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Intercomparison of three microwave/infrared high resolution line-by-line radiative transfer codes

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ABSTRACT

An intercomparison of three line-by-line (lbl) codes developed independently for atmospheric radiative transfer and remote sensing – ARTS, GARLIC, and KOPRA – has been performed for a thermal infrared nadir sounding application assuming a HIRS-like (High resolution Infrared Radiation Sounder) setup. Radiances for the 19 HIRS infrared channels and a set of 42 atmospheric profiles from the “Garand dataset” have been computed.

The mutual differences of the equivalent brightness temperatures are presented and possible causes of disagreement are discussed. In particular, the impact of path integration schemes and atmospheric layer discretization is assessed. When the continuum absorption contribution is ignored because of the different implementations, residuals are generally in the sub-Kelvin range and smaller than 0.1 K for some window channels (and all atmospheric models and lbl codes). None of the three codes turned out to be perfect for all channels and atmospheres. Remaining discrepancies are attributed to different lbl optimization techniques. Lbl codes seem to have reached a maturity in the implementation of radiative transfer that the choice of the underlying physical models (line shape models, continua etc) becomes increasingly relevant.

1. Introduction

Radiative transfer plays an important role in atmospheric science. For the analysis of an increasing number of high resolution microwave and infrared (IR) spectroscopic observations of Earth’s or planetary atmospheres as well as for the generation and verification of low resolution models, line-by-line (lbl) models are indispensable. Clearly, the quality of remote sensing products critically depends on the accuracy of the radiative transfer codes used as a forward model in the inversion process. Accordingly, verification and validation [1] of these codes is crucial, and several code intercomparisons were performed in the past, e.g. Fischer et al. [2], Ellingson and Fouquart [3], Glatthor et al. [4], Soden et al. [5], Garand et al. [6], von Clarmann et al. [7,8], Tjemkes et al. [9], Kratz et al. [10], Melsheimer et al. [11], Buehler et al. [12], Saunders et al. [13]. Further intercomparisons in the context of planetary science and climate modeling were presented by, e.g., Sromovsky et al. [14], Yang et al. [15].

To our knowledge, in most of these studies one of the participating models has been selected as reference code in case difference spectra were shown. This is clearly a natural approach when the number of models to be analyzed is “large”. For example, five independent radiative transfer codes have been intercompared against the Karlsruhe Optimized & Precise Radiative transfer Algorithm (KOPRA) [16] in the AMIL2DA (Advanced MIpas Level 2 Data Analysis; MIPAS = Michelson Interferometer for Passive Atmospheric Sounding) forward model intercomparison experiment [7]. Likewise, the Atmospheric Radiative Transfer Simulator (ARTS) [17,18] served as the “truth” in the intercomparison of microwave codes [11] in the context of the “Third International Radiative Transfer Modeling Workshop” (IRTMW3).

Some years later Milz [19] presented a comparison of the ARTS and KOPRA models in the IR spectral range. Here we extend this intercomparison with GARLIC, the Generic Atmospheric Radiation Line-by-line Infrared Code [20], whose Fortran 77 predecessor “MIRART–SQuIRRL” (Modular InfraRed Atmospheric Radiative Transfer – Schwarzschild Quadrature IR Radiation Lbl) had been participating in both the AMIL2DA and IRTMW3 studies. First results of the intercomparison have been presented at the International Radiation Symposium 2012 [21].

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This paper is organized in five sections: In the next section, we introduce the essentials of infrared radiative transfer with high spectral resolution (i.e., lbl modeling) and continue with a brief review of the three codes considered here. The setup of the intercomparison study is described in Section 3, and the results are presented in Section 4. A summary and conclusions are given in Section 5.

2. Theory and methods

2.1. Atmospheric infrared radiative transfer

In a gaseous, non-scattering atmosphere in local thermodynamic equilibrium radiative transfer [22] is described by the Schwarzschild equation [23–25], and the intensity (radiance) I at wavenumber ν is given by the integral along the line-of-sight

$$I(\nu) \;=\; I_\mathrm{b}(\nu)\,\mathrm{e}^{-\tau_\mathrm{b}(\nu)} \;+\; \int_0^{\tau_\mathrm{b}(\nu)} B(\nu, T(\tau'))\,\mathrm{e}^{-\tau'}\,\mathrm{d}\tau', \qquad (1)$$

where B denotes Planck's function for a black-body with temperature T and $I_\mathrm{b}(\nu)$ describes a background contribution (e.g., due to the surface in case of a nadir-viewing observer). The optical depth τ (measured relative to the observer at position $s = 0$, equivalent to $\tau = 0$) is closely related to the monochromatic transmission

$$\begin{aligned}\mathcal{T}(\nu, s) &= \mathrm{e}^{-\tau(\nu,s)} \\ &= \exp\left(- \int_0^s \mathrm{d}s' \sum_m k_m\big(\nu, p(s'), T(s')\big)\, n_m(s') \right), \qquad (2)\end{aligned}$$

where p is the atmospheric pressure and the integrand constitutes the absorption coefficient, essentially determined by the sum of the absorption cross sections k_m scaled by the molecular number densities n_m. Note that the contribution of the pressure and temperature dependent continuum absorption [26], slowly varying with wavenumber, has not been included in Eq. (2).

In high resolution lbl models, the absorption cross section of molecule m is given by the superposition of many lines l with line center positions $\hat{\nu}_l$, each described by the product of a temperature–dependent line strength S_l and a normalized line shape function g describing the broadening mechanism(s) (for brevity the subscript m is omitted),

$$k(\nu, p, T) \;=\; \sum_l S_l(T)\, g(\nu;\; \hat{\nu}_l, \gamma_l(p, T)). \qquad (3)$$

For the infrared and microwave spectral regime, the combined effect of pressure broadening (corresponding to a Lorentzian line shape g_L) and Doppler broadening (corresponding to a Gaussian line shape g_G) can be represented by a convolution of both, i.e. the Voigt line profile [27]

$$g_\mathrm{V}(\nu - \hat{\nu}, \gamma_\mathrm{L}, \gamma_\mathrm{G}) \;=\; g_\mathrm{L}(\nu - \hat{\nu}, \gamma_\mathrm{L}) \otimes g_\mathrm{G}(\nu - \hat{\nu}, \gamma_\mathrm{G}). \qquad (4)$$

where the Lorentz width γ_L is depending on pressure and temperature and the Gaussian width γ_G depends on temperature and the molecular mass. It should be noted that the increasing quality of ground-based and, more recently, space-based spectrometers has indicated the approximative nature of the Voigt (and Lorentz) profile, i.e. effects due to Dicke narrowing, speed-dependent broadening, or line mixing have to be taken into account by more sophisticated line profiles [e.g., 28,29] and a corresponding extension of the line parameter databases [e.g., 30].

Instrumental effects are modeled by convolution of the monochromatic intensity (1) or transmission (2) with appropriate spectral response functions (SRF) $\mathcal{S}(\nu)$. The equivalent brightness temperatures shown below are computed from the convolved radiances $\hat{I}$ using the inverse of Planck's function $T_\mathrm{B} \equiv B^{-1}(\nu, \hat{I})$ with the wavenumber given by the (tabulated) SRF center position. Furthermore, the effect of the finite aperture can be simulated by numerical integration of the radiances over the finite instantaneous field of view.

2.2. ARTS – Atmospheric Radiative Transfer Simulator

ARTS is a publicly available radiative transfer code published under the GNU license agreement (see also http://www.radiativetransfer.org/). It is an open-source project driven by the University of Hamburg, Germany and Chalmers University, Gothenburg, Sweden [17,18,31]. ARTS was originally developed for applications in the microwave range but is also suitable for applications in the mid- and far-infrared range [see e.g., 32,33]. In this study we used the stable version 2.2 [18]. ARTS was included in intercomparisons for microwave radiative transfer (up, down, and limb) [11] as well as infrared radiative transfer models simulating AIRS (Atmospheric Infrared Sounder) radiances [13]. It is able to treat clear sky conditions with lbl and continuum absorption as well as different scattering schemes for hydrometeors. For this study, the Mlawer–Tobin–Clough–Kneizys–Davies (MT-CKD) 1.0 continua for O_2, N_2, H_2O, and CO_2 have been used [34,35].

Absorption in ARTS is level based. For efficiency, the lbl absorption can be stored in a frequency, pressure, temperature, and water vapor dependent lookup table and reused for many subsequent radiative transfer simulations [36]. Besides, for instrument simulation as in this study, ARTS can also be used to compute atmospheric radiative energy fluxes and heating rates [37,38].

2.3. GARLIC – Generic Atmospheric Radiation Line-by-Line Infrared Code

GARLIC [20,39] has been developed for high resolution infrared-microwave atmospheric radiative transfer modeling with a modular approach appropriate for simulation and retrieval in Earth [40,41] and planetary science [42]. Unlike ARTS, GARLIC is not open source, however, Py4CAtS – Python for Computational Atmospheric Spectroscopy [43] a lightweight implementation of GARLIC, is publically available at https://atmos.eoc.dlr.de/tools/Py4CAtS/.

In addition to the lbl absorption, the "CKD" continua [34] and collision-induced absorption (CIA) [44] are implemented. For the computation of the Voigt function GARLIC uses a combination of the Humlíček [45] and the Weideman [46] rational approximations [47]. For further speed-up of the lbl calculation a multigrid algorithm is used [48]. In contrast to most other lbl codes treating the inhomogeneous atmosphere in a layer-by-layer approach, GARLIC is level-oriented and employs numerical quadrature techniques to solve the path integrals. More specifically, the Planck function is assumed to vary either linearly or exponentially with optical depth between two adjacent levels and the Schwarzschild integral (1) is approximated by the trapezoid rule (the linear in τ mode was termed "trapezoid-Laguerre quadrature" in [20]). Note that in contrast to KOPRA and ARTS no intermediate levels are introduced for the path integration along the line-of-sight.

2.4. KOPRA – Karlsruhe Optimized & Precise Radiative Transfer Algorithm

KOPRA [16] is a line-by-line, layer-by-layer model for forward calculation of infrared atmospheric transmittance and radiance spectra for various geometries and was initially developed for the analysis of MIPAS mid infrared limb emission sounder data [49]. It is also applicable to upward and nadir looking instruments using thermal emission as well as solar and lunar absorption modes for high resolution spectroscopic and radiometer applications with