Atmospheric raypath modeling for radiative transfer algorithms

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Abstract: A general method for the determination of raypaths as well as resulting path segments and partial gas columns within a layered atmosphere is presented. Any singularity at the tangent point is avoided. No use is made of the gross spherical symmetry of the Earth's atmosphere. Hence, deviations from symmetry due to the Earth's oblate shape and atmospheric disturbances can be taken into account in a straightforward manner. It is additionally explained how KOPRA calculates integrated path quantities like Curtis-Godson values, path column amounts and their derivatives. The inclusion of horizontal gradients into this scheme is shown.

1 Introduction

Inference of atmospheric trace gas concentration profiles from observed infrared spectra relies on the comparison with synthetic spectra which are calculated from a set of relevant variables describing the state of the atmosphere. Their values are varied until the best possible agreement between the observed and the calculated spectra is achieved. The calculation of spectra requires first of all the determination of the refracted raypath through the atmosphere [1][2]. Since the usual set of variables consists of temperatures and gas concentrations at a number of discrete atmospheric levels, the path segments and partial gas column amounts for the enclosed layers have to be calculated.

2 Usual methods for raytracing in the Earth's atmosphere

A simple method is to refract the ray at the borders of discrete atmospheric layers. If the ray crosses the border, it is deviated according to Snell's law:

$$n_1 \times \sin\alpha_1 = n_2 \times \sin\alpha_2 \tag{1}$$

with n_1,n_2 denoting the refractive indices of the adjacent layers (assumed to be homogeneous) and α_1, α_2 denoting the angles of the light ray with the normal of the enclosed boundary. The method works reasonably well as long as the ray does not cross the boundary almost tangentially. This situation occurs in limb-sounding observations. In this case, the path segments in the layers near the tangent point become excessively large and the computational error increases. A further subdivision of the layers can be introduced around the tangent point, but this even increases the chance of just touching a layer near the tangent height under an angle of nearly 90° and, thus, undermining numerical stability. In any case, the region around the tangent point requires special attention. The usual solution is to insert a straight line around the tangent point.
It can be shown that in the case of spherical symmetry the construction of a constant of motion is possible [3][4]:

$$const = n(r) \times r \times \sin\alpha(r) \tag{2}$$

with $n(r)$ denoting the refractive index as a function of the radius and $\alpha(r)$ denoting the zenith angle. If $n(r)$ and the tangent height or any angle α to a certain value of r are given, the overall raypath is determined. In the vicinity of the tangent height care must be taken, because in the calculation of the distance traveled by the ray ds the quotient ds/dr diverges at the tangent point.
It is possible to take the ellipsoidal shape of the Earth approximately into account by using an appropriate radius of curvature determined by the tangent point's latitude and related azimuthal direction of view instead of the mean Earth radius. With the location of the tangent point given a priori, this causes no problems. However, in practice the given variables are the observer's position and the direction of view. The tangent point and related radius of curvature have to be sought iteratively by shooting back to the observer's position. If horizontal inhomogeneities of the atmosphere along the raypath are not negligible, the formulation's attraction disappears completely.
Therefore, a method free of numerical problems near the tangent point, avoiding symmetry requirements and capable to start raytracing at the observer's position with a given direction of sight is preferable.

3 Method of tangential displacement

Imagine a light ray propagating through a smoothly varying refractive index distribution $n(\vec{r})$ as represented in Fig. 1. A gradient $\nabla n(\vec{r})$ not parallel to the ray deviates it. The new direction of propagation $\vec{e}_{tn}$ lies in the plane defined by the old tangent vector $\vec{e}_t$ and $\nabla n(\vec{r})$. After traveling the infinitesimal distance ds, the angle $d\alpha$ between $\vec{e}_t$ and $\vec{e}_{tn}$ is

$$d\alpha = ds \times |\vec{e}_s \cdot \nabla n|/n \tag{3}$$

with $\vec{e}_s$ denoting the direction perpendicular to $\vec{e}_t$ in the plane defined by $\vec{e}_t$ and $\nabla n(\vec{r})$. This can be seen by constructing the tilt of a locally plane wavefront over

the infinitesimal distance of travel ds : $\vec{e}_s \cdot \nabla n$ is the component of the refractive index gradient along the wavefront and, thus, $|\vec{e}_s \cdot \nabla n|/n$ can be interpreted as the ratio of propagation velocities per unit length along the wavefront. Obviously, the wavefront is bent into the region where $n(\vec{r})$ becomes larger. The path of a light ray in any smooth distribution $n(\vec{r})$ can be followed by adding up together many sufficiently small displacements of this kind.
Due to the high expenditure needed when constructing the vector $\vec{e}_s$ for each displacement, we use the fact that $\nabla n(\vec{r})$ in the terrestrial atmosphere is an extremely small quantity. Then, $\vec{e}_{tn}$ can be constructed in the following way:
Calculate the auxiliary vector $\vec{e}_{ta}$ by

$$\vec{e}_{ta} = (n \times \vec{e}_t + ds \times \nabla n)/|n \times \vec{e}_t + ds \times \nabla n| \tag{4}$$

This vector can be used instead of $\vec{e}_{tn}$, as can be seen by multiplying equation (4) by $\vec{e}_s$:

$$\vec{e}_s \cdot \vec{e}_{ta} = ds \times (\vec{e}_s \cdot \nabla n)/|n \times \vec{e}_t + ds \times \nabla n| \tag{5}$$

The denominator is nearly $n(\vec{r})$ and, therefore, the value for the bending is in good agreement with the exact calculation. For a horizontal displacement of 100 m near the Earth's surface, the relative error in $d\alpha$ does not exceed 10^{-9}. For a nearly vertical displacement the relative error reaches 10^{-5}, but the absolute deviation becomes minute.

4 Implementation into a radiative transfer model

The starting point for the implementation of the method of tangential displacement into a radiative transfer model is the transformation of the observer coordinates (latitude, longitude, altitude) and the direction of view (elevation angle, azimuth) into Cartesian coordinates. All further raytracing operations will be performed in this coordinate system. Hence, given a point on the line of sight $\vec{r}_i = (x_i, y_i, z_i)$ and a tangent vector $\vec{e}_{t,i}$, the subsequent point $\vec{r}_{i+1}$ is:

$$\vec{r}_{i+1} = \vec{r}_i + 0.5 \times ds \times (\vec{e}_{t,i} + \vec{e}_{t,i+1}) \tag{6}$$

with:

$$\vec{e}_{t,i+1} = \frac{\vec{e}_{t,i} \times n(\vec{r}_i) + ds \times \nabla n(\vec{r}_i + 0.5 \times ds \times \vec{e}_{t,i})}{|\vec{e}_{t,i} \times n(\vec{r}_i) + ds \times \nabla n(\vec{r}_i + 0.5 \times ds \times \vec{e}_{t,i})|} \tag{7}$$

The gradient of the refractive index $n = 1 + \varepsilon$ at the location $\vec{r}_i + 0.5 \times ds \times \vec{e}_{t,i}$ is computed numerically by repeated use of a function $\varepsilon(x, y, z)$ giving the related ε for each coordinate (x, y, z).
Since radiative transfer models usually operate with predefined atmospheric layers, the crossing points of the ray with the level altitudes must be determined: Given a function $h(\vec{r})$ which returns for each Cartesian point $\vec{r}$ in the atmosphere the altitude h above the ground, the crossing point is determined by the linear approximation:

$$\vec{r}\,' = \vec{r}_i + (\vec{r}_{i+1} - \vec{r}_i) \times (h(\vec{r}_i) - H_j)/(h(\vec{r}_i) - h(\vec{r}_{i+1})) \tag{8}$$

with $h(\vec{r}_i) > H_j$ and $h(\vec{r}_{i+1}) < H_j$ or vice versa. H_j is the altitude of the atmospheric level j. Since $h(\vec{r})$ is nearly linear along the path over the distance ds, Eq. 8 should be a good approximation. Eq. 8 can be used iteratively (substituting $\vec{r}_{i+1}$

by $\vec{r}\,'$) to obtain a better estimate $\vec{r}\,''$, if necessary.
For limb sounding observations the determination of the tangent altitude is of interest as well. A first estimation of the tangent point is obviously $\vec{r}_{i,min}$ with $h(\vec{r}_{i,min})$ reaching a minimum. This result can be improved by parabolic interpolation taking the adjacent altitudes into account using ds as the horizontal distance between the three points. The minimum of the parabola is taken as the value for the tangent altitude.
Another important issue regarding the computation time is the choice of the increment ds. For satellite limb sounding experiments, $ds = 10$km is sufficient to obtain an accuracy of the trace gas amounts of better than 0.1%.

5 Curtis-Godson values, path column amounts and their derivatives

In this section we describe the calculation of integrated values of atmospheric state parameters for each path segment along the refracted line-of-sight. The following mean quantities are computed for each path j, each molecular species g, and in the case of non-LTE applications for each vibrational state n:

$$s_j = \int_{path_j} ds, \tag{9}$$

$$u_{jg} = \int_{path_j} \rho_g(s)ds, \tag{10}$$

$$T_{jg} = \frac{1}{u_{jg}} \int_{path_j} T(s)\rho_g(s)ds, \tag{11}$$

$$p_{jg} = \frac{1}{u_{jg}} \int_{path_j} p(s)\rho_g(s)ds, \tag{12}$$

$$r_{jgn} = \frac{1}{u_{jg}} \int_{path_j} r_{gn}(s)\rho_g(s)ds, \tag{13}$$

where s is the path length along the line-of-sight, u the partial column amount, T the kinetic temperature, p the pressure, $\rho \propto vmr_g p/T$ the number density (vmr = volume mixing ratio), and r the fractional population of each vibrational state n between non-LTE and LTE. r is connected to the vibrational temperature T_{vib} by

$$r_{gn} = f_{Q,g} \exp\left(\frac{hcE_{gn}}{k_B}\left[\frac{1}{T} - \frac{1}{T_{vib,gn}}\right]\right), \tag{14}$$

where E is the state energy, h Planck's constant, k_B Boltzmann's constant, and c the velocity of light. $f_{Q,g}$ is the non-LTE correction factor of the partition sum. Both, vibrational temperature or population ratio profiles are supported as input quantities. Since internally KOPRA only handles population ratios, vibrational temperatures will be converted at the beginning directly after read-in.
Additionally, the following derivatives of the integrated path values with respect to atmospheric retrieval parameters are determined:

$$\frac{du_{jg}}{dq_{vmr,gm}}, \frac{dT_j}{dq_{T,m}}, \frac{dp_j}{dq_{p,m}}, \frac{du_{jg}}{dq_{p,m}}, \frac{dr_{jgn}}{dq_{r,gnm}}, \tag{15}$$

where m is the index on the retrieval parameters, $q_{vmr,g}$ the retrieval parameters for vmr (or vmr gradients) of species g, q_T the retrieval parameters for temperature

(or temperature gradient), q_p the retrieval parameters for pressure, and $q_{r,gn}$ the retrieval parameters for the population ratios of state n for species g.
For the calculation of absorption coefficients and during radiative transfer in the following steps of KOPRA only the mean path quantities are needed. Therefore, by also having calculated the derivatives of these quantities with respect to the retrieval parameters the basis is provided for the flexible handling of the retrieval parameterization. I.e. that after radiative transfer the derivatives of the spectra with respect to the mean path values can be combined with (15) to construct the requested Jacobian matrix.

The integrals (9-13) are solved numerically when the end of each path segment j (i.e. the layer boundary) is reached. The steps are as following:

(a) Transformation of $\vec{r}_i = (x_i, y_i, z_i)$ into altitude $h(\vec{r}_i)$, latitude $lat(\vec{r}_i)$, and longitude $lon(\vec{r}_i)$ at each grid point i along the line-of-sight inside the actual path segment j.

(b) Calculation of atmospheric state parameters at each location $\vec{r}_i$ by calling the 'give'-functions. These functions perform the interpolation from discrete input-profiles to any location in the atmosphere.

- $T_i = give\_T(h(\vec{r}_i), lat(\vec{r}_i), lon(\vec{r}_i))$
- $p_i = give\_p(h(\vec{r}_i), lat(\vec{r}_i), lon(\vec{r}_i))$
- $vmr_{ig} = give\_vmr(h(\vec{r}_i), lat(\vec{r}_i), lon(\vec{r}_i), g)$
- $r_{ign} = give\_Tvib(h(\vec{r}_i), lat(\vec{r}_i), lon(\vec{r}_i), g, n)$

(c) Numerical integration using the grid values $T_i, p_i, vmr_{ig}, r_{ign}$ to obtain the integrated path values (9-13).

To obtain greatest flexibility in parameterization of retrieval quantities the derivatives of the integrated path quantities (15) are calculated numerically by: (for further details about derivative see Part XIII: 'Derivatives and interface to the retrieval')

(a) Change of each retrieval parameter by some increment.

(b) Recalculation of the integrated layer value with the changed parameter.

(c) Determination of the numerical derivative by using the previously determined path value for the undisturbed case.

If new parameterizations for the retrieval quantities should be implemented only the transformation rules in the 'give'-functions have to be changed and KOPRA automatically delivers the Jacobian matrix with respect to the new quantities.

6 Horizontal gradients

If the horizontal gradients are switched off ($5.9 of the main input-file) the arguments lat and lon have no effects in the 'give'-functions and the interpolation is only performed for the altitude coordinate h.
If horizontal gradients are switched on, the 'give'-functions use the altitude profiles and the altitude gradient profiles to determine the value of the atmospheric state at the point $\vec{r}_i$ with altitude h, latitude lat, and longitude lon as described in Part III: 'Geophysical model and atmospheric layering'. Therefore, the integrated values for each path segment comprise the horizontal gradients.

azimuth	spherical Earth with gradient	elliptical Earth without gradient	elliptical Earth with gradient
airmass: $2.165 \times 10^{30}/\mathrm{m}^2$			
0°	$+2.421\times 10^{-2}$	$+1.722\times 10^{-4}$	$+2.440\times 10^{-2}$
90°	$+5.789\times 10^{-4}$	$+1.728\times 10^{-3}$	$+2.311\times 10^{-3}$
180°	-2.386×10^{-2}	$+3.550\times 10^{-4}$	-2.352×10^{-2}
refraction angle: 0.219°			
0°	$+2.422\times 10^{-2}$	$+1.723\times 10^{-4}$	$+2.442\times 10^{-2}$
90°	$+5.799\times 10^{-4}$	$+1.729\times 10^{-3}$	$+2.316\times 10^{-3}$
180°	-2.387×10^{-2}	$+3.554\times 10^{-4}$	-2.353×10^{-2}

Table 1: Relative azimuthal variation of airmass and refraction angle along a ray starting tangentially at a height of 10km in 50° N. The azimuth is measured from south. The atmosphere is assumed to be isothermal (220 K) with a pressure at the tangent point of 265 hPa in a height of 10 km. For the elliptical Earth a minor axis of 6357 km and a major axis of 6378 km is assumed. In the spherical calculations a radius of 6370 km is used.

Derivatives of the integrated values with respect to the horizontal gradient parameters are determined exactly in the same way as the derivatives with respect to the altitude profile parameters by changing the (gradient)parameter-value, recalculating the integral and numerical differentiation.

7 Illustrative raytracing results

The presented method is especially suitable for raytracing in the presence of the ellipsoidal Earth shape and locally variable atmospheric state. To illustrate the effects, the azimuthal variation of airmass and refraction along a ray starting tangentially at a height of 10km were studied. The tangent point is located at 50° northern latitude and a southwards directed pressure gradient is constructed by vertical displacement of the isobars by a rate of 100 m/°. Such values can be found at the boundary of the polar vortex and near pronounced weather systems.
As can be seen from Table 1, the resulting effects are quite small in general. The relative variation in airmass and refraction angle are nearly the same. The variable atmosphere has a much stronger impact as compared to the Earth's oblateness. In the presence of both effects, the combined result is a linear superposition.

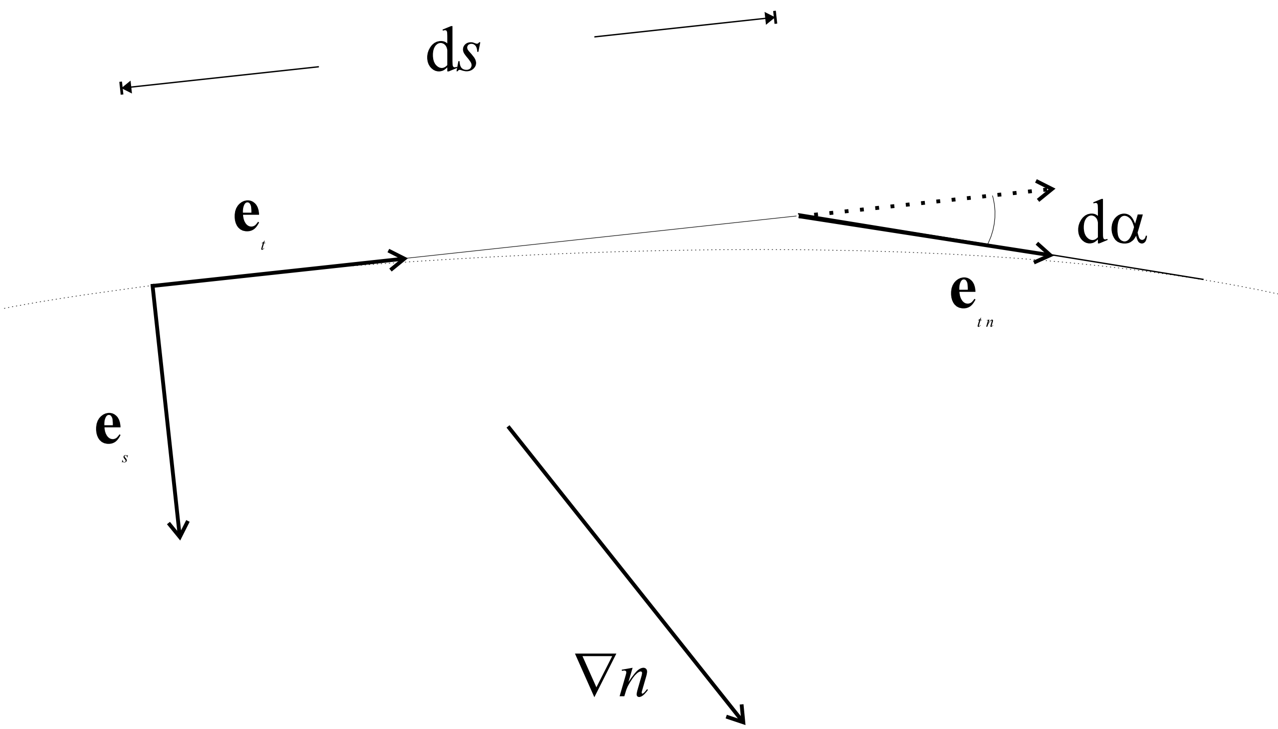

Figure 1: Method of tangential displacement: construction of the new tangent vector.

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