Atmospheric radiative transfer modeling using the Monte Carlo method

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April 2010

Contents

1 Simulation of random variables

Assume that a continous random variable ξ is defined by its probability density function p(x), defined on the interval $x_{min} \leq x \leq x_{max}$. The normalized cumulative distribution $F(x)$ is defined as

$$F(x) = \frac{\int_{x_{\rm min}}^{x} p(x')dx'}{\int_{x_{\rm min}}^{x_{\rm max}} p(x')dx'} \tag{1}$$

If we want to generate a sample of random numbers which are distributed according to $p(x)$, we may use a random number generator that produces uniformly distributed random numbers r between 0 and 1 and solve

$$F(\xi) = r \tag{2}$$

Inversion of F gives

$$\xi = F^{-1}(r) \tag{3}$$

1.1 Rayleigh phase function

The scattering phase function can be interpreted as the probablity density function for the scattering direction.
If the particles are small compared to the wavelength of the radiation (Rayleigh scattering), the phase function $P_{\rm R}$ is

$$P_{\rm R}(\theta) = \frac{3}{4}(1+\cos^2\theta) \tag{4}$$

or with $\mu = \cos\theta$

$$P_{\rm R}(\mu) = \frac{3}{4}(1+\mu^2) \tag{5}$$

Here θ is the scattering angle. Scattering of solar radiation in the atmosphere by molecules is described by Rayleigh scattering.
In order to calculate a random sample of scattering angles we have to solve

$$r = F(\mu) = \frac{\int_{-1}^{\mu} \frac{3}{4}(1+\mu'^2)\mathrm{d}\mu'}{\int_{-1}^{1} \frac{3}{4}(1+\mu'^2)\mathrm{d}\mu'} \tag{6}$$

This yields the following cubic equation:

$$\mu^3 + 3\mu - 8r + 4 = 0 \tag{7}$$

The solution of a cubic equation is given by Cardano's formula.

$$\mu = u - 1/u \tag{8}$$

with

$$u = (-q/2 + \sqrt{D})^{1/3} \tag{9}$$
$$q = -8r + 4 \tag{10}$$
$$D = 1 + q^2/4 \tag{11}$$

Figure 1 shows the Rayleigh phase function, the integated (cumulative) phase function and a histogram of randomly sampled μ-values.

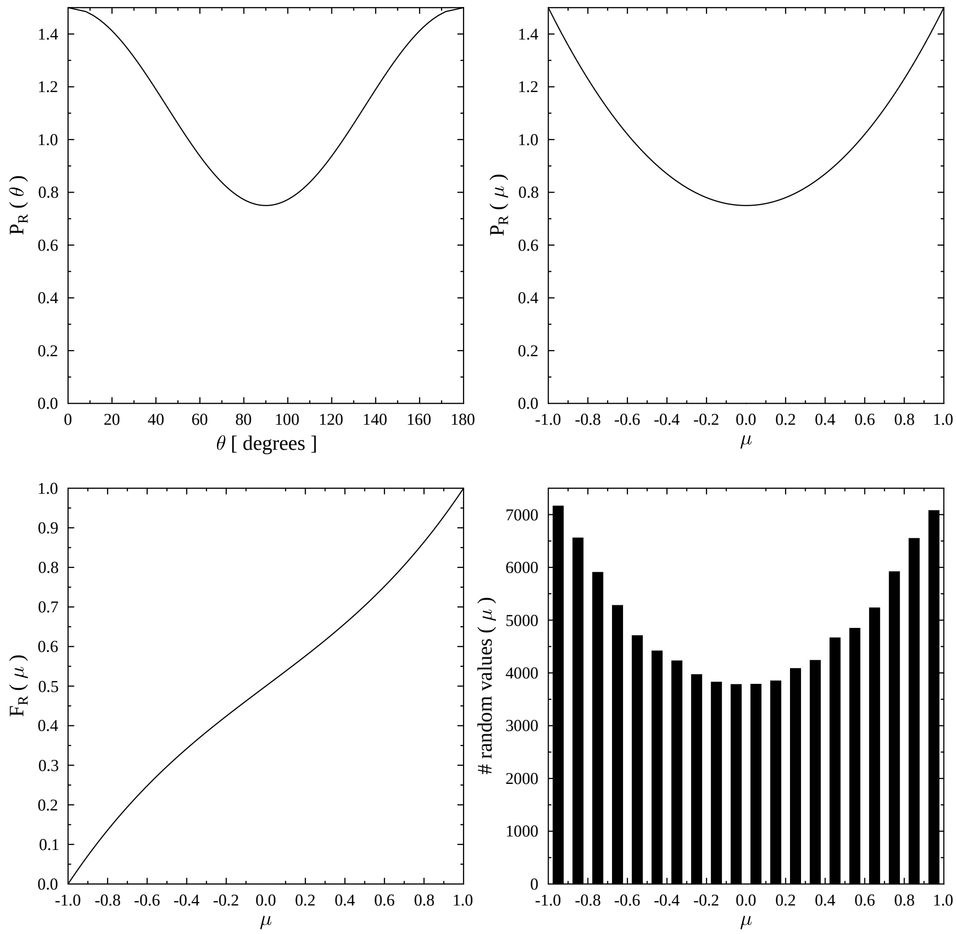

Figure 1: Top left: P_{R} as a function of the scattering angle θ. Top right: P_R as a function of the cosine of the scattering angle $\mu = cos(\theta)$. Bottom left: Cumulative probability density function for Rayleigh scattering. Bottom right: Histogram of randomly sampled values of μ using 100.000 random numbers.

1.2 Henyey-Greenstein phase function

For larger particles in the atmosphere like cloud droplets/particles or aerosols the scattering phase functions can be rather complex (see Fig. 2). An analytical approximative fit for this kind of phase functions has been proposed by *Henyey and Greenstein* [1941]:

$$P_{\mathrm{HG}}(\mu) = \frac{1-g^2}{(1+g^2-2g\mu)^{3/2}} \tag{12}$$

Here g is the asymmetry parameter which describes the distribution of forward and backward scattering. $g \to 1$ means complete forward scattering, $g = 0$ means isotropic scattering and for $g = -1$ we have complete backward scattering.

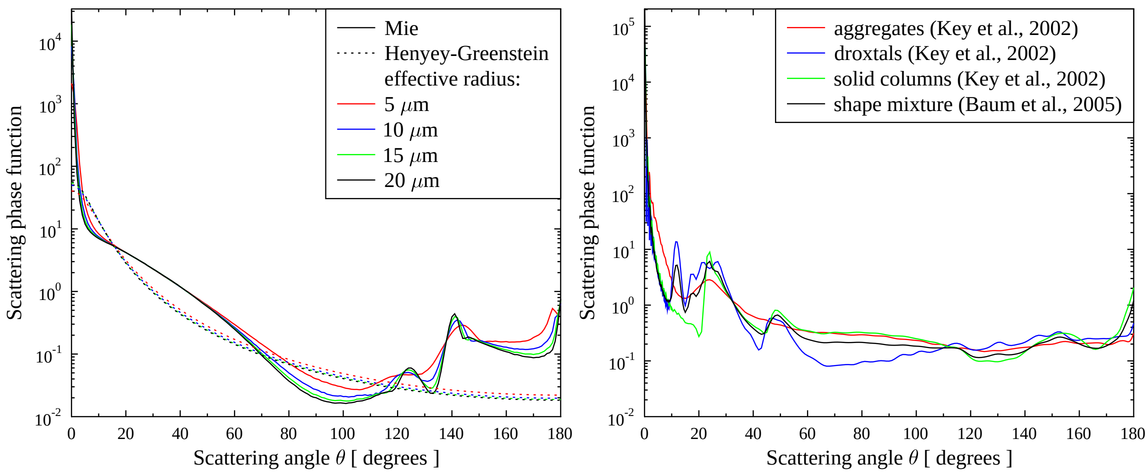

Figure 2: (Left) Mie scattering phase functions for water clouds with effective radii 5, 10, 15, and 20 μm (solid lines). Also shown are the respective Henyey-Greenstein approximations for the four cases, as provided by the parameterization of *Hu and Stamnes* [1993] (dashed lines). (Right) Ice cloud scattering phase functions for an effective radius of 50μm using different parameterizations; (red) parameterization by *Key et al.* [2002] for rough aggregates; (blue) same but for droxtals; (green) same for solid columns, (black) parameterization by *Baum et al.* [2005]; the figure shows the typical behaviour of non-spherical particles, in particular the large difference in the sideward scattering direction compared to spherical particles.

1.3 Optical thickness and photon path

The distance s that a photon travels between two interactions with the medium is related to the optical thickness of the medium. However, theoretically it is possible that the photon reaches the surface without any interactions, even if the medium has a very large optical thickness.

The transmission T is defined as

$$T = \exp(-\int_0^s \beta_{\text{ext}} ds') = \exp(-\tau) \tag{13}$$

where β_{ext} is the extinction coefficient, s the distance and τ the optical thickness. The transmission may be interpreted as the probabily that the photon travels the distance τ without interactions:

$$P(\tau) = \exp(-\tau) \tag{14}$$

1.4 Surface reflection

The reflection of most surfaces depends on the incoming direction of the photon as well as on the direction of the reflection. This is modeled using Bidirectional Reflectance Distribution Functions (BRDFs). There are simpler approximations, for instance the Lambertian reflection. Lambert's cosine law says that the radiant intensity observed from a "Lambertian" surface is proportional to the cosine of the angle θ between the observer's line of sight and the surface normal. This means that when a surface is viewed from any angle it has the same apparent radiance (see Fig.: 3).

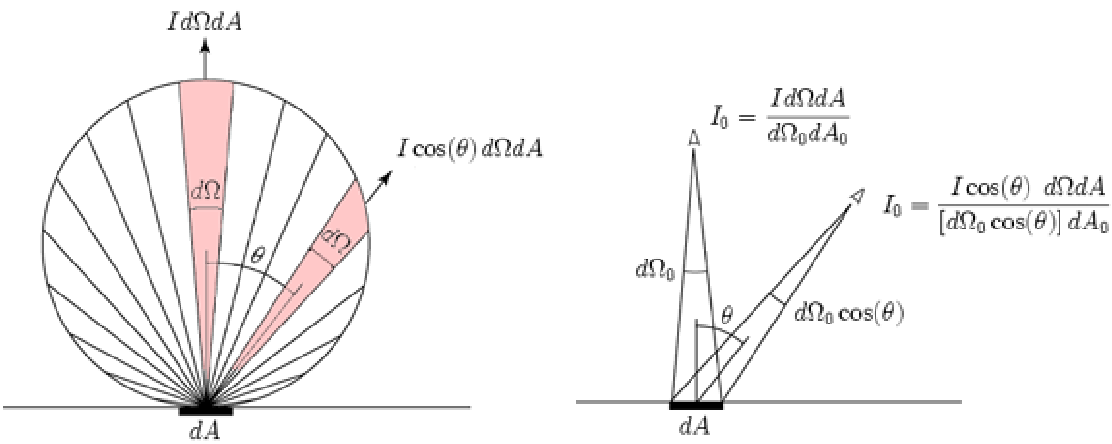

Figure 3: Illustration of a Lambertian surface: (Left) Emission/reflection in normal and off-normal direction. (Right) Observed intensity for a normal and off-normal observer; dA_0 is the area of the observing aperture and $d\Omega_0$ is the solid angle subtended by the aperture from the viewpoint of the emitting area element. Source: Wikipedia.

The probability distribution for the reflected direction of a Lambertian surface is given by:

$$p(\theta) = \cos\theta \tag{15}$$

1.5 Tasks

1. Verify Eq. 7. Write a function that generates random scattering angles for Rayleigh scattering and reproduce Fig. 1.

2. Plot the Henyey-Greenstein phase function for various asymmetry parameters. Generate random values of scattering angles for an asymmetry parameter of 0.85 (typical value for water clouds).

3. Generate random values of optical thickness τ corresponding to the distance s that a photon travels without interaction with the scattering medium.

4. Generate random values of the reflection direction by a Lambertian surface.

   Verify the results by plotting histograms of the sampled random numbers.

2 Cloud scattering

2.1 Setup: Homogeneous cloud layer

We would like to calculate the transmittance and reflectance of a homogeneous horizontally infinite cloud layer. We make the following assumptions: The geometrical thickness of the cloud layer is Δz. The scattering of the cloud droplets can be described by a Henyey-Greenstein phase function with asymmetry parameter g. The vertical optical thickness of the cloud layer is $\tau_c = \beta_{ext}\Delta z$. We assume that there is no absorption, i.e., energy is conserved. This simple setup is depicted in Fig.4.

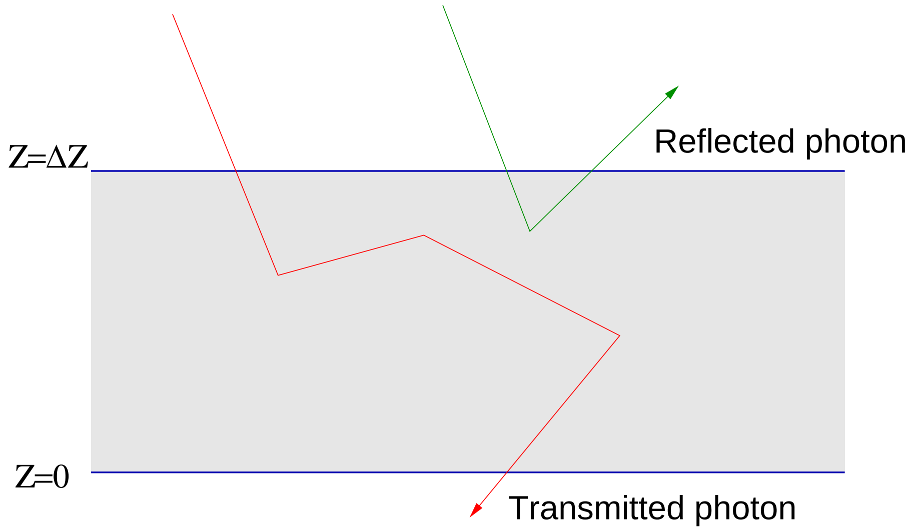

Figure 4: Schematic of homogeneous horizontally infinite cloud layer.

2.2 How to program a simple Monte Carlo model

In a Monte Carlo model a large number of photons are traced through the model domain following probabilistic assumptions about the interaction with the medium. The following steps are required to describe the photon path:

1. Initialization: As position only the vertical coordinate z is required since the medium is homogeneous and infinite in the horizontal. Starting point is the top of the cloud layer, $z = \Delta z$. The direction is given by the solar zenith angle θ_0. It is convenient to define a direction vector $\vec{dx}$.

2. Generate a random optical thickness τ and calculate the distance corresponding to this τ given the direction of the photon $\vec{dx}$ and the vertical optical thickness of the cloud τ_c. Calculate the new position z_p after the photon has traversed the optical thickness τ.

3. Scattering: Calculate the direction of the photon after it is scattered. Suppose that the probability distribution of scattering angles μ is given by the Henyey-Greenstein phase function. In addition to μ a random azimuthal angle ϕ is required to calculate the new direction after the scattering process.

4. Go back to step 2.

5. Repeat steps 2 and 3 until the photon reaches the top of the cloud layer or the bottom. Here count the photon.

Repeat this procedure for a large number of photons. Finally the transmittance of the cloud layer is defined as

$$T = \frac{N_{z=0}}{N_{tot}} \cos\theta_0 \tag{16}$$

and the reflectance is

$$R = \frac{N_{z=\Delta z}}{N_{tot}} \cos\theta_0 \tag{17}$$

where N_{tot} is the total number of photons, $N_{z=0}$ is the number of photons counted at the bottom of the layer and $N_{z=\Delta z}$ is the number of photons at the top of the layer. To calculate the irradiance the transmittance/reflectance is just multiplied with the extraterrestrial solar irradiance.

The accuracy of the Monte Carlo method depends only on the number of photons. If the number of photons is sufficiently large, it follows from Gaussian statistics that the relative error (1σ) is given by:

$$\sigma = \sqrt{\frac{N_{tot} - N}{N_{tot} N}} \tag{18}$$

where N is the number of counted photons for the quantity to be computed.

2.3 Tasks

1. Write a Monte Carlo code following the steps described above.

2. All photons must end up either at the top of the layer or at the bottom, otherwise your model would not fullfill energy conservation. Check whether $N_{z=0} + N_{z=\Delta z} = N_{tot}$.

3. Calculate transmittance and reflectance of the cloud layer using various different input values of N_{tot}, τ_c, θ_0 and g and validate your model by comparing the results to the values in Table 1 and to Fig. 5.

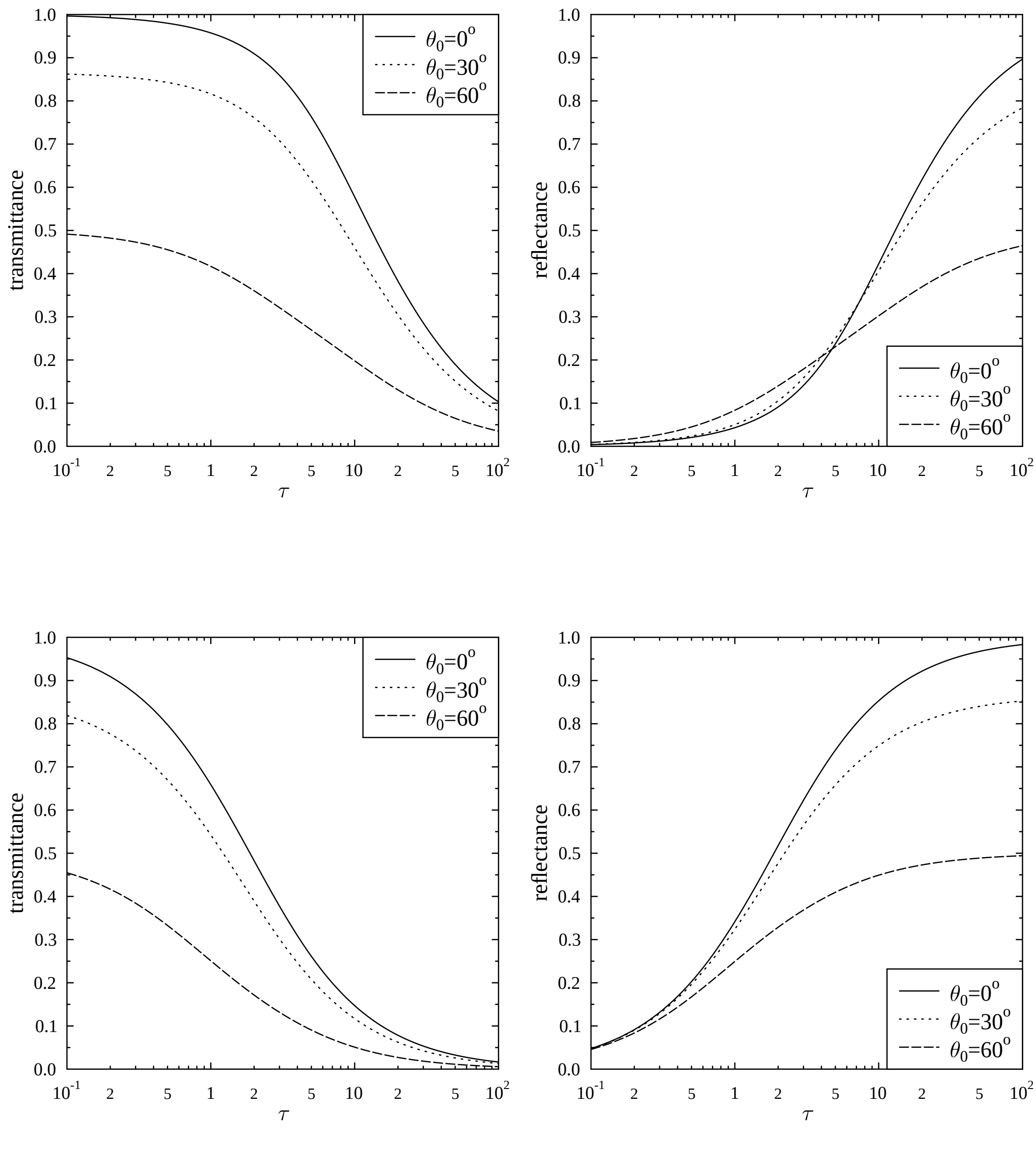

Figure 5: Reflectance and transmittance as a function of optical thickness. Different curves correspond to different solar zenith angles θ_0. The top figures show the results for a Henyey-Greenstein phase function with an asymmetry parameter of $g = 0.85$ and the bottom figures show the same calculation for isotropic scattering $g = 0$. The results are computed using a discrete ordinate radiative transfer code (DISORT) which is one of the solvers implemented in the libRadtran radiative transfer package [*Mayer and Kylling*, 2005].

optical thickness τ_c	solar zenith angle θ_0 [$^\circ$]	transmittance	reflectance
1	0	0.957	0.043
10	0	0.578	0.422
100	0	0.103	0.897
1	30	0.816	0.050
10	30	0.460	0.406
100	30	0.082	0.784
1	60	0.417	0.084
10	60	0.198	0.302
100	60	0.035	0.465

Table 1: Transmittance and reflectance of a 1D cloud layer assuming a Henyey-Greenstein phase function with g=0.85.

3 Rayleigh scattering and gas absorption

3.1 Setup: Cloudless sky Earth atmosphere

The Earth's atmosphere consists of various gas species, e.g. N_2, O_2, O_3 etc. Molecules are small compared to the wavelength of solar radiation, hence they interact as Rayleigh scatterers. The number density of air molecules decreases exponentially with height according to the hydrostatic equation. Therefore the clearsky atmosphere can not be treated as a homogeneous medium. We may assume that the atmosphere consists of homogeneous plane-parallel vertical layers (see Fig. 6). For simplicity we assume that the surface absorbs all photons, i.e. the surface albedo is 0. This is realistic for a water surface. Molecules interact with solar radiation by scattering and also by absorption. The extinction of a layer is given by

$$\beta_{\mathrm{ext}} = \beta_{\mathrm{sca}} + \beta_{\mathrm{abs}} \tag{19}$$

where β_{sca} is the volume scattering coefficient and β_{abs} is the volume absorption coefficient.

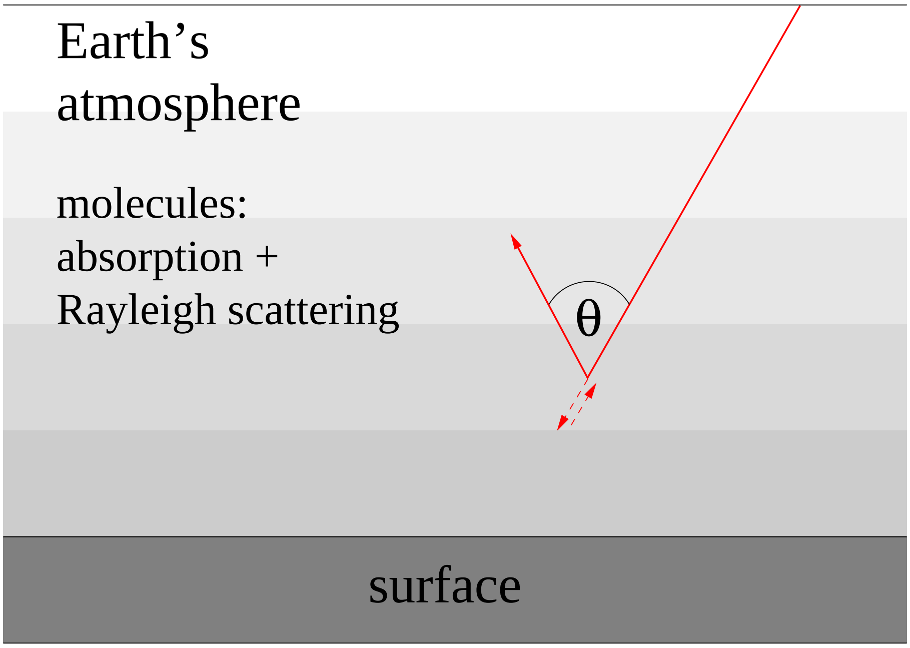

Figure 6: Schematic of cloudless Earth atmosphere.

In order to obtain profiles of β_{sca} and β_{abs} one can use reference atmospheres which contain profiles of pressure, temperature and the constituent concentrations. Several such reference atmospheres have been compiled by *Anderson et al.* [1986]. In addition the absorption cross sections of the molecules are required. These can be obtained from databases, for instance from the HITRAN database [*Rothman et al.*, 1987].

3.2 Implementation of Rayleigh scattering

In order to calculate the transmittance of a vertically inhomogeous atmosphere, the model domain is devided into a discrete number of plane-parallel layers. The implementation of Rayleigh scattering is then very similar to the procedure described in section 2. The only differences are the scattering phase function and the calculation of the free path of the photon. To sample the scattering angle, of course we have to use the Rayleigh phase function here. To calculate the free path corresponding to a randomly sampled τ, we have to go through the discrete layers step by step.

3.3 Implementation of molecular absorption

When a photon interacts with a molecule by absorption, the molecule uses the energy of the photon to be transfered to an activated state. For a photon in the Monte Carlo Model this means that it is eliminated immediately. One way to implement absorption is to use the single scattering albedo

$$\omega_0 = \frac{\beta_{\text{sca}}}{\beta_{\text{ext}}} \tag{20}$$

ω_0 is a number between 0 and 1; 0 means that there is only absorption and 1 means that there is only scattering. Now we may use a random number to decide whether the photon interacts with the medium via scattering or via absorption. If the random number is larger than $1-\omega_0$ the interaction is a scattering event and else the photon is absorbed.
A problem of this approach is that it is not very efficient. All photons that are absorbed do not contribute to the result of the Monte Carlo calculation and therefore the statistical error increases. To treat absorption in a more efficient way we may assign a weight to each photon. In the beginning the weight is 1 and absorption decreases the weight but does not eliminate the photon. The weight w_{abs} of the photon due to absorption is given by

$$w_{\text{abs}} = \exp(-\tau_{\text{abs}}) \tag{21}$$

In this case we have to use the probability density function

$$P(\tau_{\text{sca}}) = \exp(-\tau_{\text{sca}}) \tag{22}$$

in order to sample the free pathlength of the photons. Finally, when we sum up the photons to get the transmittance, we calculate

$$T = \frac{\sum_1^{N_{z=0}} w_i}{N_{\text{tot}}} \cos\theta_0 \tag{23}$$

3.4 Tasks

1. Tables of pre-calculated β_{sca} and β_{abs} profiles are provided. The tables correspond to different wavelengths. Read these tables to define your model atmosphere.

2. Extend your photon tracing function to allow vertical inhomogeneous extinction and absorption coefficient profiles.

3. Sample random scattering angles according to the Rayleigh phase function.

4. Implement molecular absorption using one of the methods described above (use single scattering albedo or assign a photon weight). If you have time implement both and compare the results.

5. Calculate the transmittance and reflectance for different wavelenghts and various solar zenith angles and compare your results with Fig. 7 and Table 2.

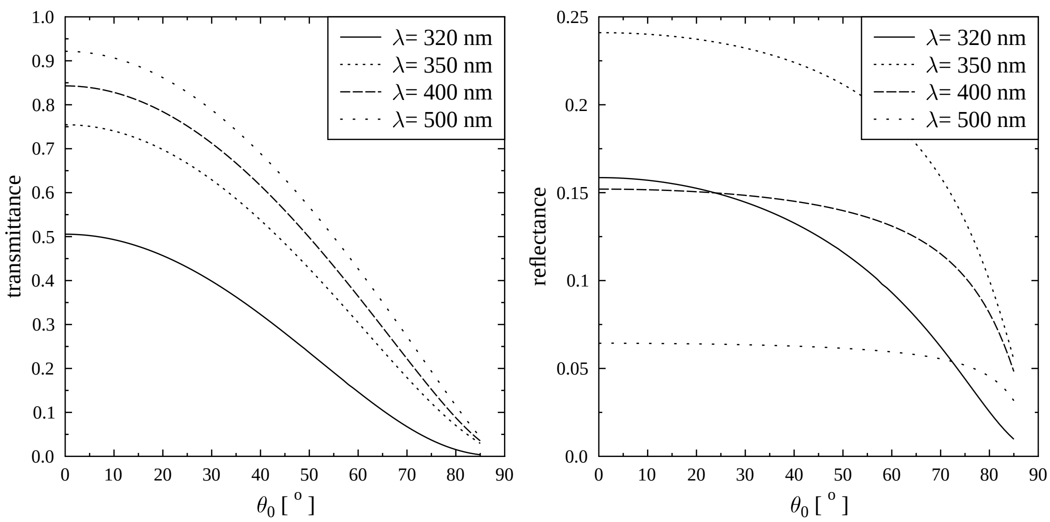

Figure 7: Reflectance and transmittance of a typical Rayleigh atmosphere as a function of solar zenith angle. Different curves correspond to different wavelengths λ. The results are computed using a discrete ordinate radiative transfer code (DISORT) which is one of the solvers implemented in the libRadtran radiative transfer package [*Mayer and Kylling*, 2005].

wavelength λ [nm]	solar zenith angle θ_0 [$^\circ$]	transmittance	reflectance
320	0	0.505	0.159
350	0	0.755	0.241
400	0	0.843	0.152
500	0	0.922	0.064
320	30	0.397	0.145
350	30	0.621	0.232
400	30	0.712	0.148
500	30	0.788	0.063
320	60	0.147	0.096
350	60	0.304	0.192
400	60	0.364	0.131
500	60	0.427	0.059

Table 2: Transmittance and reflectance of a typical clearsky Rayleigh atmosphere.

4 Atmosphere with clouds and molecules

4.1 Lambert surface

So far we have neglected reflection at the surface. We have already discussed how to sample the direction of the reflection for a Lambertian surface in section 1.4. To include surface reflection in the Monte Carlo model we may use another random number r when the photon hits the surface. If $r < a$, where a is the surface albedo, the photon is absorbed by the surface and otherwise it is reflected. Another more efficient method is to always reflect the photon at the surface and to multiply the photon weight with the surface albedo.

4.2 Rayleigh atmosphere with clouds

In the real atmosphere there may be clouds and molecules at the same time. Again we may use a random number r to decide whether the photon interacts with a cloud droplet or a molecule. If the random number is smaller than the ratio between the Rayleigh scattering coefficient and the total scattering coefficient, the photon interacts with the molecule:

$$r \leq \frac{\beta_{\text{sca,r}}}{\beta_{\text{sca,r}} + \beta_{\text{sca,c}}} \tag{24}$$

Here $\beta_{\text{sca,r}}$ is the Rayleigh scattering coefficient and $\beta_{\text{sca,c}}$ is the cloud scattering coefficient. Else, if the random number is larger than this ratio the photon interacts with the cloud droplet.

4.3 Calculation of irradiance

We have calculated the transmittance and reflectance of the atmosphere. These quantities cannot be compared directly to the measurements. A quantity that can be measured is the irradiance. It is defined as the flow of radiative energy per unit area per wavelength. The unit of irradiance is W/(m^2 nm). To obtain the irradiance we just have to multiply the transmittance and the reflectance with the extraterrestrial irradiance (Fig. 9).

4.4 Tasks

1. Implement surface reflection assuming a Lambertian surface.
2. Calculate transmittance and reflectance for various surface albedos for a clearsky atmosphere and compare the results with Fig. 10.
3. Include a cloud layer in your model.
4. Compute transmittance and reflectance for the cloudy Earth atmosphere.
5. Multiply the transmittance and reflectance values with the extraterrestrial irradiance (Fig. 9) to obtain the radiative flux at the surface and at the top of the atmosphere.

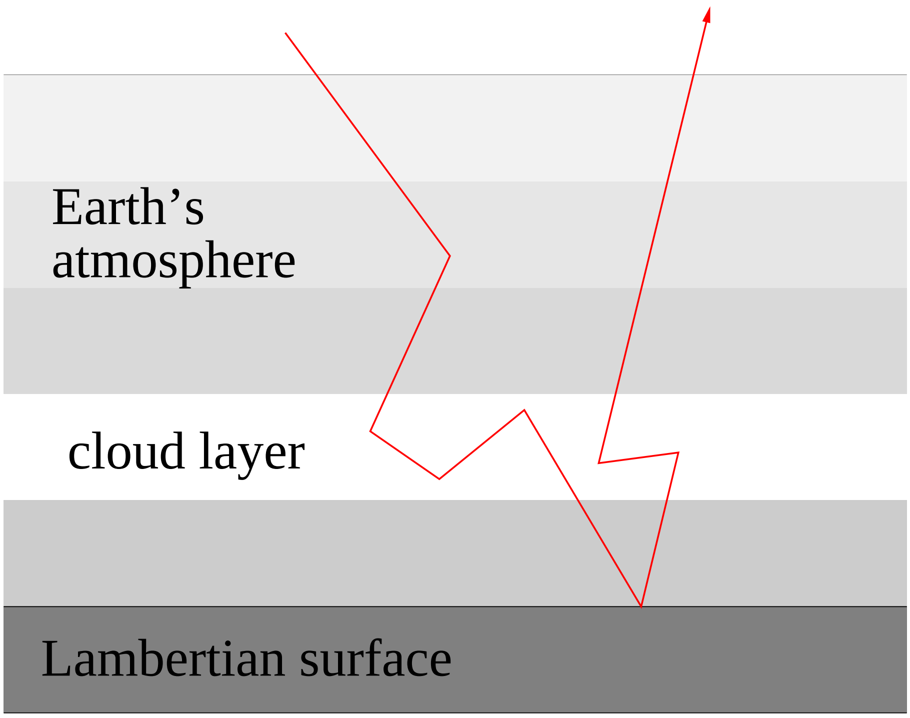

Figure 8: Schematic of a 1D-plane-parallel model with a cloud layer and a Lambertian surface.

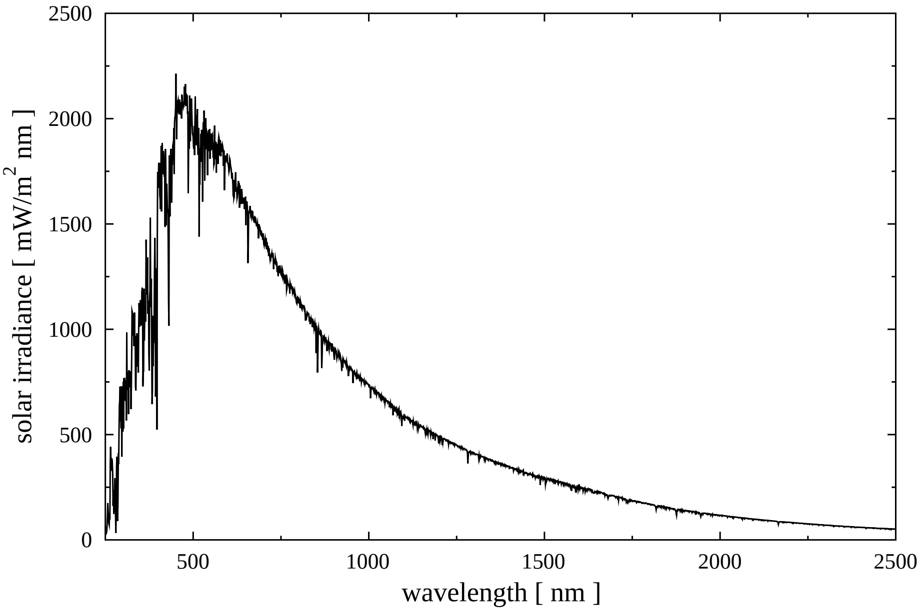

Figure 9: Extraterrestrial solar spectrum [*Kurucz*, 1992].

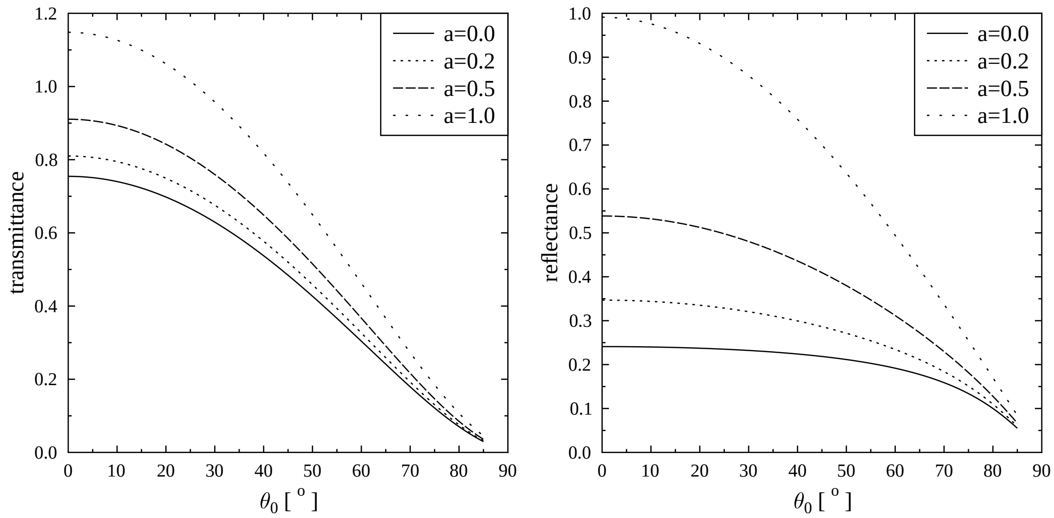

Figure 10: Transmittance and reflectance at a wavelength of 350 nm for as a function of solar zenith angle different surface albedos. The results are computed using the discrete ordinate radiative transfer code DISORT.

5 Calculation of radiance

5.1 Cone sampling

So far we have computed solar irradiances which in case of transmittance include all photons reaching the surface no matter from which direction. Another quantity that is frequently measured is the radiance. The radiance is the flow of energy per unit area per unit solid angle. The unit of radiance is W/(m^2 nm sr). A simple method to compute the radiance is to sample photons into a cone centered around the desired direction (see figure 11). The problem with this method is that the probability that the photon hits the cone is

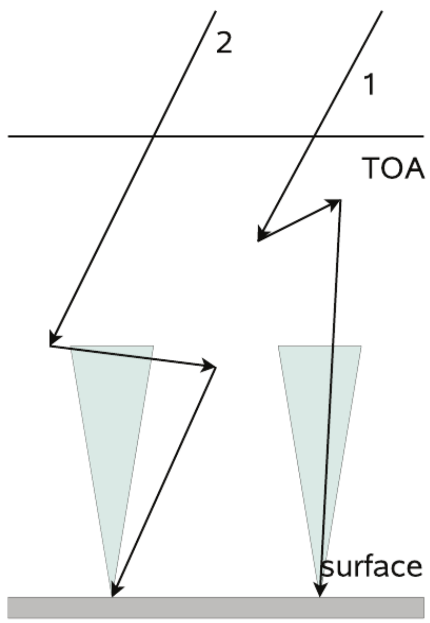

Figure 11: Cone sampling to compute radiances (from *Mayer* [2009]). Photon 1 is counted whereas photon 2 misses the cone and does not contribute to the result.

very very small. A second disadvantage is that we do not really calculate the radiance in the desired direction, but an average over the solid angle interval formed by the cone.

5.2 Local or directional estimate techniques

A much more efficient method is the so-called local or directional estimate technique [*Mayer*, 2009; *Marshak and Davis*, 2005]. Here we calculate at each scattering point the probability that the photon is scattered into the direction of the sensor (see figure 12). Note that the actual photon path is not affected by this technique. The probability for scattering into the direction of the sensor is given by the phase function taking into account the extinction between scattering and detector. In order to compute the radiance,

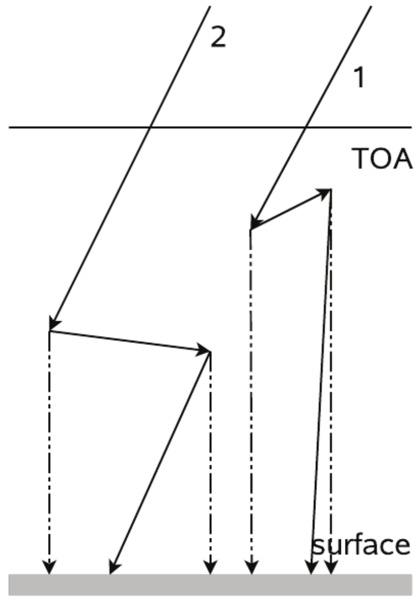

Figure 12: The local/directional estimate technique (from *Mayer* [2009]).

we just sum up the following weights calculated at each scattering point:

$$w = w_0 \cdot P(\theta_p) \cdot \exp(-\tau_{\text{ext}}) / \cos(\theta_d) \tag{25}$$

where w_0 is the photon weight (which includes absorption and may be also the surface reflection). θ_p is the angle between photon direction (before scattering) and the radiance direction. The phase function $P(\theta_p)$ gives the probability that the photon is scattered into the direction of the detector. To calculate the probability that the photon actually reaches the detector the Lambert-Beer term for extinction $\exp(-\tau_{\text{ext}})$ needs to be included. We need to devide by the zenith angle of the detector direction θ_d to account for the slant area in the definition of the radiance. The same needs to be done when a photon hits the surface, using the albedo for the photon weight instead of the scattering phase function. Using this method each photon contributes several times to the radiances.

5.3 Tasks

1. Implement the local estimate technique to compute radiances.
2. Perform calculations for various setups (clear-sky atmosphere, cloudy atmosphere, different surface albedo).
3. Investigate the contributions of individual scattering orders to the result.

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