ФУНДАМЕНТАЛЬНЫЕ ПРОБЛЕМЫ ТЕОРИИ ПЕРЕНОСА ИЗЛУЧЕНИЯ, РАСПРОСТРАНЕНИЕ ИЗЛУЧЕНИЯ И ПОДВОДНОЕ ВИДЕНИЕ

МОДЕЛИРОВАНИЕ ЯРКОСТНОГО ПОЛЯ В СИСТЕМАХ «АТМОСФЕРА-ОКЕАН»: АККУРАТНЫЙ УЧЕТ АНИЗОТРОПИИ РАССЕЯНИЯ В ЗАДАЧАХ ОПРЕДЕЛЕНИЯ ПАРАМЕТРОВ ОКЕАНА

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MODELING OF THE RADIANCE FIELD IN THE COUPLED ATMOSPHERE-OCEAN SYSTEMS: ACCURATE ACCOUNT FOR SCATTERING ANISOTROPY IN WATER PROPERTY RETRIEVALS

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В этом вкладе мы обсуждаем проблемы численного моделирования рассеянного излучения в связанных системах атмосфера-океан. Анализ выполнен в рамках дискретной теории переноса излучения. Для линеаризованной системы получено решение обратных задач.

In this contribution we discuss the problems of numerical modeling of the scattered radiance field in the coupled atmosphere-ocean systems. The analysis is performed in the framework of the discrete theory of radiative transfer. For the linearized system, the solution of inverse problems is obtained.

Introduction

Accurate and efficient modeling of radiative transfer is important for studies of Earth's climate my means of remote sensing. Essentially, such modeling comprises the forward model itself and the inverse model. The forward modeling is performed by means of radiative transfer models (RTMs). They provide the radiance field for given optical parameters of the system. In the inverse problems, the atmospheric/water body constituents are retrieved from the measured spectral radiance. Usually, an inverse problem is severely ill-posed. Typically it is reduced to an exercise in optimization, so that the retrieved parameters have to minimize the Tikhonov function. To find a corresponding minimum by using the Gauss-Newton method, the forward model (RTM in our case) has to be linearized. The linearized model provides the so called weighting functions, i.e. the partial derivatives of the radiance with respect to parameters to be retrieved. Note, that the initial forward model is still nonlinear, but it is linearized around a given atmospheric state vector by using the weighting functions.

Of a special interest are the radiative transfer models formulated for coupled atmosphere-ocean systems, i.e. models in which both atmosphere and ocean are treated as scattering mediums. Despite of the significant increase of computational capabilities, the radiative transfer computations for such coupled systems may still introduce a performance bottleneck in the retrieval algorithms. Given extreme accuracy requirements of remote sensing measurements, the error of the forward models as well as the trace gas retrieval algorithms should not exceed 1 %. Several approximations are used in order to improve the performance of both forward and inverse models. Most of these approximations have to deal with certain assumptions regarding the radiance field inside the medium. In particular, the real phase function is substituted by a less forward peaked one in order to reduce the computational time. However, this step distorts the initial problem and, thus, may introduce a bias in retrieval results. This problem is especially important in the coupled models, as the water body is characterized by a strong anisotropy of the phase function [1]. For instance, Mobley demonstrated, that the phase functions in natural waters may have the average cosine of scattering close to 0.98 (while in aerosol and cloud remote sensing, the asymmetry parameter hardly exceeds 0.9). The accurate modeling of the radiance field requires a large number of discrete ordinates N. This leads to a significant grow in computational time (which approximately scales as $N^{2.5}$). Note, that the water body requires more

discrete ordinates than the atmosphere.

Our goal in this paper is to present a general approach which is free from these shortcomings and is suitable for solving inverse problems of remote sensing of the ocean.

Brief description of the forward model for coupled systems

In the RTMs for coupled atmosphere/ocean modes, there is a distinction between flat and rough oceanic surfaces. The flat surface acts like a mirror preserving both specular and diffuse components of the radiance according to Snell's law. The rough surface scatters the specular (direct) component of the radiance and thus converts it into a diffuse one following a given reflection law, e.g. the Cox-Munk model [2].

Despite of variety of published models, they all follow one computational strategy, which can be summarized as follows. We consider the 1D radiative transfer equation (RTE):

$$\mu\frac{dL(\tau,\mu,\varphi)}{\mathrm{d}\tau}=-L(\tau,\mu,\varphi)+\frac{\omega(\tau)}{4\pi}\int_0^{2\pi}\int_{-1}^{1}P(\tau,\mu,\varphi,\mu',\varphi')L(\tau,\mu',\varphi')\mathrm{d}\mu'\mathrm{d}\varphi', \tag{1}$$

where L is the radiance, τ is the optical depth, μ the viewing zenith angle cosine, φ is the relative azimuth angle, ω is the single scattering albedo, P is the single scattering phase function. The boundary conditions for L read as follows:

$$\begin{cases}L\left(0,\mu>0,\varphi\right)=\delta\left(\mathbf{l}-\mathbf{l}_0\right),\\ L\left(\tau_A+\tau_O,\mu<0,\varphi\right)=0,\end{cases} \tag{2}$$

where τ_A and τ_O are the optical thicknesses of the atmosphere and ocean, respectively, $\mathbf{l}_0=\left\{\sqrt{1-\mu_0^2},0,\mu_0\right\}$, $\mathbf{l}=\left\{\sqrt{1-\mu^2}\cos\varphi,\sqrt{1-\mu^2}\sin\varphi,\mu\right\}$, μ_0 is the solar zenith angle cosine. Due to the singularity in (2), the initial problem cannot be solved numerically. To remove the singularity, the radiance is represented as

$$L(\tau,\mu,\varphi)=L_a(\tau,\mu,\varphi)+L_r(\tau,\mu,\varphi). \tag{3}$$

Here L_a is the anisotropic part comprising the singularity, while L_r is the regular (smooth) part. In our works, L_a is computed analytically by using the small-angle approximation [2]. In [3] it was shown that such an approach can be regarded as generalization of the delta-M and TMS correction techniques. By using this idea, previously we developed the modified discrete ordinate method (MDOM) [3,4]. In our companion talk [5] we made an analysis of the forward models. The main conclusions can be summarized as follows:

1. The initial RTE is converted into a system of linear differential equations,

$$\frac{d\mathbf{L}_{m,j}}{d\tau}(\tau)=\mathbf{A}_{m,j}\mathbf{L}_{m,j}(\tau)+\mathbf{b}_{m,j}(\tau),\quad \tau_j\le\tau\le\tau_{j+1}, \tag{4}$$

where $\mathbf{L}_{m,j}(\tau)=[\mathbf{L}^{+}_{m,j}(\tau)\quad \mathbf{L}^{-}_{m,j}(\tau)]^T$ is the radiance vector in the discrete ordinate space, $[L_m^{\pm}(\tau)]_k=L_m(\tau,\pm\mu_k)$, while τ_j and τ_{j+1} denote the boundaries of the layer *j*, **A** is a layer matrix which encapsulates the scattering properties of the layer, and *m* is the Fourier expansion index.

2. Equation (4) can be solved by using the matrix exponential approach by making use of the eigenvalue decomposition of the layer matrix:

$$\exp(-\mathbf{A}\Delta\tau_j)=\mathbf{X}\exp(-\Lambda\Delta\tau_j)\mathbf{X}^{-1}, \tag{5}$$

where **X** is the right eigenvector matrix, Λ is a diagonal matrix of eigenvalues, and $\Delta\tau_j=\tau_{j+1}-\tau_j$

3. The forward model implementation is based on the matrix operations, e.g. summation, multiplication, eigenvalue decomposition.

Integrating (4) and taking into account (5), the equation of the following form with respect to unknown radiances at the layer boundaries can be derived:

$$\mathbf{U}^1_{m,j}\mathbf{L}_{m,j}+\mathbf{U}^2_{m,j}\mathbf{L}_{m,j+1}=\mathbf{B}_{m,j}. \tag{6}$$

Equations in the form of (6) are written for each layer. The resulting system equipped with the boundary conditions can be solved as it is. That is the whole atmosphere approach. The matrix for entire system has a band structure. It can be compressed into band storage and then inverted using standard methods. The second option is to apply the matrix operator method. In this case, the entries in

(6) can be regrouped in the way that the left part contains only unknown vectors

$$\begin{bmatrix} \mathbf{L}^{+}_{m,j} \\ \mathbf{L}^{-}_{m,j+1} \end{bmatrix} = \begin{bmatrix} \mathbf{R}^{+}_{m,j} & \mathbf{T}^{+}_{m,j} \\ \mathbf{T}^{-}_{m,j} & \mathbf{R}^{-}_{m,j} \end{bmatrix} \begin{bmatrix} \mathbf{L}^{-}_{m,j} \\ \mathbf{L}^{+}_{m,j+1} \end{bmatrix} + \begin{bmatrix} \mathbf{\Sigma}^{+}_{m,j} \\ \mathbf{\Sigma}^{-}_{m,j} \end{bmatrix}, \tag{7}$$

where $\mathbf{R}^{\pm}_{m,j}$ and $\mathbf{T}^{\pm}_{m,j}$ are the reflection and transmission matrices, respectively, $\mathbf{\Sigma}^{\pm}_{m,j}$ is the source vector. The expressions for them can be found in [3]. Using the interaction principle, two layers can be merged into a single layer. The computational process is organized recursively until all the layers are merged into a single layer. The same scheme is valid for the polarized model formulated for the Stokes vector.

Such a scheme is valid for both pure atmospheric and coupled atmosphere-ocean models. In the latter case, the all Gaussian quadrature directions defined in the atmosphere are refracted into the ocean according to Snell's law (see Region I in Fig. 1). Consequently, for region II an additional set of Gaussian quadrature points is required.

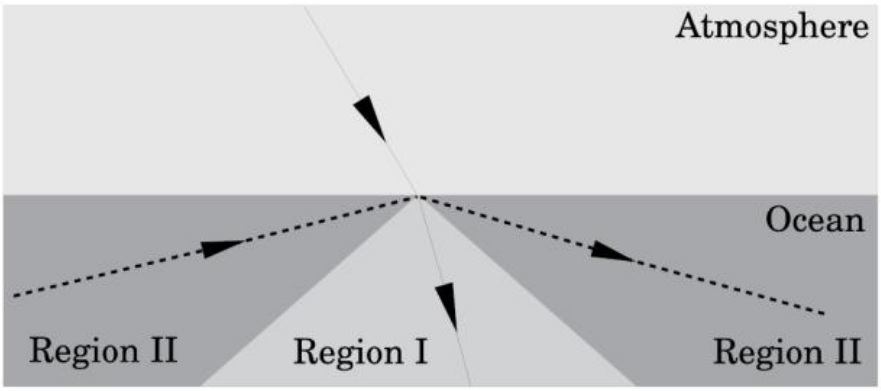

Fig.1. Two sets of Gaussian quadrature points in the ocean: the shadow zone stands for the region of total reflection

Linearization of the forward model

To retrieve a given parameter of interest by using non-linear least square fitting, the corresponding forward model has to be linearized. Now, we consider the computations of the derivatives of the radiance with respect to parameter of interest ς. In this work, the analytical linearization method is used. Essentially, this approach is based on the fact that the forward model is implemented as a sequence of differentiable functions. The differential operator is applied, first, to the input parameters of the model. Then, by applying a chain rule, it propagates through the code until the derivatives of the radiances are computed. The linearization of the basic matrix operations is straightforward. The multiplication is linearized by Leibniz rule, e.g.

$$\frac{\partial(\mathbf{A}_1\mathbf{A}_2)}{\partial\varsigma} = \frac{\partial\mathbf{A}_1}{\partial\varsigma}\mathbf{A}_2 + \mathbf{A}_1\frac{\partial\mathbf{A}_2}{\partial\varsigma}, \tag{8}$$

while the linearization of the inverse matrix is performed by two matrix multiplications:

$$\frac{\partial\mathbf{A}^{-1}}{\partial\varsigma} = -\mathbf{A}^{-1}\frac{\partial\mathbf{A}}{\partial\varsigma}\mathbf{A}^{-1}. \tag{9}$$

The linearization of the eigenvalue problem is not straight forward. As suggested in [4], we consider the eigenvalue problem for one eigenvector **x** equipped with the normalization condition:

$$\begin{cases} \mathbf{A}\mathbf{x} = \lambda\mathbf{x}, \\ \mathbf{x}^T\mathbf{x} = 1. \end{cases} \tag{10}$$

Here λ is the eigenvalue corresponding to the eigenvector $\mathbf{x}$. Applying the differential operator to Eq. (10) and using the orthogonality condition for eigenvectors, one can get a following equation:

$$\begin{bmatrix} \mathbf{x} & \lambda\mathbf{E}-\mathbf{A} \\ 0 & \mathbf{x}^T \end{bmatrix} \begin{bmatrix} \dfrac{\partial\lambda}{\partial\varsigma} \\ \dfrac{\partial\mathbf{x}}{\partial\varsigma} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial\mathbf{A}}{\partial\varsigma}\mathbf{x} \\ 0 \end{bmatrix} \tag{11}$$

The derivatives for the initial eigenvalue problem for the matrix **A** are expressed in terms of the solution of the system (11), which has to be solved for each layer and each azimuth harmonics number. Then, following the rules (8) and (9), one can get the linearization of Eq. (6).

The linearization of the matrix operator method is organized using the concept of a "stack". The stack which contains n layers is described by matrices $\mathbf{R}_{\pm}^{(n)}$, $\mathbf{T}_{\pm}^{(n)}$ and $\mathbf{\Sigma}_{\pm}^{(n)}$. To add a layer number $j=n+1$ to the stack with n layers, one has to perform two steps:

- to compute the derivatives for reflection and transmission matrices $\partial\mathbf{R}_j^{\pm}/\partial\varsigma_j$ and $\partial\mathbf{T}_j^{\pm}/\partial\varsigma_j$ for the layer j and a source vector $\left\{\partial\Sigma_j^{\pm}/\partial\varsigma_p\right\}_{p=1,\ldots,j}$ (note, that a latter has derivatives over the parameters of upper layers);
- having a linearized stack of n layers $\left\{\partial\mathbf{R}_{\pm}^{(n)}/\partial\varsigma_p, \partial\mathbf{T}_{\pm}^{(n)}/\partial\varsigma_p, \partial\mathbf{\Sigma}_{\pm}^{(n)}/\partial\varsigma_p\right\}_{p=1,\ldots,n}$, to compute $\left\{\partial\mathbf{R}_{\pm}^{(n+1)}/\partial\varsigma_p, \partial\mathbf{T}_{\pm}^{(n+1)}/\partial\varsigma_p, \partial\mathbf{\Sigma}_{\pm}^{(n+1)}/\partial\varsigma_p\right\}_{p=1,\ldots,n+1}$ in the framework of interaction principle.

Thus, the derivatives of reflection and transmission matrices should be recomputed after each adding the layer.

Numerical aspects

Computing the anisotropic part of the radiance using the small-angle approximation allows to keep the number of discrete ordinates in the atmosphere as low as two. For the ocean, thus, at least 4 discrete ordinates are required. Note, that the computations do not involve additional assumptions on the phase functions (i.e. no truncation procedures). The linearized model is just as accurate for the derivatives as the forward model for the radiances. Since all differentiations are performed "by hand", no additional assumptions are needed.

The coupled model MDOM has been compared with the coupled code LIDORT [6]. The results of the comparison are shown in Fig. 2. The agreement up to the 6^{th} digit has been obtained. The computations have been performed for the coupled model with the flat oceanic surface. The ocean has been modelled as a two-layer system with the dissolved organic matter in the upper oceanic layer. The atmosphere was modelled as a 14-layer system containing the trace gases (O_3, NO_2) as well as urban aerosol.

We have compared the efficiency of models implemented by using the matrix operator method and the whole atmosphere approach. The computational time for forward modeling is similar with slight advantage of the matrix operator method (small sizes of matrices in the matrix operator method are compensated by the banded array storage in the whole atmosphere approach). However, there is a notable difference in the linearized models, as shown in Fig.2. In the matrix operator method, the linearization of the stack is done after each adding of the layer to the stack. Thus, the number of linearization operations grows quadratically with the number of layers. In addition, the matrix operator method encapsulates several matrix inversions (note that linearization of the matrix inversion requires two additional matrix multiplications, see Eq. (9)). In this regard, the whole atmosphere approach seems to be more suitable for linearized models.

An additional validation can be performed keeping in mind an intimate connection between radiative transfer in turbid media and electron transport in solids [7]. Since the governing equations for radiative transfer and electron transport are similar, the models designed for retrieval of atmospheric or oceanic constituents can be used for retrieving the parameters of solid samples by means of electron spectroscopy. Such a methodological transition is beneficial for remote sensing, since it gets an efficient tool for the experimental validation of the designed methods by performing the retrieval exercises on solid samples with known properties.

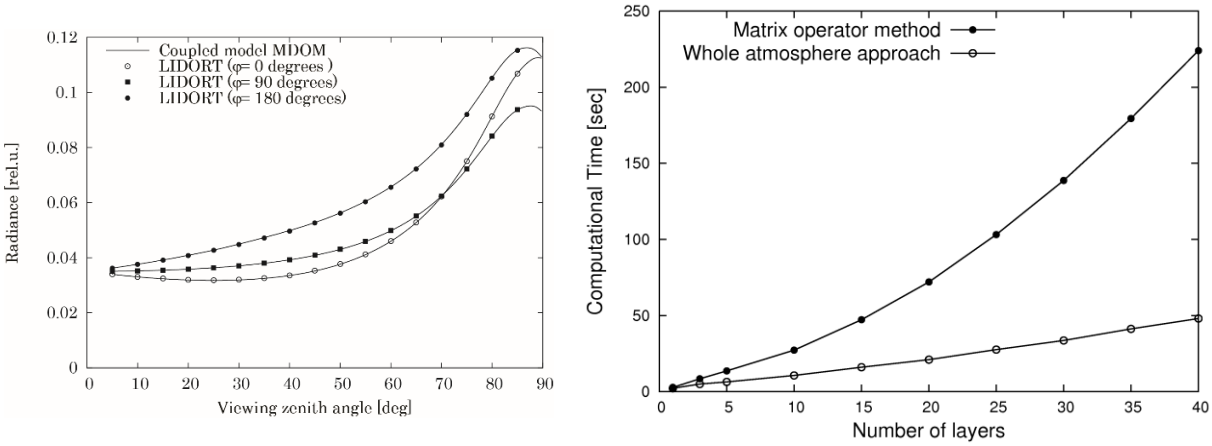

Fig.2. Validation of the coupled MDOM model against the coupled LIDORT model (left). The solar zenith angle is 35 degrees; (right) computational time of the linearized models, implemented on the base of the whole atmosphere approach and the matrix operator method for 20-layer model (2 of which are oceanic layers)

In this work we consider the retrieval of solid properties from the angular distributions of the elastically reflected electrons. As shown in Fig. 3, a chemically homogeneous sample is a multiplayer structure due to depth-dependent plasmon properties, which leads to the depth-dependent single scattering albedo. Typically, two or three layers are used to describe the depth change in the absorption cross-sections. We consider the measurements of electron fluxes reflected by Ag samples from [8]. The following parameters have been retrieved from these data in the three-layer model: the single scattering albedos for all layers, the optical thicknesses of two upper layers, the first and second expansion coefficients of the Ag phase function. The retrieval was made by using the Gauss-Newton nonlinear fitting with the weighting functions provided by the linearized MDOM. The fitting results are shown in Fig.3. An agreement within 0.5% as compared to the table values of electron properties has been achieved.

Note, that the splitting of the total radiance field into two components (see Eq. (3)) made it possible to operate with the real phase functions, and no post-processing steps for phase function correction was required. Since the small-angle term is dominant for strongly forward peaked phase functions, as shown in [9], good retrieval results can be achieved just by using the small-angle component. In this case, the forward model is very fast and the minimization of the Tikhonov function can be performed manually.

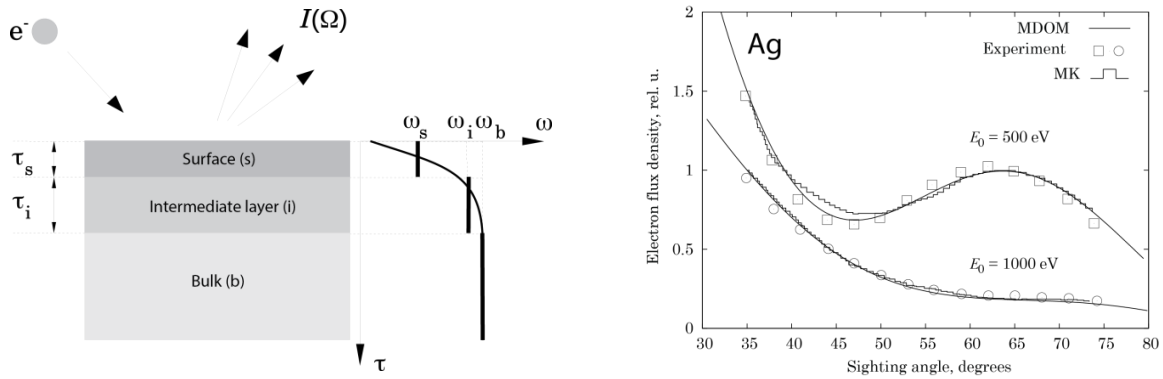

Fig.3. Three-layer model of the solid (left). The optical thicknesses and the single scattering albedos are retrieved from the angular distributions of the elastically reflected electrons by using the linearized MDOM; (right) the angular distributions of elastically scattered electrons, Ag sample: the non-linear fitting by using MDOM for retrieving the parameters of the target, the experimental data and Monte-Carlo calculations are taken from [8]

Conclusions

In this work, we consider the linearized radiative transfer model. It has been implemented on the basis of the forward model MDOM, which incorporates the small-angle approximation for describing

the anisotropic part, and the discrete ordinate method for computing the regular part of the radiance field. For computing the weighting functions (i.e. derivatives) with respect to the parameters of interest, the analytical differentiation technique is applied to the model MDOM.

Two implementations of the linearized model have been considered. The first implementation is based on the whole atmosphere approach, in which the radiances at the boundaries of the layers are computed simultaneously as a solution of the linear system of equations. In this case, the system matrix has a banded form. The second implementation is based on the matrix operator method, which exploits the concept of the layer stack. While the efficiency of these implementations for forward modeling is comparable (with slight advantage of the matrix operator method), the whole atmosphere approach for derivative computations is faster. For instance, for 40-layer coupled atmosphere-ocean system the difference can be of about 4 times.

A unique feature of the designed linearized model is that the computations are performed for realistic phase functions, and neither truncations nor post-processing steps are required. The linearization procedure is analytically exact and does not require ad hoc assumptions except those made for the boundary value problem formulation (see Eqs (1) and (2)).

The MDOM model was validated against the coupled version of the LIDORT model and an agreement up to the 6^{th} digit has been obtained. In addition, the retrieval exercises have been performed with the experimental data on elastic reflection of electrons by solid samples. It has been shown that the MDOM model can reproduce the experimental results, and so, can be used for retrieval of absorption properties of multilayer systems. The designed model is computationally very efficient: e.g. the retrieval procedure takes about 1 second on Intel Xeon CPU E-5-1620 3.60GHz. An important aspect of the designed model is that it can be simultaneously used in both remote sensing and electron spectroscopy retrieval problems. In such a way, the remote sensing retrieval algorithms can be validated on the basis of high-precision experimental setups by using the samples with known properties.

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