Multi-coupled single scattering method of solving vector radiative transfer equations*

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A new method of multi-coupled single scattering (MCSS) for solving a vector radiative transfer equation is developed and made public on Internet. Recent solutions from Chandrasekhar's X–Y method is used to validate the MCSS's result, which shows high precision. The MCSS method is theoretically simple and clear, so it can be easily and credibly extended to the simulation of aerosol/cloud atmosphere's radiative properties, which provides effective support for research into polarized remote sensing.

Keywords: vector radiative transfer, multi-coupled single scattering method

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1. Introduction

With the growth of remote sensing on the Earth's aerosol[1−3] and cloud,[4] especially in polarizing detection,[5−7] the classical radiative transfer theory constantly plays a fundamental role in scheme development of optical remote sensing and verification of an inversion result on atmospheric properties.[2,4,8,9]

The radiative transfer theory originated in astrophysicists' investigations on stellar structure in the early 20's century, and is well founded by Chandrasekhar's classical monograph,[10] in which the Chandrasekhar's X–Y method of solving radiative transfer equations (RTE) for general phase function is given, solutions of RTE in isotropic and Rayleigh scattering atmosphere is tabulated for both cases of finite and infinite optical depth with a Lambert's ground. Until recently, effort was still devoted in finding the precise solutions of RTE in the Rayleigh atmosphere, using the X–Y method.[11,12]

Though Chandrasekhar's X–Y method is the most accurate one in solving radiative transfer equation, it is mathematically complicated, and will be more complex when dealing with an aerosol atmosphere, as the scattering phase function's Legendre polynomial expression grows longer.

We provide a multi-coupled single scattering (MCSS) method as an alternative. The approximation principle is discussed, and results got from MCSS are plotted and made public on Internet in comparison with the accurate solution of Natraj and Hovenier.[11,12] We follow the definitions and notations of Chandrasekhar[10] for basic physical and geometrical quantities in theory formulation, which are considered elegant and classic.

2. Model and method

2.1. Single scattering approximation

For a plane-parallel atmosphere of optical thickness τ_1, RTE admits a formal solution[2] for emergent intensities at the border

$$\begin{aligned} & I(0,+\mu,\varphi) \\ &= I(\tau_1,\mu,\varphi)\,\mathrm{e}^{-\tau_1/\mu} \\ &\quad + \int_0^{\tau_1} \Im(t,\mu,\varphi)\,\mathrm{e}^{-t/\mu}\frac{\mathrm{d}t}{\mu}, \quad (1 \geqslant \mu > 0), \quad (1) \\ & I(\tau_1,-\mu,\varphi) \\ &= I(0,-\mu,\varphi)\,\mathrm{e}^{-\tau_1/\mu} + \int_0^{\tau_1} \Im(t,-\mu,\varphi) \\ &\quad \times \mathrm{e}^{-(\tau_1-t)/\mu}\frac{\mathrm{d}t}{\mu}, \quad (1 \geqslant \mu > 0). \quad (2) \end{aligned}$$

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For the scattering atmosphere we considered in this paper, the source function $\Im(\tau;\vartheta,\varphi)$ is

$$\begin{aligned}&\Im(\tau;\vartheta,\varphi)\\&=\frac{1}{4\pi}\oint_{4\pi}p(\vartheta,\varphi;\vartheta',\varphi')I(\tau;\vartheta',\varphi')\,\mathrm{d}\Omega'\\&\quad+\frac{1}{4}F_0\exp\left(-\frac{\tau}{|\mu_0|}\right)p(\vartheta,\varphi;\vartheta_0,\varphi_0),\end{aligned}\tag{3}$$

where πF_0 is the energy flux of solar.[10]

When optical depth is small, single scattering is dominant, multiple scattering can be approximately neglected.[10,13−16] Thus, equations (1), (2), and (3) change to a simpler form

$$\begin{aligned}&I(\tau,\mu,\varphi)\\&=I(0,\mu,\varphi)\exp\left(-\frac{\tau}{|\mu|}\right)+\int_0^\tau\Im(t,\mu,\varphi)\frac{\mathrm{d}t}{|\mu|},\\&(-1\geqslant\mu\geqslant 1,\mu\neq 0),\end{aligned}\tag{4}$$

$$\begin{aligned}&\Im(\tau;\vartheta,\varphi)\\&=\frac{1}{4\pi}\oint_{4\pi}p(\vartheta,\varphi;\vartheta',\varphi')I(0;\vartheta',\varphi')\\&\quad\times\exp\left(-\frac{\tau}{|\mu'|}\right)\mathrm{d}\Omega'+\frac{1}{4}F_0\exp\left(-\frac{\tau}{|\mu_0|}\right)\\&\quad\times p(\vartheta,\varphi;\vartheta_0,\varphi_0).\end{aligned}\tag{5}$$

Note that in the single scattering approximation, the source function is away from extinction, so we are mathematically free to choose the border $\tau=0$ as where light is penetrating, and τ grows in the direction incident light propagates. Now the second part of Eq. (4) can be expressed analytically as

$$\begin{aligned}&\int_0^\tau\Im(t,\vartheta,\varphi)\frac{\mathrm{d}t}{\mu}\\&=\frac{1}{4\pi}\int_0^{2\pi}\mathrm{d}\varphi'\int_0^\pi\left|\frac{\mu'}{\mu}\right|I(0,\vartheta',\varphi')\\&\quad\times\left[1-\exp\left(-\frac{\tau}{|\mu'|}\right)\right]p(\vartheta,\varphi;\vartheta',\varphi')\sin\vartheta'\,\mathrm{d}\vartheta'\\&\quad+\frac{1}{4}\left|\frac{\mu_0}{\mu}\right|\left[1-\exp\left(-\frac{\tau}{|\mu_0|}\right)\right]\\&\quad\times p(\vartheta,\varphi;\vartheta',\varphi')F_0.\end{aligned}\tag{6}$$

Every factor in Eq. (6) gets a clear physical meaning: $\mu' I(0,\vartheta',\varphi')\sin\vartheta'\,\mathrm{d}\vartheta'\,\mathrm{d}\varphi'$ means the loss of Z-direction energy flux of incident light at direction (ϑ',φ') in solid angle $\mathrm{d}\Omega=\sin\vartheta'\,\mathrm{d}\vartheta'\,\mathrm{d}\varphi'$, $p(\vartheta,\varphi;\vartheta',\varphi')/4\pi$ describes the redistribution of damped light energy, and $1/\mu$ is the inclined coefficient of optical thickness.

The fact that phase function $p(\vartheta,\varphi;\vartheta',\varphi')$ enters Eq. (6) in a linear way, guarantees every kind of phase function being of the same complexity in the numerical calculation of integral (6).

2.2. Multi-coupled procedure

Single scattering approximation is valid in a small optical depth but no more in optical thick conditions. So atmospheres must be divided into slices in order to use the single scattering approximation. Single scattered light of each layer will be the incident light of its neighbor, we call this the multi-coupled (MC) procedure. A computer program may be used to solve the complicated problem brought by multi-scattering.

In this procedure, damped solar flux and scattered light is simulated to transfer from one layer to another according to Eqs. (4) and (6), finally it damps to a small threshold value because not all light energy is reflected at the ground, also light will escape at the top of atmosphere (Fig. 1). Then the scattered light's intensity of any direction at every layer's border can be gained by summing up the intensity value each time light transfers through.

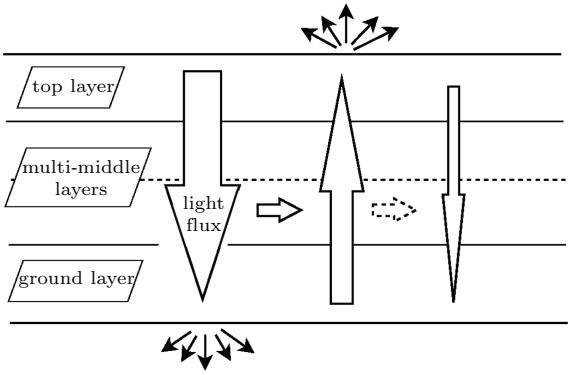


Fig. 1. Schematic plot of a multi-coupled procedure, the scattered light damps to 0 after several trips in the atmosphere.

Note that the MC procedure describes the response of the solar flux "at one moment", it means the solar flux ends its life when it hits the ground and changes into reflected light, while scattered light stimulated by a "previous" solar flux is still transmitting everywhere until it is absorbed by the ground or escaped out of the atmosphere. Because solar flux is constantly entering the atmosphere at approximately fixed intensity and direction in a short time interval, the scattered light intensity achieved by the MC procedure is also constant and is naturally what the sensors detect.

2.3. Vector radiative transfer

Polarized light is commonly characterized by the Stocks vector $\boldsymbol{I}=(I,Q,U,V)$, accordingly, the phase

function changes to the phase matrix $\boldsymbol{P}(\Theta)$. The vector version of RTE can be found by simply replacing the scalar symbol to its vector version, except that the phase matrix needs to further transform to a fixed reference plane of Stocks vector, that is $\boldsymbol{L}(\chi_2) * \boldsymbol{P}(\Theta) * \boldsymbol{L}(\chi_1)$, where rotate transforming matrix $\boldsymbol{L}(\chi)$ is defined as[15]

$$\boldsymbol{L}(\chi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(2\chi) & \sin(2\chi) & 0 \\ 0 & -\sin(2\chi) & \cos(2\chi) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{7}$$

$\boldsymbol{L}(\chi_1)$ means transforming the incident light's reference plane to the scatter plane, and $\boldsymbol{L}(\chi_2)$ means the scatter plane to the scatter light's reference plane. It is conveniently chosen as the plane determined by light direction and Z axis as the reference plane. Usually, transform angles χ_1 and χ_2 are obtained by spherics geometry which is suffered from the confusing signs of angles, remembering that χ cannot be specified by a single arcsin or arccos function because the field of definition of χ is $(-\pi, \pi]$ for clockwise and anti-clockwise rotation. So we adopt a pure analytic geometry way, the final result is (the deduction can be downloaded at project's website):

$$\cos(2\chi_1) = \frac{[\cos(\theta_i)\cos(\phi_i-\phi_s)\sin(\theta_s) - \cos(\theta_s)\sin(\theta_i)]^2 - \sin^2(\theta_s)\sin^2(\phi_i-\phi_s)}{\sin^2(\Theta)}, \tag{8}$$

$$\cos(2\chi_2) = \frac{[\cos(\theta_s)\cos(\phi_i-\phi_s)\sin(\theta_i) - \cos(\theta_i)\sin(\theta_s)]^2 - \sin^2(\theta_i)\sin^2(\phi_i-\phi_s)}{\sin^2(\Theta)}, \tag{9}$$

$$\sin(2\chi_1) = \frac{2\sin(\theta_s)\sin(\phi_i-\phi_s)[\cos(\theta_i)\cos(\phi_i-\phi_s)\sin(\theta_s) - \cos(\theta_s)\sin(\theta_i)]}{\sin^2(\Theta)}, \tag{10}$$

$$\sin(2\chi_2) = \frac{2\sin(\theta_i)\sin(\phi_i-\phi_s)[\cos(\theta_s)\cos(\phi_i-\phi_s)\sin(\theta_i) - \cos(\theta_i)\sin(\theta_s)]}{\sin^2(\Theta)}. \tag{11}$$

3. Algorithm realization

Transform Eqs. (4) and (6) to vector version and approximate the integral by summation

$$\begin{aligned} &\boldsymbol{I}(\tau,\theta_s,\phi_s) \\ &= \boldsymbol{I}(0,\theta_s,\phi_s)\exp\left(-\frac{\tau}{|\mu_s|}\right) \\ &\quad + \frac{1}{4\pi}\sum_{\theta_i=0}^{\pi/2}\sum_{\phi_i=0}^{2\pi}\frac{\mu_i}{\mu_s}\left[1-\exp\left(-\frac{\tau}{|\mu_i|}\right)\right] \\ &\quad \times \boldsymbol{L}_2 * \boldsymbol{P}(\Theta) * \boldsymbol{L}_1 * \boldsymbol{I}(0,\theta_i,\phi_i)\Delta\Omega_i \\ &\quad + \frac{\mu_0}{4\,\mu_s}\left[1-\exp\left(-\frac{\tau}{|\mu_0|}\right)\right] \\ &\quad \times \boldsymbol{L}_2 * \boldsymbol{P}(\Theta) * \boldsymbol{L}_1 * \boldsymbol{F}_0. \end{aligned} \tag{12}$$

This equation alone describes how one layer's polarized scattered light is coupled to its neighbor, causing further more the neighbor's outward scattering light. Calculation of scatter light $\boldsymbol{I}(\tau,\theta_s,\phi_s)$ at all directions needs a loop of rank 4, for θ_s, ϕ_s, θ_i, and ϕ_i, respectively.

The overall procedure of calculating program is quite straight as depicted in Fig. 1 and 2. There are 6 major steps listed below.

(i) Initialization: arrange a bunch of layers with a top-layer and a ground-layer;

(ii) The top-layer receives downward solar incident light, start calculating the procedure according to steps (iii)–(vi);

(iii) Each layer's emergent scattered light and the damped solar flux (if present) serve as the incident light of its neighbor layer, light is simulated to transfer layer by layer according to the MC procedure Eq. (12), as depicted by Fig. 1;

(iv) When light reaches ground layer, calculate the up-scattered light according to the user specified BRDF model;

(v) When light reaches the top layer, up-emergent light will not enter our calculation any more, while down-scattered light goes on transmitting to the lower layers;

(vi) Scattered light finally damps to a small threshold because of the energy lost in top and ground layers, the calculation is over. Collect all scattered light through the border of the top and ground layers (or any other interesting layers) for the final result.

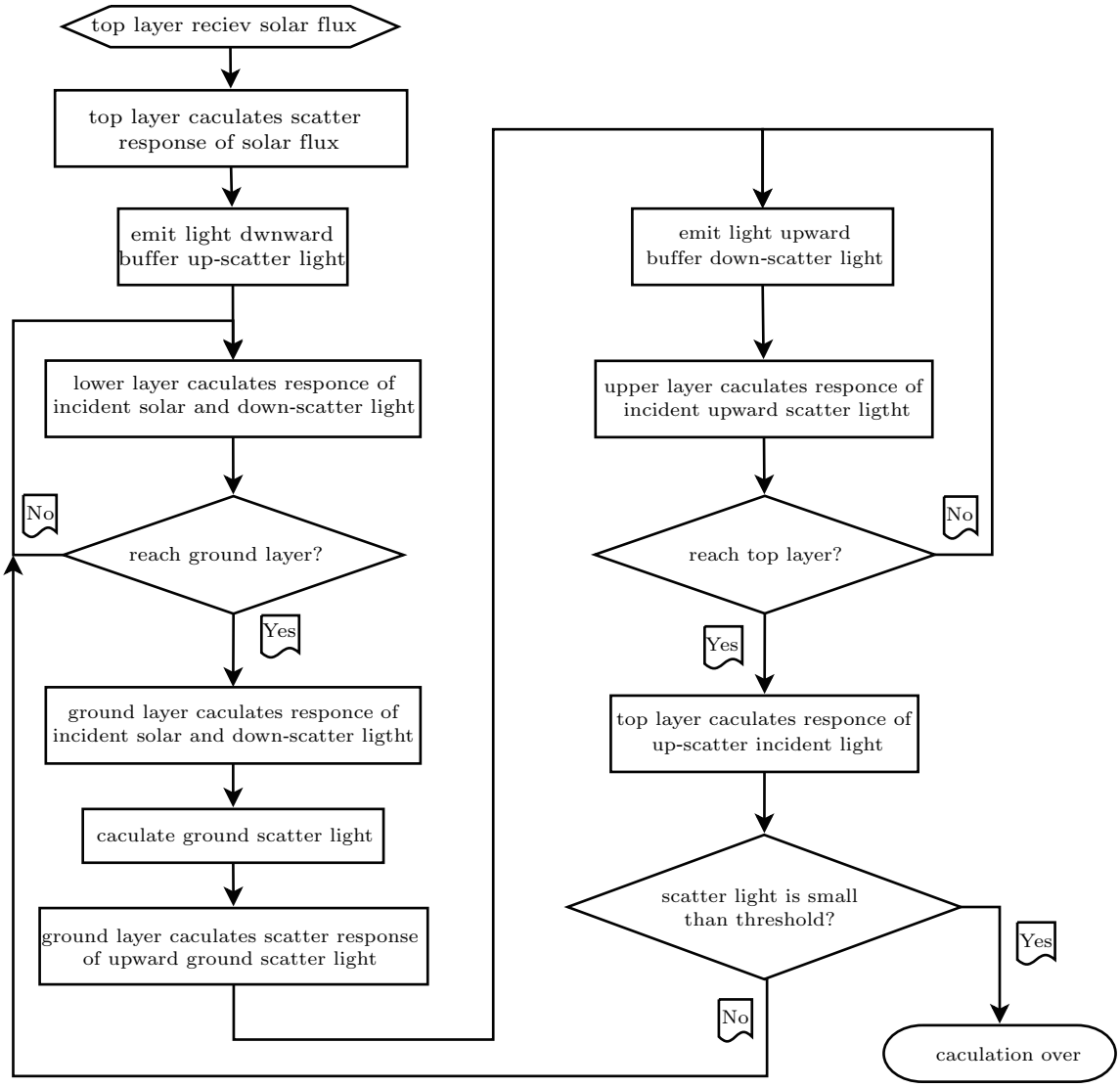


Fig. 2. Calculation procedure of the MCSS algorithm.

4. Validation

4.1. Conservation of energy

The radiative transfer equation describes the differential variation of light intensity, conservation of energy is the principle law hidden behind it. In the case of a conservative plane parallel to the atmosphere, conservation of energy is equivalent to

$$\frac{\mathrm{d}\boldsymbol{F}_z}{\mathrm{d}z} = 0 \quad \text{or} \quad \boldsymbol{F}_z = \text{constant}. \tag{13}$$

It is easy to prove that equations (4) and (6) satisfy conservative condition (13) theoretically, while the error in realization depends on how many angles in Eq. (12) are divided.

4.2. Comparison with Chandrasekhar's X–Y function method

The creditability of this MCSS algorithm focuses on how well the multi-coupled procedure corrects the approximation of single scattering.

We use a 2° step in Eq. (12), and up to 1600 layers are divided for two given optical thicknesses $\tau = 1$ and 2 of Rayleigh atmosphere ($\tau = 0.00125$ for single scattering layer). Only the result for the case of Lambert's ground with albedo 0.8 is plotted (Fig. 3), where more multiple scattering happens compared to dark ground and small optical thickness, hence this can serve as a rigorous test condition. More tabulated results can be downloaded at project's website.

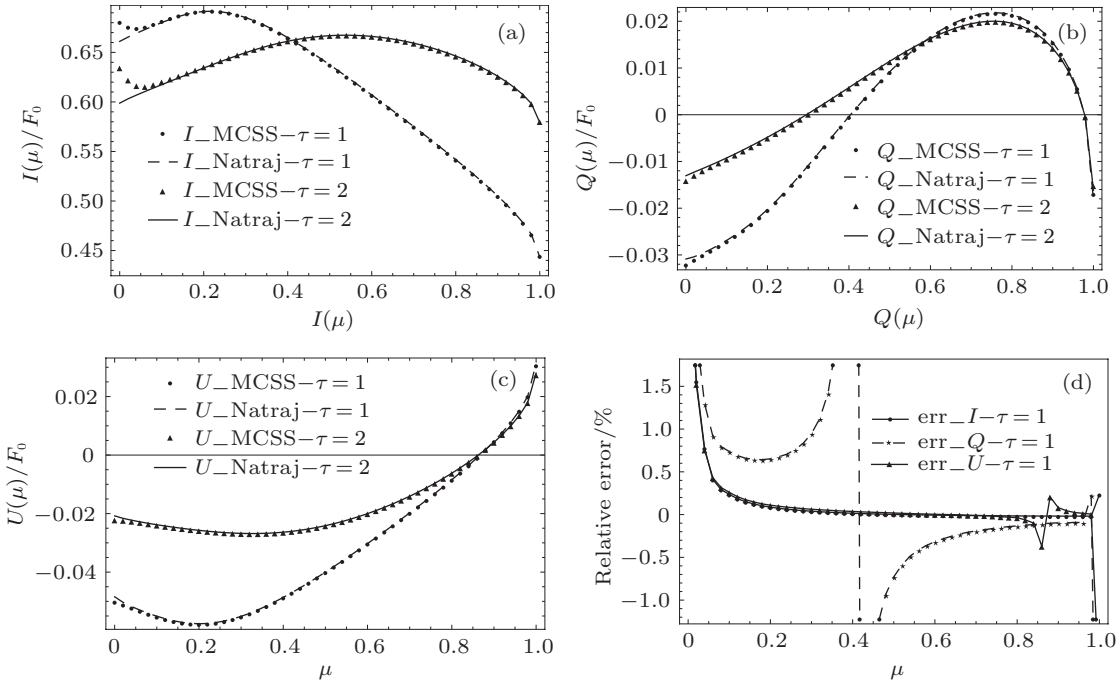


Fig. 3. Downward I, Q, U for $\tau = 1$ and 2, ground albedo 0.8, $\mu_0 = 0.8$, at azimuth $\phi = 30°$ relative to solar direction (MCSS results are interpolated to μ of Natraj's result in order to compare). The increase of relative error of Q and U near $\mu = 0.4$ and 0.85 is because Q and U cross 0, where a pole generates in Eq. (14).

The result shows an accurate approximation to Natraj's which is considered an exact solution, the relative difference defined as:

$$\text{Rel_err} = \frac{\boldsymbol{I}_{\text{MCSS}} - \boldsymbol{I}_{\text{Natraj}}}{\boldsymbol{I}_{\text{Natraj}}} \tag{14}$$

is below 0.1% for zenith 3.5° away from the horizontal direction, with an error of about 5% for horizon.

This can be interpreted clearly as follows: the optical thickness tends to be infinite as zenith angle $\vartheta \to \pi/2$, so multiple scattering will be dominant. The rising on the curve near to zenith $\pi/2$ shows the extinction caused by multiple scattering is insufficiently simulated by the MCSS algorithm near horizontal direction, and accordingly, there will be a little negative error of light intensity at directions near the vertical one because of conservation of energy.

5. Calculation speed and accuracy

Calculation speed and accuracy depend on only two approximations in an MCSS algorithm, that is, 1) N_l: the number of layers in the atmosphere is divided; 2) N_p: the number of summation points used in Eq. (12).

Theoretically, the finer the atmosphere layer is divided (bigger N_l), the more multi-scattering progress is simulated in the algorithm; meanwhile, better precision will be obtained if more N_p are used to approximate the integral in Eq. (6).

However, because the multiple scattering process is insufficiently simulated by the MCSS near the horizontal direction, the number of layers and summation points have a subtle relationship: if we increase N_p, there will be more points near the horizon (e.g. $\mu < 0.1$), as a result, more N_l are needed in order to gain accurate results in the horizontal direction and consequently other directions. Table 3 shows a counter-example, where the calculation error of the case $N_\text{p} = 90$ is slightly bigger than $N_\text{p} = 60$ for the same $N_\text{l} = 1000$.

As tabulated in Table 1, the calculation time depends linearly on N_l, while exponentially depends on N_p, asymptotically N_p^4.

The relationship between calculation accuracy and N_l is tabulated in Table 2, it is shown that a bigger N_l will always gain more precise results, regardless how many N_p are used.

The subtle relationship between N_p and N_l is shown in Table 3. For Rayleigh atmosphere, the phase function varies smoothly, so the precision effect of N_p is not as remarkable as the effect of N_l is.

The current version of the MCSS code uses the Newton–Cotes method of 1st rank (the trapezoidal rule) in Eq. (12). It is well known that Gaussian quadrature can improve the calculating efficiency,

while special consideration is needed in practice according to the above analyses: 1) there should be more points in zeniths away from the horizontal direction; 2) there should be more points near the solar direction as the phase function of aerosol varies greatly in forward peak.

Table 1. Comparison of calculation time for different number of layers (N_l) and points (N_p), time unit is in minutes.

$N_\mathrm{l}\backslash N_\mathrm{p}$	50	60	70	80	90
10	0.18	0.33	0.55	0.93	1.47
50	1.02	2.02	3.23	5.35	8.68
100	2.03	4.32	6.38	10.72	17.32
500	9.93	20.50	33.32	53.48	84.57
1000	19.72	38.37	68.47	110.88	184.55

Table 2. Comparison of relative error for different N_l, same $N_\mathrm{p} = 90$ is used here. Relative error is got by average $|\mathrm{Err}(\mu)|$ for $\mu > 0.1$ at one azimuth plane $\phi = 90°$ relative to solar azimuth, Rayleigh atmosphere, $\tau = 1$, ground albedo 0.

err $\backslash N_\mathrm{l}$	10	50	100	500	1000
rel_err_I %	6.116	1.187	0.590	0.116	0.057
rel_err_Q %	50.255	9.456	4.764	1.078	0.624
rel_err_U %	8.546	1.635	0.811	0.157	0.076

Table 3. Comparison of relative error at different N_p. Relative error is calculated in the same way as Table 2, Rayleigh atmosphere, $\tau = 1$, ground albedo 0. $N_\mathrm{l} = 1000$ layers are divided in every case.

$N_\mathrm{p}\backslash$err	rel_err_I %	rel_err_Q %	rel_err_U %
90	0.05720489	0.62361654	0.07556234
80	0.05910936	0.58414837	0.07469279
70	0.0556337	0.69448626	0.0736686
60	0.05406751	0.80079541	0.07020558
50	0.0520473	0.94289578	0.16381802

So, a self-adaptive piecewise Gaussian quadrature with the above two guiding rules is the most suitable for the MCSS algorithm, which is under development and will be released soon with the next version's code for better computational efficiency.

6. Conclusion

The MCSS algorithm is constructed and well validated for the case of an ideal Rayleigh atmosphere. The realization of MCSS (using C++) and some typical results are made public on the web: http://code.google.com/p/vrt-calculate. It is a simple, yet effective method dealing with complicated atmosphere and ground conditions, which will be helpful to the quantification of polarized remote sensing.

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