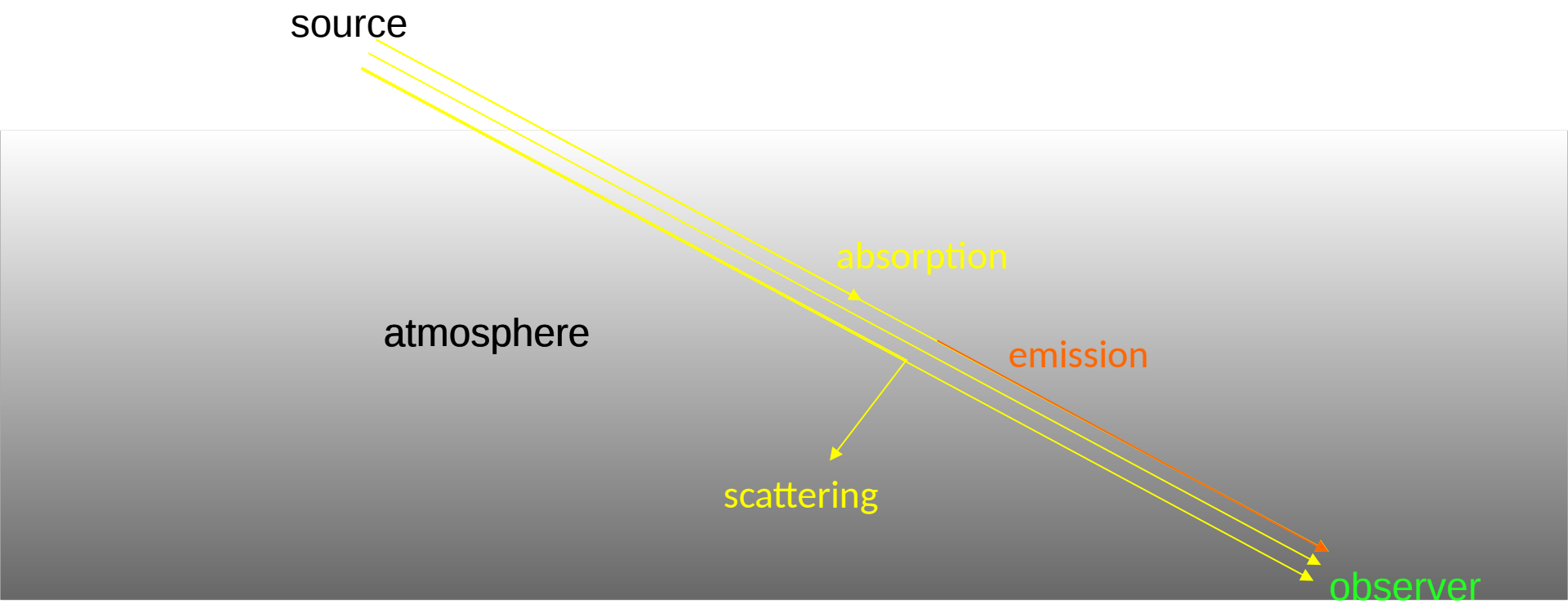
Molecfit

http://www.eso.org/sci/software/pipelines/skytools/molecfit

Sabine Moehler

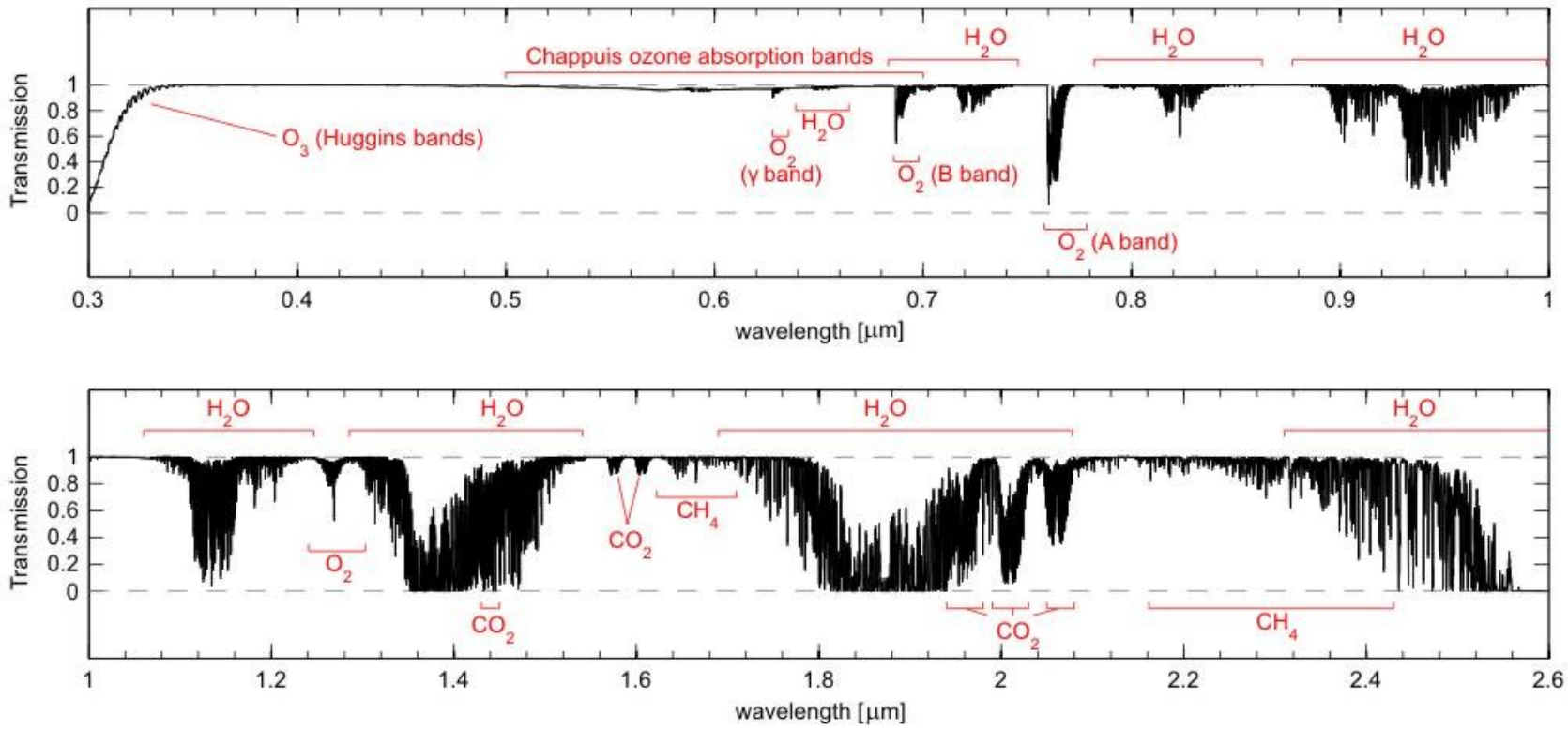
Based on a presentation by
Wolfgang Kausch
(Innsbruck, Austria)

Atmospheric Correction



Atmospheric Correction

Atmospheric absorption / optical + NIR

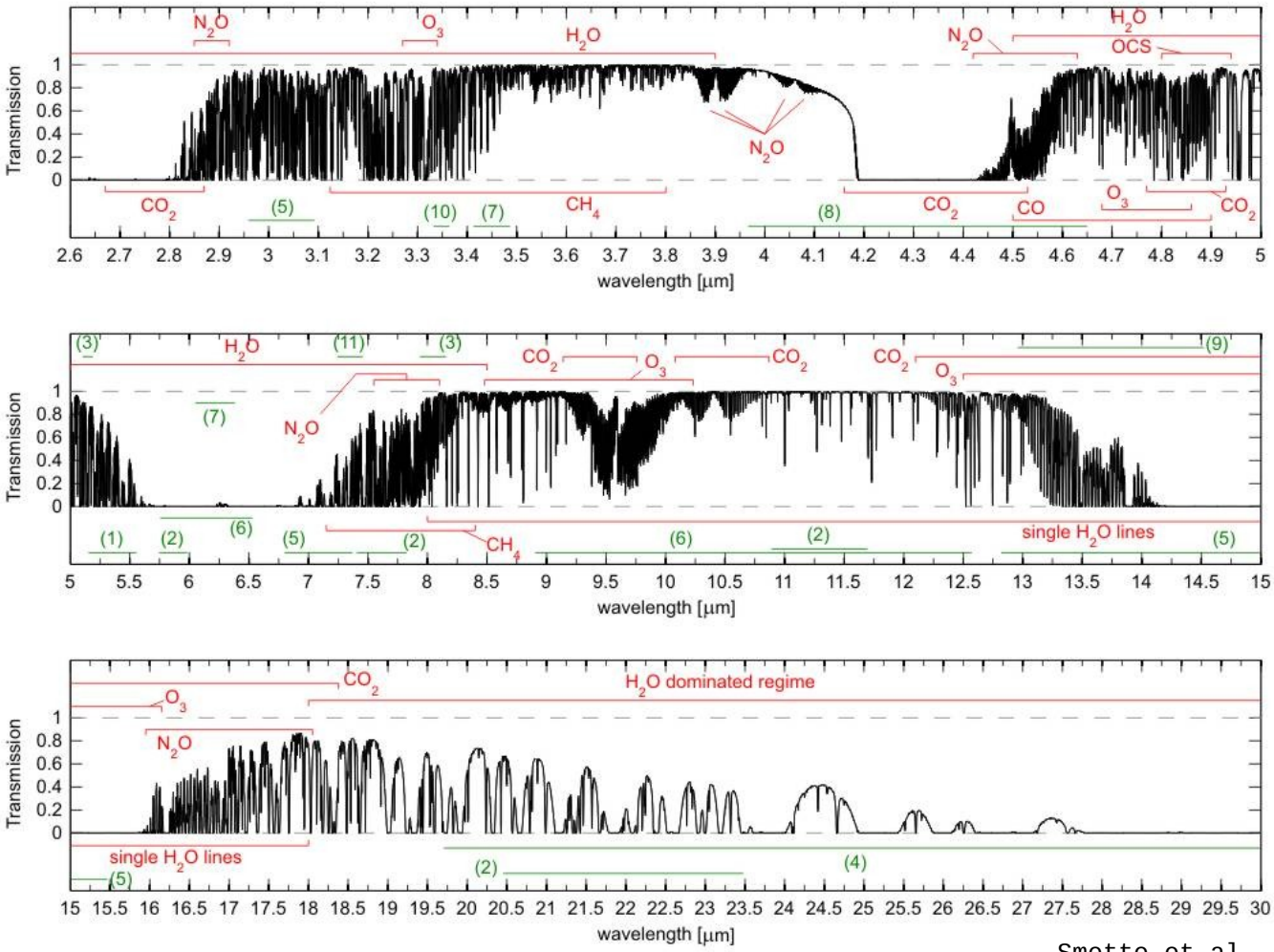


Smette et al., 2015, A&A 576, A77

Based on a presentation by Wolfgang Kausch

Atmospheric Correction

Atmospheric absorption / MIR



Trace gases: (1) NO, (2) HNO_3, (3) COF_2, (4) H_2O_2, (5) HCN, (6) NH_3, (7) NO_2, (8) N_2, (9) C_2H_2, (10), C_2H_6, (11) SO_2.

Smette et al., 2015, A&A 576, A77

Atmospheric Correction

How can we get rid of this?

Plan A:
Supplementary calibration frames
„Classical method“

Atmospheric Correction

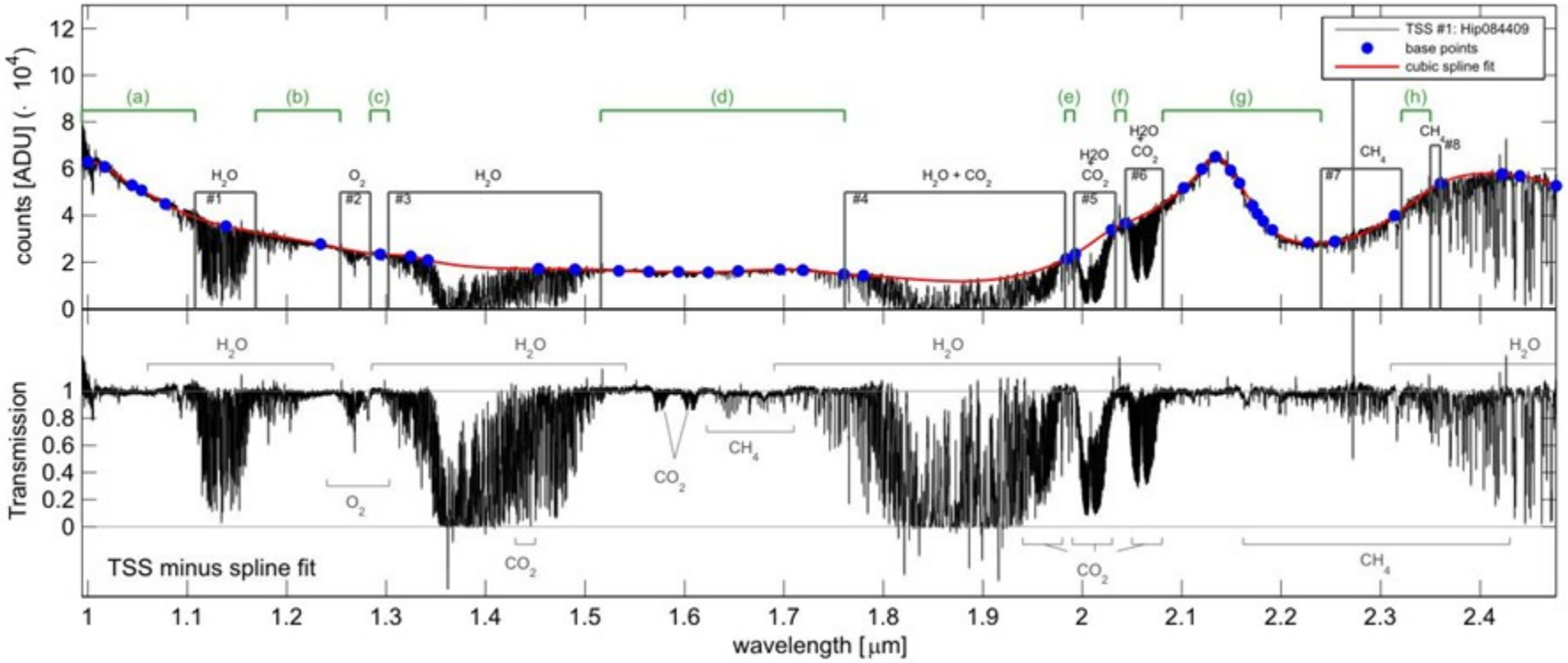
Required: transmission spectrum

Telluric Standard Stars:

- hot stars without/with few, well known intrinsic spectral features (B-type) or solar analogs
- observation in the vicinity, very similar airmass as science target
- observation directly before/after the science target

– expensive in telescope time
– conditions sometimes vary too fast
+ instrument line spread function is the same as for science

Atmospheric Correction



Kausch et al, 2015, A&A 576, A78

Based on a presentation by Wolfgang Kausch

Atmospheric Correction

How can we get rid of this?

Plan α:
Modelling

molecfit

Atmospheric Correction

Telluric absorption correction with `molecfit`

Basic idea ([1],[2]):

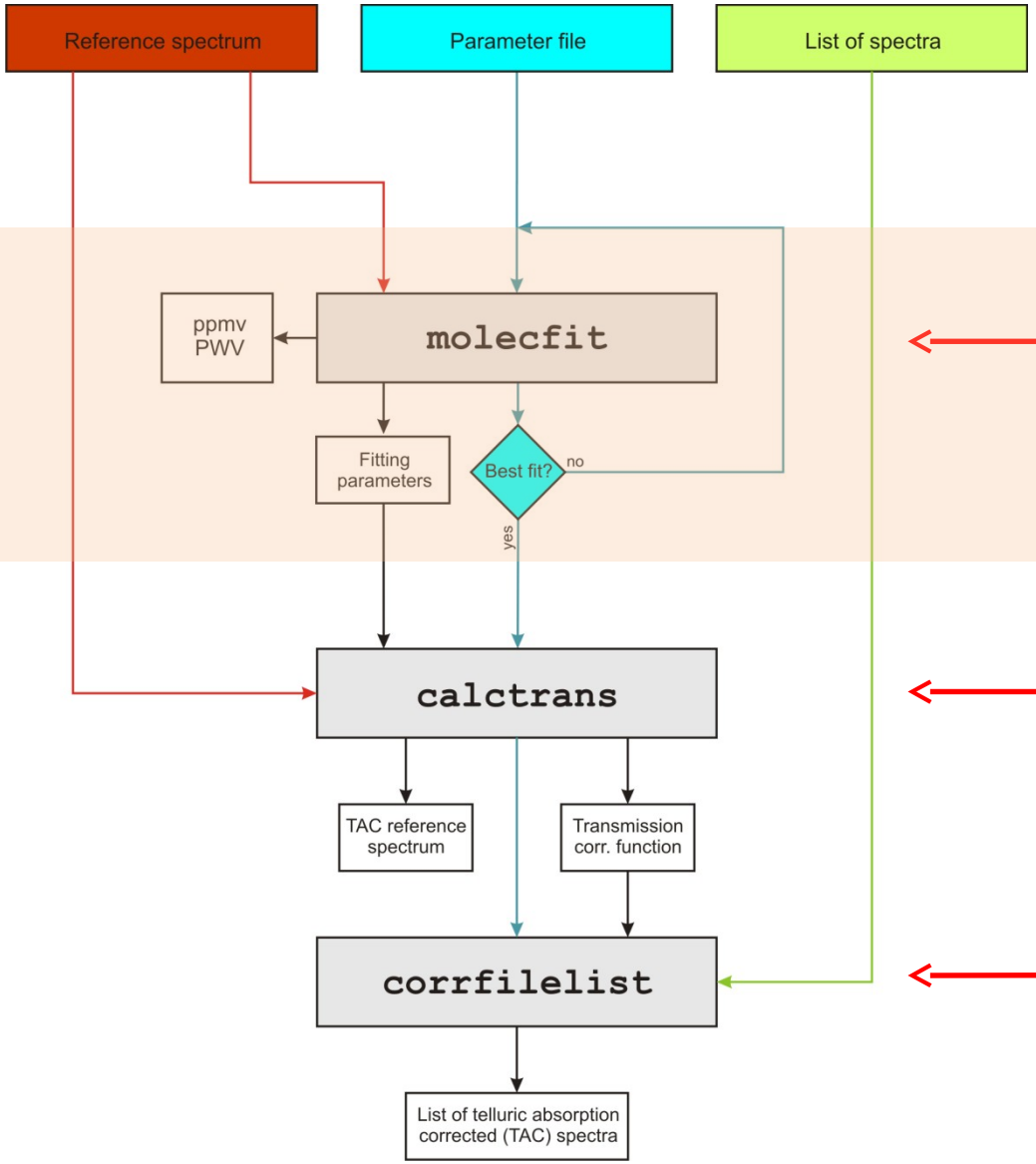
- Derive the atmospheric state from its fingerprint in the science spectra
- Calculate synthetic transmission spectra corresponding to this state by means of a radiative transfer code
- Fit these spectra iteratively to absorption features in science spectra
- Use the best-fit transmission for the telluric absorption correction

Features:

- Comprehensive software suite for telluric absorption correction
- Instrument independent
- world-wide use
- based on Ansi-C → high compatibility (Linux+MacOS)
- freely available*

[1] Smette et al., 2015, A&A 576, A77
[2] Kausch et al, 2015, A&A 576, A78
*http://www.eso.org/pipelines/skytools

Atmospheric Correction



fitting of spectral features in the fitting ranges → best fit solution

Calculation of the transmission based on the fit + application of the telluric abs. correction

Application of the correction to other files.

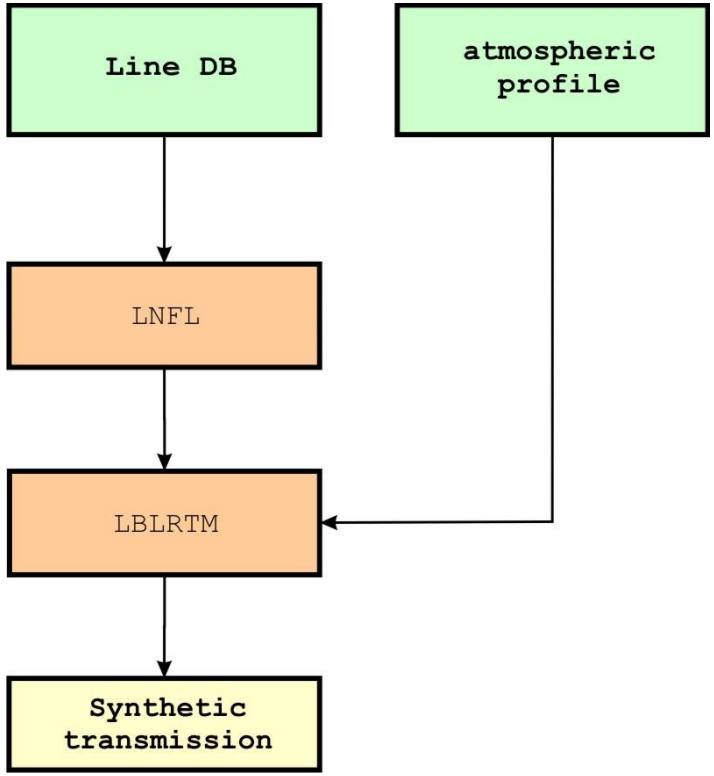
Based on a presentation by Wolfgang Kausch

Atmospheric Correction

Radiative transfer code

LBLRTM ([1],[2]):

- Line-By-Line-Radiative-Transfer-Model
- third party code [3]
- V12.2
- widely used in atmospheric research
- still being further developed
- uses LiNeFiLe to retrieve line information from the High Resolution Transmission database



[1] Clough et al., 2005, *J. Quant. Spectrosc. Radiat. Transfer*, **91**, 233-244
[2] Clough et al., 1992, *J. Geophys. Res.*, **97**, 15761-15785
[3] http://rtweb.aer.com/lblrtm_frame.html

Atmospheric Correction

Radiative transfer code / line database

HITRAN database([1],[2],[3]):

- 39 different molecules
- 2,713,968 spectral lines
- calculated & observed data
- V13 (HITRAN 2008)

[1] Atomic and Molecular Physics Division, Harvard-Smithsonian Center for Astrophysics
[2] Rothman et al., 2009, Journal of Quantitative Spectroscopy and Radiative Transfer, vol. **110,** pp. 533-572
[3] http://www.cfa.harvard.edu/HITRAN/

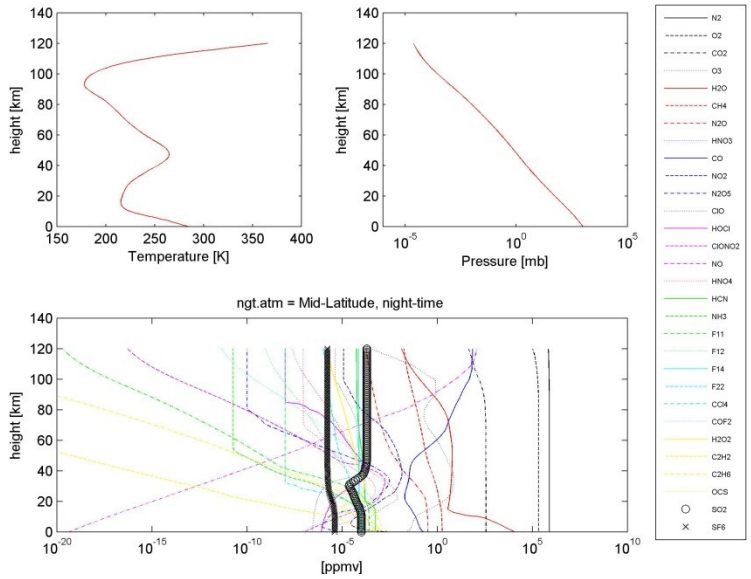
Atmospheric Correction

Radiative transfer code / atmospheric profile

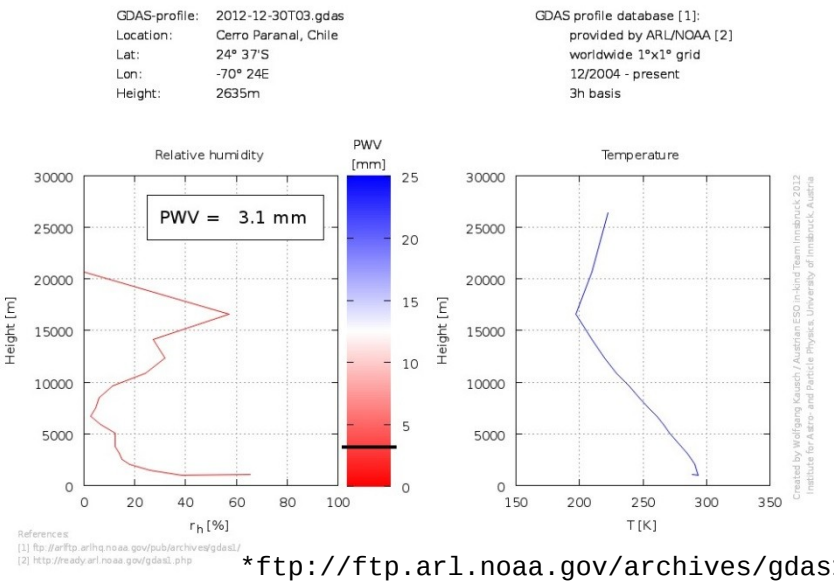
- Static atmospheric standard profile (P, T, mixing ratios for many molecules)
- Global GDAS* weather model: 1° x 1° grid, every 3 h, profiles for P, T, r_H

Local meteorological data for height of site: P, T, and r_H (taken from FITS header if present) → ESO MeteoMonitor

atmospheric standard profile



GDAS profile: 2012-12-30T03.gdas

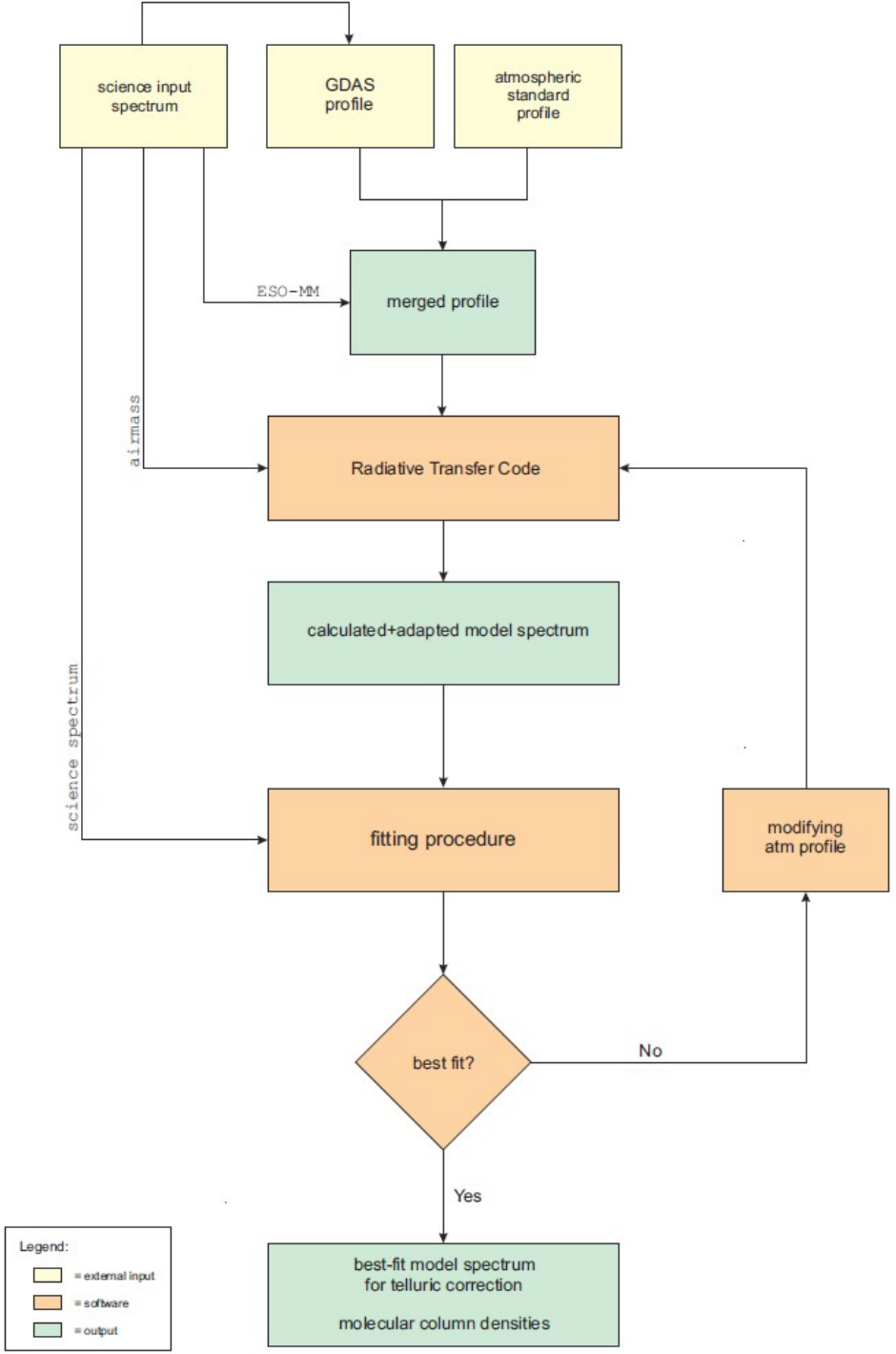


*ftp://ftp.arl.noaa.gov/archives/gdas1/

ppmv = parts per million volume

Based on a presentation by Wolfgang Kausch

molecfit workflow

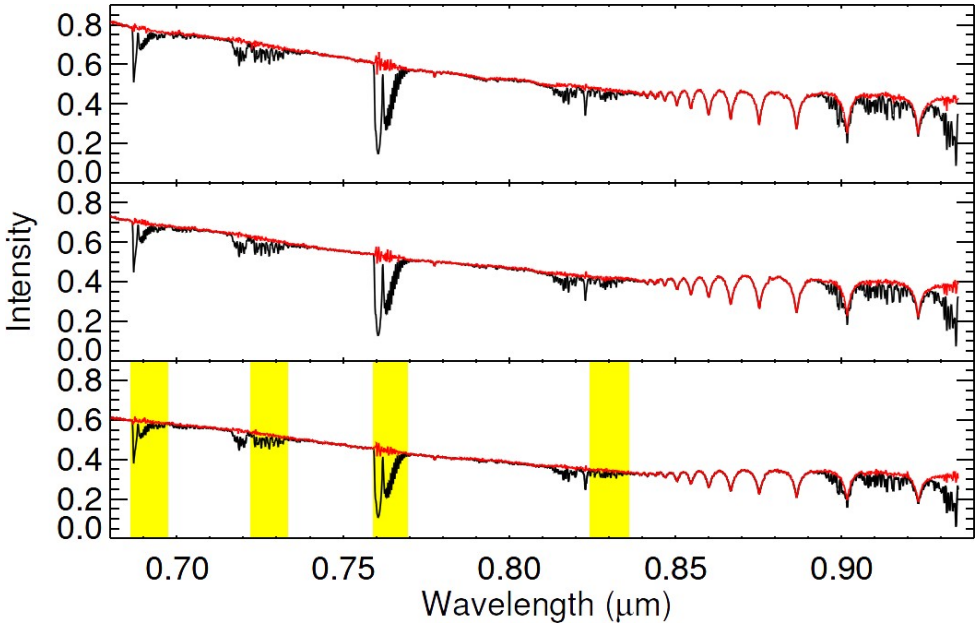


Atmospheric Correction

Fitting procedure

Fitting ranges: lines of intermediate strength; good coverage of wavelength range; as narrow as possible (better continuum fit and shorter code run times)

Exclusion regions: no fitting of bad pixels (or other instrumental defects) and object features



Smette et al., 2015, A&A 576, A77

Atmospheric Correction

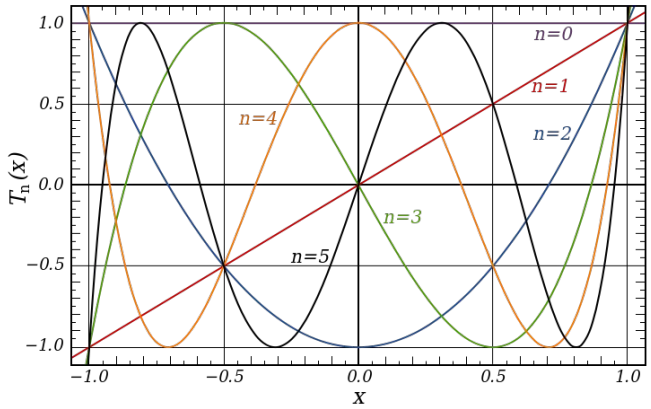
Fitting procedure

χ^2 minimisation by a Levenberg-Marquardt technique (MPFIT [1])

Fitting parameters:

- Scaling factors for molecular profiles
- Coefficients of polynomials for continuum fit
- Coefficients of Chebyshev polynomials for modification of wavelength grid
- Widths of boxcar, Gaussian, and Lorentzian for instrumental profile (alternative: user-provided kernel → no fit)
- Emissivity of greybody (only for fit of sky emission spectra in the thermal IR)

Chebyshev polynomials

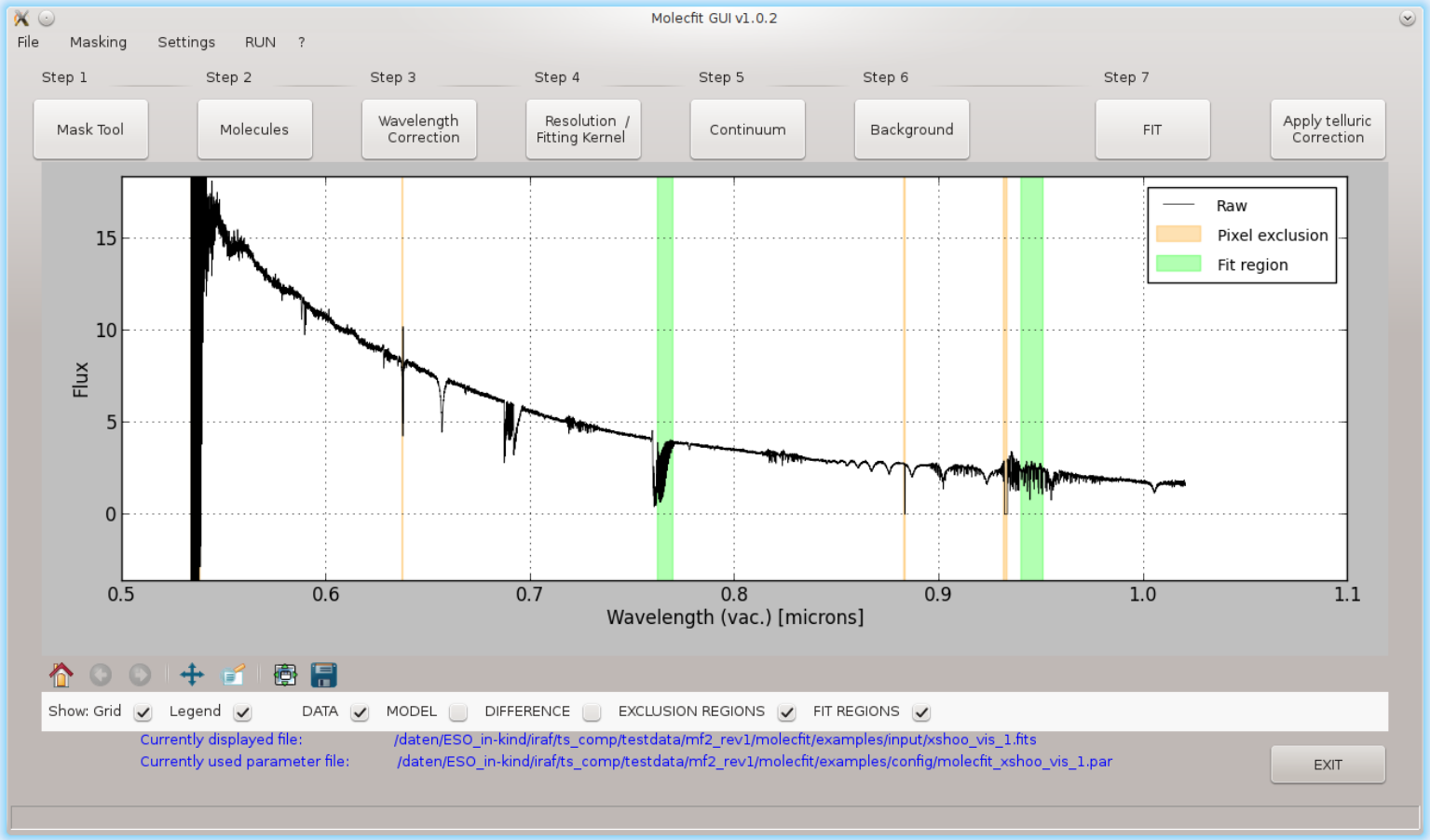


[1] Markwardt, C. B. 2009, in Astronomical Society of the Pacific Conference Series, Vol. 411, Astronomical Data Analysis Software and Systems XVIII, ed. D. A. Bohlender, D. Durand, & P. Dowler, 251

Atmospheric Correction

Invoking `molecfit`

- **GUI:** `<inst_dir>/bin/molecfit_gui <parameterfile>`



Atmospheric Correction

Parameter file: plain ASCII file → text editor

```
### Driver for MOLECFIT
## DIRECTORY STRUCTURE
# Base directory (default: ".") for the following folder structure:
#
# |--bin/
# |
# |--config/
# <basedir>----|
# |--data/
# |
# |--output/
#
# A relative or an absolute path can be provided. In the former case MOLECFIT
# has to be started in <basedir>.
basedir: .

## INPUT DATA
# Data file name (path relative to basedir or absolute path)
filename: examples/input/crires_spec_jitter_extracted_0000.fits

# ASCII list of files to be corrected for telluric absorption using the
# transmission curve derived from the input reference file (path of list and
# listed files relative to basedir or absolute path; default: "none")
listname: none

# Type of input spectrum -- 1 = transmission (default); 0 = emission
trans: 1

.
.
.
```

Sections

comments (‚#‘)

parameter:

<parname>: <parvalue>

- or -

<parname>

Atmospheric Correction

Parameter file: plain ASCII file → text editor

X-shooter

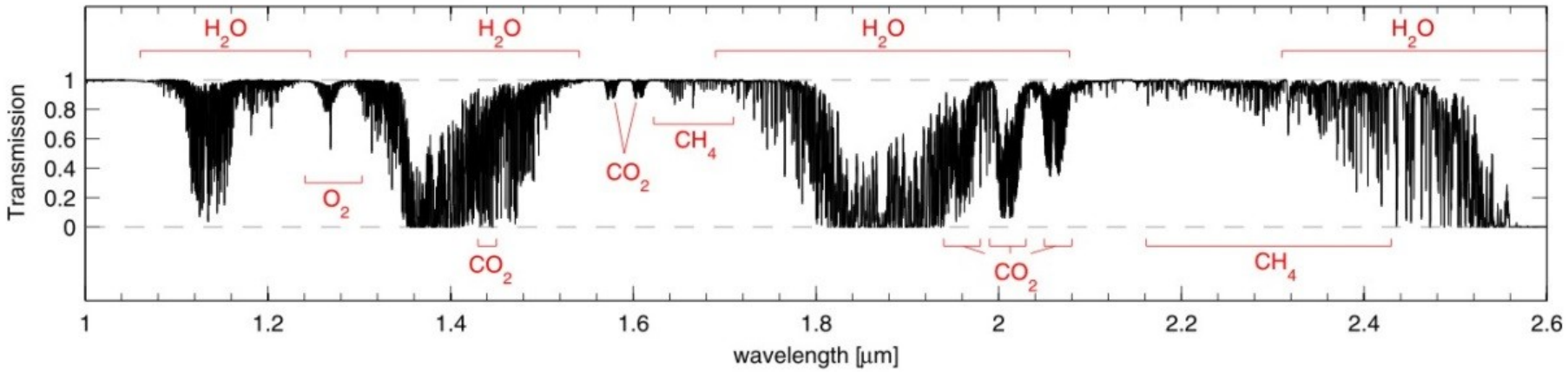
`varkern: 1` (variable kernel, linear increase with wavelength)

`columns: NULL FLUX ERRS QUAL` (MERGE1D)

`columns: WAVE FLUX ERR QUAL` (IDP)

`H2O O2` (VIS, fit only `H2O`)

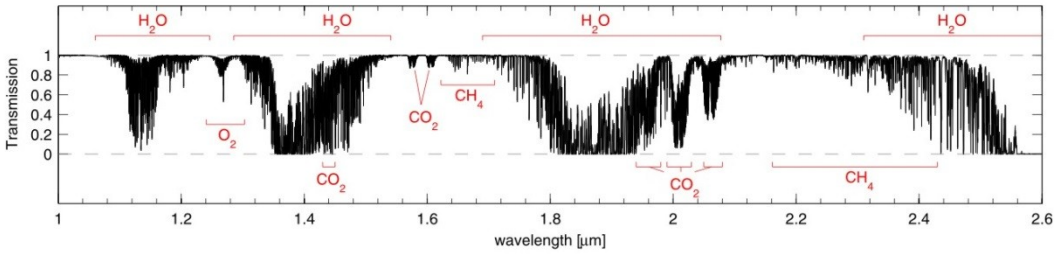
`H2O O2 CO CH4 CO2` (NIR fit only `H2O`)



Atmospheric Correction

Parameters: Section „Molecular column“

```
[…]

# List of molecules to be included in the model
# (default: 'H2O', N_val: nmolec)
list_molec: H2O CH4 O3

# Fit flags for molecules -- 1 = yes; 0 = no (N_val: nmolec)
fit_molec: 1 1 1

# Values of molecular columns, expressed relatively to the input ATM profile
# columns (N_val: nmolec)
relcol: 1. 1. 1.

[…]
```



list_molec: List of molecules to be considered by the radiative transfer code; Depends on the chosen fitting range
fit only molecules present in spectrum

fit_molec: Defines, whether a molecular column should be fitted or assumed to be constant

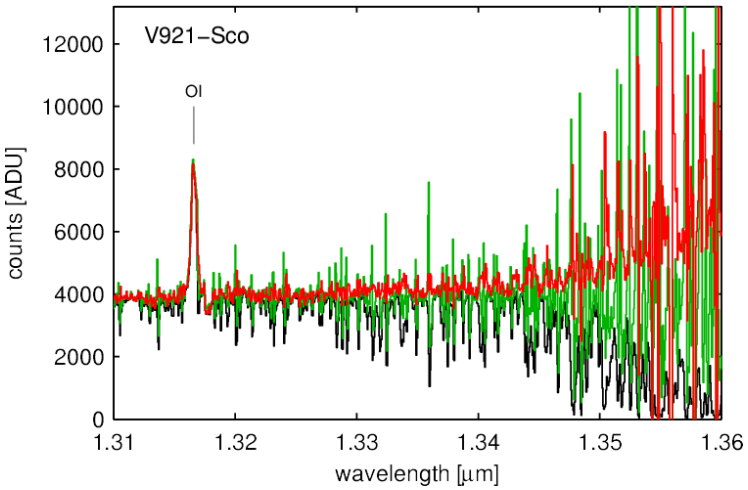
relcol: Scaling factor for the molecular column (starting value);

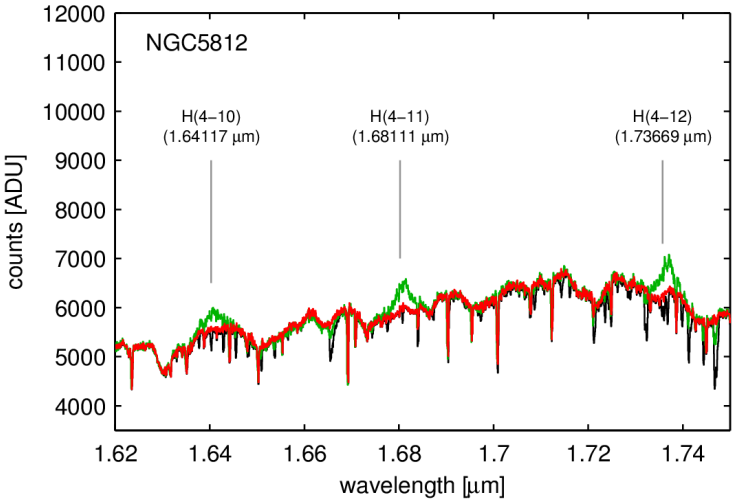
NOTE: # of values in *fit_molec* and *relcol* must be equal to number of molecules (order!);

Atmospheric Correction

Results / comparison

Comparison with Telluric Standard Star

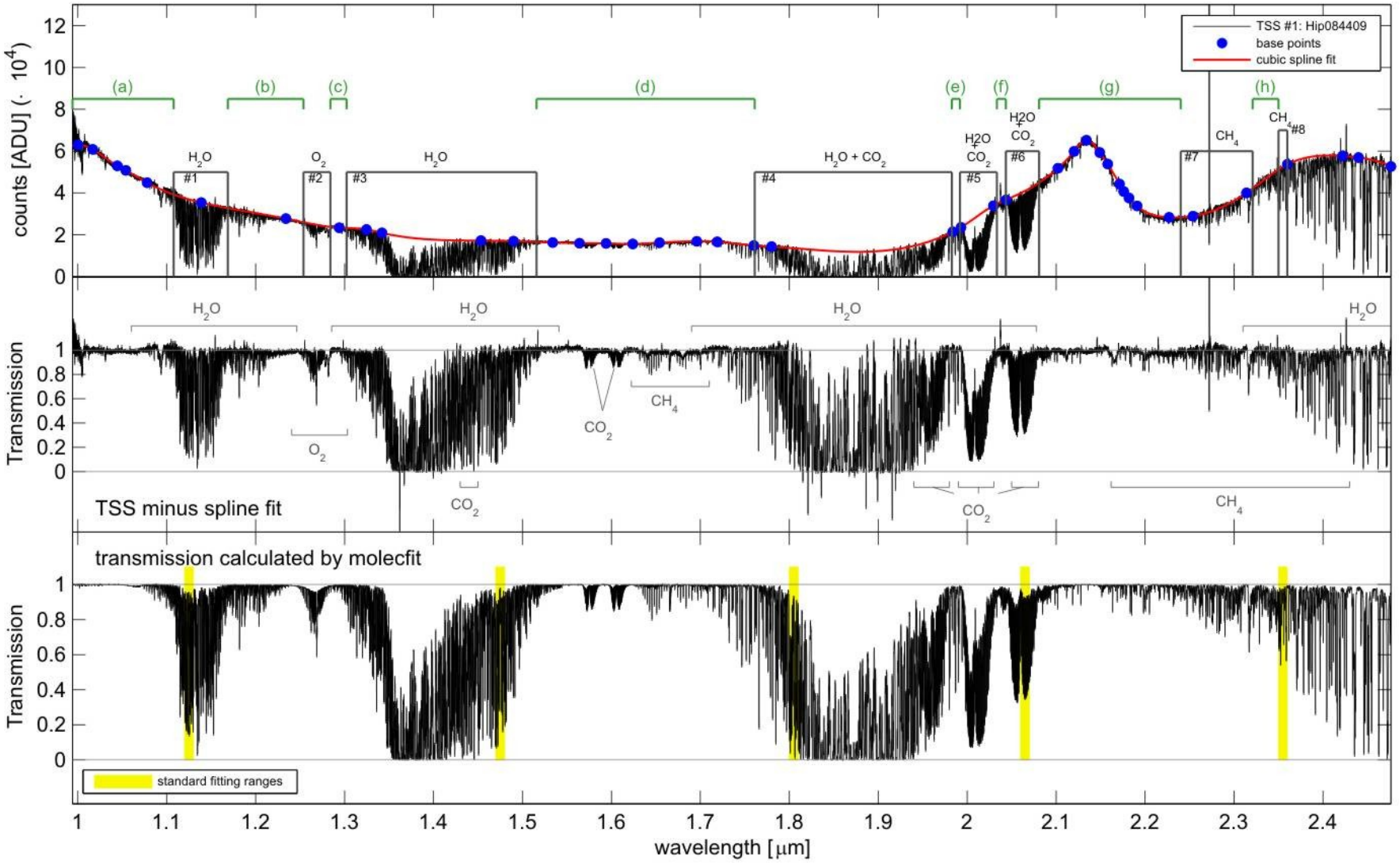




Object spectrum
molecfit correction
Classical method correction

Kausch et al, 2015, A&A 576, A78

Atmospheric Correction



Kausch et al, 2015, A&A 576, A78

Based on a presentation by Wolfgang Kausch

Atmospheric Correction

Limitations

External:

- Accuracy of the line database
- Radiative transfer code accuracy
- Initial atmospheric profile

Internal:

- No correction for very low T possible
- Low S/N spectra cannot be fitted reliably
- Number of fitting parameters (λ-fit, continuum, LSF,….)
- Intrinsic spectral features of the object
- Resolution

Kausch et al, 2015, A&A 576, A78

Atmospheric Correction

Summary + Outlook

Modelling is a good alternative to supplementary observations

`molecfit` and `skycorr` are

- Instrument independent
- world-wide use
- based on Ansi-C → high compatibility
- high flexibility
- freely available*

Will be implemented in future pipelines

* *Licenses for outside code to be respected*

Molecfit details

- Molecfit User Manual
  ftp://ftp.eso.org/pub/dfs/pipelines/skytools/molecfit/VLT-MAN-ESO-19550-5772_Molecfit_User_Manual.pdf
- Molecfit Tutorial
  ftp://ftp.eso.org/pub/dfs/pipelines/skytools/molecfit/VLT-MAN-ESO-19550-5928_Molecfit_GUI_and_Tutorial.pdf

Atmospheric Correction

Invoking `molecfit`:

- Reflex
- GUI
- **console:**

```
<inst_dir>/bin/molecfit  <parameterfile>
```

`<parameterfile>`:

contains all information required for the telluric absorption correction for a specific file, i.e. filenames, fitting parameters, output,....

Atmospheric Correction

Parameters: Sections „Directory“ and „Input Data“

```
[…]

# A relative or an absolute path can be provided. In the former case MOLECFIT
# has to be started in <basedir>.
basedir: .

## INPUT DATA
# Data file name (path relative to basedir or absolute path)
filename: examples/input/crires_spec_jitter_extracted_0000.fits

# ASCII list of files to be corrected for telluric absorption using the
# transmission curve derived from the input reference file (path of list and
# listed files relative to basedir or absolute path; default: "none")
listname: none

[…]
```

basedir: In all cases either absolute paths can be given, or paths relative to *basedir*

filename: File, which is to be corrected. This file is the reference, which is usually used for fitting and for the correction

listname: ASCII file containing a list of other spectra, which should be corrected with the same transmission spectrum

Atmospheric Correction

Parameters: Sections „Directory“ and „Input Data“

```
[…]

# Type of input spectrum -- 1 = transmission (default); 0 = emission
trans: 1

# Names of the file columns (table) or extensions (image) containing:
# Wavelength Flux Flux_Err Mask
# - Flux_Err and/or Mask can be avoided by writing ’NULL’
# - ’NULL’ is required for Wavelength if it is given by header keywords
# - parameter list: col_lam, col_flux, col_dflux, and col_mask
columns: Wavelength Extracted_OPT Error_OPT NULL

# Default error relative to mean for the case that the error column is missing
default_error: 0.01

[…]
```

trans: molecfit can fit both emission and transmission features;

columns: column names of the input file

default_error: If no error column is present one can give a default error here

Atmospheric Correction

Parameters: Sections „Directory“ and „Input Data“

```
[…]

# Multiplicative factor to convert wavelength to micron
# (e.g. nm -> wlgtomicron = 1e-3)
wlgtomicron: 1e-3

# Wavelengths in vacuum (= vac) or air (= air)
vac_air: vac

[…]
```

wlgtomicron: Molecfit calculates internally in [µm]. Thus one needs to specifiy the wavelength unit in the input spectrum

vac_air: Wavelength regime; depends on the pipeline output

Atmospheric Correction

Parameters: Sections „Directory“ and „Input Data“

```
[…]

# ASCII or FITS table for wavelength ranges in micron to be fitted
# (path relative to basedir or absolute path; default: "none")
wrange_include: none

# ASCII or FITS table for wavelength ranges in micron to be excluded from the
# fit (path relative to basedir or absolute path; default: "none")
wrange_exclude: none

# ASCII or FITS table for pixel ranges to be excluded from the fit
# (path relative to basedir or absolute path; default: "none")
prange_exclude: examples/config/exclude_crires.dat

[…]
```

Definition of the range files

wrange_include: Path to the file defining the fitting ranges

wrange_exclude: Exclusion range in λ space

prange_exclude: Exclusion range in pixel space

Atmospheric Correction

Parameters: Section „Results“

```
[…]

## RESULTS
# Directory for output files (path relative to basedir or absolute path)
output_dir: output

# Name for output files
# (supplemented by "_fit" or "_tac" as well as ".asc", ".atm", ".fits",
# ".par, ".ps", and ".res")
output_name: molecfit_crires

# Plot creation: gnuplot is used to create control plots
# W - screen output only (incorporating wxt terminal in gnuplot)
# X - screen output only (incorporating x11 terminal in gnuplot)
# P - postscript file labelled '<output_name>.ps', stored in <output_dir>
# combinations possible, i.e. WP, WX, XP, WXP (however, keep the order!)

# all other input: no plot creation is performed
plot_creation: XP

# Create plots for individual fit ranges? -- 1 = yes; 0 = no
plot_range: 0

[…]
```

output_dir: directory where all output files are stored in

output_name: Defines name space for output files

plot_creation: Defines type of output plots

plot_range: Defines whether plots for ALL fitting ranges should be created individually

Atmospheric Correction

Parameters: Section „Fit Precision“

```
[…]

## FIT PRECISION
# Relative chi2 convergence criterion
ftol: 1e-2

# Relative parameter convergence criterion
xtol: 1e-2

[…]
```

mpfit stops the fitting procedure as soon as either the χ^2-value or the fitting parameters change less than a given certain limit

ftol: Convergence criterion for the variation of the χ^2-value

xtol: Convergence criterion for the variation of the fitting parameters

Note: Use with care!

Atmospheric Correction

Parameters: Section „Background and continuum“

```
[…]

## BACKGROUND AND CONTINUUM
# Conversion of fluxes from phot/(s*m2*mum*as2) (emission spectrum only) to
# flux unit of observed spectrum:
# 0: phot/(s*m^2*mum*as^2) [no conversion]
# 1: W/(m^2*mum*as^2)
# 2: erg/(s*cm^2*A*as^2)
# 3: mJy/as^2
# For other units, the conversion factor has to be considered as constant term
# of the continuum fit.
flux_unit: 0

# Fit of telescope background -- 1 = yes; 0 = no (emission spectrum only)
fit_back: 0

# Initial value for telescope background fit (range: [0,1])
telback: 0.1

[…]
```

flux_unit: Same as wlgtomicron, but for the flux (internal units: photons/(s*m²*µm*as²))

fit_back: Defines, whether the telescope background should be fitted (greybody). Only important for emission spectra (parameter: *trans*: 0)

telback: Initial value for the telescope background (greybody factor)

Atmospheric Correction

Parameters: Section „Background and continuum“

```
[…]

# Polynomial fit of continuum --> degree: cont_n
fit_cont: 1

# Degree of coefficients for continuum fit
cont_n: 3

# Initial constant term for continuum fit (valid for all fit ranges)
# (emission spectrum: about 1 for correct flux_unit)
cont_const: 1.

[…]
```

fit_cont: Defines whether the continuum should be fitted as poynomial

cont_n: degree of continuum polynomial

cont_const: Initial constant continuum value; Can be only roughly in the order of the continuum level

Atmospheric Correction

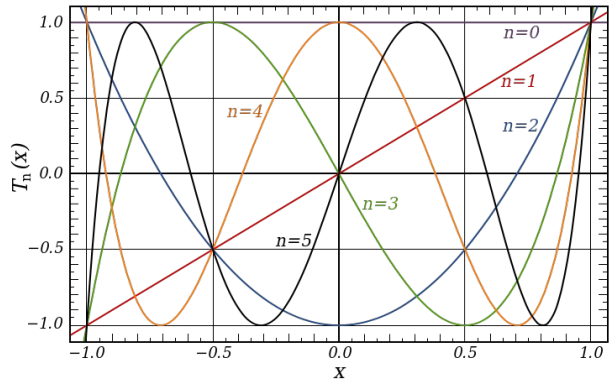
Parameters: Section „Wavelength solution“

```
[…]

## WAVELENGTH SOLUTION
# Refinement of wavelength solution using a polynomial of degree wlc_n
fit_wlc: 1

# Polynomial degree of the refined wavelength solution
wlc_n: 3

# Initial constant term for wavelength correction (shift relative to half
# wavelength range)
wlc_const: 0.

[…]
```

fit_wlc: Defines whether the wavelegth grid should be fitted with a Chebyshev polynome

wlc_n: degree of Chebyshev polynomial

wlc_const: Initial constant term for the wavelength correctopm



Atmospheric Correction

Parameters: Section „Resolution“

```
[…]

## RESOLUTION
# Fit resolution by boxcar -- 1 = yes; 0 = no
fit_res_box: 0

# Initial value for FWHM of boxcar relative to slit width (>= 0. and <= 2.)
relres_box: 0.

# Voigt profile approximation instead of independent Gaussian and Lorentzian
# kernels? -- 1 = yes; 0 = no
kernmode: 0

[…]
```

fit_res_box: Defines whether the Line Spread Function (LSF) kernel should contain a boxcar component

relres_box: Initial value for the BOXCAR component relative to the slit width

kernmode: molecfit can fit the line profile by either a Voigt profile, or by independent Gaussian/Lorentzian kernel

Atmospheric Correction

Parameters: Section „Resolution“

```
[…]

# Fit resolution by Gaussian -- 1 = yes; 0 = no
fit_res_gauss: 1

# Initial value for FWHM of Gaussian in pixels
res_gauss: 1.

# Fit resolution by Lorentzian -- 1 = yes; 0 = no
fit_res_lorentz: 0

# Initial value for FWHM of Lorentzian in pixels
res_lorentz: 0.5

[…]
```

fit_res_gauss:

rel_gauss: Initial value for FWHM of the GAUSSIAN component

fit_res_lorentz:

res_lorentz: Initial value for FWHM of the LORENTZIAN component

Atmospheric Correction

Parameters: Section „Instrumental parameters“

```
[…]

## INSTRUMENTAL PARAMETERS
# Slit width in arcsec (taken from FITS header if present)
slitw: 0.4
slitw_key: ESO INS SLIT1 WID

# Pixel scale in arcsec (taken from this file only)
pixsc: 0.086
pixsc_key: NONE

[…]
```

slitw: Slit width in arcsec (taken from FITS header if present)

slitw_key: fitsheader keyword describing the slit width

pixsc: Pixel scale in arcsec

pixsc_key: fitsheader keyword describing the pixel scale

Atmospheric Correction

Parameters: Sections „Ambient parameters“ and „Atmospheric profiles“

These sections incorporate parameters describing the date/time of the observations, the airmass, atmopsheric state during the time of the observations (r_H, P, T, M1 temperature,…), longitude/latitude of observatory, ….

Mostly taken from fits header keyword („<parameter>_key“), or should not be modified.