Prescriptions to generate Modtran and LibRadtran predictions for air transparency at LSST site

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Abstract

This note aims specifying a set of atmospheric configurations, in order to compare the air transparencies predictions by Modtran and LibRadtran for LSST site. Starting from similar atmospheric model, we want to check the level of agreement between both predictions within the accuracies of LSST photometry as well as auxiliary telescope wavelength resolution.

1 Introduction

We want to compare air-transparency predicted by Modtran and LibRadtran for LSST observatory site. This comparison can be done only if we choose common configuration parameters for the kind of atmosphere from which both simulators can calculate air attenuation.

2 Common configuration parameters

2.1 Wavelength range and accuracy

Wavelength : $\lambda \in [250, 1200]$ nm, $\Delta\lambda$ =1 nm

It must be noticed that every light interaction process may not be defined over this whole range. For example, in LibRadtran, one cannot simulate with wavelength smaller than 250 nm, except for special cases.

2.2 LSST site

Altitude : $h = 2.680$ km.

2.3 Zenith angle

We want to compare the air shower simulator over a wide range of airmass values. Thus we recommends to simulate air-transparencies for

Airmass : z computed for 31 points in steps of 0.1 : $z \in [1, 3]$.

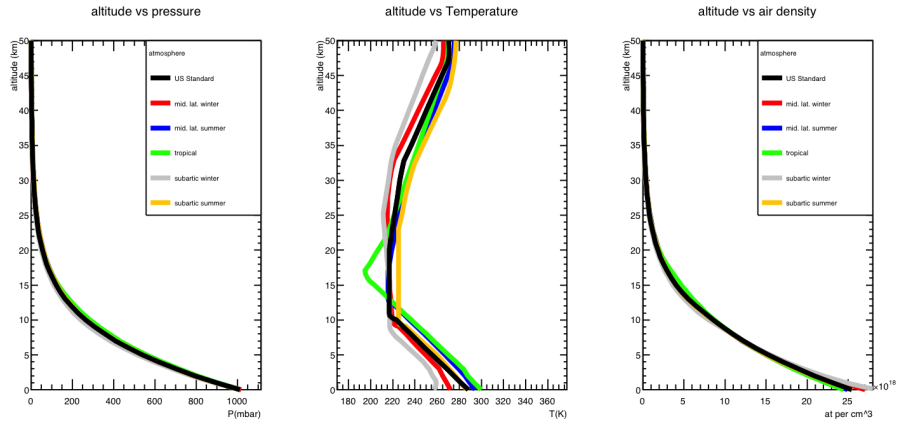

Figure 1: Vertical profiles for Temperature, Pressure and Air density for typical atmospheres in LibRadtran.

Usually, simulation programs need the zenith angle θ_z as input parameter. Then we should use the simple relation between θ_z and z :

$$z = \sec \theta_z = \frac{1}{\cos \theta_z} \tag{1}$$

3 Solvers and Geometry options

Because we want to compare calculations at high airmass, we have to compare calculations performed either under the standard parallel plane approximation and also under the pseudo-spherical correction. The we recommends to select two Radiative Transfer Equation (RTE) solvers :

Two RTE solvers : "*disort*" for Parallel Plane approximation and "*sdisort*" for Pseudo-Spherical correction.

4 Atmospheric models

There are several pre-defined atmospheres in both simulation packages. These atmospheres are defined by their vertical profile of the Temperature, Pressure and Air densities. The typical profiles expected are shown on figure 1.

If pressure and air density may not vary a lot from one atmospheric model to another, Temperature profiles may be quite different, especially at ground and also at temperature inversion altitude at $h = 15 - 20$ km. We will see that Temperature has an impact on absorption coefficient but has little effect on scattering processes like Rayleigh and Aerosols.

Then looking at molecular species vertical profiles densities on figure 2, we can notice the large dispersion between the various atmosphere on precipitable water level close to ground and also on ozone at $h = 15 - 20$ km, precisely where Temperature has significant variations.

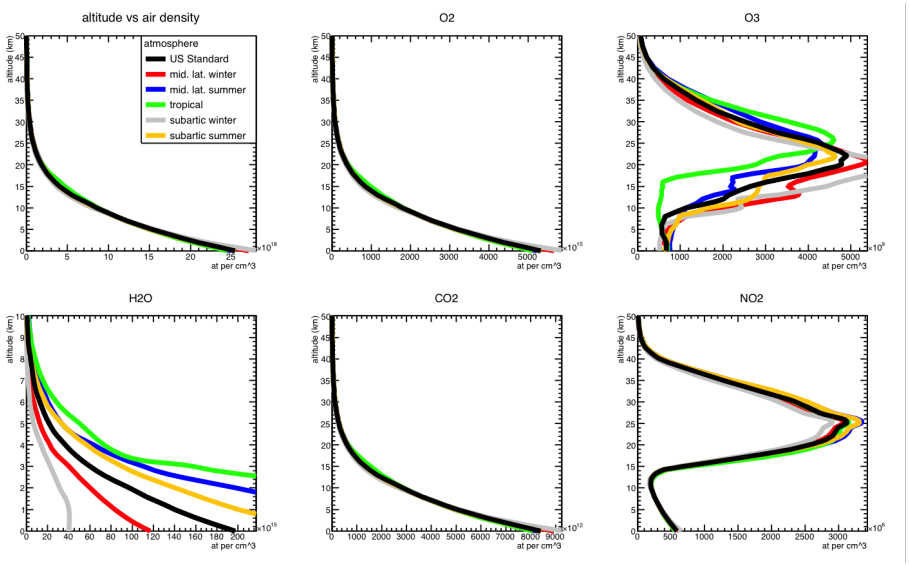

Figure 2: Densities profiles for different molecules in air for typical atmospheres in LibRadtran.

Thus we propose to use the two standard atmospheres (AFGL-TR-86-0110 [3], which are probably both defined in Modtran and LibRadtran, the standard US atmosphere and also the subarctic winter the driest climate which may be well suited to LSST.

Atmospheric models : AFGL atmospheric constituent profile : U.S. standard atmosphere 1976 and Subarctic Winter.

The US atmosphere is shown as the black line in figure 1 and 2. This US atmosphere is a good choice because it is not a extreme case. Really it can be considered as an average of all other atmospheric models. It shows an average PWV at ground and also an average Temperature at the 20-25 km altitude.

5 Comparison of Rayleigh Scattering

Rayleigh scattering is also called molecular scattering. It is an elastic scattering of light on the molecules of the atmosphere. The proposition is to simulate a pure Rayleigh atmosphere by switching off any other scattering process like the particle or Mie scattering also called the Aerosols scattering.

The Figure 3 hows the air transparencies obtained by LibRadtran for the 10 selected air-masses.

The comparison of Rayleigh Scattering in Modtran and LibRadtran is not difficult. Indeed, the air optical index τ can be easily approximated by two formula as follow

$$\begin{cases} \tau & = & \frac{X_v(h)\cdot z}{2770 g/cm^2} \left(\frac{400nm}{\lambda}\right)^4 \\ \tau & = & \frac{X_v(h)\cdot z}{3102 g/cm^2} \left(\frac{400nm}{\lambda}\right)^4 \frac{1}{1-0.0722\left(\frac{400nm}{\lambda}\right)^2} \end{cases} \quad (2)$$

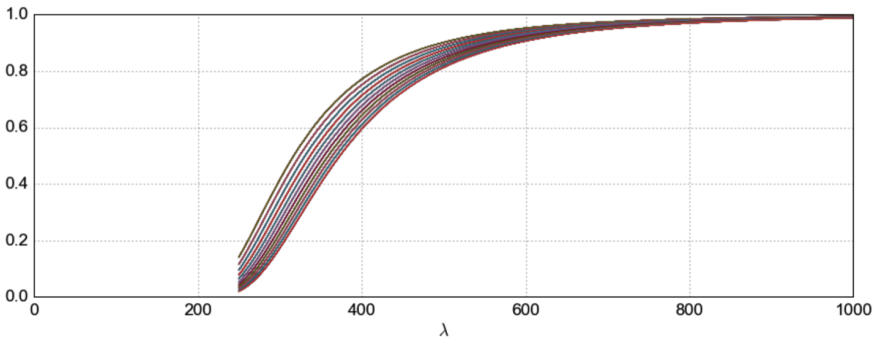

Figure 3: Air transparencies attenuation predicted by LibRadtran for US standard atmosphere, when only Rayleigh scattering is selected and all other processes like aerosols scattering and molecular absorption are switched off. The different lines are obtained by varying the airmass $z = 1., 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0$.

where is $X - v(h)$ is the atmospheric column depth at altitude h expressed in unit g/cm^2 and z is the airmass. The air transparency is given by $T = e^{-\tau}$.

In our case, we have to choose h as the LSST altitude.

By fitting the simulated air transmittance curve as a function of the wavelength λ,

$$\ln T(\lambda) = -\tau(\lambda) = -\frac{C \cdot z}{\left(\frac{400nm}{\lambda}\right)^4} \tag{3}$$

one can compare the fitted value of the C parameter derived from Modtran and LibRadtran for each of the 10 airmass values z. C should depend only on air density or pressure at altitude h. Thus C values are expected to be very similar within the computer errors.

Pure molecular scattering : Simulate a pure molecular scattering atmosphere for pre-selected airmass and climate, without absorbing component and without aerosols.

6 Comparison of Absorption predictions

We want to compare atmospheric absorption prediction by switching off any scattering process. An example of such prediction for each of the 10 airmass values z is shown on figure 4.

Several molecular species in the air show either few strong absorption lines like O_2 or wide absorption bands like H_2O (PWV) or O_3.

6.1 Various Absorption Models

Because bands consist in tens of thousand lines that may overlap, it is usually impossible to compute the absorption line by line. Instead one has to select different kinds of models which implement absorption in the bands. These

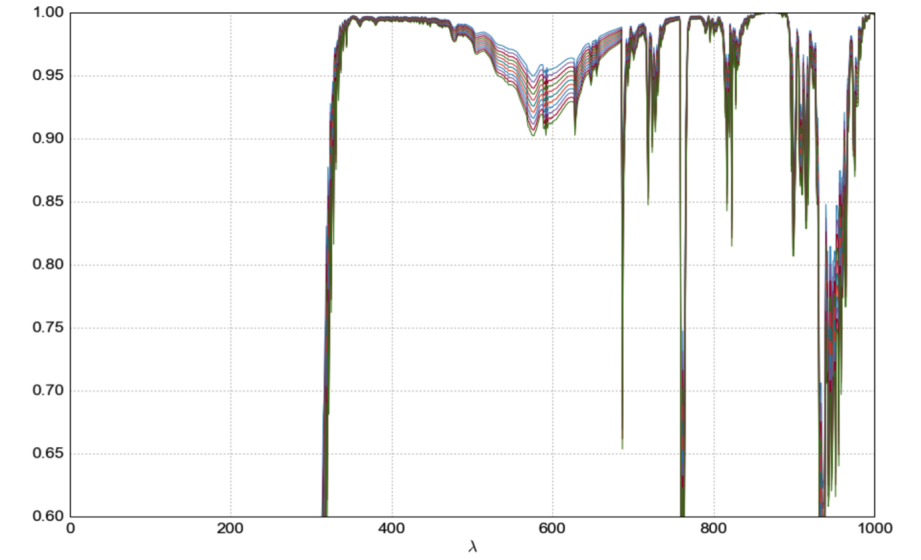

Figure 4: Air transparency predicted by LibRadtran, when only molecular absorption is selected.

models are probably implemented both in Modtran an LibRadtran as well. However, those models implementation need to be compared.

In the LibRadtran documentation, such models are referred as :

- **Spectrally resolved calculation**,
- **Line-by-line calculation**,
- **The correlated-k method**,(Kato and Kato2),
- **Representative wavelengths parameterization (REPTRAN)**,
- **Pseudo-spectral calculation adapted from LOWTRAN**.

Probably, there is no need for perfectly well resolved lines calculations (which consumes much simulation time) for LSST broad band photometric measurements. We suggest to simulate only the "correlated-k method", the "Representative wavelengths parameterization" and the "Pseudo-spectral calculation".

Absorption models : 1) REPTRAN, 2) LOWTRAN, 3) KATO2, 4) KATO

6.2 Variable component specifications

Once the absorption models, one has to specify the amount of variable components in the selected atmosphere. The two variable molecular component of interest for LSST are the precipitable water vapor (PWV) and Ozone (O_3). Even if the standard atmosphere include a default value for such component, we strongly recommend to overwrite the standard value by a set of pre-defined values.

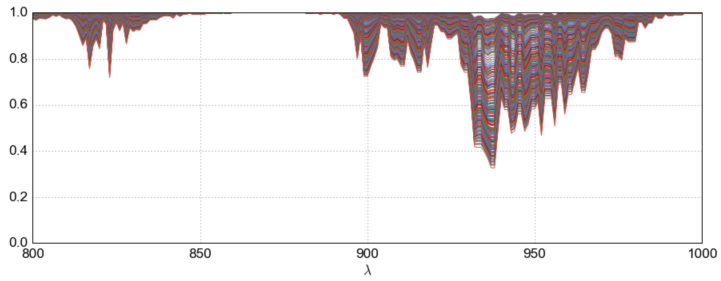

Figure 5: Simulation of absorption by PWV for PWV ranging from $0.1, 0.2, 0.3, \cdots 9, 8, 9.910$ mm.

6.2.1 Precipitable Water Vapour

We can vary the H_2O pwv in a wide range of values as shown on figure **??**.

H_2O **PWV :** Generate Modtran/LibRadtran absorption profiles for 31 points $pwv \in [0 \text{ mm}, 15 \text{ mm}]$ in steps of 0.5 mm (and fix O_3 to 300 Dobson unit).

6.2.2 Ozone

Again we can vary the amount of Ozone in the atmosphere we have selected :

O_3 **absorption bands** : Generate Modtran/LibRadtran absorption profiles in grids of 21 points $O_3 \in [200 \text{ Dobson}, 600 \text{ Dobson}]$ (and fix pwv to 3 mm).

7 Combination of scattering and absorption

We have to combine the molecular scattering process with the molecular absorption processes.

Combined light interaction processes : simulate pure molecular scattering, pure molecular absorption, combined molecular scattering and absorption.

8 Comparison of Aerosols

The simulation of aerosols may be done by specifying the Aerosol Optical Depth (AOD) τ_0 at a given wavelength λ_0 and giving the value of the Angstrom exponent α such the effective optical depth $\tau_{aer}(\lambda)$ is :

$$\tau_{aer}(\lambda) = \tau_0 \cdot \left(\frac{\lambda_0}{\lambda}\right)^{\alpha} \tag{4}$$

Aerosols : $\tau_0 \in [0, 0.5]$ in steps of 0.01, $\alpha \in [0, 4]$ in steps of 0.5, $\lambda_0 = 532$ nm. We suggest to simulate this with a pure molecular scattering atmosphere.

9 Summary

9.1 Summary with color conventions

The list of the settings for the simulations are listed below :

Simulation parameters summary and analysis to compare Modtran and LibRadtran.

9.2 Numbers of runs and files

Number of	Variable name	Number	Range	Step	Comment
Airmass	z	31	$[1, 3]$	0.1	Check PP wrt PS
Solvers	rte	2	(PP, PS)		Radiative transfer Eq.
Atmosphere	atm	2	(us, sw)		out of 6 standards def.
Light inter. procs	$procs$	4	$(mol\_scatt, mol\_abs, mol\_all)$		no aerosols
Abs Models	$amod$	4	$(rept, lowt, kato2, kato)$		
Water vapor	pwv	31	$[0, 15]$	0.5	O_3 set to 300 Dobson
Ozone	O_3	21	$[200, 600]$	20	pwv set to 3 mm
Aerosols1	τ_0	51	$[0, 0.5]$	0.01	
Aerosols2	α	17	$[0, 4]$	0.25	

9.3 Counting the files

9.3.1 Pure molecular scattering files (Rayleigh)

$$\begin{aligned} N_{molscat}^{files} &= N_z \times N_{rte} \times N_{atm} \\ &= 31 \times 2 \times 2 = 124 \end{aligned} \tag{5}$$

9.3.2 Pure molecular absorption files

The number of pure molecular absorption files with varying $H2_0$:

$$\begin{aligned} N_{molabs}^{files}(H_2O) &= N_z \times N_{rte} \times N_{atm} \times N_{proc} \times N_{amod} \times N_{pwv} \\ &= 31 \times 2 \times 2 \times 4 \times 4 \times 31 = 61504 \end{aligned} \tag{6}$$

The number of pure molecular absorption files with varying O_3 :

$$\begin{aligned} N_{molabs}^{files}(O_3) &= N_z \times N_{rte} \times N_{atm} \times N_{proc} \times N_{amod} \times N_{O3} \\ &= 31 \times 2 \times 2 \times 4 \times 4 \times 21 = 41664 \end{aligned} \tag{7}$$

9.3.3 Combined molecular scattering and absorption

In this case we double the number of files we had to simulate for pure molecular absorption. Thus we would have another 103168 files.

In total we would generate 206460 files.

9.3.4 Variation of aerosols

For the aerosols, we assure to use a single configuration of molecular scattering and absorption. We have to simulate aerosols over a two parameter grid :

$$\begin{aligned} N_{molabs}^{files}(H_2O) &= N_z \times N_{rte} \times N_{atm} \times N_{\tau} \times N_{alpha} \\ &= 31 \times 2 \times 2 \times 31 \times 21 \times 31 = 80724 \end{aligned} \tag{8}$$

9.3.5 File size and total file size

For LibRadtran, the output is a file of two columns. First column is the wavelength. The second column is the air transmittance. In total, there are 1101 lines.

The typical file size is 25kB.

- We need at least 5.2 GB storage, without aerosols.
- If we want to simulate an aerosols grid, we would need at least 2 GB.

10 File naming conventions

We can propose a file naming convention accounting for the selected parameters for the simulation :

P_O_{rte}_{atm}_{proc}_{mod}_zXX_wvXX_ozXX.extension

P : **RT** or **MT** for LibRadtran or Modtran,

O : Observatory site **LS** or **HP** or **GM** or **MK** for LSST, OHP, Gemini South, Mauna Kea,...

{rte} : **pp** or **ps**,

{atm} : **us** or **sw**,

{proc} : **sc** for pure molecular scattering, **ab** for pure molecular absorption, **sa** for the combination of molecular scattering and absorption,

{mod} : **rt** for Reptran model, **lt** for Lowtran model, **k2** for Kato2 model, and **kt** for Kato model.

zXX : Airmass z, where XX is the value of the airmass on 2 digit $XX = 2 \times z$,

wvXX : Precipitable water vapour pwv, where XX is the value of the pwv on 3 digit $XXX = 10 \times pwv$, pwv in mm unit,

ozXX : Ozone oz, where XX is the value of the oz on 2 digit $XX = oz/10$, oz is Dobson unit.

File extension may be chosen to be $extension = dat$ or $extension = txt$.
For example a filename for LibRadtran, for LSST could be :

$$RT\_LS\_pp\_us\_sa\_rt\_z15\_wv030\_oz30.txt$$

where $pwv = 3$ mm and $oz = 300$ Dobson unit and $z = 1.5$.

11 Files organisation

We may suggest a hierarchical structure of the files in embedded directories. Each leaf directory provides the set of simulated files of varying z and pwv or oz in case of molecular absorption, for a given atmospheric and absorption model configuration.

rootdir	top directory
rootdir/RT/VXX/LS/pp/us/sc/	pure molecular scattering
rootdir/RT/VXX/LS/pp/us/ab/rep/pwv/	pure molecular absorption for varying pwv
rootdir/RT/VXX/LS/pp/us/ab/rep/oz/	pure molecular absorption for varying oz
rootdir/RT/VXX/LS/pp/us/sa/rep/pwv/	molecular absorption and scattering for varying pwv
rootdir/RT/VXX/LS/pp/us/sa/rep/oz/	molecular absorption scattering for varying oz
rootdir/RT/VXX/LS/pp/us/sc/ae/	pure molecular scattering and aerosols scattering
rootdir/RT/VXX/LS/pp/us/sa/rep/ae/	molecular absorption scattering and aerosols scattering

VXX is the version number of Radtrran or Modtran.

In a leaf directory, interpolation of spectra in z and either pwv or oz is possible.

A Minutes

Kirk, Sylvie et al,

Below are short minutes of our Friday meeting. I think we had a productive discussion, thank you all for your time. I try to be short. Please email me if you think I have forgotten something.

Atmosphere models : MODTRAN / libRadTran comparison
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(*) Sylvie is finishing up a note, where she discusses input parameters for libRadtran. The goal is to define a standard atmosphere, not too different from what we have at Cerro Pachon, and to generate a grid of libRadTran models around this standard atmosphere.

(*) Regarding the atmosphere profiles: there are several standard options available in libRadTran (and MODTRAN). For the moment, Sylvie is going to pick "US standard" and "Arctic Winter" and generate the same grid of model for each of these profiles.

(*) Sylvie has not yet explored the aerosols options (in particular, everything regarding the typical particle sizes) in detail. The atmosphere models will have an aerosol component, which may require further refinements in the future.

(*) Sylvie will produce the transmission curves of the individual components alongside her full models.

(*) Kirk is going to generate the same grid of models, (same parameters, same assumptions, same atmosphere profiles) with MODTRAN.

(*) These grids of models will be uploaded on the github repository of Key Task #5 (atmospheric models). Sylvie and Kirk have code too, that will be uploaded there.

(*) in a second step, similar grids will be produced for an atmosphere that is typical of OHP.

Modeling the telescope <-> stardice line of sight at OHP
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(*) Kirk is going to produce a grid of atmospheric transmissions for the configuration we have at OHP : horizontal line of sight, L=250-m, pressure, PWV, Ozone, aerosol opt. depth to be transmitted by Sebastien.

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Preliminary model comparisons
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 (*) The first step, when comparing libRadtrans vs.  MODTRAN
     transmission, is to determine, for any given transmission generated
     with one model, how well (and for what value of its parameters) the
     other can reproduce this transmission.

 (*) Sylvie has sent models typical of the atmosphere at OHP to
     Sebastien, who has performed a preliminary comparison with the
     Buton et al model (tuned on observations performed at Mauna Kea)

 (*) Sebastien has shown that the Buton model can reproduce the
     transmissions sent by Sylvie well.

CTIO spectroscopic data
=======================

 (*) Kirk presents the data he has taken at CTIO. These are
     spectroscopic observation of (CALSPEC?) stars, followed
     during the night, over a wide range of airmass.

 (*) an interesting goal is to explore whether one can describe the
     variations of atmospheric absorption with MODTRAN.

 (*) Kirk is going to produce a data release (files + models + current
     version of his fit code + readme)

TODO:
=====

 (*) Nicolas creates a git repository for Key Task #5

 (*) Sylvie and Kirk generate grids of libRadTran and MODTRAN models
     around a typical Cerro Pachon atmosphere.

 (*) In a second step, they produce similar grid for a typical
     atmosphere at OHP and Mauna Kea.

 (*) Kirk produces a grid of model for the horizontal line of sight at
     OHP.

 (*) Kirk prepares a data release for the CTIO / Pachon data.

Nicolas.
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Github

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Dear all,
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Just letting you know that I have created a new git repository for the PCWG work on the atmospheric extinction.

It is here:

https://github.com/DarkEnergyScienceCollaboration/PC5AtmosphericExtinction

At the moment, the repository is private. Shall I make it public ? It think it can be public. If the consensus is that it should be kept private, please send me your github usernames, so that I can grant access to it.

Regards,

Nicolas.

References

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