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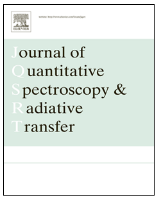

Fast radiative transfer using monochromatic look-up tables

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ABSTRACT

Line-by-line (LBL) methods of numerically solving the equations of radiative transfer can be inhibitingly slow. Operational trace gas retrieval schemes generally require much faster output than current LBL radiative transfer models can achieve. One option to speed up computation is to precalculate absorption cross sections for each absorbing gas on a fixed grid and interpolate. This work presents a general method for creating, compressing, and validating a set of individual look-up tables (LUTs) for the 11 most abundant trace gases to use the Reference Forward Model (RFM) to simulate radiances observed by the Infrared Atmospheric Sounding Interferometer (IASI) at a more operational pace. These LUTs allow the RFM to generate radiances more than 20 times faster than LBL mode and were rigorously validated for 80 different atmospheric scenarios chosen to represent variability indicative of Earth's atmosphere. More than 99% of all IASI simulated spectral channels had LUT interpolation errors of brightness temperature less than 0.02 K, several factors below the IASI noise level. Including a reduced spectral grid for radiative transfer speed up the computation by another factor of six at the expense of approximately doubling interpolation errors, still factors below IASI noise. Furthermore, a simple spectral compression scheme based upon linear interpolation is presented, which reduced the total LUT file size from 120 Gbytes to 5.6 Gbytes; a compression to just 4.4% of the original. These LUTs are openly available for use by the scientific community, whether using the RFM or to be incorporated into any forward model.

1. Introduction

The retrieval of atmospheric temperature and composition from infrared measurements is usually an iterative process requiring repeated calculations of the radiative transfer equation to simulate the observations. In its simplest form the radiance L reaching the satellite at wavenumber ν from viewing geometry (e.g., tangent height, scan angle) z can be expressed as the sum of atmospheric and background terms:

$$L(\nu,z)=\int_{\tau_0}^{1} B(\tau)\,d\tau+B_0\tau_0, \tag{1}$$

where τ is the transmittance along the line-of-sight from the satellite ($\tau=1$) to the remote boundary of the atmosphere ($\tau=\tau_0$), B is the Planck function along this path, and B_0 is the Planck function of the background at the far side of or beyond the atmospheric path.

The measurement itself, R_{ij}, for nominal wavenumber ν_i and viewing geometry z_j, is modelled as a convolution of this radiance with the appropriate instrument functions

$$R_{ij}=\iint L(\nu,z)\Phi(z-z_j)\Psi(\nu-\nu_i)\,d\nu\,dz. \tag{2}$$

Φ_j represents the instrument field-of-view (usually omitted with nadir-viewing) and Ψ_i represents the spectral response (the instrument line shape for Fourier transform spectrometers, or channel response for radiometers).

The three main geometries for infrared remote sensing can be distinguished by the relative importance of the

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background term in the radiative transfer equation; for solar occultation $B_0\tau_0$ is dominant, for limb-viewing it is negligible and for nadir-viewing it is comparable to the atmospheric term. However, in all cases, since B is only a function of wavenumber and temperature, information on the composition and pressure (as well as temperature) is derived from the transmittance.

Calculating transmittance is usually the time-consuming part of the retrieval process. The most accurate method is to use a line-by-line (LBL) model. However, this is slow and only feasible in real-time data processing for solar occultation measurements, which typically have a maximum of 28 profile acquisitions per day.

Nadir-viewing instruments, such as those commonly used for operational weather forecasting, provide measurements at typically 10^5–10^6 locations per day and this presents a greater challenge. With (spectrally broad) measurements from filter radiometers, the usual method is to apply the radiative transfer to pre-computed spectrally integrated quantities, effectively:

$$R_i = \int \overline{B}\, d\overline{\tau} + \overline{B}_0\overline{\tau}_0 \tag{3}$$

where

$$\overline{\tau} = \int \tau(\nu)\Psi(\nu-\nu_i)\, d\nu \tag{4}$$

and similarly for $\overline{B}$ [1,2]. This differs fundamentally from the monochromatic approach in that Beer's Law does not hold for spectrally integrated transmittances. In other words, the net transmittance of a composite path is no longer simply the product of the transmittances of the component paths when dealing with averaged quantities. This can be readily appreciated if one considers the net transmittance through two consecutive identical cells, each opaque over the lower half of the spectral range and transparent in the upper half. The spectrally averaged transmittance of each cell is 0.5, but the transmittance of the two cells combined is, clearly, also 0.5, rather than the product $0.5 \times 0.5 = 0.25$. To overcome this it is necessary to parametrise spectrally averaged transmittances not only as a function of the 'natural' quantities such as pressure and temperature, but also a number of ad hoc 'predictors' such as geometry and contaminants, relating to each channel and generally obtained by statistical regression from a large sample (with all the risks that entails when dealing with anomalous atmospheric cases) [3].

The recent trend has been towards replacing broad band filter radiometers, such as the High-resolution Infrared Radiation Sounder (HIRS; order of 10 channels of widths $\sim$10's of cm^{-1}), with Fourier transform or grating spectrometers (order of 1000 channels with resolution $\sim 1\ \text{cm}^{-1}$). Extending the spectrally averaged approach requires treating each spectral sample as an independent channel with its own set of tailored predictors. While this remains the 'fast' solution, it becomes unwieldy and, noting the steady increase in computing speeds, it is anticipated that a monochromatic approach will gradually be adopted even for the operational nadir-viewing instruments.

Significant time savings can be made by using the line-by-line model to pre-compute monochromatic transmittances $\tau(\nu)$ (or, more usually, a related quantity such as absorption cross section), over a variety of atmospheric conditions, and storing these in a 'look-up table' (LUT) for use in the retrieval forward model. Such an approach has, for example, been used for the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) [4] limb-sounding instrument and the nadir-viewing Infrared Atmospheric Sounding Interferometer (IASI) [5]. The use of monochromatic LUTs of absorption cross sections is not new [6]. However, in many cases the LUTs themselves are closely tied to their application and details of their generation, testing, and optimisation are not widely published.

The aim of this paper is to review the criteria required to construct such LUTs and the various methods chosen for their implementation. Simulations of IASI radiances are used as a test case. Furthermore, a detailed description is given of the construction and testing of LUTs which can be implemented in the Reference Forward Model (RFM) for radiative transfer [7] as a direct replacement for the line-by-line calculation, which therefore allows comparisons of the speed/accuracy trade-off.

Finally, given that these LUTs require a relatively simple file format (even if the files are large) it is hoped that this paper might encourage such LUTs to be regarded as independent databases, decoupled from their originating line-by-line models and any particular instrumental application.

2. Calculating transmittance

It will be assumed that a generic atmospheric radiative transfer model (RTM) represents the transmittance of a line-of-sight path from the satellite through an inhomogeneous atmosphere as the product of the monochromatic transmittances of the component path segments,

$$\tau = \prod_l \tau_l. \tag{5}$$

Each segment (l) is defined, for example, by the intersection of the line-of-sight with the internal vertical grid on which the atmospheric profile is represented. In turn, the transmittance of each segment is related to the optical depth (χ_g) of each absorbing species (g) through

$$\tau_l = \exp\left(-\sum_g \chi_{gl}\right). \tag{6}$$

The optical depths themselves are computed from

$$\chi_{gl} = k_{gl}u_{gl}, \tag{7}$$

where k is the absorption cross section (e.g., units of $\text{m}^2\ \text{mol}^{-1}$) and u is the integrated absorber amount within the segment (inverse units of k). As an example, Fig. 1 shows the contribution to optical depth for a water vapour spectral line in a tropical atmospheric scenario for each 100 hPa tropospheric layer. Notice that the optical depth shape changes depending upon the physical atmospheric conditions of that layer. The total optical depth is then the sum of the optical depths from each layer.

The absorption cross section itself, as well as its spectral dependence, is also a function of pressure, temperature and, sometimes, absorber concentration if the absorbing