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 : $h = 2.75$ 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 : $z \in [1, 3]$.

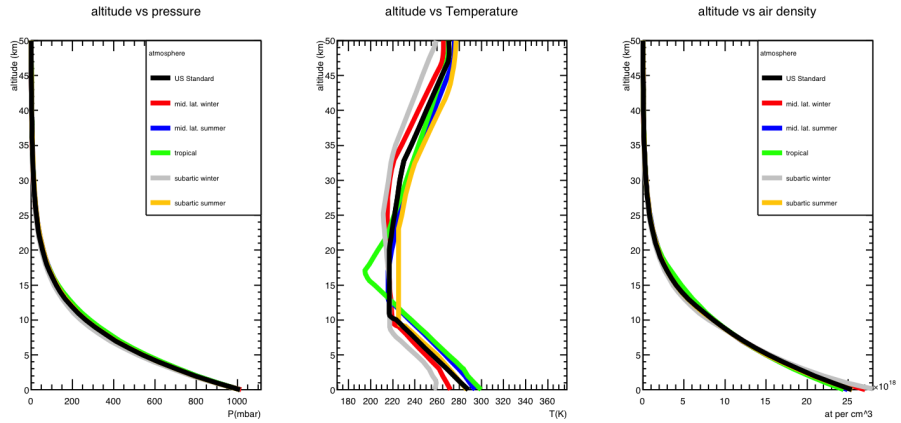

Figure 1: Vertical profiles for Temperature, Pressure and Air density for typical atmospheres in LibRadtran.

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.

It is possible that only the RTE solver "disort" is available in Modtran. In a first stage, we focus on a Parallel Plane and disort comparison.

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

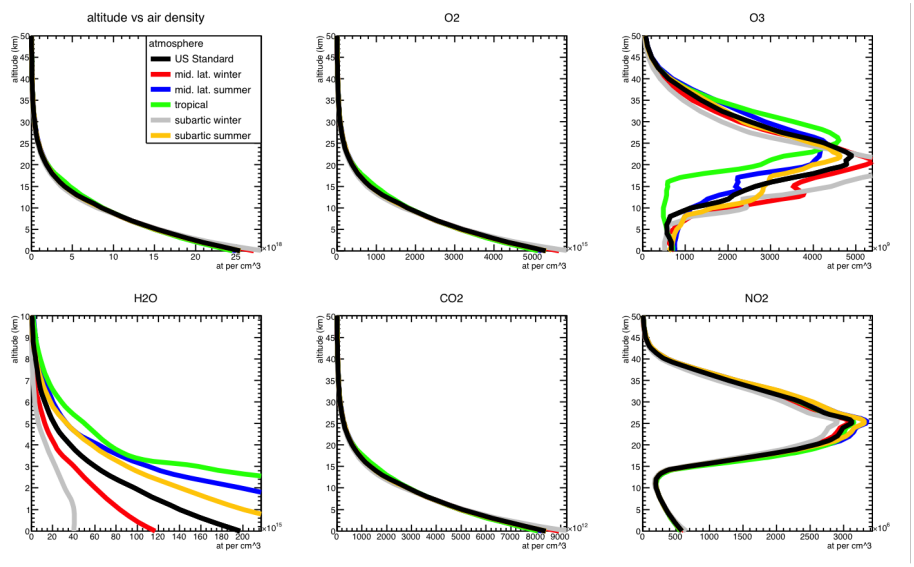

Figure 2: Densities profiles for different molecules in air for typical atmospheres in LibRadtran.

water level close to ground and also on ozone at $h = 15 - 20$ km, precisely where Temperature has significant variations.

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.

The above atmospheric models are both available in Modtran(Data Card : Card1.MODEL) and LibRadTran (Data Card : atmosphere_file.)

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

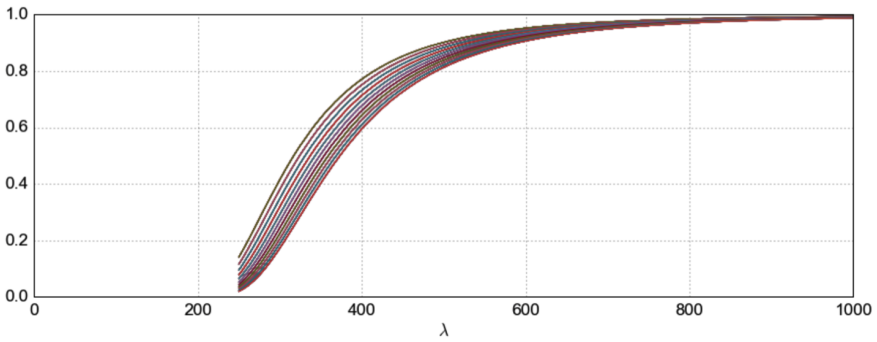

Figure 3: Air transparencies attenuation predicted by LibRadtran for US standard atmosphere, when only Rayleigh scattering is selected and all other processes like aerosols scattering and molecular absorption are switched off. The different lines are obtained by varying the airmass $z = 1., 1.1, 1.2,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

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

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.

It is not sure it is possible to switch on only molecular scattering and switching off molecular absorption in Modtran.

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.

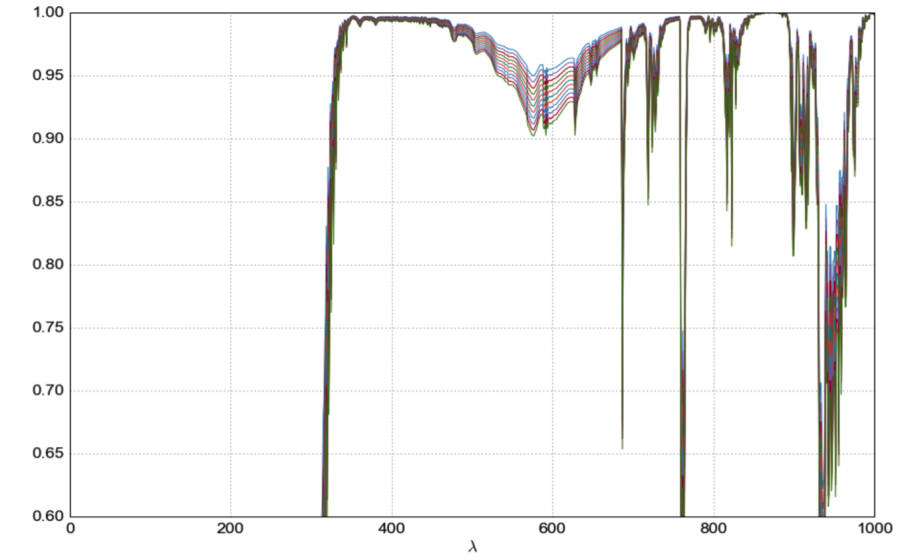

Figure 4: Air transparency predicted by LibRadtran, when only molecular absorption is selected.

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

6.1.1 Absorption models in LibRadTran :

In the LibRadtran documentation, such models are referred as :

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

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" [1]

[1]For the moment, I can generate absorption spectra with REPTRAN, LOWTRAN and CRS. Apparently CRS parameterize only ozone.

Absorption models in LibRadTran : 1) REPTRAN, 2) LOWTRAN, 3) CRS, 4) Fu 5) KATO, 6) KATO2, 7) KATO2.96

The Data card for specifying the absorption model in LibRadTran is *mol_abs_param* . One should provides the values *reptran fine* or *reptran medium*, *reptran coarse* or *lowtran*,...

6.1.2 Absorption models in Modtran:

In ModTran, the absorption models are refered as :

- **Band models methods**, The Modtran or Lowtran models,
- **The correlated-k method**, The Modtran and Lowtran either in slow or medium modes.

Absorption models in Modtran : 1) MODTRAN band Model, 2) LOWTRAN Band Model , 3) MODTRAN correlated-k and slow speed, 4) MODTRAN correlated-k and slow speed, 5) MODTRAN correlated-k and medium speed.

The Data card for specifying the absorption model in Modtran is *CARD1 MODTRN* . One should provides the values *T,M,C,K,F,L* and *CARD1 SPEED* is *S* or blank.

6.1.3 Summary on Models comparison

Probably we should compare the standard absorption model REPTRAN of LibRadTran (available in FINE, MEDIUM and COARSE modes) to the MODTRAN model in Band and correlated-k calculations provided by Modtran program on the one side and compare LOWTRAN in LibRadTran to LOWTRAN in band model as well as correlated-k calculation provided by Modtran. The question remains: can we switch off the molecular scattering is Modtran program to focus only to absorption features.

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.

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.

Data card for Precipitable Water Vapour in LibRadTran: Typically to overwrite the default Precipitable Water Vapour of the atmospheric model, one should specify the following Data Card in LibTadTran : *mol_modify H2O XX mm*, where *XX* is the column depth of precipitable water in millimeters.

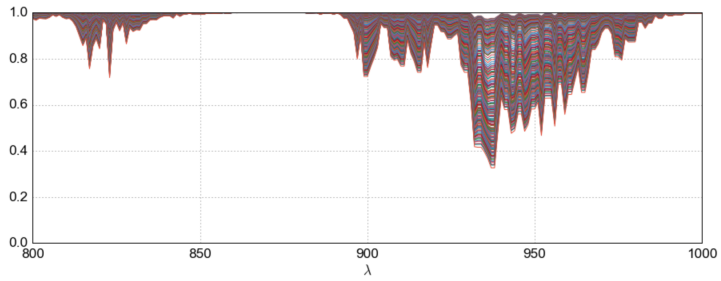

Figure 5: Simulation of absorption by PWV for PWV ranging from $0.1, 0.2, 0.3, \cdots 9, 8, 9.910$ mm.

Data card for Precipitable Water Vapour in Modtran: Typically to overwrite the default Precipitable Water Vapour of the atmospheric model, one should specify the following Data Card in ModTran : *CARD1A H2OSTR XX*, where XX is the column depth of precipitable water in g/cm^2.

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 $O_3 \in [200 \text{ Dobson}, 600 \text{ Dobson}]$.

Data card for Ozone in LibRadTran: Typically to overwrite the default Precipitable Water Vapour of the atmospheric model, one should specify the following Data Card in LibTadTran : *mol_modify O3 XX DU*, where XX is the column depth of Ozone in Dobson Units.

Data card for Ozone in Modtran: Typically to overwrite the default Precipitable Water Vapour of the atmospheric model, one should specify the following Data Card in ModTran : *CARD1A O3STR XX*, where XX is the column depth of Ozone in g/cm^2.

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.

If the molecular scattering cannot be swithed off in Modtran, then this combination of scattering and absorption will be the only way to compare Modtran and LibRadTran.

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.

Aerosols, to be defined later.

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	Name	Nb.	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	$(rept, lowt, crs, fu, kato2, kato)$		
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} in LibRadTran : **rt** for Reptran model, **lt** for Lowtran model, **cr** for CRS model, **fu** for the Fu and Liou model, **k2** for Kato2 model, and **kt** for Kato model.

{mod} in ModTran : **mt** for Modtran band model, **mk** for Modtran correlated-k model, **lt** for Lowtran 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 $z = 1.5$.

A more accurate definition of *mod* in ModTran could be :

{mod} : in ModTran :

- **mt** for Modtran band model (CARD1.MODTRN='T'),

- **mm** for Modtran band model (CARD1.MODTRN='M'),,
- **lt** for Lowtran band model (CARD1.MODTRN='L' or 'F'),
- **mks** for Modtran correlate-k in slow mode (speed), (CARD1.MODTRN='K' or 'C and CARD1.SEED='S'),
- **mkm** for Modtran correlate-k in medium mode (speed), (CARD1.MODTRN='K' or 'C and CARD1.SEED='M'),

For example a filename for Modtran, for LSST could be :

$$MT\_LS\_pp\_us\_sa\_mt\_z15\_wv030\_oz30.txt$$

where $pwv = 3$ mm and $oz = 300$ Dobson unit[2] 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/rt/wv/	pure molecular absorption for varying pwv
rootdir/RT/VXX/LS/pp/us/ab/rt/oz/	pure molecular absorption for varying oz
rootdir/RT/VXX/LS/pp/us/sa/rt/wv/	molecular absorption and scattering for varying pwv
rootdir/RT/VXX/LS/pp/us/sa/rt/oz/	molecular absorption scattering for varying oz
rootdir/RT/VXX/LS/pp/us/sc/ae/	pure molecular scattering and default aerosols scattering
rootdir/RT/VXX/LS/pp/us/sa/rt/ae/	molecular absorption scattering and default aerosols scattering
rootdir/RT/VXX/LS/pp/us/sc/as/	pure molecular scattering and special aerosols scattering
rootdir/RT/VXX/LS/pp/us/sa/rt/as/	molecular absorption scattering and special aerosols scattering

VXX is the version number of Radtrran or Modtran. Special aerosols scattering means not standard. The exact definition will be provided.

In a leaf directory, interpolation of spectra in z and either pwv or oz is possible. Notice that under the above directories, it is proposed to keep input configuration parameter and output results in parallel directories :

```
in/ : input files for configuration
out/: files results of the simulation
```

[2]In Modtran Dobson Unit Ozone has to be given in g/cm^2. Thus Dobson Unit has to be converted into equivalent g/cm^2 units.

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
==========

(*) 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
==========

(*) 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.

```
Preliminary model comparisons
=============================

 (*) 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.
```

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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