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An ultrafast line-by-line algorithm for calculating spectral transmittance and radiance

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ABSTRACT

An ultrafast line-by-line algorithm for calculating spectral transmittance and radiance of gases is presented. The algorithm is based on fast convolution of the Voigt line profile using Fourier transform and a binning technique. The algorithm breaks a radiative transfer calculation into two steps: a one-time pre-computation step in which a set of pressure independent coefficients are computed using the spectral line information; a normal calculation step in which the Fourier transform coefficients of the optical depth are calculated using the line of sight information and the coefficients pre-computed in the first step, the optical depth is then calculated using an inverse Fourier transform and the spectral transmittance and radiance are calculated. The algorithm is significantly faster than line-by-line algorithms that do not employ special speedup techniques by a factor of 10^3–10^6. A case study of the 2.7 μm band of H_2O vapor is presented.

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1. Introduction

Various radiative transfer (RT) models have been developed in the last a few decades for numerical calculation of spectral transmittance and radiance of gases. These numerical models are generally classified into two major categories, line-by-line (LBL) models e.g., [1–9] and band models, depending on whether the real spectral lines of the gases are directly used or a set of band parameters derived from the line information of the gases are used in the calculation. Although band models are several orders of magnitudes faster than LBL models, they suffer from the accuracy problem that is inherent within the statistical framework of these models. Moreover, using band models for an inhomogeneous line of sight (LOS) requires more approximations that further reduce their accuracy.

As a consequence of the rapid advance of computational power in the past two decades, LBL models have received many applications due to their high accuracy. In order to reduce computational cost, modern LBL models generally make use of some sort of speedup techniques while calculating the line function. This includes, for example, decomposition of the line function into sub-functions spanning finite domains e.g., [4–6], interpolation over regions where the line function varies slowly e.g., [7–9], and use of approximate but easy-to-evaluate functions to represent the line function e.g., [10–13]. In spite of all the efforts, LBL models are still notoriously slow while dealing with problems in which large number of spectral lines are involved. For example, in modeling molecular emission from plasma, rocket plume, or atmospheric emission of hot gas giants, the number of spectral lines can easily exceed hundreds of millions or even billions. Under these conditions, LBL models quickly become prohibitively expensive.

In this paper, we describe a new LBL model that is dramatically faster than any existing LBL models and is comparably to band models in speed. This model still calculates the optical depth line by line but it does so in the Fourier transform space. It achieves the unprecedented speed by separating out the computationally expensive line-by-line calculation into a one-time pre-computation step in which a set of pressure-independent coefficients

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are calculated and stored in computer disk. A normal RT calculation requires only minimal calculations using these pre-computed coefficients and an inverse Fourier transform.

This paper is organized as follows. The theoretical framework of the model is given in Section 2. The time complexity and accuracy considerations are analyzed in Section 3. A case study using the new model for the 2.7 μm band of H_2O vapor is presented in Section 4. Further discussions are presented in Section 5. We will use the term "algorithm" rather than "model" hereafter in the paper to refer to the new LBL algorithm since it is presented in a way that can be directly implemented into a computer program.

2. Theoretic framework

Solutions to the equation of radiative transfer [14] for calculating spectral transmittance and radiance require calculation of the optical depth as a function of the path though the LOS. In numerical approaches, this calculation is decomposed into calculations of the optical depth through a number of homogenous segments along the LOS. Within each of these LOS segments, temperature, pressure, and gas mole fractions are assumed to be uniform. In a LBL model, the wavelength-dependent optical depth for a gas mixture in a homogeneous segment is given by

$$\tau(\tilde{\nu};T,P,U_1,U_2,\ldots,U_{N_s})=\sum_{\alpha}^{N_s}U_\alpha\sum_{i}^{N_\alpha}S_{\alpha,i}V(\sigma_{\alpha,i},\gamma_{\alpha,i};\tilde{\nu}-\tilde{\nu}_{\alpha,i}) \quad (1)$$

where $\tau(\tilde{\nu};T,P,U_1,U_2,\ldots,U_{N_s})$ is the optical depth that depends on the wavenumber $\tilde{\nu}$, temperature T and total pressure P, and the column densities $U_1,U_2,\ldots,U_{N_s}$ of the N_s gas species in the segment; $S_{\alpha,i}$ is the line strength for the ith line of gas α that has N_α lines in total; $V(\sigma_{\alpha,i},\gamma_{\alpha,i};\tilde{\nu}-\tilde{\nu}_{\alpha,i})$ is the Voigt line profile for the ith line of gas α whose central wavenumber is $\tilde{\nu}_{\alpha,i}$; $\sigma_{\alpha,i}$ and $\gamma_{\alpha,i}$ are the Doppler width and the collision broadened half width (HWHM) for the ith line of gas α, respectively.

The Doppler width $\sigma_{\alpha,i}$ is given by

$$\sigma_{\alpha,i}=\sqrt{\frac{k_BT}{m_\alpha}}\frac{\tilde{\nu}_{\alpha,i}}{c} \quad (2)$$

where k_B is the Boltzmann constant, c is the speed of light in the vacuum, and m_α is the molecular mass of the gas α. The collision broadened width $\gamma_{\alpha,i}$ of the same line is given by

$$\gamma_{\alpha,i}=\left[\gamma_{\alpha,i}^{a0}(1-r_\alpha)\left(\frac{T^0}{T}\right)^{n_{\alpha,i}^a}+\gamma_{\alpha,i}^{s0}r_\alpha\left(\frac{T^0}{T}\right)^{n_{\alpha,i}^s}\right]\left(\frac{P}{P^0}\right) \quad (3)$$

where $\gamma_{\alpha,i}^{a0}$ and $\gamma_{\alpha,i}^{s0}$ are the air- and self-broadened half widths for the ith line of gas α at the reference temperature T^0 and pressure P^0, respectively; r_α is the mole fraction of the gas species; $n_{\alpha,i}^a$ and $n_{\alpha,i}^s$ are temperature-dependent exponents for the air- and self-broadened widths for the ith line of gas α, respectively.

The line strength $S_{\alpha,i}$ in Eq. (1) is given by

$$S_{\alpha,i}=S_{\alpha,i}^0\frac{Q_\alpha^0}{Q_\alpha(T)}\exp\left[-c_2E_{\alpha,i}\left(\frac{1}{T}-\frac{1}{T^0}\right)\right]\left[\frac{1-\exp(-c_2\tilde{\nu}_{\alpha,i}/T)}{1-\exp(-c_2\tilde{\nu}_{\alpha,i}/T^0)}\right] \quad (4)$$

where $S_{\alpha,i}^0$ is the line strength at the reference temperature; Q_α^0 and $Q_\alpha(T)$ are the total partition functions of the gas species at the reference temperature T^0 and the temperature of T, respectively; $E_{\alpha,i}$ is the total lower state energy of the spectral line; c_2 is a constant that equals to hc/k_B, where h is the Planck constant.

Instead of calculating the optical depth using Eq. (1) directly, which requires a lot of computational power when N_αs are large (e.g., $>10^8$ while dealing with molecular transmission and emission problems at temperatures higher than 1000 K for common atmospheric species such as H_2O, CO_2, NH_3, etc.), we seek a solution to Eq. (1) in Fourier transform space and exploit properties of such a solution for dramatic speed improvement. Eq. (1) can be easily rewritten in Fourier transform space using the convolution theorem, as shown by Mendenhall [15]:

$$\tilde{\tau}(k;T,P,U_1,U_2,\ldots,U_{N_s})=\sum_{\alpha}^{N_s}U_\alpha\sum_{i}^{N_\alpha}S_{\alpha,i}\exp(-\sigma_{\alpha,i}{}^2k^2-\gamma_{\alpha,i}|k|-ik\tilde{\nu}_{\alpha,i}) \quad (5)$$

where k is the Fourier transform variable of wavenumber $\tilde{\nu}$. If the LOS information (i.e., $T,P,U_1,U_2,\ldots,U_{N_s}$) and the spectral line information (i.e., $S_{\alpha,i}$ for all lines of all species) are known, one can sum over all the terms in the right side of Eq. (5) to get the Fourier transform coefficients of the optical depth and then performs an inverse Fourier transform to get the real optical depth. Note that Eq. (5) is exactly correct, and in practice one has to use an approximate discrete Fourier transform such as the fast Fourier transform (FFT) to calculate Eq. (5). Although this FFT based approach is much faster than the calculation of Eq. (1) directly, the summation over all spectral lines in Eq. (5) is still very computationally expensive when N_αs are large.

Note that the left side of Eq. (5) is a function of temperature and total pressure. While temperatures for common RT problems vary from a few K to a few thousand K, the total pressures could vary in a much wider range (e.g., 10^{-1}–10^8 Pa). The dependence of $\tilde{\tau}(k;T,P,U_1,U_2,\ldots,U_{N_s})$ on temperature can be easily treated with a relatively small temperature grid and with interpolation. It is the pressure dependence of $\tilde{\tau}(k;T,P,U_1,U_2,\ldots,U_{N_s})$ that makes it difficult for us to employ a pre-computation technique to boost performance. To overcome this difficulty, we employ a low-resolution binning (LRB) technique. The principle of LRB is to bin the pressure-entangled quantities in Eqs. (3) and (5) (i.e., $\gamma_{\alpha,i}^{a0}$, $\gamma_{\alpha,i}^{s0}$, $n_{\alpha,i}^a$, and $n_{\alpha,i}^s$) so that we can factor pressure-related terms out of the last summation in Eq. (5) and enable a pre-computation approach.

By applying LRB to the temperature-dependent exponents $n_{\alpha,i}^a$ and $n_{\alpha,i}^s$, we assume that these quantities take values only from a number of preset bin values. In the extreme case where there is only one bin, we have

$$n_{\alpha,i}^a=\overline{n_\alpha^a}, \quad (6)$$

and

$$n_{\alpha,i}^s=\overline{n_\alpha^s} \quad (7)$$

where $\overline{n_\alpha^a}$ and $\overline{n_\alpha^s}$ are the average temperature-dependent exponents for the air- and self-broadening for gas α, respectively. This special case of LRB is called the average temperature-dependent pressure-broadening approximation

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