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Computation of Green's function for radiative transfer

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Abstract

In an accompanying paper, we develop the computational expressions for the higher order perturbation of the radiative transfer equation, and present some numerical results for typical cases. In this article, we discuss a number of issues regarding the implementation of the HOP computation: obtaining the Green's function, its expansion as a double series of Legendre polynomials, and obtaining the adjoint radiance of more general sources such as those for the fluxes at arbitrary altitudes. Examples of Green's function and its expansion coefficients are presented.

Keywords: Radiative transfer; Green's function; Higher order perturbation

1. Introduction

In the accompanying paper, Qin et al. [1] develop the computational expressions for the higher order perturbation (HOP) for the radiative transfer equation for azimuthally independent radiative effects in parallel plane atmosphere models. Results of some typical cases are presented in that paper, indicating the success of the computation.

There are, however, several issues which need be solved in order to implement the HOP computation. The key one is the Green's function, which requires solving a large number of radiative transfer problems for sources of arbitrary vertical position and illumination direction. Trautmann and Box [2] have presented some results of the Green's function for a special atmosphere model. In this article, we present an approach to efficiently obtain the azimuthally averaged Green's function for general (plane parallel) atmosphere models.

It is shown in the accompanying paper, and will be further discussed in this paper, that by expanding the Green's function into a double series of Legendre polynomials, the HOP computational expressions, and therefore the computer code, can be greatly simplified. However, expanding the

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Green's function directly is very time consuming. In Section 3 we will introduce a much more efficient scheme to expand the function.

In Section 4, we will briefly discuss the method to obtain the adjoint radiance for sources that illuminate as a continuous function of zenith angle in a hemisphere and are located at an arbitrary vertical position, for example, sources corresponding to fluxes. Finally, we will present some numerical examples of the Green's function and its expansion.

2. Green's function

The Green's function, initially introduced in the neutron transport literature [3], has been found to be a clear concept that can be used to express the general reciprocity principle of atmospheric radiative transfer [4–6], is also a key element in HOP theory [1,7]. The Green's function, $G(r,\Omega;r',\Omega')$, is effectively the intensity observed at (r,Ω) due to a parallel beam source of unit flux at (r',Ω'), i.e., the intensity of the source may be expressed as

$$I_0(r,\Omega) = \frac{1}{|\mu|}\,\delta(r-r')\delta(\Omega-\Omega'), \tag{1}$$

where the absolute value of μ is used because it could be negative. We would like to point out that there are two different formulations for expressing the radiative transfer equation (RTE), which consequently result in different expressions for the source term. In the first formulation [8–13], only the diffusely transmitted radiance—the radiance transmitted from the source to the observation point after being scattered at least once—is considered. In the second formulation [3,6,7], as well as the diffusely transmitted radiance, the directly transmitted radiance—the radiance transmitted from the source to the observation point after being attenuated only—is also considered. The second formulation, which often appears in the radiative transfer operator form, i.e., $LI = Q$, is more convenient for the development of the radiative perturbation theory, while the first formulation is probably more suitable for solving radiative transfer problems. However, the source term in these two formulations is expressed differently, which may cause some confusion. In the first formulation the source—for example, the solar beam—is expressed in intensity, while in the second formulation the source term is expressed as a flux. While the source shown by Eq. (1) is suitable for the first formulation, when it is used in the second formulation it should be expressed as

$$Q(r,\Omega) = |\mu| I_0(r,\Omega) = \delta(r-r')\delta(\Omega-\Omega'). \tag{2}$$

Care should be taken to distinguish the two formulations, with the proper form of the source being used. Box et al. [6] have discussed this same problem from another perspective by using the terms "volume source" and "surface source".

Once the Green's function is obtained, by applying the linearity property of atmospheric radiative transfer, the intensity field due to an arbitrary source, $Q(r',\Omega')$, can be obtained from [6]

$$I(r,\Omega) = \langle G(r,\Omega;r',\Omega'), Q(r',\Omega')\rangle, \tag{3}$$

where the angular brackets denote integration over the whole phase space of the source, (r',Ω').

In our HOP computation [1], due to the assumption of a plane parallel atmosphere model and azimuthally independent radiative effect, only the azimuthally averaged Green's function for a plane parallel atmosphere model is required. In this case, r and r' are reduced to τ and τ', and Ω and Ω'

are reduced to μ and μ', and the averaged Green's function is denoted as $\bar{G}(\tau,\mu;\tau',\mu')$. (Note that we use the optical thicknesses, τ and τ', rather than the altitude, z and z', as the measure of vertical position.) The diffusely transmitted component of this function then satisfies (cf. [11,14, Section 6.1])

$$\mu\frac{\mathrm{d}\bar{G}^{(\mathrm{dif})}(\tau,\mu;\tau',\mu')}{\mathrm{d}\tau}=\bar{G}^{(\mathrm{dif})}(\tau,\mu;\tau',\mu')-\frac{\tilde{\omega}_0}{2}\sum_l\chi_l P_l(\mu)\int_{-1}^{1}P_l(\mu'')\bar{G}^{(\mathrm{dif})}(\tau,\mu'';\tau',\mu')\,\mathrm{d}\mu''$$
$$-\frac{\tilde{\omega}_0}{4\pi|\mu'|}t(\tau,\tau',\mu')\sum_l\chi_l P_l(\mu)P_l(\mu'), \tag{4}$$

which is the azimuthally independent case of the (first formulation) radiative transfer equation due to a parallel beam source whose intensity may be expressed as $1/|\mu'|\delta(\tau-\tau')\delta(\mu-\mu')$. In Eq. (4), χ_l are the coefficients of the phase function's Legendre polynomial expansion [14], and,

$$t(\tau,\tau',\mu')=U((\tau'-\tau)/\mu')\mathrm{e}^{-(\tau'-\tau)/\mu'}, \tag{5}$$

where

$$U((\tau'-\tau)/\mu')=\begin{cases}1 & (\tau'-\tau)/\mu'\geqslant 0,\\ 0 & \text{other},\end{cases} \tag{6}$$

where μ and μ' are positive if the corresponding direction is upward, otherwise they are negative. The total (averaged) Green's function may then be written as

$$\bar{G}(\tau,\mu;\tau',\mu')=\bar{G}^{(\mathrm{dif})}(\tau,\mu;\tau',\mu')+\frac{\delta(\mu-\mu')}{2\pi|\mu'|}t(\tau,\tau',\mu'), \tag{7}$$

where the second term on the right-hand side represents the azimuth average of the directly transmitted radiance (see discussion following Eq. (1)). Because this Green's function will be involved in integrations over (τ,μ) and (τ',μ') in HOP computation, we need to obtain $\bar{G}$ at a grid that is fine enough in order to compute the integration numerically with sufficient accuracy. That is, Eq. (4) needs to be solved at a fine grid of (τ',μ').

For altitude integration, we have used the trapezoidal rule by evenly dividing each model atmosphere layer into sub-layers [1]. For the zenith angle integration, Gaussian quadrature has been used. In our computation, we have used the same grid for both (τ,μ) and (τ',μ'). The size of the grid is decided experimentally, depending on the balance between the accuracy and the amount of computation. For example, for a single layer model atmosphere having an optical thickness of 10.0, the proper sub-layer thickness might be 0.04 and the number of streams (which also is the order of the Gaussian quadrature) might be 8. Generally, for optically thicker atmospheres, we may use a smaller Gaussian quadrature order and thicker sub-layers, and vice versa. The shape of the phase function may also influence the Gaussian quadrature order.

While several algorithms and computer codes are available to solve the radiative transfer equation [15], efficiency is a key issue to obtain the detailed Green's function. For the example mentioned above, the radiative transfer equation will need to be solved 2000 times. This certainly requires special considerations. As well as efficiency, obtaining the Green's function also requires solving the radiative transfer equation for sources of arbitrary vertical position and illumination direction, as is the case of Eq. (4).

To accomplish such a task and achieve efficiency at the same time, and for other adjoint radiance and radiative perturbation calculations as well, the Discrete-Ordinate Method (DOM) [9–13] has been extended. The extended algorithm (EDOM) and its implementation has been discussed by Qin et al. [8]. By expanding Eq. (43) of [8] for the cases of upward and downward parallel surface sources (PSS), the numerical solution to Eq. (4) can be expressed in terms of DOM components as

$$\bar{G}^{\ell,(\mathrm{dif})}(\tau,\mu;\tau',\mu') = \sum_{j=\pm 1}^{\pm N_s} L_j^{\ell}(\mu')\Phi_j^{\ell}(\mu)\mathrm{e}^{\lambda_j^{\ell}(\tau_\ell-\tau)} + Z^{\ell}(\mu,\mu')t(\tau,\tau',\mu'), \tag{8}$$

where Φ_j^{ℓ} and λ_j^{ℓ} are the general solution, Z^{ℓ} is the particular solution, and L_j^{ℓ} are the integral constants. The superscript ℓ denotes the model layer, i.e., $\tau_{\ell-1} < \tau < \tau_\ell$ where $\tau_{\ell-1}$ and τ_ℓ are the optical depth at the boundaries of layer ℓ.

The EDOM code has considered the efficiency problem as well. By solving the radiative transfer equation simultaneously for multiple sources, this code is capable of obtaining the solutions using only about 15% of the time of full solutions.

3. Expansion of Green's function

It has been shown [1] that by expanding the Green's function into a double series of Legendre polynomials, i.e.,

$$\bar{G}^{\ell}(\tau,\mu;\tau',\mu') = \sum_m \sum_n g_{mn}(\tau,\tau')P_m(\mu)P_n(\mu') \tag{9}$$

with the coefficients being expressed as

$$g_{mn}(\tau,\tau') = \frac{(2m+1)(2n+1)}{4}\int_{-1}^{1} P_m(\mu)\,\mathrm{d}\mu \int_{-1}^{1} \bar{G}^{\ell}(\tau,\mu;\tau',\mu')P_n(\mu')\,\mathrm{d}\mu' \tag{10}$$

the HOP computational expressions can be greatly simplified. The amount of computation has actually also been reduced. However, expanding directly using Eq. (10) could be very time consuming. In this section, we introduce a much more efficient scheme for this task, which shows us another benefit of using a DOM-based code.

Eq. (8) shows that any radiance is a summation of terms composed of factors that mostly depend on only one of the phase space variables—τ, μ, τ' or μ'. This characteristic can be utilized to analytically carry out integrations over some of the phase space variables. In the first-order perturbation calculation, integration over altitude has been carried out analytically which has led to significant improvement of precision as well as reduction of the amount of calculation.

This idea can also be applied in the expansion of the Green's function. By inserting Eq. (7) into Eq. (10) and considering Eq. (8), we obtain the expansion coefficients for the total Green's function, $\bar{G}(\tau,\mu;\tau',\mu')$:

$$g_{mn}(\tau,\tau') = \frac{(2m+1)(2n+1)}{4}\left[\sum_{j=\pm 1}^{\pm N_s} \tilde{\Phi}_{jm}^{\ell}\tilde{L}_{jn}^{\ell}\mathrm{e}^{\lambda_j^{\ell}(\tau_\ell-\tau)} + g_{mn}^{\ell,p}(\tau,\tau')\right], \tag{11}$$

where

$$\tilde{\Phi}^{\ell}_{jm} = \int_{-1}^{1} \Phi^{\ell}_{j}(\mu) P_m(\mu)\,\mathrm{d}\mu,$$

$$\tilde{L}^{\ell}_{jn} = \int_{-1}^{1} L^{\ell}_{j}(\mu') P_n(\mu')\,\mathrm{d}\mu'. \tag{12}$$

The expression for $g^{\ell,p}_{mn}(\tau,\tau')$ depends on the relation between τ' and τ. Specifically, when $\tau=\tau'$, i.e., the source and the observation point are at the same vertical position:

$$g^{\ell,p}_{mn}(\tau,\tau') = \int_{0}^{1} P_n(\mu')\left\{\tilde{Z}^{\ell}_{m}(\mu') + (-1)^n \tilde{Z}^{\ell}_{m}(-\mu') + [1+(-1)^{m+n}]\,\frac{P_m(\mu')}{2\pi\mu'}\right\}\mathrm{d}\mu'; \tag{13}$$

when $\tau<\tau'$, or the source is below the observation point:

$$g^{\ell,p}_{mn}(\tau,\tau') = \int_{0}^{1} P_n(\mu')\left[\tilde{Z}^{\ell}_{m}(\mu') + \frac{P_m(\mu')}{2\pi\mu'}\right]\mathrm{e}^{-(\tau'-\tau)/\mu'}\,\mathrm{d}\mu' \tag{14}$$

and when $\tau>\tau'$, or the source is above the observation point:

$$g^{\ell,p}_{mn}(\tau,\tau') = (-1)^n \int_{0}^{1} P_n(\mu')\left[\tilde{Z}^{\ell}_{m}(-\mu') + (-1)^m\,\frac{P_m(\mu')}{2\pi\mu'}\right]\mathrm{e}^{(\tau'-\tau)/\mu'}\,\mathrm{d}\mu'. \tag{15}$$

In the above three equations:

$$\tilde{Z}^{\ell}_{m}(\pm\mu') = \int_{-1}^{1} Z^{\ell}(\mu,\pm\mu') P_m(\mu)\,\mathrm{d}\mu. \tag{16}$$

We note that $\tilde{\Phi}^{\ell}_{j,m}$, $\tilde{L}^{\ell}_{j,n}$ and $\tilde{Z}^{\ell}_{m}(\pm\mu')$ depend on the model layer, rather than sub-layer. Because each model layer has to be divided into many sub-layers in order to perform integrations over altitude, comparatively the number of model layers is small, and the overhead to obtain the above three quantities is therefore small, especially when the total optical thickness is large. Compared to Eq. (10) which involves a two-level integration over angle, Eq. (11) is a one-level integration. We therefore have reduced the amount of computation to roughly the square root of the original Eq. (10).

Through the development of the HOP computational expression [1] and the development of the above expressions, we see that the expansion of the Green's function brings us a number of benefits: it leads to the simplification of the computational expressions; following that, it also greatly reduces the amount of computation; it hides the delta function in Eq. (7) and the step function in Eq. (5). The last point would introduce great complexity into the HOP computational expressions, and consequently into the computer code, if the expansion was otherwise not used.

In the developed HOP computational expressions the adjoint Green's function is required rather than the forward one. Recall the relation between the adjoint and the forward Green's function, and the general reciprocity principle [3,7]:

$$\bar{G}^{+}(z,\mu;z',\mu') = \bar{G}(z,-\mu;z',-\mu') = \bar{G}(z',\mu';z,\mu). \tag{17}$$

Therefore,

$$g^{+}_{mn}(z,z') = g_{nm}(z',z) = (-1)^{m+n} g_{mn}(z,z') \tag{18}$$

which might be used to avoid repeated calculation and reduce storage requirements.

4. The adjoint radiance

Another issue regarding the implementation of the HOP computation that we would like to discuss briefly is the adjoint radiance for sources that have arbitrary vertical location and illuminate continuously in the upper or lower hemisphere as a function of zenith angle. Most codes do not directly provide for such sources, including the EDOM code.

This problem can be solved by simulation as has been generally discussed by Qin et al. [8]. For an azimuthally independent source function, $Q(\tau',\mu')$, which is a continuous function of μ', we can represent it using a vector of sources:

$$[Q(\tau',\mu'_1), Q(\tau',\mu'_2), \ldots, Q(\tau',\mu'_n)], \tag{19}$$

where μ'_j, $j = 1,2,\ldots,n$, are the Gauss quadrature abscissas, and each of the $Q(\tau',\mu'_j)$ is a parallel beam illuminating in a single direction. The radiance due to these sources, $\bar{I}_j(\tau,\mu)$, can readily be obtained using the EDOM code. The radiance due to $Q(\tau',\mu')$ can therefore be simulated using

$$\bar{I}(\tau,\mu) = 2\pi \sum_{j=1}^{n} w_j \bar{I}_j(\tau,\mu), \tag{20}$$

which is a reduced form of Eq. (51) in [8] and where w_j, $j = 1,2,\ldots,n$, are the Gauss quadrature weights.

To compute adjoint radiance, we firstly write the adjoint source function as $Q^{+}(\tau,\mu) = R(\tau,\mu)/\mu$ where $R(\tau,\mu)$ is the response function [6]. For example, if the effect is flux, the response function is $R(\tau,\mu) = \mu\delta(\tau-\tau')$, therefore the adjoint source function should be $Q^{+}(\tau,\mu) = \delta(\tau-\tau')$, where τ' is the vertical location where the flux is computed. Now we reverse the zenith direction of the adjoint source, i.e., $Q(\tau,\mu) = Q^{+}(\tau,-\mu)$, and simulate the radiance $I(\tau,\mu)$ due to the source $Q(\tau,\mu)$ using Eq. (20). The adjoint radiance can then be obtained by reversing the zenith direction of $I(\tau,\mu)$, i.e., $I^{+}(\tau,\mu) = I(\tau,-\mu)$.

5. Examples of Green's function and its expansion

We finally present some examples of the Green's function and the coefficients of its double series in Legendre polynomials. Shown in Figs. 1 and 2 are samples of the diffuse component of the averaged Green's function, $\bar{G}^{(\mathrm{dif})}(\tau,\mu;\tau',\mu')$, for an atmosphere model of a single homogeneous layer of optical thickness 1.0, single scattering albedo 1.0 and a two-term Henyey–Greenstein (TTHG) phase function [16] of parameters $\alpha = 0.965$, $g_1 = 0.75$ and $g_2 = 0.65$. The (Lambertian) surface albedo for this example is 0.2. In Fig. 1 we show $\bar{G}^{(\mathrm{dif})}$ when both the source and the observer are at fixed altitude (optical thickness). The saddle pattern observed in the upper left and lower right panels shows the forward peak of the radiance around the direction of the source, and this forward

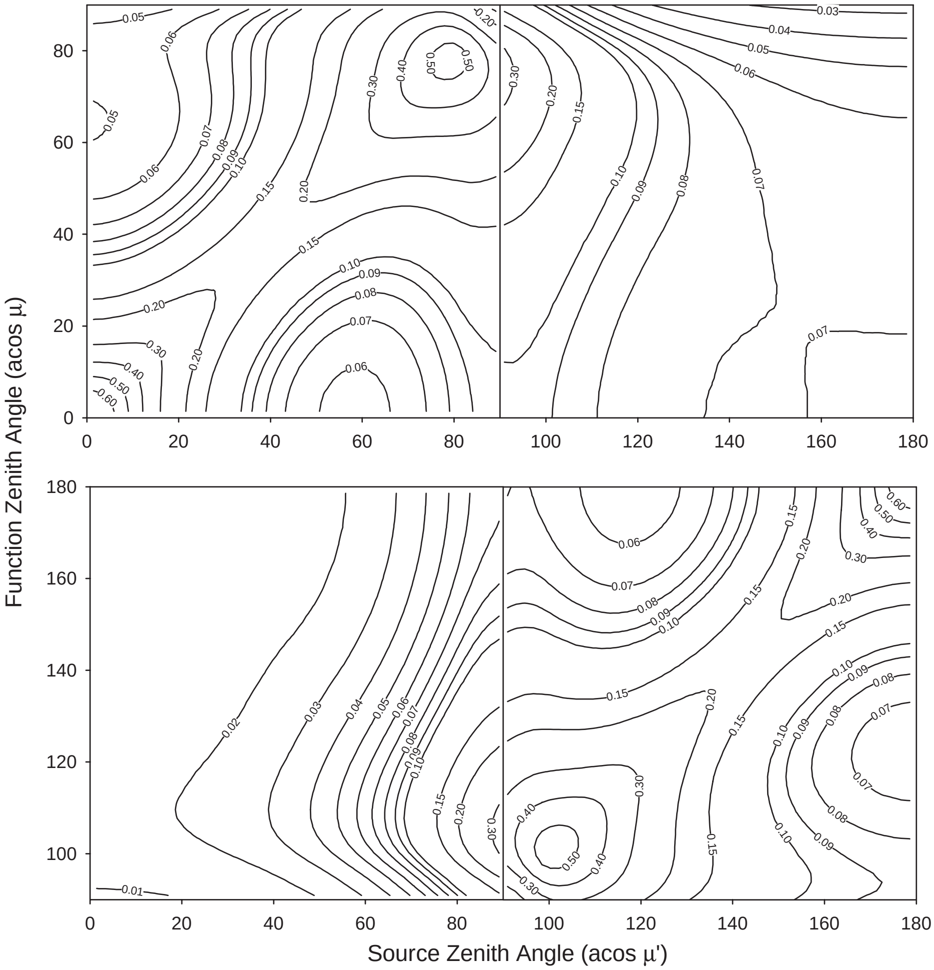

Fig. 1. The averaged Green's function $\bar{G}(\tau,\mu;\tau',\mu')$ for a model atmosphere of single homogeneous layer (see text for the model parameters) and sources located at the middle of the atmosphere. The upper panels are the function in the upper hemisphere at the top of the atmosphere and the lower panels are the function in the lower hemisphere at the bottom of the atmosphere.

peak becomes stronger when the source is approaching either the horizontal or the vertical direction. In Fig. 2 we show a full picture of $\bar{G}^{(\mathrm{dif})}$ for a fixed source (illuminating direction and location). It shows that the upward radiance (left panel) becomes less variable when the observer moves towards the surface. Eventually, it becomes a constant at the bottom of the atmosphere—at this point the radiance is just the radiance reflected by the surface which is assumed to be a Lambertian reflector and therefore reflects isotropically. The downward radiance (right panel) also shows similar trend but in the reverse direction—it becomes less variable when the observer moves towards the upper boundary of the atmosphere and eventually it becomes zero indicating that no radiance enters the atmosphere from above.

In Figs. 3 and 4 we present examples of the expansion coefficients of the Green's function, which show us how the coefficients may behave. Note that these two figures show the coefficients of the

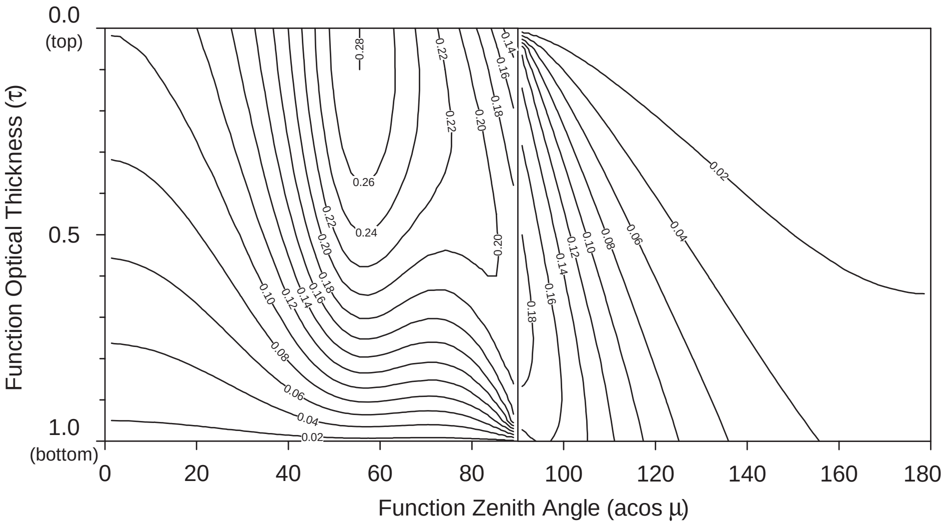

Fig. 2. The averaged Green's function $\bar{G}(\tau,\mu;\tau',\mu')$ for the same atmosphere model as Fig. 1 and for a fixed source at the bottom of atmosphere ($\tau' = 1.0$) and illuminating in the zenith angle (a $\cos\mu'$) of 53.63°.

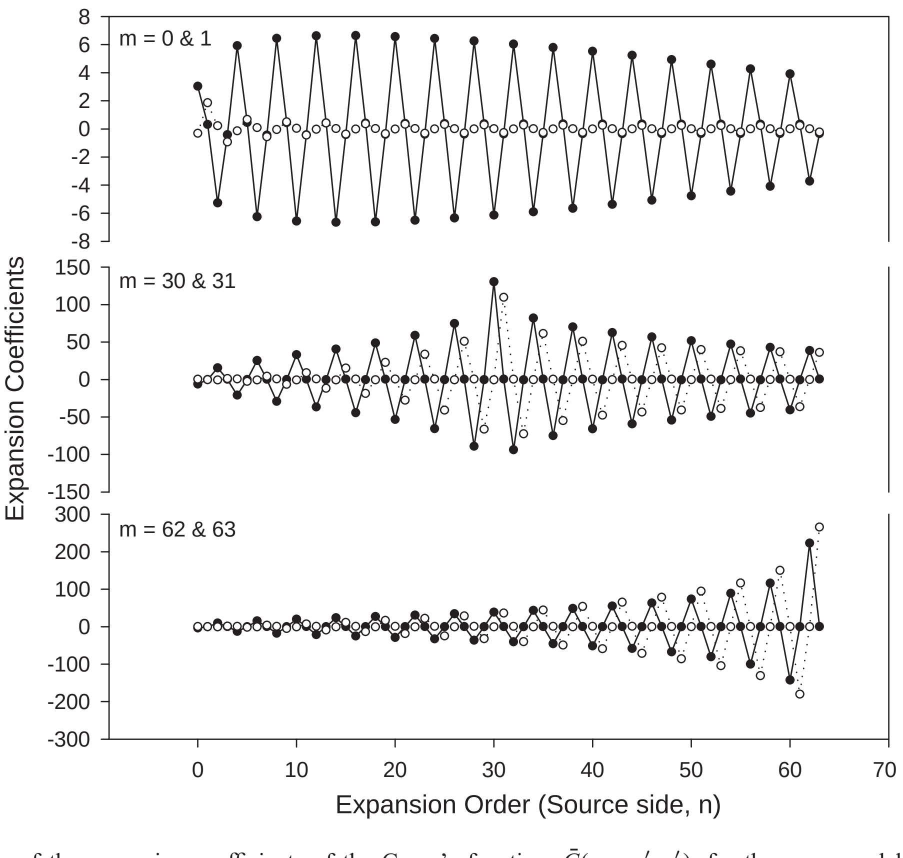

Fig. 3. Examples of the expansion coefficients of the Green's function, $\bar{G}(\tau,\mu;\tau',\mu')$, for the same model atmosphere as Figs. 1 and 2. Here m is the function side expansion order and both τ and τ' are 0.0 (i.e. at the top of the atmosphere). The solid circles represent the even order terms and the empty circles the odd order terms.

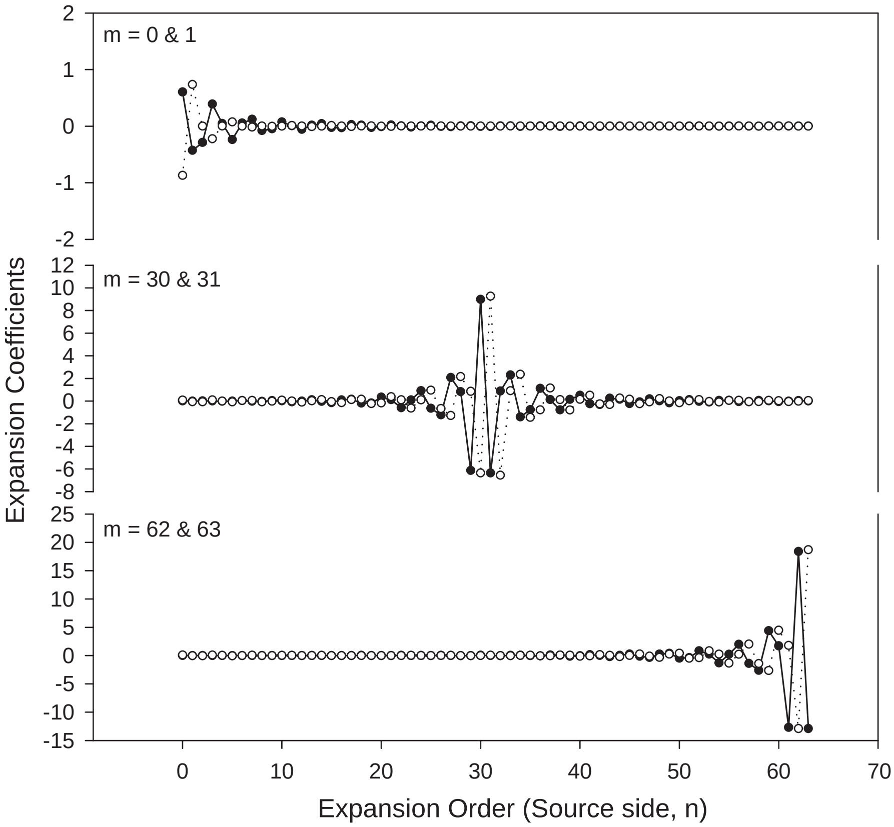

Fig. 4. Examples of the expansion coefficients of the Green's function, $\bar{G}(\tau, \mu; \tau', \mu')$, for the same model atmosphere as Figs. 1 and 2. Here m is the function side expansion order and $\tau = 0.0$ and $\tau' = 0.5$ (i.e. the middle of the atmosphere). The solid circles represent the even order terms and the empty circles the odd order terms.

total function, rather than the diffuse component only as was the case of Figs. 1 and 2. Fig. 3 shows a typical case when both the source and the observation point are at the same altitude, while Fig. 4 shows the case when the two sides are at different altitudes. The most noticeable characteristic shown is that when the two sides are at different altitudes, which is the majority of cases, the number of significant terms is rather limited and the significant terms are centered around the term when the expansion order of the observation side, m, equals the source side expansion order, n.

6. Summary

In this article, we discussed two key issues regarding the implementation of the HOP computational expressions developed in the accompanying paper [1]. The most important of these is the detailed Green's function, which requires solving radiative transfer problems with sources of arbitrary vertical location and illuminating direction. With the support of the EDOM code [8], we are able to obtain this function with high efficiency. Another issue discussed is the expansion of the Green's function into a double series of Legendre polynomials. It is found that such expansion has brought us a number of benefits, both theoretically and computationally. However, it has been found that a direct expansion using Eq. (10) is very time consuming—it takes more time than to obtain the Green's function. Therefore a much more efficient scheme has been introduced and significant reduction of the amount of computation involved in the expansion is achieved. We also discussed very briefly the calculation of adjoint radiance when the adjoint source has arbitrary vertical location and illuminates continuously in a hemisphere, such as those corresponding to flux and heating rate.

Examples of the averaged Green's function and its expansion coefficients are presented. Complex patterns of the Green's function are observed in the figures which indicates that, to compute integrations over the source and radiance phase space accurately, it is necessary to obtain the value of the function at a very fine grid of the source and radiance phase spaces. The coefficient figures show that, when the source and the observer are at different altitudes, only a very limited number of terms is significant, which may be used to reduce the storage requirement and improve computational efficiency.

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