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Accelerated higher order radiative perturbation computation: an application of GDOM

Yi Qin[a], Michael A. Box[a,*], Thomas Trautmann[b]

[a]School of Physics, University of New South Wales, Sydney, NSW 2052, Australia
[b]Institute of Meteorology, University of Leipzig, Germany

Abstract

In a previous paper by the authors, the computational expressions for the higher order terms of the radiative perturbation series have been developed, and numerical results have been obtained. In this paper, new computational expressions are developed that use the analytic Green's function and the GDOM code, which were developed recently by Qin and Box. Our analysis and numerical computations indicate that the new scheme dramatically improves the efficiency of the computation (by reducing the CPU-time to less than 2% of that required by the previous scheme), and the huge demand on memory usage has been completely removed. This new scheme allows us to expand the high order perturbation computations to more general cases, for example, to include azimuth dependence, and to use the perturbation theory in more potential applications.

Keywords: Perturbation theory; Green's function; Radiative transfer

1. Introduction

In a recent paper by Qin and Box [1], an algorithm has been developed to compute the Green's function for radiative transfer, and a Fortran 90 computer code, GDOM, has been developed to implement this algorithm. The GDOM code also includes a special implementation of the

*Corresponding author. Tel.: +61-2-9385-4545; fax: +61-2-9385-6060.
E-mail address: m.box@unsw.edu.au (M.A. Box).

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Discrete-Ordinate Method (DOM) [2,3] on the basis of the EDOM [4] with a number of improvements, especially on the particular solution [5]. This integrated code package provides us with the comprehensive functionalities that allow us to compute simultaneously the Green's function and the DOM solution for multiple sources of different types.

This GDOM code gives us a new opportunity to accelerate the computation of the high order terms of the radiative perturbation series [6,7]. In this paper, new computational expressions for higher order perturbation will be developed that use the new Green's function expression [1]. As in previous computation [7], we assume that the radiative effect for which the perturbation is to be computed is azimuth independent, such as flux and heating rate, and the atmosphere model is plane-parallel.

In Section 2, the newly developed Green's function will be presented and expanded into a double Legendre polynomial series. In Section 3, we will present the forward and adjoint intensities and expand them into Legendre polynomials. The new computational expression for higher order perturbation will be developed in Section 4. Validation of the new computation, and a detailed comparison with the previous computation in terms of efficiency will be given in Section 5.

2. The adjoint Green's function and its expansion

The Green's function for radiative transfer in a plane-parallel atmosphere over a reflecting surface has been developed by Qin and Box [1], which can be written as

$$\mathbf{G}^{l,l_0}(\tau,\tau_0)=[\mathbf{\Phi}_+^l \quad \mathbf{\Phi}_-^l]\mathbf{\Lambda}^l(\tau)\tilde{\mathbf{T}}_\mathrm{s}^{l,l_0}(\tau,\tau_0)\mathbf{\Lambda}_0^{l_0}(\tau_0)\begin{bmatrix} {}_-\mathbf{\Phi}_0^{l^\mathrm{T}} \\ {}_+\mathbf{\Phi}_0^{l^\mathrm{T}} \end{bmatrix}, \tag{1}$$

where τ is the optical thickness, and τ_0 represents the position of the source in terms of the optical thickness. We assume the atmosphere is composed of multiple layers and l denotes the layer where the radiation field is being computed, and l_0 denotes the source layer, i.e., $\tau^{l-1}<\tau<\tau^l$ and $\tau^{l_0-1}<\tau_0<\tau^{l_0}$ where τ^l denotes the optical thickness at the bottom of layer l. Suppose N_s is the number of intensity streams in a hemisphere, $\mathbf{\Phi}_\pm^l$ are $2N_\mathrm{s}$ by N_s matrices whose columns are the eigenvectors of the coefficient matrix of the radiative transfer equation for layer l (cf. Section A2.1 in [1]), and the coefficient matrix is related (only) to the phase function and the single scattering albedo of layer l. ${}_\pm\mathbf{\Phi}^{l^\mathrm{T}}$ are the transpose of $\mathbf{\Phi}_\pm^l$. $\mathbf{\Lambda}^l$ and $\mathbf{\Lambda}_0^{l_0}$ are $2N_\mathrm{s}$ by $2N_\mathrm{s}$ diagonal matrices defined as

$$\mathbf{\Lambda}^l(\tau)=\begin{bmatrix}\mathbf{\Lambda}_+^l(\tau,\tau^{l-1}) & \mathbf{0}\\ \mathbf{0} & \mathbf{\Lambda}_-^l(\tau,\tau^l)\end{bmatrix}=\begin{bmatrix}\mathrm{e}^{\mathbf{\lambda}_+^l(\tau^{l-1}-\tau)} & \mathbf{0}\\ \mathbf{0} & \mathrm{e}^{\mathbf{\lambda}_-^l(\tau^l-\tau)}\end{bmatrix}, \tag{2}$$

$$\mathbf{\Lambda}_0^{l_0}(\tau_0)=\begin{bmatrix}\mathbf{\Lambda}_-^{l_0}(\tau^{l_0-1},\tau_0) & \mathbf{0}\\ \mathbf{0} & \mathbf{\Lambda}_+^{l_0}(\tau^{l_0},\tau_0)\end{bmatrix}=\begin{bmatrix}\mathrm{e}^{\mathbf{\lambda}_-^{l_0}(\tau_0-\tau^{l_0-1})} & \mathbf{0}\\ \mathbf{0} & \mathrm{e}^{\mathbf{\lambda}_+^{l_0}(\tau_0-\tau^{l_0})}\end{bmatrix}, \tag{3}$$

where $\mathbf{\lambda}_\pm^l$, $\mathbf{\lambda}_\pm^l\equiv-\mathbf{\lambda}_\mp^l$, are N_s by N_s diagonal matrices composed, respectively, by the positive and negative eigenvalues of the coefficient matrix of layer l (cf. Section A2.1 in [1]). $\tilde{\mathbf{T}}_\mathrm{s}^{l,l_0}$ can be written as

$$\tilde{\mathbf{T}}_{\mathrm{s}}^{l,l_0}(\tau,\tau_0) = \mathbf{T}_{\mathrm{s}}^{l,l_0} + \delta_{l,l_0}\mathbf{\Lambda}_{+}^{l}(\tau^{l-1},\tau^{l})\begin{bmatrix} \mathbf{0} & \boldsymbol{\xi}_{+}^{l}H(\tau-\tau_0) \\ \boldsymbol{\xi}_{+}^{l}H(\tau_0-\tau) & \mathbf{0} \end{bmatrix}, \tag{4}$$

where $\mathbf{T}_{\mathrm{s}}^{l,l_0}$ is a $2N_{\mathrm{s}}$ by $2N_{\mathrm{s}}$ matrix that depends on l and l_0, but it does not depend on τ or τ_0. H is the step function and $\boldsymbol{\xi}_{+}^{l}$ is an N_{s} by N_{s} diagonal matrix defined as

$$\xi_{+jj}^{l} = -\frac{1}{2\pi}\left(\boldsymbol{\varphi}_{+j}^{l^{\mathrm{T}}}\boldsymbol{\mu}\mathbf{w}\boldsymbol{\varphi}_{+j}^{l}\right)^{-1}, \quad j=1,\ldots,N_{\mathrm{s}}, \tag{5}$$

where $\boldsymbol{\varphi}_{+j}$ is the jth column of $\mathbf{\Phi}_{+}^{l}$.

All the components in the Green's function expressions, $\mathbf{\Phi}_{\pm}^{l}$, $\boldsymbol{\lambda}_{\pm}^{l}$ and $\mathbf{T}_{\mathrm{s}}^{l,l_0}$, can be obtained using the GDOM code [1]. Depending mainly on the number of layers and the stream number, the time needed to compute these values ranges from less than to a few times of that required to compute the radiation field produced by a single beam source using a standard implementation of the DOM algorithm.

We now expand the Green's function into a double Legendre polynomial series using the following definition:

$$g_{mn}^{l,l_0}(\tau,\tau_0) = \frac{(2m+1)(2n+1)}{4}\int_{-1}^{1} p_m(\mu)\,\mathrm{d}\mu \int_{-1}^{1} G^{l,l_0}(\tau,\mu,\tau_0,\mu_0)p_n(\mu_0)\,\mathrm{d}\mu_0,$$
$$m,n = 0,1,\ldots,N_{\mathrm{xpd}}, \tag{6}$$

where $p_i(\mu)$ is the Legendre polynomial, and N_{xpd} is the order of the expansion. By replacing the integrations with Gaussian quadrature, and writing the resulting equation in matrix form, we have

$$\mathbf{g}^{l,l_0}(\tau,\tau_0) = \mathbf{mpwG}^{l,l_0}(\tau,\tau_0)\mathbf{wp}^{\mathrm{T}}\mathbf{m}, \tag{7}$$

where $\mathbf{g}$ is an $N_{\mathrm{xpd}}+1$ by $N_{\mathrm{xpd}}+1$ matrix function of τ and τ_0, $\mathbf{m}$ is an $N_{\mathrm{xpd}}+1$ by $N_{\mathrm{xpd}}+1$ diagonal matrix defined by $m_{ii}=(2i+1)/2$, $\mathbf{p}$ is an $N_{\mathrm{xpd}}+1$ by $2N_{\mathrm{s}}$ matrix defined by $p_{ij}=p_i(\mu_j)$, the ith order Legendre polynomial at μ_j, and $\mathbf{w}$ is a $2N_{\mathrm{s}}$ by $2N_{\mathrm{s}}$ diagonal matrix composed of the Gaussian quadrature weights. Insert Eq. (1) into Eq. (7), we have:

$$\mathbf{g}^{l,l_0} = \mathbf{X}^{l}\mathbf{\Lambda}^{l}(\tau)\tilde{T}_{\mathrm{s}}^{l,l_0}\mathbf{\Lambda}_{0}^{l_0}(\tau_0)\mathbf{X}_{0}^{l_0}, \tag{8}$$

where

$$\mathbf{X}^{l} = [\mathbf{X}_{+}^{l} \quad \mathbf{X}_{-}^{l}], \quad \mathbf{X}_{0}^{l_0} = \begin{pmatrix} \mathbf{X}_{-}^{l_0^{\mathrm{T}}} \\ \mathbf{X}_{+}^{l_0^{\mathrm{T}}} \end{pmatrix}, \tag{9}$$

where

$$\mathbf{X}_{\pm}^{l} = \mathbf{mpw\Phi}_{\pm}^{l}. \tag{10}$$

Finally, we convert $\mathbf{g}^{l,l_0}$ to $\mathbf{g}^{+l,l_0}$—the expansion of the adjoint Green's function. Because the adjoint Green's function differs from the Green's function only by the direction of the source and the radiation field zenith angles, $\mathbf{g}^{+l,l_0}$ can be written as:

$$\mathbf{g}^{+l,l_0} = \mathbf{X}^{+l}\mathbf{\Lambda}^l(\tau)\tilde{\mathbf{T}}_{\mathrm{s}}^{l,l_0}\mathbf{\Lambda}_0^{l_0}(\tau_0)\mathbf{X}_0^{+l_0}, \tag{11}$$

where $\mathbf{X}^{+l} = \mathbf{s}\mathbf{X}^l$ and $\mathbf{X}_0^{+l_0} = \mathbf{X}_0^{l_0}\mathbf{s}$, where $\mathbf{s}$ is a diagonal matrix defined by $s_{ii} = (-1)^i$.

Compared to the previous approach that uses DOM to compute Green's function [8], it is now very simple to compute and expand the (adjoint) Green's function, and it is much more efficient and much less demanding on memory. Since it does not require us to evaluate Eq. (11) to compute the higher order perturbation as will be seen in Section 4, there is no need to store the expansion coefficients of the Green's function, and the $\mathbf{X}$ matrix defined in Eq. (9) is the only computation required. We will also see in the next section that this matrix can be reused in the forward and adjoint intensity expansion, which further saves us some time.

3. The intensities and their expansions

In this section, we present the forward and adjoint intensity, and expand them into Legendre polynomial series.

3.1. The forward intensity

In the DOM algorithm, the intensity produced by a solar beam source is composed of three terms: the general solution, the particular solution and the directly transmitted radiance. The general solution and the directly transmitted radiance are standard [2,3], and an analytic particular solution has been derived in [5]. Putting all three terms together, the forward intensity can be written as

$$\mathbf{I}^l(\tau) = \mathbf{\Phi}^l\mathbf{Y}^l\mathrm{e}^{-\boldsymbol{\lambda}^l(\tau-\tau^{l-1})} + \mathbf{\Phi}^l\mathbf{y}^l\mathrm{e}^{(\tau-\tau^{l-1})/\mu_{\mathrm{src}}} + \frac{\delta(\mu-\mu_{\mathrm{src}})}{2\pi}I_{\mathrm{src}}\mathrm{e}^{(\tau-\tau^{l-1})/\mu_{\mathrm{src}}}, \tag{12}$$

where $\mathbf{I}^l$ is a $2N_{\mathrm{s}}$ vector function of τ, $\mathbf{\Phi}^l = [\mathbf{\Phi}_+^l \;\; \mathbf{\Phi}_-^l]$ is a $2N_{\mathrm{s}}$ by $2N_{\mathrm{s}}$ matrix (see the previous section), $\mathbf{Y}^l$ is a $2N_{\mathrm{s}}$ by $2N_{\mathrm{s}}$ diagonal matrix composed of the integral constants, and $\boldsymbol{\lambda}^l$ in Eq. (12) is a $2N_{\mathrm{s}}$ vector composed of the eigenvalues of the coefficient matrix of the radiative transfer equation for layer l (compared to the diagonal matrices, $\boldsymbol{\lambda}_\pm^l$, in Eqs. (2)–(3)), $\mathbf{y}^l$ is a $2N_{\mathrm{s}}$ vector, and $\mu_{\mathrm{src}} < 0$ is the cosine of the source zenith angle.

The intensity can be expanded into a Legendre polynomial series using

$$\xi_m^l(\tau) = \frac{(2m+1)}{2}\int_{-1}^{1} p_m(\mu)I^l(\tau,\mu)\,\mathrm{d}\mu, \quad m = 0, 1, \ldots, N_{\mathrm{xpd}} \tag{13}$$

which can also be written in matrix form, after replacing the integration with Gaussian quadrature, as $\boldsymbol{\xi}^l(\tau) = \mathbf{mpwI}^l$. By merging all the components, we have

$$\boldsymbol{\xi}^l(\tau) = \mathbf{A}^l\mathrm{e}^{-\boldsymbol{\lambda}_b^l(\tau-\tau^{l-1})}, \tag{14}$$

where $\mathbf{A}^l$ is an $N_{\text{xpd}} + 1$ by $2N_\text{s} + 1$ matrix defined by

$$A_{ij}^l = \begin{cases} X_{ij}^l Y_j^l, & j \neq 0, \\ \mathbf{Xy} + \dfrac{i+1}{2} \dfrac{I_{\text{src}}}{2\pi} p_i(\mu_{\text{src}}), & j = 0, \end{cases} \quad i = 0, \ldots, N_{\text{xpd}}, \; j = -N_\text{s}, \ldots, -1, 0, 1, \ldots, N_\text{s}, \tag{15}$$

where $\mathbf{X}$ is defined in Eq. (9). $\boldsymbol{\lambda}_b^l$ in Eq. (14) is a column vector defined as

$$\boldsymbol{\lambda}_b^l = [\lambda_{-N_\text{s}}^l, \ldots, \lambda_{-1}^l, -1/\mu_{\text{src}}, \lambda_1^l, \ldots, \lambda_{N_\text{s}}^l]^\text{T}. \tag{16}$$

3.2. The adjoint intensity

As in previous computation [7], the adjoint intensity here corresponds to a flux style response function—it is azimuth independent and is a continuous function of the zenith angle, so the adjoint source can be represented by an Angularly Distributed Source (ADS), for which an analytic particular solution has been derived in [5].

Because an ADS is a continuous function of the zenith angle, there is no need to separate the directly transmitted radiance from the source term of the radiative transfer equation as in the case of a solar beam source (in which the Dirac delta function contained in the source function causes numerical difficulties). Therefore, the ADS intensity is composed of only two terms: the general solution and the particular solution. The general solution is the same as that of the solar beam source [2,3], and the particular solution has been derived in [5]. Putting the two terms together, we write the ADS intensity as

$$\mathbf{I}_{\text{ads}}^l(\tau, \mu) = \boldsymbol{\Phi}^l(\mu)\mathbf{Y}^l \mathrm{e}^{-\boldsymbol{\lambda}^l(\tau - \tau^{l-1})} + \mathbf{I}_{p,\text{ads}}^l(\tau, \mu), \tag{17}$$

where

$$\mathbf{I}_{p,\text{ads}}^l(\mu) = \delta_{l,l_{\text{obs}}} \boldsymbol{\Phi}_\pm^l(\mu)\mathbf{y}_\pm^l \mathrm{e}^{-\boldsymbol{\lambda}_\pm^l(\tau - \tau^{l-1})}, \tag{18}$$

where the subscript, $\pm$, corresponds to $\tau > \tau_{\text{obs}}$ and $\tau < \tau_{\text{obs}}$ respectively, where τ_{obs} is the vertical position of the adjoint source and $\tau^{l_{\text{obs}}-1} < \tau_{\text{obs}} < \tau^{l_{\text{obs}}} \cdot \mathbf{y}_\pm^l$ is a diagonal matrix, and $\boldsymbol{\lambda}_\pm^l$ is a column vector composed of the positive or negative eigenvalues of the coefficient matrix of the transfer equation for layer l. From the ADS intensity, the adjoint intensity is simply

$$\mathbf{I}^{+l}(\tau, \mu) = \mathbf{I}_{\text{ads}}^l(\tau, -\mu). \tag{19}$$

We note that to obtain the adjoint intensity, the response function should be multiplied by $1/\mu$ to normalize it to unit flux, and its zenith angle should be reversed. After solving the transfer equation, the radiation field zenith angle should be reversed again as shown in Eq. (19). An outline of the steps required to compute the adjoint intensity using a normal radiative transfer code has been given in [9].

As for the forward intensity, we expand the adjoint intensity into Legendre polynomial series as

$$\boldsymbol{\xi}^{+l} = \mathbf{A}^{+l} \mathrm{e}^{-\boldsymbol{\lambda}^l(\tau - \tau^{l-1})}, \tag{20}$$

where $\mathbf{A}^{+l}$ is an $N_{\text{xpd}} + 1$ by $2N_{\text{s}}$ matrix

$$\mathbf{A}^{+l} = \mathbf{X}^{+l}\mathbf{Y}^{l} + \delta_{l,l_{\text{obs}}}[H(\tau - \tau_{\text{obs}})\mathbf{X}_{+}^{+l} \quad H(\tau_{\text{obs}} - \tau)\mathbf{X}_{-}^{+l}] \begin{bmatrix} \mathbf{y}_{+}^{l} & \mathbf{0} \\ \mathbf{0} & \mathbf{y}_{-}^{l} \end{bmatrix}, \tag{21}$$

where $\mathbf{X}_{\pm}^{l}$ are matrices defined following Eq. (11), and H is the step function.

4. Higher order perturbation

Box et al. [6] have shown that any radiation effect, such as flux or heating rate, can be expanded into a series as

$$E = E_0 + \sum_{k=1}^{\infty} (-1)^k \Delta_k E, \tag{22}$$

where E_0 is the radiation effect corresponding to a base atmosphere model, E is the same effect corresponding to a model that is perturbed from the base model, and $\Delta_k E$ represent the perturbation orders of the radiation effect due to the perturbation of the atmosphere model.

In the previous computation [7], the computational expression for the higher order perturbation terms, $\Delta_k E\,(k \geqslant 2)$, have been developed and implemented that use the DOM algorithm to provide the intensities as well as the Green's function. Although it was possible to perform the computation, it was, however, not efficient. With the new Green's function, we are now able to develop a new computational expression for the higher order terms. It has been shown that $\Delta_k E$ can be computed using the following recursion relation [7]:

$$\mathbf{A}_2^{l}(\tau) = \sum_{l'=1}^{N_{\text{p}}} \int_{\tau^{l'-1}}^{\tau^{l'}} \mathrm{d}\tau' \mathbf{g}^{+l,l'}(\tau, \tau') \Delta\mathbf{V}^{l'} \boldsymbol{\xi}^{+l'}(\tau'), \tag{23}$$

$$\mathbf{A}_k^{l}(\tau) = \sum_{l'=1}^{N_{\text{p}}} \int_{\tau^{l'-1}}^{\tau^{l'}} \mathrm{d}\tau' \mathbf{g}^{+l,l'}(\tau, \tau') \Delta\mathbf{V}^{l'} \mathbf{A}_{k-1}^{l'}(\tau'), \tag{24}$$

$$\Delta_k E = \sum_{l=1}^{N_{\text{p}}} \int_{\tau^{l-1}}^{\tau^{l}} \mathrm{d}\tau (\xi^{l}(\tau))^{\mathrm{T}} \Delta\mathbf{V}^{l} \mathbf{A}_k^{l}(\tau), \quad k = 2, 3, \ldots, \tag{25}$$

where $\Delta\mathbf{V}$, a diagonal matrix characterizing the perturbation, is defined by:

$$\Delta V_{jj}^{l} = \frac{4\pi}{2j+1} \left\{ \left[\frac{(\Delta\tau^{l})^{\text{p}}}{(\Delta\tau^{l})^{\text{b}}} \right] (1 - \tilde{\omega}_0^{l^{\text{p}}} \chi_j^{l^{\text{p}}}) - (1 - \tilde{\omega}_0^{l^{\text{b}}} \chi_j^{l^{\text{b}}}) \right\}, \tag{26}$$

where the superscripts, p and b, denote the perturbed model and the base model, respectively, $\Delta\tau^{l}$, $\tilde{\omega}_0^{l}$ and χ_j^{l} are the optical thickness, the single scattering albedo and the coefficients of the phase function's Legendre polynomial series for the lth atmosphere layer. Note that, for convenience, we have converted all integrations over altitude to integrations over optical thickness in this paper.

Insert Eqs. (8), (14) and (20) into Eqs. (23)–(25), we have

$$\mathbf{B}_2^l(\tau) = \sum_{l'=1}^{N_\mathrm{p}} \int_{\tau^{l'-1}}^{\tau^{l'}} \mathrm{d}\tau' \tilde{\mathbf{T}}_\mathrm{s}^{l,l'}(\tau,\tau')\boldsymbol{\Lambda}_0^{l'}(\tau')\boldsymbol{\Omega}_0^{+l'}\mathrm{e}^{-\boldsymbol{\lambda}^{l'}(\tau'-\tau^{l'-1})}, \tag{27}$$

$$\mathbf{B}_k^l(\tau) = \sum_{l'=1}^{N_\mathrm{p}} \int_{\tau^{l'-1}}^{\tau^{l'}} \mathrm{d}\tau' \tilde{\mathbf{T}}_\mathrm{s}^{l,l'}(\tau,\tau')\boldsymbol{\Lambda}_0^{l'}(\tau')\boldsymbol{\Omega}^{l'}\boldsymbol{\Lambda}^{l'}(\tau')\mathbf{B}_{k-1}^{l'}(\tau'), \tag{28}$$

$$\Delta_k E = \sum_{l=1}^{N_\mathrm{p}} \int_{\tau^{l-1}}^{\tau^{l}} \mathrm{d}\tau \mathrm{e}^{-(\boldsymbol{\lambda}_\mathrm{b}^l)^\mathrm{T}(\tau-\tau^{l-1})}\boldsymbol{\Omega}_0^l\boldsymbol{\Lambda}^l(\tau)\mathbf{B}_k^l(\tau), \tag{29}$$

where

$$\boldsymbol{\Omega}_0^{+l} = \mathbf{X}_0^{+l}\Delta\mathbf{V}^l\mathbf{A}^{+l}, \tag{30}$$

$$\boldsymbol{\Omega}^{l} = \mathbf{X}_0^{+l}\Delta\mathbf{V}^l\mathbf{X}^{+l}, \tag{31}$$

$$\boldsymbol{\Omega}_0^{l} = (\mathbf{A}^l)^\mathrm{T}\Delta\mathbf{V}^l\mathbf{X}^{+l}. \tag{32}$$

Insert Eq. (4) into Eq. (27) and Eq. (28), recall that $T_\mathrm{s}^{l,l'}$ does not depend on optical thickness and that H is the step function, we obtain

$$\mathbf{B}_k^l(\tau) = \sum_{l'=1}^{N_\mathrm{p}} \mathbf{T}_\mathrm{s}^{l,l'} \int_{\tau^{l'-1}}^{\tau^{l'}} \mathrm{d}\tau' \mathbf{r}_k^{l'}(\tau') + \boldsymbol{\xi}_+^l\boldsymbol{\Lambda}_+^l(\tau^{l-1},\tau^l)\begin{bmatrix} \int_{\tau^{l-1}}^{\tau} \mathbf{r}_{k,2}^l(\tau')\,\mathrm{d}\tau' \\ \int_{\tau}^{\tau^l} \mathbf{r}_{k,1}^l(\tau')\,\mathrm{d}\tau' \end{bmatrix}, \tag{33}$$

where $\mathbf{r}_k$ is a $2N_\mathrm{s}$ column vector defined by

$$\mathbf{r}_k^l(\tau) = \begin{cases} \boldsymbol{\Lambda}_0^l(\tau)\boldsymbol{\Omega}_0^{+1}\mathrm{e}^{-\boldsymbol{\lambda}^{l(\tau-\tau^{l-1})}}, & k=2, \\ \boldsymbol{\Lambda}_0^l(\tau)\boldsymbol{\Omega}^l\boldsymbol{\Lambda}^l(\tau)\mathbf{B}_{k-1}^l(\tau), & k>2 \end{cases} \tag{34}$$

and $\mathbf{r}_{k,1}^l$ and $\mathbf{r}_{k,2}^l$ are the upper and lower half of $\mathbf{r}_k^l$.

We note that the variable τ of Eq. (33) appears only as an integral limit, therefore Eq. (33) can be computed much more efficiently than Eq. (23/24). We rewrite Eq. (33) as

$$\mathbf{B}_k^l(\tau) = \sum_{l'=1}^{N_\mathrm{p}} \mathrm{T}_\mathrm{s}^{l,l'} \begin{bmatrix} \bar{\mathbf{r}}_{k,1}^l(\tau^{l'-1}) \\ \bar{\mathbf{r}}_{k,2}^l(\tau^{l'}) \end{bmatrix} + \boldsymbol{\xi}_+^l\boldsymbol{\Lambda}_+^l(\tau^{l-1},\tau^l)\begin{bmatrix} \bar{\mathbf{r}}_{k,2}^l(\tau) \\ \bar{\mathbf{r}}_{k,1}^l(\tau) \end{bmatrix}, \tag{35}$$

where

$$\bar{\mathbf{r}}^l_{k,1}(\tau) = \int_{\tau}^{\tau^l} \mathbf{r}^l_{k,1}(\tau')\,\mathrm{d}\tau', \tag{36}$$

$$\bar{\mathbf{r}}^l_{k,2}(\tau) = \int_{\tau^{l-1}}^{\tau} \mathbf{r}^l_{k,2}(\tau')\,\mathrm{d}\tau'. \tag{37}$$

Suppose layer l is evenly divided into N_l sub-layers at the nodes τ_i, $i = 0, \ldots, N_l$, where $\tau_0 = \tau^{l-1}$ and $\tau_{N_l} = \tau^l \cdot \bar{\mathbf{r}}^l_{k,2}$ can be computed using the trapezoidal rule as:

$$\bar{\mathbf{r}}^l_{k,2}(\tau_i) = \bar{\mathbf{r}}^l_{k,2}(\tau_{i-1}) + \frac{\Delta\tau^l}{2}[\mathbf{r}^l_{k,2}(\tau_{i-1}) + \mathbf{r}^l_{k,2}(\tau_i)], \quad \bar{\mathbf{r}}^l_{k,2}(\tau_0) = 0, \quad i = 1, \ldots, N_l, \tag{38}$$

where $\Delta\tau^l$ is the sub-layer thickness. $\bar{\mathbf{r}}^l_{k,l}$ can be computed similarly but in reverse order.

We see that the number of operations (multiplications and additions) required to compute Eq. (35) is proportional to N_{ps}, the total number of sub-layers for the whole atmosphere. In contrast, the number of operations required to compute Eq. (23/24) for the previous computation is proportional to N^2_{ps}. The efficiency of the current computation, compared to the previous one, will be discussed in detail in the next section.

5. Validation and discussion

This paper concentrates on the acceleration of the computation. It performs exactly the same computation as previously [7], and therefore, the new code should have similar accuracy to the previous one. To make a comparison, the three cases used previously (Table 1, [7]) for validation have been re-computed. The results, together with the previous results (Table 2, [7]), are listed in Table 1. It shows that the results are very similar: the small differences may be caused by different implementation details.

More validation of the new code was carried out by comparing the perturbation predicted by the code with that calculated directly, for another four cases (Table 2). M_1 and M_2 are two

Table 1
The perturbations of reflected and transmitted flux predicted by the previous and the current computations, $\Delta E^{(\mathrm{Pred.})}$, for the three cases used previously (Table 1, [7])

Flux/Perturbation	Case 1		Case 2		Case 3	
	Ref.	Trans.	Ref.	Trans.	Ref.	Trans.
$\Delta E^{(\mathrm{Pred.})}$						
Previous	6.74E−02	−1.33E−01	5.61E−02	−5.61E−02	−1.41E−01	−1.05E−01
Current	6.74E−02	−1.33E−01	5.63E−02	−5.63E−02	−1.42E−01	−1.05E−01
$\Delta E^{(\mathrm{Dir})}$	6.71E−02	−1.33E−01	5.60E−02	−5.60E−02	−1.42E−01	−1.06E−01
E_0	1.22E−01	5.85E−01	4.86E−01	2.21E−01	4.86E−01	2.21E−01

Shown also are the directly computed flux perturbation, $\Delta E^{(\mathrm{Dir})}$, and the base model flux, E_0.

Table 2
Computation cases used for validation (Table 3) and CPU-Time comparison (Table 4)

Parameters	Case 1	Case 2	Case 3	Case 4
N_p	10	10	1	1
N_s	16	4	16	4
Base Model				
P^l	M_1[1–10]	M_1[1–10]	M_1[10]	M_1[10]
$\tilde{\omega}_0^l$	M_1[1–10]	M_1[1–10]	M_1[10]	M_1[10]
τ^l	0.5 to 5.0 step 0.5	1.0 to 10.0 step 1.0	1.0	10.0
Perturbed Model				
P^l	M_2[1–10]	M_2[1–10]	M_2[10]	M_2[10]
$\tilde{\omega}_0^l$	M_2[1–10]	M_2[1–10]	M_2[10]	M_1[10]
τ^l	1.0 to 10.0 step 1.0	1.5 to 15.0 step 1.5	2.0	15.0

M_1 and M_2 are two ten-layer atmosphere models used to construct the base model and the perturbed model. In cases 1 and 2, the base model and the perturbed model have ten layers ($N_p = 10$). Each layer has equal optical thickness. In cases 3 and 4 ($N_p = 1$), only the 10th layer of M_1 and M_2 are used. N_s is the hemisphere stream number.

Table 3
The perturbation of reflected and transmitted flux predicted by the new code, $\Delta E^{(\mathrm{Pred.})}$, and that directly calculated, $\Delta E^{(\mathrm{Dir})}$, for the 4 cases listed in Table 2

	Case 1		Case 2		Case 3		Case 4	
	Ref.	Trans.	Ref.	Trans.	Ref.	Trans.	Ref.	Trans.
$\Delta E^{(\mathrm{Pred.})}$	−1.03E−01	−1.89E−01	3.28E−02	−4.11E−02	6.95E−02	−1.07E−01	4.82E−02	−6.04E−02
$\Delta E^{(\mathrm{Dir})}$	−1.02E−01	−1.89E−01	3.26E−02	−4.09E−02	6.93E−02	−1.07E−01	4.79E−02	−6.01E−02
E_0	5.19E−01	2.35E−01	5.94E−01	1.42E−01	2.35E−01	5.90E−01	5.28E−01	2.24E−01

Shown also is the base model flux, E_0.

ten-layer atmosphere models that are used to construct the phase function and single scattering albedo of the base and perturbed models. M_1 and M_2, in turn, are generated from the following three scattering models:

(1) Rayleigh scattering with single scattering albedo $\tilde{\omega}_0 = 1.0$;
(2) TTHG phase function [10] with $\alpha = 0.965$, $g_1 = 0.75$, $g_2 = 0.65$ and $\tilde{\omega}_0 = 1.0$;
(3) Phase function and single scattering albedo calculated from the Haze M aerosol model [11], with wavelength $\lambda = 1.0\,\mu\mathrm{m}$ and refractive index $r_x = 1.5–0.00001i$.

These scattering models are then mixed together using varying mixing ratios as shown below:

(1) $\mathbf{M}_1 : r \times \mathrm{Rayleigh} + (1 - r) \times \mathrm{TTHG}$, $r = 1.0, 0.9, \ldots, 0.1$,
(2) $\mathbf{M}_2 : r \times \mathrm{Rayleigh} + (1 - r) \times \mathrm{Haze\,M}$, $r = 1.0, 0.9, \ldots, 0.1$,

Table 4
CPU-Time comparison between the current and the previous computations

Component	$N_{ps} = 100$			$N_{ps} = 500$		
	GF/Xpd	Pert.	Total	*GF/Xpd*	Pert.	Total
$N_s = 4$, $N_p = 1$						
Previous	0.2501	0.3437	0.5938	4.1719	7.9219	12.0938
Current	0.0002	0.0032	0.0034	0.0001	0.0143	0.0144
Reduced by	99.9%	99.1%	99.4%	100.0%	99.8%	99.9%
$N_s = 4$, $N_p = 10$						
Previous	0.5937	0.3751	0.9688	5.9687	7.8594	13.8281
Current	0.0031	0.0091	0.0122	0.0032	0.0199	0.0231
Reduced by	99.5%	97.6%	98.7%	99.9%	99.7%	99.8%
$N_s = 16$, $N_p = 1$						
Previous	13.9375	4.8437	18.7812	252.9375	209.7031	462.6406
Current	0.0034	0.0291	0.0325	0.0038	0.1104	0.1142
Reduced by	100.0%	99.4%	99.8%	100.0%	99.9%	100.0%
$N_s = 16$, $N_p = 10$						
Previous	35.6406	6.0156	41.6406	371.9531	222.4063	594.3594
Current	0.0830	0.2673	0.3502	0.0821	0.3540	0.4361
Reduced by	99.8%	95.6%	99.2%	100.0%	99.8%	99.9%

Column “GF/Xpd” is the time needed to compute and expand the Green’s function and the intensities, column “Pert.” is the time needed to compute the (10) perturbation terms. All times are in seconds. The reduction of time (in percentage) is shown in the third rows. Other parameters are: N_s—the hemisphere stream number, N_p—the number of atmosphere layers, and N_{ps}—the total number of sub-layers.

where r is the mixing ratio for the ten layers. The surface model is Lambertian with an albedo of 0.2.

Table 3 shows the perturbation of transmitted and reflected flux predicted by the new code and that computed directly. For cases 1 and 2, the computations use 500 sub-layers for optical thickness integration. For cases 3 and 4, the sub-layer number is 100. Ten perturbation terms are computed for all four cases. We can see that the predicted perturbation is very close to that calculated directly.

We have found that, by using the newly developed analytic Green’s function and the GDOM code, computing the higher order terms of the radiative perturbation series has indeed been accelerated dramatically, which is shown in Table 4. (The base and perturbed models used for this testing are those shown in Table 2). Cases of different hemisphere stream number ($N_s = 4$ and 16), atmosphere layer number ($N_p = 1$ and 10) and sub-layer number ($N_{ps} = 100$ and 500) are tested. The two major steps, i.e., computing and expanding the Green’s function and the intensities, and computing the perturbation terms, are timed separately. Other parameters used are: 2 adjoint sources, 1 forward source, and the number of perturbation terms computed is 10. The testing is conducted on a PC with a 1.8 GHz Intel Pentium 4 CPU and 256 megabytes memory running

Windows XP. Both codes are compiled using Compaq Visual Fortran version 6.5 with full level optimisation.

The new code is not only much faster, it also relieves the huge demand of memory usage by the previous computation, which requires the whole Green's function expansion be computed and stored. For the case $N_p = 10$, $N_{ps} = 500$ and $N_s = 16$ and if double precision is used, the storage required for the Green's function alone will be about two gigabytes. In contrast, for the current computation and for the same case mentioned above, the peak memory usage reported by the system is less than four megabytes which includes the code itself. Therefore, we have much more freedom to optimise the current computation to further improve its performance.

Our testing shows that the higher order terms of the radiative perturbation series can be computed efficiently using the new code, which allows us to expand the computation to more general cases, for example, to include azimuthal dependence. This provides us the opportunity to expand the applications of the perturbation theory.

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