Examination Project on 1-D Plane-Parallel models Computational Methods for the Interaction of Light and Matter (WS2019/20)

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Earth Atmosphere Model

The basic idea of this project

In recent months the topic of climate change has gained center stage in the political arena. The main issue is the anthropogenic CO_2 emission, which increases the abundance of this greenhouse gas globally. Before industrial times the CO_2 concentration in the Earth Atmosphere was 280 parts per million (ppm). Today we are at 415 ppm, and this concentration is expected to increase strongly in the coming decades. The way the CO_2 concentration affects the Earth's climate is through the greenhouse effect: the Sunlight (short wavelength radiation) is transmitted to the surface, but the thermal cooling radiation (long wavelength radiation) is trapped by the opacity of H_2O and CO_2. An increase of CO_2 means more radiative trapping of heat, less cooling of the Earth's lower atmosphere, and thus increase of temperature.

In this lecture we discussed various methods for computing radiative transfer, and we applied it to a simple model of an exoplanet atmosphere. Now let's apply our skills to the Earth's atmosphere. There are several major differences, however, compared to the exoplanet atmosphere we discussed in the lecture:

- The Earth's atmosphere has a clear lower boundary: the surface of the Earth.
- A cloud-free Earth atmosphere is in some wavelengths optically thin, so we then expect fast convergence.
- The lower 10 km of the atmosphere is not in radiative equilibrium: instead, it is very close to adiabatic. Instead of finding an equilibrium solution, we have to compute net heating/cooling rates to compute the effect on the climate.
- Gas opacities consist of millions of transitions ("lines"), and thus require a special technique to handle in an efficient way.
- Clouds will strongly affect the heating/cooling rates, so Lambda Iteration on scattering will be necessary.

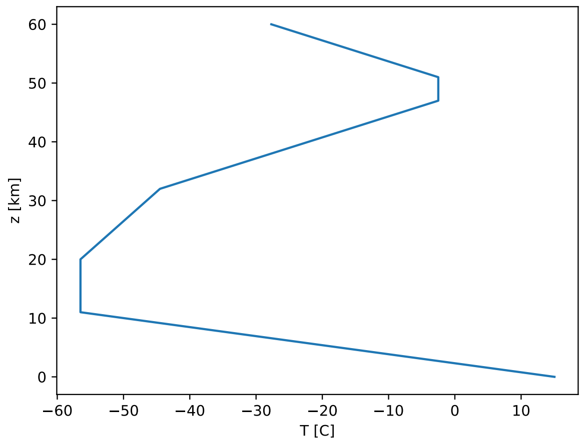
The idea of this project is to make a simple radiative transfer model of the Earth's atmosphere, and investigate what the effects of CO_2 and of clouds are.

A simple Earth Atmosphere Model

To keep things as simple as possible (but not simpler than necessary), we will fix the temperature and pressure structure of the atmosphere, rather than calculate it. We use the

International Standard Atmosphere model[1]. This is a simple model of the temperature $T(z)$ as a function of height z, made up of several linear parts, so it can be easily reconstructed in a computer program.

z [km]	T [°C]
-0.61	+19.0
11	56.5
20	56.5
32	44.5
47	2.5
51	2.5
71	58.5



The temperature at any given height z is simply the linear interpolation of the points in the above table. The pressure $P(z)$ as a function of z then follows from the hydrostatic equilibrium equation:

$$\frac{dP(z)}{dz} = -g\rho(z) \tag{1}$$

where the equation of state is that of an ideal gas:

$$P = \rho \frac{k_B}{\mu m_p} T \tag{2}$$

where $k_B = 1.3807 \times 10^{-23}$ J/K is Boltzmann's constant, $m_p = 1.6726 \times 10^{-27}$ kg the mass of the proton, and $\mu = 28.9$ is the mean molecular weight of air in units of the proton mass. In this equation, the pressure P is in Pascal, the density ρ is in kg/m^3 and the temperature T is in Kelvin. Note that the conversion of Celcius to Kelvin is: 0 °C = 273.15 K. The conversion of Pascal to bar is: 1 bar = 10^5 Pa.

For your convenience, we provide you with a text file that contains this model:

```
earth_atmosphere_model.txt
```

In Python you can read this file with:

```python
import numpy as np
data=np.loadtxt('earth_atmosphere_model.txt')
```

and `data` is now an array containing the data. You can look at the first line of this text file to see what the columns mean. Note that this file also contains abundance information of water, carbon dioxide and ozone, but more about that later.

[1] `https://en.wikipedia.org/wiki/International_Standard_Atmosphere`

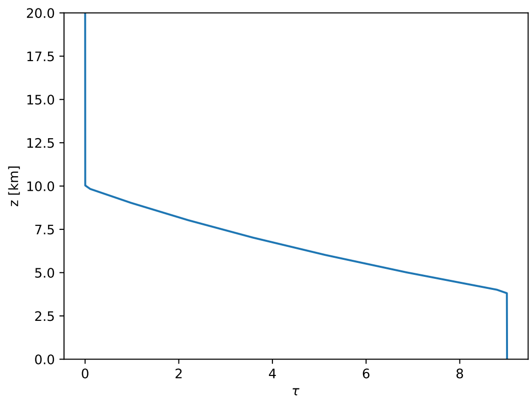
PART 1: A first radiative transfer model: only scattering by clouds

In one of the previous exercises of this lecture, you already created a computer program to perform Lambda Iteration on a scattering problem in a plane-parallel geometry. Using this program, you can calculate how much the mean intensity of sunlight is on a cloudy day compared to a cloud-free day.

Let us assume that clouds consist of water droplets with a radius of 30 μm. The density of liquid water is $\rho_{\mathrm{liq}} = 10^3$ kg/m^3, so that the mass of each cloud droplet is $m = (4\pi/3)\rho_{\mathrm{liq}}a^3 = 4.19 \times 10^{-12}$ kg. We assume that raindrops have albedo 1 (i.e. they do not absorb; they only scatter), and that the scattering is isotropic. The cross section of scattering is assumed to be geometric: πa^2. With this information, the scattering opacity (i.e. scattering cross section per unit cloud mass) is:

$$\kappa_{\mathrm{cloud}} = \frac{\pi a^2}{(4\pi/3)\rho_{\mathrm{liq}}a^3} = 25\frac{\mathrm{m}^2}{\mathrm{kg}} \tag{3}$$

where kilogram here stands for "kilogram of water" (not of air). Let us assume that a cloud has a liquid water content (in the form of the above mentioned droplets) of 0.1 gram per kg of air. We now fill the atmosphere with this cloud opacity between $z = 4$ km and $z = 10$ km. Below 4 km and above 10 km we assume the air to be perfectly transparent. The total vertical optical depth, for this model (with the above described atmospheric structure) is $\tau = 9$.



We now illuminate this atmosphere from above with a solar flux of $F_* = 1.36\mathrm{kW/m}^2$. This is called the the "solar constant", and it plays a central role in any studies of the Earth's climate. We assume that the Sun's rays impinge on the atmosphere under a zenith angle i with $\cos(i) = 0.5$.

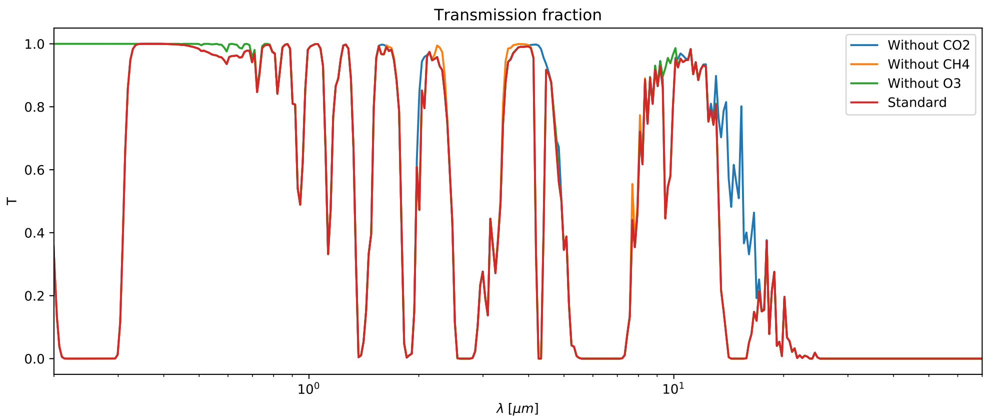
At the ground $z = 0$ we assume, for convenience, that the ground has albedo 0, meaning all radiation is immediately absorbed. We will be concerned with visual radiation only (not infrared), so that we do not need to include the thermal blackbody radiation from the ground at this point.

Assignment: Apply your computer program to this problem and find out what the mean intensity $J(z = 0)$ at ground level is in units of $\mathrm{J\,s^{-1}\,m^{-2}\,ster^{-1}}$ (the usual unit of intensity, integrated over frequency). Compare this value to that of the case without cloud cover. As you will see, cloud cover strongly suppresses the sunlight at ground level, even though it does not absorb anything: instead, it reflects most of it back into space.

PART 2: Molecular opacities

Apart from clouds, most of the opacity of the Earth's atmosphere comes from millions of "molecular lines", i.e. quantum transitions between different rotational states of molecules, primarily H_2O, CO_2, O_3 and CH_4. Even on a cloud-free day, most of the spectral region between the ultraviolet and the far-infrared is covered by these lines, with the most notable exception being the visual wavelength range between about 0.4 and 0.8 micrometers (which is precisely why Nature has chosen this wavelength range for our eyes) and the microwave and radio range (which is why our cell phones and car radios work).

To give a qualitative impression of this "forest of lines": here is the (low resolution) "transmission spectrum":



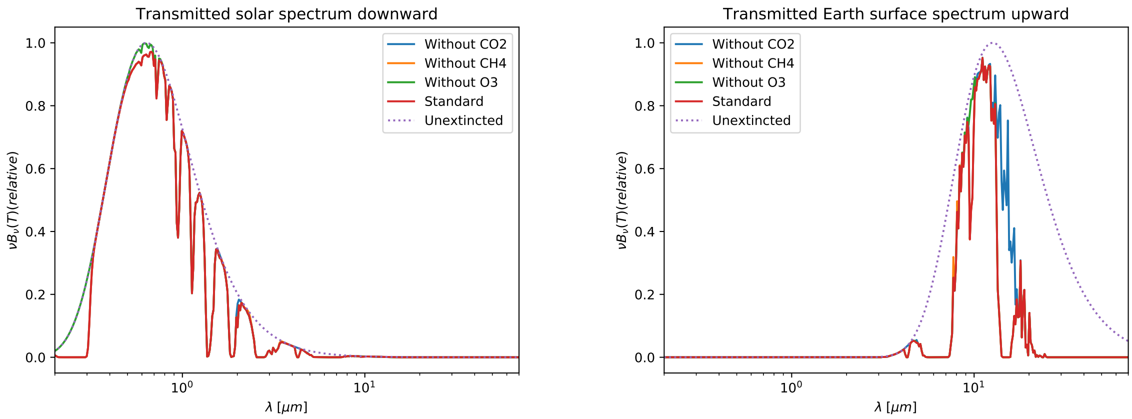
It shows, as a function of wavelength, the fraction of the radiation that can pass through the atmosphere. Where $T = 1$ the atmosphere is transparent. Where $T = 0$ the atmosphere is opaque. Where $0 < T < 1$ part of the radiation is absorbed, while part is passing through. All of this extinction is *absorption*, not scattering. So while clouds have an albedo of 1, molecules have an albedo of zero[2]. As you can see, in addition to the 0.4 and 0.8 micrometers "window" there are also some smaller windows through the atmosphere (where T is close to 1 in the above figure).

Most of the extinction seen in the above figure is caused by H_2O lines. But some of it is also caused by CO_2, O_3 and CH_4. To see this, you can compare the curve marked "Standard" (which contains all molecules) with the curve marked "Without CO2" (which contains all molecules *except* CO_2). The main difference is between $13.5\,\mu$m and $16.5\,\mu$m. Without CO_2 the transmission in this wavelength range is moderate (between 20% and 80%). But with CO_2 this wavelength range is completely opaque: no radiation can escape to outer space.

The question is now: how does this transmission spectrum affect the climate? Answering this is the million-dollar question. But to get a first impression, let us compute two things: the solar spectrum that reaches the ground (assuming the Sun stands at zenith), and the ground thermal spectrum that reaches outer space (assuming that that radiation goes straight upward). Let us approximate the Sun's spectrum with a Planck curve at $T_\odot = 5780\,\mathrm{K}$, and the thermal spectrum of the ground with a Planck curve at $T_{\mathrm{ground}} = 17°C = 290.15\,\mathrm{K}$. We then multiply these spectra with the transmission $T(\lambda)$.

[2]To be more precise: we do not have resonant line scattering because all molecules in the Earth atmosphere are in LTE (local thermodynamic equilibrium).

The result is[3]:



What do we see here? In the left figure we see how the Sun's light is mostly passing through the Earth's atmosphere, except for several wavelength bands in the near-infrared ($\lambda \gtrsim 1\mu$m). Also, as you can see, all the Sun's radiation at $\lambda < 3\mu$m (ultraviolet) is extincted by the atmosphere: this is due to the ozone (O_3) in the atmosphere. Without ozone, much of this ultraviolet radiation would pass through, and would cause serious damage to the DNA in the cells of living things on Earth. But a good portion of the Sun's radiative energy can pass through the (cloudless) sky and warm up the ground.

As the ground warms up, it starts emitting infrared radiation. The Planck spectrum for a ground of 17° C peaks in the mid-infrared (5μm $\lesssim \lambda \lesssim 50\mu$m), see the dotted line in the right figure. This thermal radiation is the way by which the Earth cools into outer space. Without it, the Earth would continue to heat up indefinitely. But, as we learned in the lecture, eventually everything will reach thermal radiative equilibrium in which the radiative heating by the Sun in the visual wavelength range is balanced by this infrared radiative cooling.

In the figure on the right we see how much of this infrared thermal radiation can pass through the atmosphere and escape into outer space. Here we can see that a substantial fraction of this thermal cooling radiation is blocked by the atmosphere. The window around 10 μm is the only part of the thermal infrared wavelength range through which the ground can emit thermal radiation to outer space, and thus radiatively cool. At all other wavelengths the radiation from the ground is absorbed by the air above it. This heats up the air, which then starts radiating back down. This is the *greenhouse effect* that climate scientists talk about! The Earth atmosphere allows most of the Sun's radiation to pass through the atmosphere and warm up the ground, but it prevents much of the ground radiation to reach outer space. Instead, the atmosphere warms up too, and radiatively warms the ground again. This combination of ground and air keeping each other warm is the main reason why we have a comfortable temperature on Earth. Again you can see the role of CO_2: though most of the extinction is by H_2O lines, without CO_2 (the blue curve) the wavelength range between 13.5 μm and 16.5 μm would be at least partly transparent. So without CO_2 a much larger fraction of the ground radiation can escape to outer space, and the equilibrium temperature of the ground would be colder.

All of this you can compute (and verify) yourself, using the "correlated k" opacity tools that will be described next.

[3]In this plot the Rayleigh scattering that makes the sky blue and the setting Sun red is not included.

The correlated-k opacity files and how to use them

As you can see from the transmission spectrum: the molecular opacities vary extremely strongly with wavelength λ. In fact, the above figure is a very low-resolution spectrum. In reality the opacity can vary by factors of 1000 within a wavelength "distance" of $\Delta\lambda/\lambda \ll 10^{-4}$. To properly account for this wildly varying opacity on a computer, one would need to define a wavelength grid with millions of grid points. For each of these wavelength grid points one then needs to integrate the formal transfer equation. This *line-by-line (LBL) radiative transfer* method can be done, but it is computationally costly.

An approximate method, which turns out to be fairly accurate nonetheless, is the *correlated-k* method. The idea is to define N wavelength bands (with N being a reasonable number, say, $N \simeq 500$, or even much smaller). Let us define the boundaries between bands i and $i+1$ as $\lambda_{i+1/2}$, where the $+1/2$ is just a way of writing to clarify that it is between i and $i+1$. That means that band i is defined to be the wavelength range between $\lambda_{i-1/2} < \lambda < \lambda_{i+1/2}$. In the correlated-k datafile that you will use (which will be described below) you have $N = 483$ bands. As an example: band $i = 300$ is between $13.36642\,\mu\text{m} < \lambda < 13.58200\,\mu\text{m}$. This is still a relatively narrow wavelength range, but not nearly as narrow as one would require for LBL radiative transfer. However, within even this narrow range, the opacity can vary by factors of 1000 or more!

The correlated-k trick is to figure out what fraction of this wavelength range is covered with opacity $10^{-3} \leq \kappa < 10^{-2}$, which fraction with $10^{-2} \leq \kappa < 10^{-1}$, which fraction $10^{-1} \leq \kappa < 10^{0}$, etc. Or more precisely, to define the *opacity distribution function* $P(\kappa)$ such that

$$\int_0^\infty P_i(\kappa)d\kappa = 1 \tag{4}$$

and

$$\int_{\kappa_1}^{\kappa_2} P_i(\kappa)d\kappa = \text{fraction of wavelength range } i \text{ with } \kappa_1 \leq \kappa < \kappa_2 \tag{5}$$

So for each of the 483 bands we need to define a function $P_i(\kappa)$. In principle this can be done by defining a grid of κ values and defining the corresponding P values for those κ values.

It turn out that a more practical way to define $P_i(\kappa)$ is by defining the *cumulative contribution function* $g_i(\kappa)$ in the following way:

$$g_i(\kappa) \equiv \int_0^\kappa P_i(\kappa')d\kappa' \tag{6}$$

This ensures that g_i is always a value between 0 and 1, with $g_i(0) = 0$ and $g_i(\infty) = 1$. Again, one could now store on the compute the values $g_i(\kappa)$ for a grid of κ values. But it is better to store the κ-values for a fixed grid of g-values. In fact, we will use a globally fixed grid of 16 g-values:

```
0.01786956, 0.09150009, 0.2135104 , 0.3674544 ,
0.5325456 , 0.6864896 , 0.8084999 , 0.8821304 ,
0.9019855 , 0.9101667 , 0.9237234 , 0.9408283 ,
0.9591717 , 0.9762766 , 0.9898333 , 0.9980145
```

We now store, for each of the 483 wavelength domains 16 values of κ, which are the κ values belonging to $g(\kappa)$ equal to the 16 values given above. The correlated-k opacity table is thus given by

$$\kappa_{i,k} \equiv \kappa(\nu_i, g_k) \qquad \text{with } 0 \le i < 483, \text{ and } 0 \le k < 16 \tag{7}$$

where $\nu_i = c/\lambda_i$ is the average frequency of wavelength range i (with $\lambda_i = (\lambda_{i+1/2} + \lambda_{i-1/2})/2$). This means we now "only" have to integrate the formal transfer equation for $483\times16 = 7728$ points in λ-g space. This is still a substantial number, but much less than a few million that the LBL method requires. The table of $\kappa_{i,k}$ values is the correlated-k opacity table.

Question: How it is calculated? Answer: we ask an expert to calculate it for us! In this case, we use the correlated-k opacity tables from the `petitCODE` radiative transfer package[4] written by Dr. Paul Molliere.

Another question: How do we work with this correlated-k opacity? Answer: by first doing the formal transfer integrations for all i and k, and then summing over the g_k-bins. Example: Suppose we wish to compute how the stellar flux F^*_ν gets extincted as it travels from the top of the atmosphere downward to the ground. After performing the FTE for all 483 wavelength bins and all 16 g-bins, we have obtained the values $F_{ik}(z=0)$. Now we are no longer interested in the k-dependence, so we can integrate over g:

$$F_i = F_{\nu_i} = \int_0^1 F_{\nu_i g} dg = \sum_{k=0}^{15} F_{ik} \Delta g_k \tag{8}$$

where Δg_k are the values:

```
0.04555284, 0.1000715 , 0.141168  , 0.1632077 ,
0.1632077 , 0.141168  , 0.1000715 , 0.04555284,
0.00506143, 0.01111905, 0.01568533, 0.01813419,
0.01813419, 0.01568533, 0.01111905, 0.00506143
```

which, as you can verify, add up to 1 (since we have to guarantee that $\int_0^1 dg = 1$). The values of the ratio $F_i(z=0)/F_i(z=z_{\mathrm{TOA}})$ (with z_{TOA} being the "top of the atmosphere" defined as 60 km) are now the values plotted in the transmission spectrum shown above.

Important note: We are only allowed to integrate over g (sum over k) *after* performing the integral of the FTE! If we would do it before the FTE, we would defeat the purpose of the correlated-k method, and we would obtain unreliable results.

Another note: from the point of view of the FTE we do not care about distinguishing between i and k: we simply treat each combination of i and k as a separate wavelength point for which a separate FTE has to be integrated. Only when we want to plot mean intensities or mean fluxes, we need to integrate over g (i.e. sum over k) to get rid of the g-dependence. So the trick is to keep working in (i,k) space (i.e. working with all $483\times16 = 7728$ bins) until the very end, and only then do the k-summation.

At this point one could think that we only need to ask our "opacity expert" to compute for us the 7728 values of k_{ik}, which is a file of only 62 kB size, and then we can start working on our atmosphere model. However, that is a bit too optimistic. The problem is that these correlated-k opacities depend on:

1. The temperature of the gas T,

[4] `http://www2.mpia-hd.mpg.de/homes/molliere/#petitcode`

2. the pressure of the gas P, and
3. the abundance of the molecular constituents H_2O, CO_2, O_3 and CH_4.

Both temperature and pressure change with height z above the ground. Even the abundance of the water vapor and the ozone changes with z (the abundances of CO_2 and CH_4 can be assumed to be independent of z). This means that we have to compute the 7728 values of κ_{ik} for each vertical grid point z_j separately. Because we have 61 vertical grid points in the `earth_atmosphere_model.txt` model definition file, this means that our correlated-k opacity table will have $7728\times 61 = 471408$ values[5]. This is a data file of about 3.8 MB size. That is still very manageable. The file containing these values is called `interpolated_correlkappa_mix.npy`. It is a datafile in the standard Python data format. You can read it from within Python in the following way[6]:

```
import numpy as np
kappa = np.load('interpolated_correlkappa_mix.npy')
```

This `kappa` is then an array of dimension `(61, 483, 16)`, i.e. 61 points in z, 483 points in frequency $\nu_i = c/\lambda_i$ and 16 points in g_k. In addition there is a file called `interpolated_correlkappa_metadata.txt` that contains a lot of useful information such as the λ_i grid, the g_k grid, as well as the values of T_j and P_j for which the opacities were computed (they correspond to the temperature and pressure at the 61 height grid points, starting at $z = 0$ and ending at $z = 60$ km).

To make it a bit easier to read the correlated-k opacities from the `interpolated_correlkappa_mix.npy` as well as the metadata from the `interpolated_correlkappa_metadata.txt` file, we provide a python code for that:

```
import read_ck as ck
opac = ck.InterpolatedCorrKapp('mix')
```

Now `opac.kappa` contains the `(61, 483, 16)` array of κ values, `opac.g_weights` the 16 values of Δg_k, `opac.opac.nu_hz` the 483 values of ν_i in units of Hz, `opac.wl_micron` the corresponding 483 values of λ_i in units of μm, `opac.opac.dnu` the $\Delta\nu_i$ that you can use for integrals over ν, and finally `opac.P` and `opac.T` being the $P_j = P(z_j)$ and $T_j = T(z_j)$ values belonging to the heights z_j above the ground. Note that the file does not explicitly contain the z_j values themselves (you can find them in the file `earth_atmosphere_model.txt`; the values of P and T should correspond to the ones in that file).

To get you started with these complicated data files, here are two little Python scripts that produce nice figures. The first one plots the $\kappa_{\nu,g=g_0}$ and $\kappa_{\nu,g=g_{15}}$ (the lowest and the highest opacity of each wavelength bin):

```
%run plot_mixed_kappas.py
```

The second computes the transmission spectrum and the transmitted solar and ground spectra (see figures above):

[5] If you would like to obtain the original data files and the code to compute these z-dependent correlated-k opacity tables from the original data files yourself, just let me know and I'd be happy to give them to you, so that you can experiment with different abundances of water, carbon dioxide, ozone and methane.

[6] IMPORTANT NOTE: The κ opacity values in this file are in CGS units, i.e. they are cm^2/g, where g stands for gram of gas. To convert to m^2/kg just multiply by 0.1.

```
%run plot_mixed_kappas_transmission.py
```

Please look into these two example codes to learn how to use the correlated-k opacities for the atmosphere model.

Assignment: We will *not* try to self-consistently compute the temperature profile as we did for the exoplanet atmosphere, because that requires a bit more physics. But what we *can* do is compute the mean intensity spectrum $J_\nu(z)$ (integrated over g) at each height z_j. Write a computer program that does this. You can start from the programs you created before. But now you have to include two extra dimensions: that of ν and that of g (i.e. 483×16). So you first compute all 61×483×16 values of $J_{\nu,g}(z)$, and then multiply by Δg_k and sum over k to obtain the 61×483 values of $J_\nu(z)$. To keep things simple and fast, use 2 values of μ (the usual $\pm 1/\sqrt{3}$). Keep the atmosphere cloud-free. No iteration is needed. Just one integration of the FTE. For the Sun you use a Planck spectrum at 5780 K and for the ground spectrum a Planck spectrum at 290.15 K (see the above example python programs to learn how). The Sun has $\cos(i) = 0.5$. Plot the resulting spectrum for different z_j and see how it changes with z_j, and try to explain what you see.

Next compute, from the same FTE calculation, the netto flux:

$$F_\nu(z) = 2\pi \int_{-1}^{+1} I_{\nu\mu}(z)\mu d\mu - \cos(i) F^*_\nu(z) \tag{9}$$

where the integral over μ is (for only two values of μ) a sum of only 2 values (at each combination of ν, z). Note that

$$I_{\nu\mu}(z) = \int_0^1 I_{\nu\mu g}(z) dg \tag{10}$$

is the g_k summed itensity (but only *after* having integrated the FTE). Now also plot this flux. Try to explain what you see, and why it changes with z the way it does. To help you check if you get the right answer, here is the result for $z = 5\,\mathrm{km}$: