Infrared radiative transfer modeling and temperature retrievals with Py4CAtS (Python for Computational ATmospheric Spectroscopy)

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Abstract

Given the increasing number and quality of spectroscopic observations of (Earth-like) extrasolar planets, the detailed characterization of their atmosphere by means of remote sensing techniques is becoming increasingly important. Infrared radiative transfer models are mandatory for the data analysis, serving as forward model for the solution of the inverse problem. Here we present Py4CAtS — Python for Computational ATmospheric Spectroscopy, a re-implementation of a Fortran line-by-line code and demonstrate its use in the context of temperature retrievals of Earth-like exoplanets.

1. Introduction

With more than 4000 exoplanets known today, including some dozen Earth-likes and super-Earths, their detailed characterization has come into the focus of current research. Despite the limited quality of currently available exoplanet spectral observations, the methodology developed for atmospheric remote sensing of Earth and solar system planets can be readily applied to the analysis of terrestrial extrasolar planet data. For the retrieval of atmospheric composition, transmission spectroscopy analyzing the attenuation of stellar light along its optical path through the planet's atmosphere is particularly suited; for the inference of atmospheric temperature, thermal infrared emission spectra (secondary eclipse) are important. In both cases the inverse problem (in general nonlinear) has to be solved by means of numerical optimization techniques combined with an efficient and accurate radiative transfer code (forward model). In this contribution we present a high resolution line-by-line (lbl) infrared (IR) radiative transfer code linked to a nonlinear least squares solver and show first results of our temperature retrievals.

2. Radiative Transfer Modeling

Py4CAtS — Python for Computational ATmospheric Spectroscopy [Schreier et al., 2019, available at `http://atmos.eoc.dlr.de/tools/Py4CAtS/`], is a Python re-implementation of the Generic Atmospheric Radiation Line-by-line Infrared Code (GARLIC) [Schreier et al., 2014]. GARLIC has been extensively verified and validated, e.g. Schreier et al. [2018a,b] and has been used for a variety of exoplanetary atmosphere studies, e.g. Vasquez et al. [2013a,b], ..., Scheucher et al. [2018]; Wunderlich et al. [2019].

Most (all?) IR lbl models (incl. GARLIC) work as a kind of black box. In contrast, in Py4CAtS the individual steps of an infrared (or microwave) radiative transfer computation are implemented in separate modules/functions: to extract lines of relevant molecules in the spectral range of interest, to compute line-by-line cross sections for given pressure(s) and temperature(s), to combine cross sections to absorption coefficients and optical depths, and to integrate along the line-of-sight to transmission and radiance/intensity. Py4CAtS can be used in two ways, from a Unix-like console or inside the (I)Python/Jupyter interpreter.

3. Temperature Retrievals

Temperature is one of the most fundamental parameters of atmospheric physics and chemistry. Remote sensing of atmospheric temperature of Earth or solar system planets is done routinely [e.g. Hanel et al., 2003], and more recently atmospheric spectroscopy and inversion techniques have also been used to infer exoplanet temperatures [e.g. Madhusudhan, 2018; Deming et al., 2019].

For the retrieval Py4CAtS has been coupled to the MINPACK nonlinear least squares solver. Temperature is a function of altitude (or pressure), but for the solution of the inverse problem a discretization is required. Our tests indicate that a representation of the profile with about five unknowns is adequate.

The retrievals have been conducted for a James Webb Space Telescope (JWST) setting, in particular we consider high resolution thermal infrared spectra as expected by the NIRSpec and MIRI instruments. For verification we have used a set of Earth climatological data (US Standard etc.). Furthermore we considered the set of M-dwarf planets of Wunderlich et al. [2019]. Even for low signal-noise-ratios (SNR) the temperature of M-dwarf planets can often be retrieved within some Kelvin, especially in the upper troposphere / lower stratosphere.

4. Summary and Conclusions

Despite the speed limitations of the Python interpreter Py4CAtS is attractive because of the flexibility, ease of use, and access to intermediate quantities. Furthermore, Py4CAtS can be easily used as forward model for the solution of inverse problems by numerical optimization. Using appropriate spectral windows in the infrared, temperature can be retrieved reasonably well for Earth-like exo-planetary atmospheres.

Acknowledgements

Financial support by the Deutsche Forschungsgemeinschaft — DFG (projects SCHR 1125/3-1 and GO 2610/1-1) is gratefully acknowledged.

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