EFFICIENT METHODS FOR COMPUTATION OF OPTICAL PROPERTIES OF GASEOUS MEDIA

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Received July 15, 1994

We present a review of the approaches to improving the efficiency of numerical techniques used in atmospheric optics. The methods of line–by–line (LBL) calculation of the parameters of selective absorption of optical radiation by gases and its scattering by spherical particles as well as the LBL methods for solving the transfer equation for long– and short–wave radiation in the atmosphere are considered. Numerical procedures for increasing the efficiency of these methods and corresponding computational algorithms together with assessments of the computation time are given.

INTRODUCTION

The methods of increasing the efficiency of the line–by–line method for calculating the selective gas absorption of optical radiation and algorithms for calculating the parameters of its scattering by aerosol (spherical) particles as well as LBL methods of solving the equations of long– and short–wave radiation transfer in the atmosphere, which are the basis of a software package, have been developed by the authors of this paper during the last decade for *ab initio* simulation of radiative processes in the atmosphere. This software package was successfully used in climatic investigations, solution of problems on sounding the atmosphere from space, and some other problems which require evaluated accuracy and detailed consideration of selective gas absorption. In some cases, their efficiency was higher then of the analogous ones by several orders of magnitude. Thus, the computation of solar radiation fields in a cloudy plane–stratified atmosphere took 30–40 hours with an IBM PC–486[1], while it took 100 hrs by CYBER–205.[2] Some details of these algorithms have already been published. However, the review of these papers can be useful both for specialists in numerical simulation of optical radiation transfer and in related sciences.

1. COMPUTATION OF ABSORBING AND SCATTERING PROPERTIES OF THE ATMOSPHERE

First, we describe the LBL technique of computation the gas absorption coefficient, which allows one to increase the computation speed by one to two orders of magnitude.

The monochromatic (volume) coefficient of gas absorption K_ν at the wavenumber ν is calculated by the formula

$$K_\nu = \sum_i f_i(\nu, \tilde{\nu}_i) , \qquad (1.1)$$

where $f_i(\nu, \tilde{\nu}_i)$ is the profile of the ith spectral line with the center at a point $\tilde{\nu}_i$. The contribution coming from far lines can be taken into account as a "continuum" using the method described by Drayson.[3] Therefore, not so distant lines, i.e., $|\nu - \tilde{\nu}_i| < D \sim 10$ cm^{-1} are summed directly by formula (1.1). The calculations of K_ν are usually carried out with an uniform or nonuniform wavenumber grid sufficiently dense to represent a line contour, i.e., with a characteristic step H comparable to the line half–width. Hence, in the LBL calculations for the real atmosphere, each contour is computed approximately $2D/H \sim 10/0.001 = 10^4$ times (0.001 cm^{-1} is the characteristic line width in the upper atmosphere) thus requiring long computer time. A nonuniform grid, which is more dense at line centers and sparse in its wings, allows one to reduce somewhat the number of contour calculations. However, in strong bands where the lines are spaced at distances comparable with their half–widths, it is practically impossible to decrease the number of contour calculation points using a single grid. The use of single grid results in overexpenditure of computer time, since any contour is calculated in extremely detailed segments of the grid near the centers of the remaining lines.

The principal feature of the described algorithm is a series of grids with doubling steps h_i

$$h_0 = H, \quad h_1 = H\cdot 2, \quad h_2 = h_1\cdot 2, \ \ldots , \quad h_l = H\cdot 2^l, \quad l = 0, 1, \ldots , L,$$

$$\nu_j^{(l)} = \nu_{\text{start}} + h_l\, j , \; j = 0, 1, \ldots , \qquad (1.2)$$

where $\nu_j^{(0)} = \nu_j$ is the most dense grid, ν_{start} is the starting wavenumber, and L is the number of the most rough grid. Only ten grids ($L = 10$) are required to extend the step from 0.001 to 1 cm^{-1}. Now, the contour of each line is calculated independently of the other lines at about 50 points of this series of grids, as shown in Fig. 1. In other words, an optimal set of interpolation nodes is formed for each line. It should be noted that summation (1.1) must be done individually for each grid $\nu_j^{(l)}$ for the corresponding segment of the contour

$$\tilde{\varphi}_j^{(l)} = \tilde{\varphi}_j^{(l)} + f_i(\nu_j^{(l)}, \tilde{\nu}_i) , \; \varphi_{j+1}^{(l)} = \varphi_{j+1}^{(l)} + f_i(\nu_{j+1}^{(l)}, \tilde{\nu}_i) ,$$

$$\tilde{\tilde{\varphi}}_{j+2}^{(l)} = \tilde{\tilde{\varphi}}_{j+2}^{(l)} + f_i(\nu_{j+2}^{(l)}, \tilde{\nu}_i) , \quad j = 0, 2, \ldots , \qquad (1.3)$$

where $\tilde{\varphi}_j^{(l)}$, $\varphi_j^{(l)}$, and $\tilde{\tilde{\varphi}}_j^{(l)}$ are the accumulated contributions from the remaining lines.

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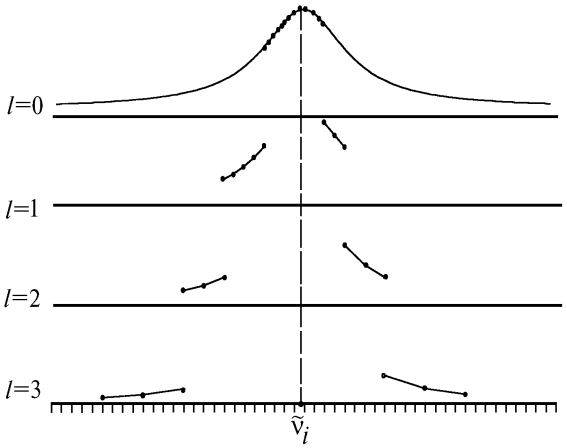

FIG. 1. An illustration of the calculational technique for K_ν using a series of grids.

At the each second point, we have to consider $\tilde{\varphi}_j^{(l)}$ and $\tilde{\tilde{\varphi}}_j^{(l)}$ individually due to "discontinuities" of the contour depicted in Fig. 1. After considering all of the lines, a recursion procedure is carried out based on simple quadratic interpolations, which enable one to obtain the unknown coefficient of gas absorption at the nodes of the most detailed uniform grid

$$\tilde{\tilde{\varphi}}_m^{(l-1)} = \tilde{\tilde{\varphi}}_m^{(l-1)} + \tilde{\tilde{\varphi}}_{m/2}^{(l)}\,, \quad \tilde{\varphi}_m^{(l-1)} = \tilde{\varphi}_m^{(l-1)} + \tilde{\varphi}_{m/2}^{(l)}\,,$$

$$\varphi_{m+1}^{(l-1)} = \varphi_{m+1}^{(l-1)} + 0.375\,\tilde{\varphi}_{m/2}^{(l)} + 0.75\,\varphi_{(m/2)+1}^{(l)} - 0.125\,\tilde{\tilde{\varphi}}_{(m/2)+2}^{(l)}\,,$$

$$\tilde{\varphi}_{m+2}^{(l-1)} = \tilde{\varphi}_{m+2}^{(l-1)} + \varphi_{(m/2)+1}^{(l)}\,, \quad \tilde{\tilde{\varphi}}_{m+2}^{(l-1)} = \tilde{\tilde{\varphi}}_{m+2}^{(l-1)} + \varphi_{(m/2)+1}^{(l)}\,, \quad (1.4)$$

$$\varphi_{m+3}^{(l-1)} = \varphi_{m+3}^{(l-1)} - 0.125\,\tilde{\varphi}_{m/2}^{(l)} + 0.75\,\varphi_{(m/2)+1}^{(l)} + 0.375\,\tilde{\tilde{\varphi}}_{(m/2)+2}^{(l)}\,,$$

$$\tilde{\varphi}_{m+4}^{(l-1)} = \tilde{\varphi}_{m+4}^{(l-1)} + \varphi_{(m/2)+2}^{(l)}\,, \quad \tilde{\tilde{\varphi}}_{m+4}^{(l-1)} = \tilde{\tilde{\varphi}}_{m+4}^{(l-1)} + \tilde{\tilde{\varphi}}_{(m/2)+2}^{(l)}\,,$$

where $m = 0, 4, 8, \ldots$ and $l = L, L-1, \ldots, 1$.

By interrupting this procedure in those spectral intervals where in the finest grids the accumulated contributions are equal to zero (between widely spaced lines), it is also possible to obtain a nonuniform grid, which is more efficient for use in the transfer problems solution. The interpolation procedure (1.3) is carried out once and, as a rule, in a time, which is negligible in comparison with the time of the entire computation. It is easy to analyze the interpolation errors of the method making advantage of an approximate proportionality of the contour to $|\nu - \tilde{\nu}_i|^{-2}$ starting from distances of several half–widths from the center. It can be shown that these errors (Fig. 2) are alternating (that results in their partial compensation) and does not exceed 7.8% (in wings). In this case, the errors related to the contour amplitude and appearing in calculation of contour area are not larger than 1%. Such accuracy is sufficient for most of practical computations. It can easily be improved by introducing a complementary central point in each grid in Eq. (1.2) and coming from Eq. (1.4) to the procedure based on the 4th–order interpolations. In this case, the error is reduced from 7.8 down to 0.4%. Finally, the procedure described increases the computational speed to $10^4/50$~100 times, though it requires a 2.5 time larger memory of a computer.[4]

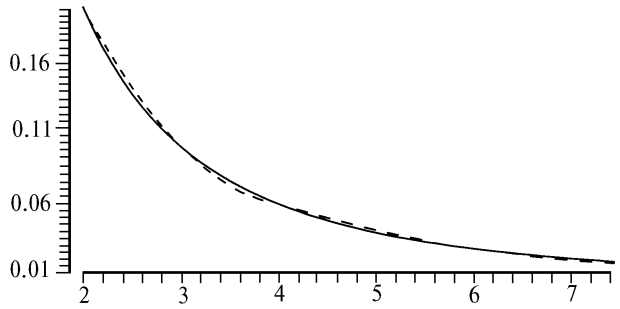

FIG. 2. The Lorentz contour (normalized to unity) calculated directly (solid line) and using the described technique (dashed line) at distances in half–width units.

To completely describe the computational algorithms of interaction between the optical radiation at the atmosphere, it is useful to consider scattering by aerosol particles or cloud drops. Here, the authors use more traditional methods. The calculation is accomplished using the Deirmendjian algorithms[5] based on the Mie series, which allow one to obtain precise parameters of scattering by spherical homogeneous particles. However, for "large particles" (the particle radius exceeds the incident wave length by one or two orders of magnitude), the optical approximation is used. Such an approach proposed by Shifrin[6] enables one not only to increase the computational speed by some orders of magnitude, but also to resolve the known computational problems caused by the need for the consideration of diffraction peak in the scattering phase function in a rather simple way.

2. SOLUTION OF THE RADIATIVE TRANSFER EQUATIONS FOR THE ATMOSPHERE

In this section the peculiarities of the solution of the radiative transfer equations in the atmosphere are briefly described based on linear interpolation of the monochromatic absorption coefficient $K_\nu(Z)$ and other values for a vertical path. This method was developed by the authors during the last several years; it revealed much higher efficiency then the traditional one connected with division of the atmosphere into homogeneous layers. First, the volume absorption coefficient is calculated at the levels Z_j (usually in one–kilometer intervals). Between the levels, the coefficient is presented in the form

$$K_\nu(Z) = \alpha_\nu^j + \beta_\nu^j Z\,, \quad 1 \le j \le N\,, \qquad (2.1)$$

where $Z_j \le Z \le Z_{j+1}$ and N is the number of levels.

The values α_ν^j and β_ν^j are easily found from the solution of the system of two linear equations obtained by considering Eq. (1.2) at the levels Z_j and Z_{j+1}. Expression (1.2) makes it possible to avoid the numerical integration over Z when calculating the optical depths. Thus, integrating Eq. (1.2) in an analytical form, we obtain an algebraic formula for the optical depth of the layer between the levels Z_j and Z_{j+1}:

$$\tau_\nu(Z_j, Z_{j+1}) = \alpha_\nu^j\,(Z_{j+1} - Z_j) + \beta_\nu^j\,\frac{1}{2}\,(Z_{j+1}^2 - Z_j^2)\,. \qquad (2.2)$$

Generalization of Eq. (2.2) for calculating the optical thicknesses of any layer, optical paths of photons, etc., seems obvious and provides sufficiently rapid computation.

Schwarzschild integrals[7] (over frequency and space) being solutions of a corresponding transfer equation neglecting the scattering process are used in the calculation of integral characteristics of long–wave radiation transfer (fluxes, intensities, and influxes). When making numerical integration, some difficulties appear, which are accounted for by a wide spread of photon free paths in the atmosphere due to selective gas absorption. Thus, the photon free path at a frequency within the center of strong line can be reduced to several centimetres. As a result, unrealistic spatial grids are needed for integration. This problem is solved using the identity

$$\int_H^{\dots} dZ\, B_{\Delta\nu}[T(Z)]\,\varphi(Z) \equiv B_{\Delta\nu}[T(H)] \int_H^{\dots} \varphi(Z)\, dZ + \\ + \int_H^{\dots} \{B_{\Delta\nu}[T(Z)] - B_{\Delta\nu}[T(H)]\}\,\varphi(Z)\, dZ\,, \qquad (2.3)$$

where $B_{\Delta\nu}(T)$ is the Planck function which is frequency–independent at small intervals $\Delta\nu$ ($\Delta\nu$ = 1–10 cm^{-1}); T is the temperature dependent on altitude Z; H is the height of a calculation point; and, $\varphi(Z)$ is the result of integration over frequency in the interval $\Delta\nu$ of the corresponding functions K_ν and τ_ν, entering into the Schwarzschild integral. The function φ is nonzero only in the region of several photon free paths around the calculation point.

The first integral in the right–hand side of Eq. (2.3) is taken analytically and the second one is taken numerically on spatial grids with the 10–100 m step determined by the characteristic scale associated with temperature stratification of the atmosphere. For strong absorption, where the photon free path becomes shorter then 1–10 m, the second integral can be neglected, since the product in the integrand is close to zero. This method is described at length in Ref. 8.

Consider now a universal technique based on the combination of line–by–line and the Monte Carlo methods. It allows us to strictly account for selective gas absorption in composite scattering media, such as cloudy and dusty atmosphere. The consideration of selectivity drastically complicates the problem that forces us to make computations with the spectral resolution of 0.001 cm^{-1} (see previous Section), often over the entire short–wave range of the order of 10^4 cm^{-1} (see the example from Ref. 2, which has been mentioned in the Introduction). This calls for consideration of $10^4/10^{-3} = 10^7$ monochromatic transfer equations. The initial is the expression for the optical path $u_\nu(M^*)$ of a simulated photon at a point M^* of its trajectory which is a broken line with vertices at scattering points at altitudes H_1, H_2, H_3, ... and cosines $\cos\alpha_1$, $\cos\alpha_2$, $\cos\alpha_3$, ... of zenith angles of the broken–line segments

$$u_\nu(M^*) = (\tau_\nu(H_2) - \tau_\nu(H_1)) / \cos\alpha_1 + (\tau_\nu(H_3) - \\ - \tau_\nu(H_2)) / \cos\alpha_2 + \dots\,, \qquad (2.4)$$

where H_1 is the altitude of the upper level of the atmosphere; $\tau_\nu(H_1) = 0$; $\tau_\nu(H_2)$, $\tau_\nu(H_3)$, $\tau_\nu(H_4)$, ... are the optical depths of scattering points obtained using the "rapid" relations of the Eq. (2.2) type. The selective gas absorption is taken into account with the help of the photon "weight"

$$Q_\nu(M^*) = \exp(-u_\nu(M^*))\,. \qquad (2.5)$$

The subsequent procedures for calculations by the Monte Carlo method are standard and depend on the type of a problem.[9] Let us point out the efficiency of combining a spatial photon grope with frequency photon grope (this was proposed by A.N. Rublev) which enables one to obtain integral characteristics in wide spectral ranges.[10] Using the aforementioned technique, the consideration of selective gas absorption could be introduced into the Monte Carlo method without increasing computer time, since due to high efficiency of LBL calculations, the total computational time does not increase substantially.

CONCLUSION

The characteristic time of complete computation of radiation field in the atmosphere or simulation of the experiment for its sounding (including that from space) over the entire long or short–wave range with the accuracy accounted for by uncertainty of contemporary atmospheric optical models is several tens of hours with IBM PC–486. The technique was used in climatic problems for studying the radiation forcing and obtaining the benchmark calculations of solar and thermal radiative fluxes serving to test radiation units of climatic models. The technique also has the potential for developing the programs for processing the data of spaceborne experiments. It is already used for the orbital IR–spectrometer ISTOK–1 (project PRIRODA, from the orbiting station "Mir" in 1995), in space research of the Earth's radiative budget, etc.[11]

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