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Acceleration techniques for the discrete ordinate method

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ABSTRACT

In this paper we analyze several acceleration techniques for the discrete ordinate method with matrix exponential and the small-angle modification of the radiative transfer equation. These techniques include the left eigenvectors matrix approach for computing the inverse of the right eigenvectors matrix, the telescoping technique, and the method of false discrete ordinate. The numerical simulations have shown that on average, the relative speedup of the left eigenvector matrix approach and the telescoping technique are of about 15% and 30%, respectively.

1. Introduction

In anticipation of the huge amount of data to be delivered by the new generation of European UV/VIS/NIR atmospheric composition sensors (Sentinel 5 Precursor, Sentinel 4 and Sentinel 5), fast and accurate radiative transfer models for simulating satellite-based measurements are required. For the retrieval of atmospheric constituents from satellite-measurements of earthshine radiation, we developed a software tool at the German Aerospace Centre (DLR), which includes as forward models the discrete ordinate method with matrix exponential (DOME) [1], and the small-angle modification (SAM) of the radiative transfer equation [2]. In the latter approach, the solution of the radiative transfer equation under the small-angle approximation is subtracted from the total radiance; the resulting radiance field is much smoother than the diffuse radiance, and the method is more appropriate for modeling strongly anisotropic scattering. In the present paper, which is a sequel to Ref. [2], we analyze the efficiency of these methods when they are equipped with several acceleration techniques, as for example, the left eigenvector matrix approach, the telescoping technique, and the method of false discrete ordinate.

The idea of computing the inverse of the right eigenvector matrix using the left eigenvector matrix is due to Waterman [3]. Essentially, in this work, the radiance field is first scaled in order to obtain a layer matrix with a symmetric block structure. The radiative transfer equation for the scaled radiance is then solved in the framework of the discrete ordinate method with matrix exponential using a spectral decomposition of the layer matrix on the basis of the right and left eigenvector matrices. The same scaling procedure yielding symmetric matrices has been used by Nakajima and Tanaka [4] and by Stamnes et al. [5].

An accurate description of the scattering characteristics of a cloud requires a large number of expansion coefficients of the phase function as compared to the number of expansion coefficients for gas molecules. A substantial improvement consisting in the reduction of the linear algebra system to the active layers of the clouds has been proposed by Spurr [6]. This efficient approach, also known as the telescoping technique, has been adopted in the discrete ordinate method with matrix exponential, and has been described in [1].

The method of false discrete ordinate has been discussed in a series of papers especially in connection with the matrix operator method [7–9]. For a viewing angle in the direction of the line of sight, an additional stream as an extra Gaussian quadrature point with zero weight is

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introduced. The upward radiance at the false discrete ordinate is exactly the upward radiance in the direction of the line of sight computed by the source function integration method.

2. Mathematical formulation

The radiative transfer equation for the diffuse radiance $I(r,\Omega)$ at the generic point r and in the direction $\Omega=(\mu,\varphi)$ reads as

$$\mu\frac{dI}{dr}(r,\Omega)=-\sigma_{\mathrm{ext}}(r)I(r,\Omega)+J(r,\Omega). \tag{1}$$

The source function J sums the contributions of the single scattering term

$$J_{\mathrm{ss}}(r,\Omega)=\frac{\sigma_{\mathrm{sct}}(r)}{4\pi}F_{\mathrm{sun}}e^{-\tau_{\mathrm{ext}}^{\mathrm{sun}}(r)}P(r,\Omega,\Omega_0)+\sigma_{\mathrm{abs}}(r)B(T(r)),$$

and of the multiple scattering term

$$J_{\mathrm{ms}}(r,\Omega)=\frac{\sigma_{\mathrm{sct}}(r)}{4\pi}\int_{4\pi}P(r,\Omega,\Omega')I(r,\Omega')\,d\Omega',$$

where, σ_{ext}, σ_{sct} and σ_{abs} are the extinction, scattering and absorption coefficients, respectively, F_{sun} is the incident solar flux, P is the scattering phase function, $\Omega_0=(-\mu_0,\varphi_0)$ with $\mu_0>0$ is the incident solar direction, $\tau_{\mathrm{ext}}^{\mathrm{sun}}$ is the solar optical depth, and B is the Planck function. In the case of a plane parallel atmosphere, the solar optical depth is given by $\tau_{\mathrm{ext}}^{\mathrm{sun}}(r)=(1/\mu_0)[\tau(r_{\mathrm{TOA}})-\tau(r)]$, where $\tau(r)=\int_{r_s}^{r}\sigma_{\mathrm{ext}}(r')\,dr'$ is the vertical optical depth. The points r_{TOA} and r_s correspond to the top and the lower surface of the atmosphere, respectively.

For the phase function, we consider the conventional expansion in terms of Legendre polynomials P_n, i.e.,

$$P(r,\mu)=\sum_{n=0}^{\infty}c_n\chi_n(r)P_n(\mu), \tag{2}$$

where $c_n=\sqrt{(2n+1)/2}$ and $\mu=\Omega\cdot\Omega'$. In practice, the infinite sum (2) is truncated to a specific expansion order N_{rank}.

In the discrete ordinate method, we assume an azimuthal expansion of the diffuse radiance ($\varphi_0=0$),

$$I(r,\Omega)=\sum_{m=0}^{M_{\mathrm{rank}}}I_m(r,\mu)\cos m\varphi,$$

and for each azimuthal component $I_m(r,\mu)$, we discretize the radiative transfer equation in the angular domain by considering a set of Gauss–Legendre quadrature points and weights $\{\mu_k,w_k\}_{k=\overline{1,N_{\mathrm{do}}}}$ in the interval (0,1); thus, N_{do} is the number of discrete ordinates per hemisphere and M_{rank} is the number of azimuthal modes. For an inhomogeneous atmosphere, we consider a spatial discretization with N layers: $r_1>r_2>\cdots>r_{N+1}$, where $r_1=r_{\mathrm{TOA}}$ and $r_{N+1}=r_s$, and assume that the optical coefficients and the phase function are constant within each layer. On the layer j, with boundary levels r_{j+1} and r_j, we are led to the linear system of differential equations

$$\frac{d\mathbf{i}_m}{dr}(r)=\mathbf{A}\mathbf{i}_m(r)+\mathbf{b}(r),\quad r_{j+1}\le r\le r_j, \tag{3}$$

where $\mathbf{i}_m(r)=\begin{bmatrix}\mathbf{i}_m^+(r)\\ \mathbf{i}_m^-(r)\end{bmatrix}$ is the radiance vector in the discrete ordinate space, and $[\mathbf{i}_m^{\pm}(r)]_k=I_m(r,\pm\mu_k)$, $k=1,\ldots,N_{\mathrm{do}}$. To simplify subsequent notation, we omit to indicate the dependency of the layer matrix $\mathbf{A}$ and of the layer vector $\mathbf{b}$ on the azimuthal index m and the layer index j. The layer matrix has a block structure

$$\mathbf{A}=\begin{bmatrix}\mathbf{A}_{11} & \mathbf{A}_{12}\\ -\mathbf{A}_{12} & -\mathbf{A}_{11}\end{bmatrix},$$

where

$$\mathbf{A}_{11}=\mathbf{M}\mathbf{S}_+\mathbf{W}-\sigma_{\mathrm{ext}j}\mathbf{M},$$
$$\mathbf{A}_{12}=\mathbf{M}\mathbf{S}_-\mathbf{W}. \tag{4}$$

Here $\mathbf{M}$ and $\mathbf{W}$ are diagonal matrices with entries $[\mathbf{M}]_{kl}=(1/\mu_k)\delta_{kl}$ and $[\mathbf{W}]_{kl}=w_k\delta_{kl}$, respectively, and

$$[\mathbf{S}_{\pm}]_{kl}=\tfrac{1}{2}\sigma_{\mathrm{sct}j}p_{mj}(\mu_k,\pm\mu_l),\quad k,l=1,\ldots N_{\mathrm{do}},$$

with

$$p_{mj}(\mu,\mu')=\sum_{n=m}^{N_{\mathrm{rank}}}\chi_{nj}P_n^m(\mu)P_n^m(\mu'), \tag{5}$$

and χ_{nj} being the expansion coefficient $\chi_n(r)$ on the layer j. It should be remarked that the symmetry relation of the associated Legendre functions $P_n^m(-\mu)=(-1)^{n+m}P_n^m(\mu)$, implies that $\mathbf{S}_+$ and $\mathbf{S}_-$ are symmetric matrices. The layer vector incorporates the solar and the thermal contributions, $\mathbf{b}=\mathbf{b}_{\mathrm{sun}}+\mathbf{b}_{\mathrm{th}}$, while the block components of $\mathbf{b}_{\mathrm{sun}}$ and $\mathbf{b}_{\mathrm{th}}$ are given by

$$[\mathbf{b}_{\mathrm{sun}}^{\pm}(r)]_k=\pm\frac{\frac{1}{\mu_k}(2-\delta_{m0})\sigma_{\mathrm{sct}j}}{4\pi}F_{\mathrm{sun}}p_{mj}(\pm\mu_k,-\mu_0)e^{-\tau_{\mathrm{ext}}^{\mathrm{sun}}(r)}, \tag{6}$$

and

$$[\mathbf{b}_{\mathrm{th}}^{\pm}(r)]_k=\pm\frac{1}{\mu_k}\delta_{m0}\sigma_{\mathrm{abs}j}B(r),$$

respectively.

2.1. Inverse of the eigenvector matrix

The discrete ordinate method makes use of a spectral decomposition of the layer matrix $\mathbf{A}$, i.e.,

$$\mathbf{A}=\mathbf{X}\Lambda\mathbf{X}^{-1}. \tag{7}$$

In [1,4], the important quantities which are required for further calculations are the eigenvalue matrix Λ, and the inverse of the eigenvector matrix $\mathbf{X}^{-1}$.

Before proceeding we recall that the computation of a spectral decomposition of $\mathbf{A}$ requires the solution of an $N_{\mathrm{do}}\times N_{\mathrm{do}}$ eigenvalue problem. In the Stamnes and Swanson procedure with real arithmetic [10], the steps for computing an eigensystem of $\mathbf{A}$ consists in the calculation of

1. the eigensystem $\{\mu_k,\mathbf{w}_k^+\}_{k=\overline{1,N_{\mathrm{do}}}}$ of the asymmetric matrix $\mathbf{A}_-\mathbf{A}_+$, where $\mathbf{A}_+=\mathbf{A}_{11}+\mathbf{A}_{12}$ and $\mathbf{A}_-=\mathbf{A}_{11}-\mathbf{A}_{12}$,
2. the eigenvalues $\lambda_k=\sqrt{\mu_k}$, $k=1,\ldots,N_{\mathrm{do}}$,
3. the eigenvectors $\mathbf{w}_k^-$ of the matrix $\mathbf{A}_+\mathbf{A}_-$, as $\mathbf{w}_k^-=(1/\lambda_k)\mathbf{A}_+\mathbf{w}_k^+$, $k=1,\ldots,N_{\mathrm{do}}$,
4. the linear combinations $\mathbf{v}_k^+=(\mathbf{w}_k^++\mathbf{w}_k^-)/2$ and $\mathbf{v}_k^-=(\mathbf{w}_k^+-\mathbf{w}_k^-)/2$ for $k=1,\ldots,N_{\mathrm{do}}$.