Latest developments and upcoming innovations in Py4CAtS - Python for Computational Atmospheric Spectroscopy

Hochstaffl, Philipp[1] and Franz Schreier[1]

[1] *DLR — German Aerospace Center, Remote Sensing Technology Institute, Oberpfaffenhofen,* GERMANY

Session.Poster: P8.10

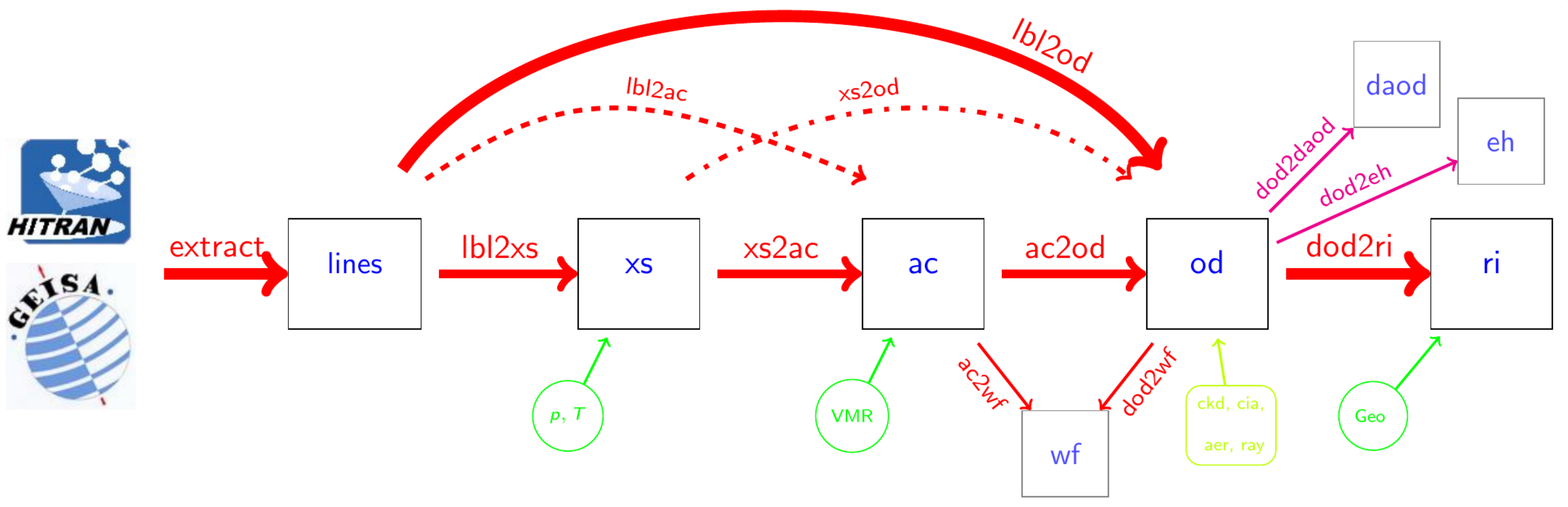
Introduction

- High resolution IR-μW atmospheric radiative transfer.
- Numeric/Scientific Python for optimized array processing.
- Rapid prototyping and testing of new algorithms.
- Study interaction of radiation with planetary atmospheres.
- Easy installation via `pip` after downloading the wheel file `https://atmos.eoc.dlr.de/tools/Py4CAtS/`

Radiative Transfer

Forward model setup (and design) using Py4CAtS:

- Schwarzschild equation and Beer's law.
- Efficient and fast multi-grid line-by-line calculations.
- Spectroscopic databases such as HITRAN and GEISA.
- Various line shapes (e.g. Voigt, Rautian [2], ...).
- Continuum absorption (water vapor MT-CKD and CIA).
- Downlooking, uplooking, limb viewing geometries.
- Spherical or plane-parallel atmospheres.
- Passive and active sensors.



Inversion

Retrieval algorithm for corresponding forward model:

- Infer atmospheric composition or/and temperature.
- Single or multiple spectral intervals.
- Weighted or classical least squares.
- Linear inversion schemes:
  - Singular Value Decomposition (SVD)
  - Matched Filter (MF) ...
- Nonlinear inversion schemes:
  - Variable Projection (VARPRO, separable least squares)
  - Levenberg-Marquardt (LM) ...

Ongoing & Outlook

- Cloud and aerosol scattering (see Fig. 2).
- Atmospheric refraction.
- Jacobians via automatic differentiation.
- Parallelization to improve computational efficiency.
- Field-of-View instead of pencil-beam calculations.

Molecular concentrations from SWIR

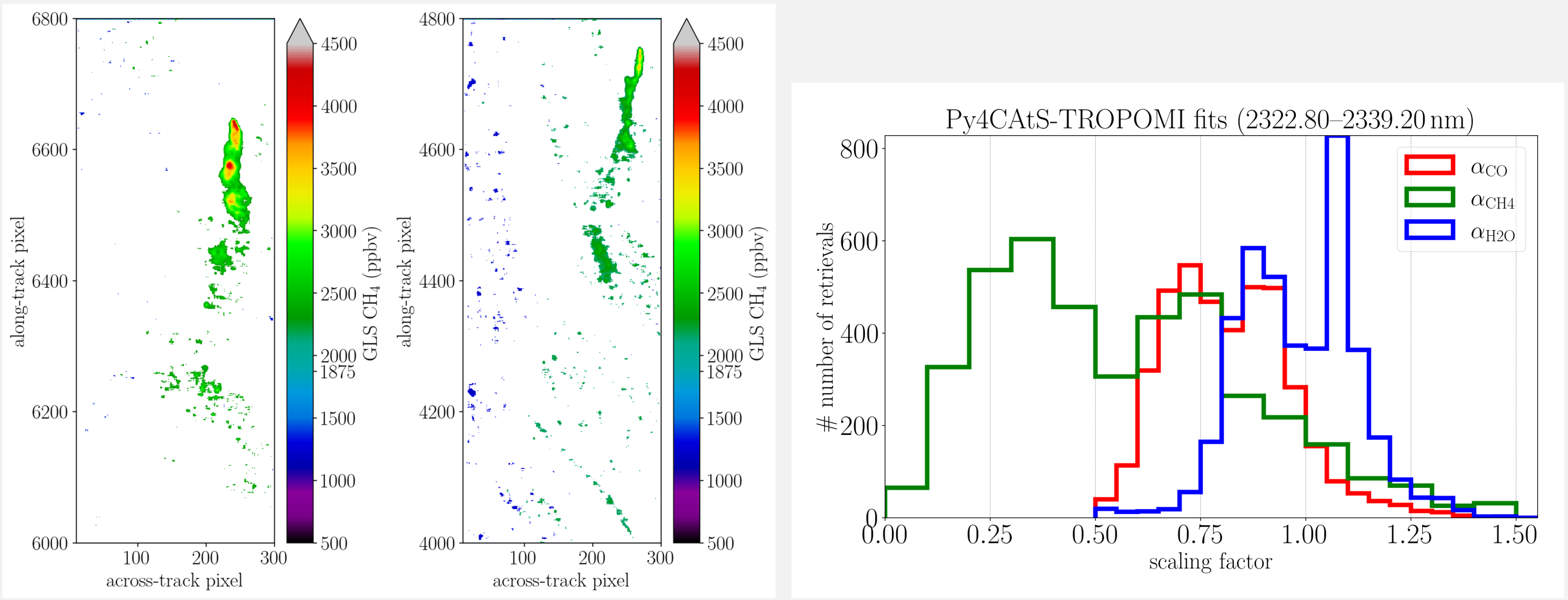


Figure 1: (Left) CH_4 plumes HySpex [1]. (Right) CO, CH_4, and H_2O fits TROPOMI.

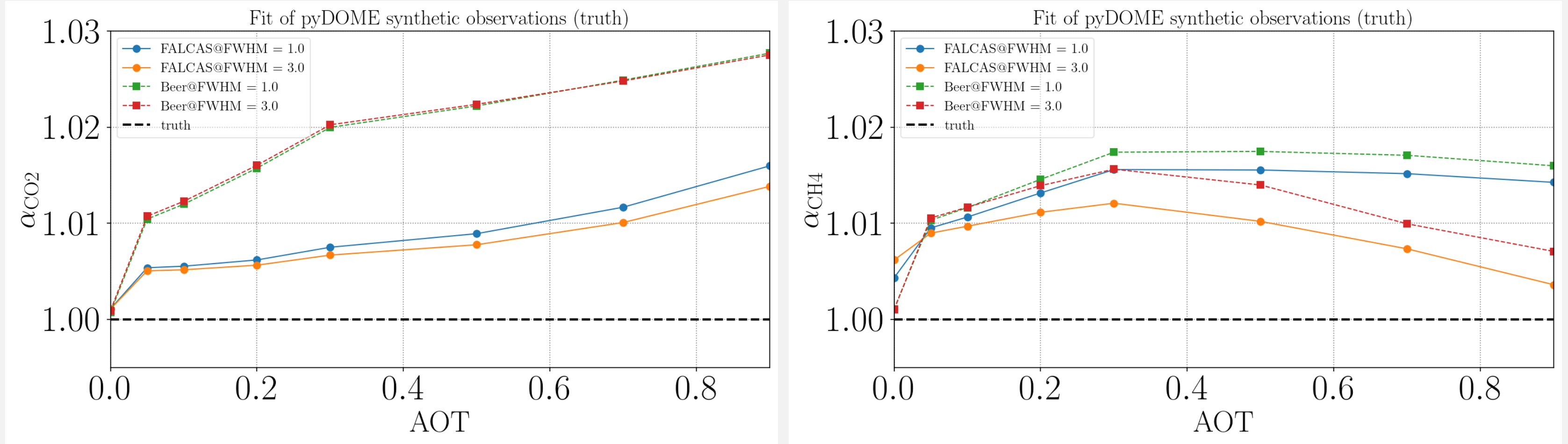


Figure 2: CO_2 and CH_4 fits with FALCAS accounting for aerosols vs. Beer model.

Temperature profiles from TIR

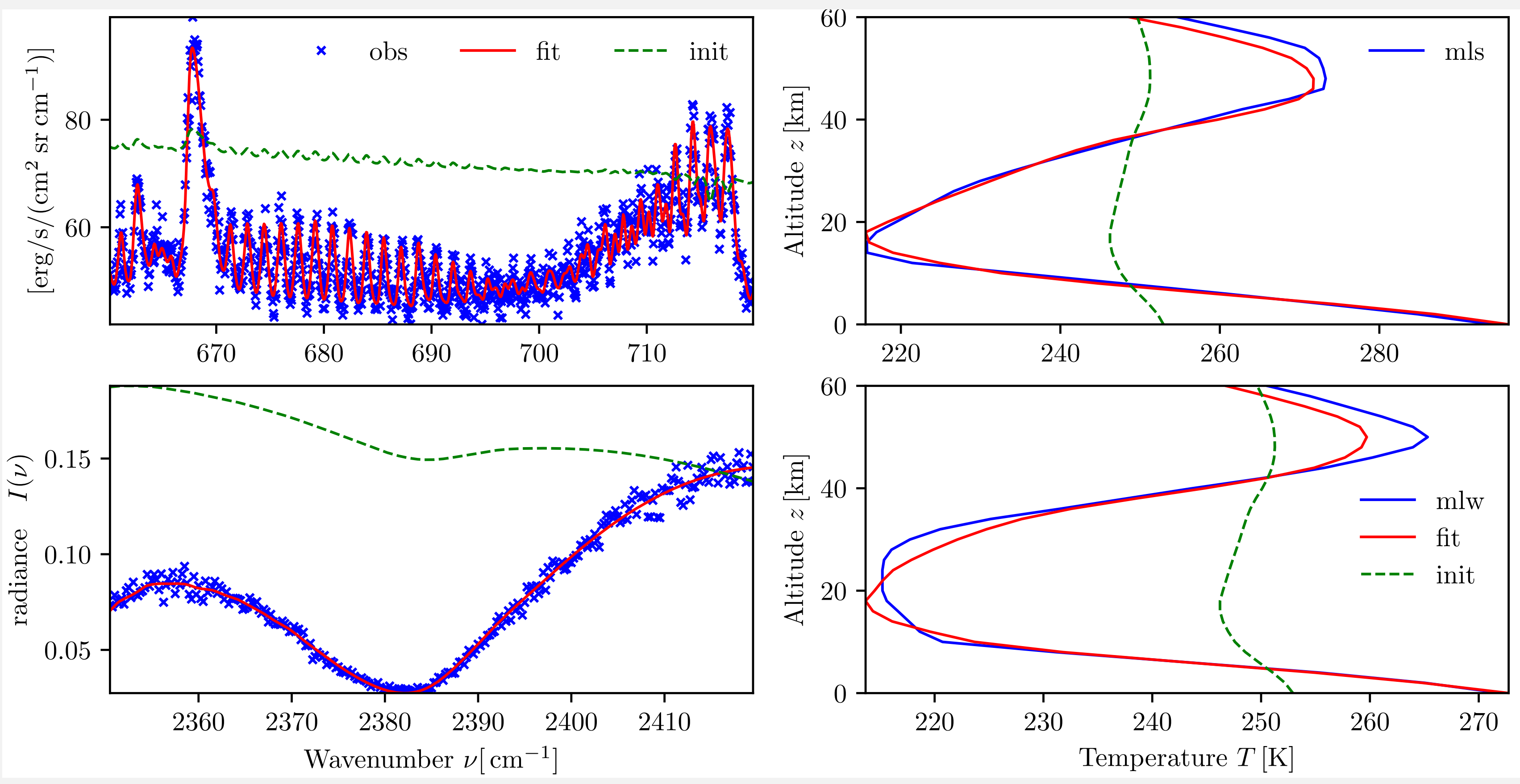


Figure 3: SVD to estimate temperatures from (exo-)planetary emission spectra [4].

LIDAR and MIR Observations

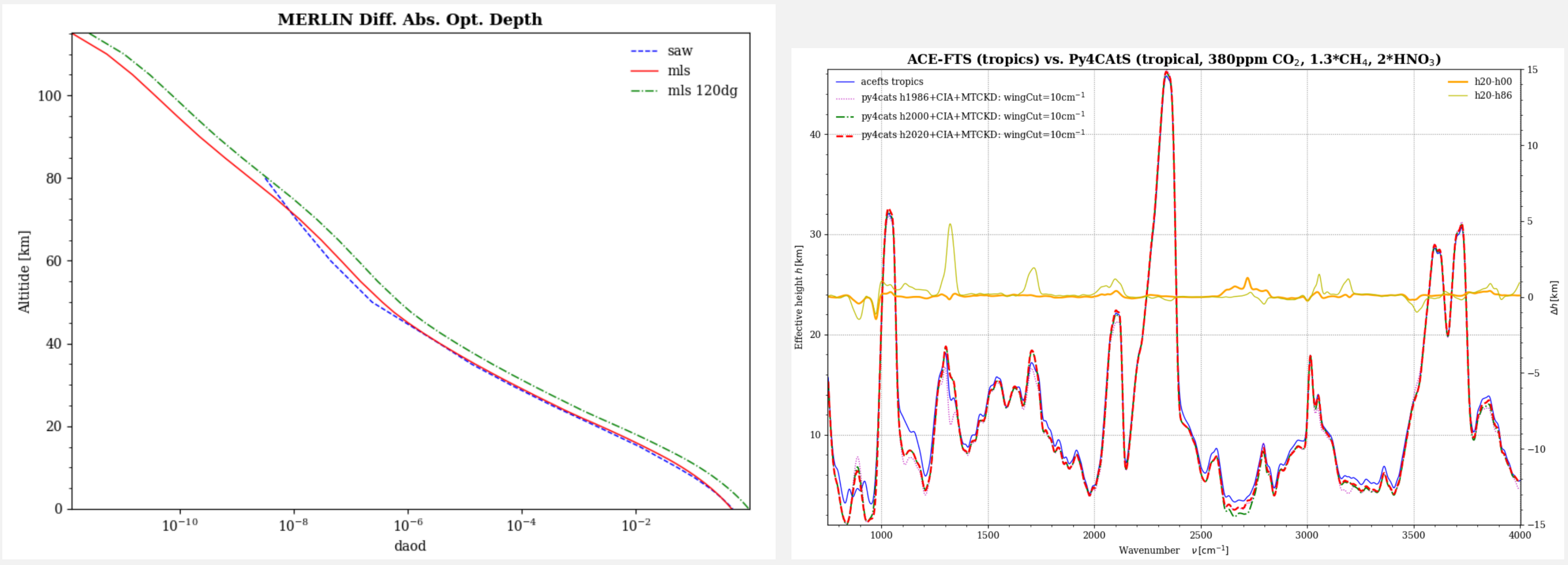


Figure 4: (Left) DAOD with center frequency ν_{on}=1645.552 nm and wing frequency ν_{off}=1645.846 nm. (Right) ACE-FTS effective heights from limb transmissions [3].

References:

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[3] F. Schreier, S. Städt, P. Hedelt, and M. Godolt. Transmission spectroscopy with the ACE-FTS infrared spectral atlas of Earth: A model validation and feasibility study. *Molec Astrophys.*, 11:1–22, 2018. doi: 10.1016/j.molap.2018.02.001.

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ATMOS 2024 | 1–5 July 2024 | Bologna, Italy