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Python Tools for Line-by-Line Modelling of Atmospheric Radiative Transfer

F. Schreier and S. Gimeno Garcia

DLR - Remote Sensing Technology Institute, Atmospheric Processors, Wessling, Germany (franz.schreier@dlr.de, +49-8153-28-1446)

Radiative transfer modeling is an important aspect of atmospheric physics and chemistry, both for Earth and planetary atmospheres. In particular, for the analysis of atmospheric remote sensing data as well as for theoretical investigations such as retrieval assessments a flexible, yet efficient and reliable radiative transfer code is mandatory. In view of the increasing number of high resolution instruments and thanks to the increasing computational power, line-by-line modeling of high resolution infrared and microwave spectra is widely used today.

Although highly optimized codes written in compiled languages such as Fortran or C/C++ are indispensable for operational processing, radiative transfer tools developed in script/interpreter languages such as Python, IDL/GDL, or MatLab/Octave/SciLab are an interesting alternative. Despite the reduced execution speed, script based tools are attractive because they allow for "rapid prototyping", can be executed on a large variety of platforms, and provide easy access to intermediate quantities, hence facilitating visualization and better understanding of the physics.

Py4CAtS — Python scripts for Computational ATmospheric Spectroscopy is a Python re-implementation of the Fortran infrared radiative transfer code MIRART/GARLIC (Schreier&Schimpf, IRS2000), where compute-intensive code sections utilize the Numeric and Scientific Python modules (numpy, scipy) allowing for highly optimized array-processing. In Py4CAtS the individual steps of an infrared or microwave radiative transfer computation are implemented in separate scripts 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. In this paper the basic design of the package, numerical and computational aspects relevant for optimization (esp. for the line-by-line computations), and a sketch of the typical workflow will be presented along with examples.