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GARLIC — A general purpose atmospheric radiative transfer line-by-line infrared-microwave code: Implementation and evaluation

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ABSTRACT

A suite of programs for high resolution infrared-microwave atmospheric radiative transfer modeling has been developed with emphasis on efficient and reliable numerical algorithms and a modular approach appropriate for simulation and/or retrieval in a variety of applications. The Generic Atmospheric Radiation Line-by-line Infrared Code — GARLIC — is suitable for arbitrary observation geometry, instrumental field-of-view, and line shape. The core of GARLIC's subroutines constitutes the basis of forward models used to implement inversion codes to retrieve atmospheric state parameters from limb and nadir sounding instruments.

This paper briefly introduces the physical and mathematical basics of GARLIC and its descendants and continues with an in-depth presentation of various implementation aspects: An optimized Voigt function algorithm combined with a two-grid approach is used to accelerate the line-by-line modeling of molecular cross sections; various quadrature methods are implemented to evaluate the Schwarzschild and Beer integrals; and Jacobians, i.e. derivatives with respect to the unknowns of the atmospheric inverse problem, are implemented by means of automatic differentiation. For an assessment of GARLIC's performance, a comparison of the quadrature methods for solution of the path integral is provided. Verification and validation are demonstrated using intercomparisons with other line-by-line codes and comparisons of synthetic spectra with spectra observed on Earth and from Venus.

1. Introduction

Radiative transfer [1–3] plays a central role in atmospheric science (e.g., remote sensing, meteorology, and climatology) and related branches of astronomy and astrophysics, and a large variety of codes have been developed differing in (level of) sophistication, spectral domain, and resolution. Thanks to increases in computational power, high resolution infrared (IR) and microwave (MW) radiative transfer calculations by means of "line-by-line" (lbl) models — once a challenge even for big machines — has become widely available.

Although lbl models are still computationally demanding, they are indispensable for the analysis of high resolution spectra delivered by a growing fleet of space-borne IR/MW sensors and some dozens of ground-based spectrometers (e.g., in the framework of NDACC, the Network for the Detection of Atmospheric Composition

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Change, http://www.ndacc.org) and several airborne or balloon-borne instruments (e.g., [4–8]). Furthermore, lbl models are mandatory to generate and verify fast parameterized radiative transfer models based on band model [9], k-distribution/correlated-k [10], exponential sum fitting [11] or emissivity-growth approximations [12] utilized for numerical weather forecasting and climate models. Finally, lbl models are required in the rapidly growing field of extrasolar planet remote sensing. Although band models etc., have been developed for other planets as well (e.g., [13–15]) and exoplanet spectra will likely be available only with limited resolution and considerable noise levels in the near future, the use of fast parameterized radiative transfer models typically developed for a limited range of atmospheric conditions (mostly Earth-like) can be dangerous and the greater flexibility of lbl models is advantageous to cope with these largely unknown atmospheric conditions.

Despite significant progress, lbl-modeling is still challenging in view of the rapidly growing number of Earth (and (exo-)planet) observation systems producing more and more data with increasing resolution and decreasing noise levels. For example, during its 10 years lifetime (2002–2012) MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) observed about 80 million spectra [16], whereas the infrared limb imager of PREMIER (PRocess Exploration through Measurements of Infrared and millimetre-wave Emitted Radiation [17]), a candidate for ESA's Earth Explorer 7 mission, would have delivered 12 000 limb images comprising 15 million radiance spectra per day. Furthermore, the amount and quality of spectroscopic line parameters is continuously increasing, from about 0.1 million in the first release (1972, then known as the AFGL tape) to about 7.5 million lines in the current 2012 edition of the HITRAN database [18], and many millions of lines in dedicated databases such as HITEMP [19] or ExoMol [20].

The lbl calculation of molecular absorption cross sections is generally the most time consuming part of a high resolution radiative transfer computation. The approach to tackle this challenge is probably the most distinct feature of the various codes developed, starting with the early works of, e.g., FASCODE and 4A [21,22]. Some widely used lbl codes developed later include GENLN2 [23], LBLRTM (based on FASCODE [24]), or ARTS [25,26].

When our code development started in the mid-90s, the number of publicly available lbl codes was quite limited, especially with retrieval applications in mind. Neither FASCODE nor GENLN2 provides analytical derivatives important for nonlinear optimization schemes, where the radiative transfer code serves as forward model. The option to evaluate analytical Jacobians has been implemented in 2004 in LBLRTM (v9.2). ARTS [25] evaluates molecular concentration derivatives analytically and uses a semi-analytic approach for some other variables. Job specification for FASCODE is cumbersome and error prone as dozens of variables have to be given in a strictly formatted input file (the so-called "TAPE5"). Furthermore, computation of a series of viewing geometries, e.g., for finite field-of-view and/or limb sequences, has to be performed manually with a series of jobs, so invariant quantities (e.g., molecular cross sections) have to be recalculated again and again. Finally note that FASCODE is closely linked to the HITRAN spectroscopic database [19], hence inclusion of molecules not covered by HITRAN is almost impossible.

In view of these shortcomings, development of a new code was started in the mid-90s (early versions of the code are described in conference proceedings [27,28]). Use of modern, efficient and accurate numerical algorithms has been an important design principle from the beginning, and verification and validation have been an integral and essential aspect of the code development that has been addressed in several ways. Apart from frequent comparisons with FASCODE, the new code has been participating in two extensive intercomparison studies assessing the performance of thermal infrared [29] and microwave [30] radiative transfer models.

This paper is organized in five sections: In the next section, we briefly review the physical basis of infrared and microwave radiative transfer with high spectral resolution, i.e. line-by-line modeling (for brevity "microwave" is not always mentioned in the following). In Section 3, we present GARLIC (Generic Atmospheric Radiation Line-by-line Infrared Code) providing an extensive discussion of numerical and computational approximations and implementation aspects. The performance is evaluated in Section 4, and a summary and outlook is given in Section 5.

2. Atmospheric radiative transfer and molecular absorption

2.1. Infrared and microwave radiative transfer

In a gaseous cloud and aerosol free atmosphere, scattering usually does not significantly contribute to IR extinction, and radiative transfer is described by the Schwarzschild equation [1–3]. For an arbitrary slant path, the intensity (radiance) I at wavenumber ν and position $s=0$ is given by the integral along the line-of-sight:

$$I(\nu) = I_b(\nu)\exp\left(-\int_0^{s_b}\alpha(\nu,s)\,ds\right) + \int_0^{s_b} J(\nu,s')\,e^{-\int_0^{s'}\alpha(\nu,s'')\,ds''}\alpha(\nu,s')\,ds' \tag{1a}$$

$$I(\nu) = I_b(\nu)\,e^{-\tau_b(\nu)} + \int_0^{\tau_b} J(\nu,\tau')\,e^{-\tau'}\,d\tau' \tag{1b}$$

$$I(\nu) = I_b(\nu)\mathcal{T}_b(\nu) + \int_{\mathcal{T}_b(\nu)}^{1} J(\nu,\mathcal{T})\,d\mathcal{T} \tag{1c}$$

where the first term describes an attenuated background contribution I_b at position s_b. In case of a nadir viewing geometry, the background is the emission and reflection from the Earth's (or planet's) surface, whereas in case of an uplooking or limb-viewing geometry the integral practically terminates at the "top-of-atmosphere" (ToA). Furthermore, assuming local thermodynamical equilibrium, the source function J depends on temperature T