Efficiency of algorithm for solution of vector radiative transfer equation in turbid medium slab

V.P.Budak\textsuperscript{1,3}, D.S.Efremenko\textsuperscript{2}, O.V.Shagalov\textsuperscript{1}

\textsuperscript{1}National research university “MPEI”, Krasnokazarmennaya, 14, Moscow, 111250, Russia
\textsuperscript{2}Remote Sensing Technology Institute, German Aerospace Centre, Oberpfaffenhofen, Wessling, Germany

BudakVP@mpei.ru

Abstract. The numerical solution of the vectorial radiative transfer equation (VRTE) is possible only by its discretization, which requires elimination of the solution anisotropic part including all the singularities. Discretized VRTE for the turbid medium slab has the unique analytical solution in the matrix form. Modern packages of matrix (linear) algebra allow only one possible algorithm of VRTE solution by computer. Various realizations of such an algorithm differ by the method of the elimination of the solution anisotropic part. Methods of the solution anisotropic part elimination are analysed in the paper. The codes created by the authors of these methods are analysed in simple situations in order to define its influence on the code efficiency. It is shown that the most effective method is based on the small angle modification of the spherical harmonics method (MSH). The code based on MSH is investigated in details by the influence of different properties of hard and software.

1. Boundary value problem

The comparison of different solution codes of scalar and vector radiative transfer equations (RTE, VRTE) has shown that results of calculations are almost the same \cite{1}. This suggests that different computational methods of polarization fields in a turbid medium slab are in fact variants of the uniform VRTE solution method \cite{2,3}. In this paper we present VRTE general solution, analysis and optimization of the solution algorithm, and its effective computer implementation on the basis of the general expression.

We have VRTE boundary problem for the turbid medium slab of optical depth $\tau_0$, on which a plane wave of the arbitrary polarized light incidents in the direction $\hat{n}$: \cite{3}:

\begin{equation}
\frac{\mu}{d\tau} \hat{L}(\tau,\hat{n}) + \hat{L}(\tau,\hat{n}) = \frac{\Lambda}{4\pi} \int \hat{R}(\chi) \hat{v}(\hat{n},\hat{n}') \hat{R}(\chi') \hat{L}(\tau,\hat{n}') d\chi',
\end{equation}

\begin{align*}
\hat{L}(\tau,\hat{n}) |_{\tau \to 0, (\omega,\hat{n}) > 0} &= \hat{L}_{0}\delta(\hat{n} - \hat{n}_0), & \hat{L}(\tau,\hat{n}) |_{\tau \to 0, (\omega,\hat{n}) > 0} &= 0;
\end{align*}

To whom any correspondence should be addressed.

Published under licence by IOP Publishing Ltd
where \( \hat{\mathbf{L}}(\tau, \hat{\mathbf{i}}) \) is the vector of Stokes parameters of the light field in the medium at the optical depth \( \tau \) in the direction \( \hat{\mathbf{i}} \). We use Cartesian coordinate system \( OXYZ \) where axis \( OZ \) is directed down perpendicularly to the slab border: 

\[
\hat{\mathbf{i}} = \left\{ \sqrt{1-\mu^2} \cos \phi, \sqrt{1-\mu^2} \sin \phi, \mu \right\}, \quad \hat{\mathbf{t}}_0 = \left\{ \sqrt{1-\mu_0^2}, 0, \mu_0 \right\},
\]

\( \mu = (\hat{\mathbf{i}}, \hat{\mathbf{z}}) \), \( \mu_0 = (\hat{\mathbf{i}}_0, \hat{\mathbf{z}}) \), \( \hat{\mathbf{z}} \) is the unit vector along \( OZ \). \( \hat{x}(\hat{\mathbf{i}}, \hat{\mathbf{t}}) \) is the phase scattering matrix, \( \Lambda \) is the single scattering albedo. \( \hat{\mathbf{R}}(\chi) \) is the change matrix (rotator) of Stokes parameters at the reference plane rotation. \( \chi \) is the dihedral angle between two planes \( (\hat{\mathbf{z}} \times \hat{\mathbf{i}}) \) and \( (\hat{\mathbf{i}} \times \hat{\mathbf{t}}) \), and \( \chi' \) is the angle between planes \( (\hat{\mathbf{i}} \times \hat{\mathbf{t}}) \) and \( (\hat{\mathbf{i}}' \times \hat{\mathbf{t}}') \). The unit vectors have a symbol “\( \hat{\mathbf{a}} \)”, the columns have the right arrow, the rows have the left arrow, the matrices have the double arrow above the symbol.

For a numerical VRTE solution the integrals should be replaced with the finite sums that could be done by one of two methods: the method of spherical harmonics (SH) and the discrete ordinates method (DOM). The DOM is the best method for implementation since VRTE gains a clear ray interpretation that essentially simplifies the definition of the composite boundary conditions. In this case VRTE and boundary conditions take a form of interacting streams of radiation for the fixed interpretation that essentially simplifies the definition of the composite boundary conditions. In this case VRTE and boundary conditions take a form of interacting streams of radiation for the fixed directions in space.

However in the initial boundary value problem (1) the replacement of the integral by the Gaussian quadrature is impossible due to the solution singularity. The singularities are an inherent feature of the ray approximation. Really, any break in the boundary conditions propagates inside the medium slab in the form of the edge between light and shadow that gives the singularity in the radiance angular distribution. Therefore, it is necessary to search the solution as the generalized function. To consider the solution singularities, the desired vector of Stokes parameters is represented as the sum of two parts: the anisotropic one that contains all the solution singularities, and the regular one – the smooth function of angular variables:

\[
\hat{\mathbf{L}}(\tau, \hat{\mathbf{i}}) = \hat{\mathbf{L}}_a(\tau, \hat{\mathbf{i}}) + \hat{\mathbf{L}}_r(\tau, \hat{\mathbf{i}}).
\]

(2)

It is assumed that the anisotropic part can be found analytically. This allows expressing its integral also analytically – a singularity elimination method. The substitution of (2) in (1) changes the boundary value problem to the equivalent one

\[
\begin{bmatrix}
\mu \frac{\partial \hat{\mathbf{L}}_r(\tau, \hat{\mathbf{i}})}{\partial \tau} + \hat{\mathbf{L}}_r(\tau, \hat{\mathbf{i}}) = \frac{\Lambda}{4\pi} \int \hat{\mathbf{R}}(\chi) \hat{x}(\hat{\mathbf{i}}, \hat{\mathbf{t}}) \hat{\mathbf{R}}(\chi') \hat{\mathbf{L}}_r(\tau, \hat{\mathbf{t}}') d\hat{\mathbf{t}}' + \hat{\Delta}(\tau, \hat{\mathbf{i}});
\end{bmatrix}
\]

(3)

with the source function on the right side of the equation

\[
\hat{\Delta}(\tau, \hat{\mathbf{i}}) = \frac{\Lambda}{4\pi} \int \hat{\mathbf{R}}(\chi) \hat{x}(\hat{\mathbf{i}}, \hat{\mathbf{t}}) \hat{\mathbf{R}}(\chi') \hat{\mathbf{L}}_a(\tau, \hat{\mathbf{t}}') d\hat{\mathbf{t}}' - \mu \frac{\partial \hat{\mathbf{L}}_a(\tau, \hat{\mathbf{i}})}{\partial \tau} - \hat{\mathbf{L}}_a(\tau, \hat{\mathbf{i}}).
\]

(4)

2. Discretization of VRTE

The effectiveness of DOM application in the case of VRTE is strongly reduced since in the scalar type it is determined by the possibility of the phase function presented by the series of the surface harmonics. This allows reducing the double integral on the basis of the addition theorem to the single one [4]. In the case of polarization the scattering matrix is surrounded by the rotator matrices \( \hat{\mathbf{R}} \) that disturbs the azimuthal symmetry and does not allow using the addition theorem for the surface harmonics. Kuščer-Ribarič [5] uses the circular basis to determine polarization

\[
\hat{\mathbf{L}}_{CP} = \left[ \begin{array}{c}
L_{+2} \\
L_0 \\
L_{-2}
\end{array} \right] = \frac{1}{2} \left[ \begin{array}{c}
Q - iU \\
I - V \\
I + V
\end{array} \right] = \frac{1}{2} \left[ \begin{array}{c}
0, 1, 1 \\
0, 1, 0 \\
0, 0, 1
\end{array} \right] \left[ \begin{array}{c}
I \\
Q \\
U
\end{array} \right] = \hat{T}_{CS} \hat{T}_{SP}, \quad \hat{T}_{SC} = \hat{T}_{CS}^{-1}.
\]

(5)
It changes the rotator form and allows using generalizes surface functions $P_{kn}^k(\cos \theta)$ for the scattering matrix representation that obey to the special form of the addition theorem

$$e^{-i\omega_T}P_{mn}^k(\hat{\mathbf{i}} \cdot \hat{\mathbf{j}})e^{-i\omega_T} = \sum_{q=-k}^k (-1)^q P_{mq}^k(\hat{\mathbf{i}} \cdot \hat{\mathbf{j}}) P_{qn}^q(\hat{\mathbf{z}} \cdot \hat{\mathbf{i}}) e^{i\Delta \varphi}, \quad \Delta \varphi = \varphi - \varphi' . \quad (6)$$

As the results, all the coefficients in VRTE become complex numbers, and this makes use of the effective numerical methods for equation system solution difficult. Therefore, after applying the addition theorem for the generalized spherical function one should return to the Stokes presentation (SP).

Let’s consider the local transformation matrix of the ray at scattering in details:

$$S(\hat{\mathbf{i}}, \hat{\mathbf{j}}) \equiv \tilde{R}(\chi) \tilde{x}(\hat{\mathbf{i}}, \hat{\mathbf{j}}) \tilde{R}(\chi') = \tilde{T}_{SC} \tilde{R}_{CP} \chi(\chi) \tilde{x}_{CP} \chi(\chi') \tilde{T}_{CS} = \tilde{T}_{SC} \tilde{S}_{CP} \chi(\chi') \tilde{T}_{CS}, \quad (7)$$

where $\tilde{x}_{CP}(\hat{\mathbf{i}}, \hat{\mathbf{j}}) = \tilde{T}_{CS} \tilde{x}_{CP}(\hat{\mathbf{i}}, \hat{\mathbf{j}}) \tilde{T}_{SC}$ is the scattering matrix, $\tilde{R}_{CP}(\chi) = \tilde{T}_{CS} \tilde{R}(\chi) \tilde{T}_{CS}$ is the rotator in the circular polarization (CP) presentation.

Then we present the elements of scattering matrix in the form of the expansion on the generalized spherical functions

$$[\tilde{x}_{CP}(\cos \gamma)]_{rs} = \sum_{k=0}^{K} (2k+1)x_{rs}^k P_{rs}^k(\cos \gamma), \quad (8)$$

where $r$ and $s$ have only values ±0 and ±2; $K$ is the number of harmonics in expansion of the scattering matrix in the generalized spherical functions.

Taking into account the addition theorem (6), one can get every element of the local transformation matrix in CP as

$$S(\hat{\mathbf{i}}, \hat{\mathbf{j}}) \equiv \tilde{R}(\chi) \tilde{x}(\hat{\mathbf{i}}, \hat{\mathbf{j}}) \tilde{R}(\chi') = \tilde{T}_{SC} \tilde{R}_{CP} \chi(\chi) \tilde{x}_{CP} \chi(\chi') \tilde{T}_{CS} = \tilde{T}_{SC} \tilde{S}_{CP} \chi(\chi') \tilde{T}_{CS}, \quad (9)$$

With the use of diagonal matrix $\tilde{Y}_{\hat{\mathbf{i}}}^q(\mu) = \text{Diag}(P_{-\delta,0}^q(\mu), P_{\delta,0}^q(\mu))$ and taking into account the reciprocal relation

$$P_{-\delta,0}^q(\mu) = P_{\delta,0}^q(\mu), \quad (10)$$

where $\delta = \pm 1$. Then

$$\tilde{S}_{CP}(\hat{\mathbf{i}}, \hat{\mathbf{j}}) = \sum_{k=0}^{K} (2k+1) \sum_{q=-k}^k (-1)^q e^{i(q \varphi - \varphi')} \tilde{T}_{SC} \tilde{Y}_{\hat{\mathbf{i}}}^q(\mu) \tilde{x}_{\hat{\mathbf{i}}} \tilde{Y}_{\hat{\mathbf{i}}}^q(\mu') \tilde{T}_{CS} = \sum_{k=0}^{K} (2k+1) \sum_{q=-k}^k e^{i(q \varphi - \varphi')} \tilde{S}_{\hat{\mathbf{i}}}^k(\mu, \mu'), \quad (11)$$

where $\tilde{x}_{\hat{\mathbf{i}}} \equiv \tilde{x}_{\hat{\mathbf{i}}} \tilde{T}_{CS}$.

Then

$$\tilde{S}_{\hat{\mathbf{i}}}^k(\mu, \mu') = (-1)^k \tilde{T}_{SC} \tilde{Y}_{\hat{\mathbf{i}}}^q(\mu) \tilde{x}_{\hat{\mathbf{i}}} \tilde{Y}_{\hat{\mathbf{i}}}^q(\mu') \tilde{T}_{CS} = \tilde{P}_{\hat{\mathbf{i}}}^k(\mu) \tilde{X}_{\hat{\mathbf{i}}} \tilde{P}_{\hat{\mathbf{i}}}^k(\mu'), \quad (12)$$

where $\tilde{X}_{\hat{\mathbf{i}}} = \tilde{T}_{CS} \tilde{x}_{\hat{\mathbf{i}}} \tilde{T}_{CS}$ is the so-called «Greek matrix»,

$$\tilde{P}_{\hat{\mathbf{i}}}^k(\mu) = (-i)^k \tilde{T}_{SC} \tilde{Y}_{\hat{\mathbf{i}}}^n(\mu) \tilde{T}_{CS} = \tilde{P}_r^k(\mu) \tilde{I}_r^k(\mu'), \quad (13)$$

$\tilde{P}_r$ and $\tilde{P}_i$ are the real parts of matrix $\tilde{P}_{\hat{\mathbf{i}}}^k(\mu)$ [6].

Finally, VRTE (1) could be written as

$$\mu \frac{\partial}{\partial \tau} L_r(\tau, \hat{\mathbf{i}}) + L_r(\tau, \hat{\mathbf{i}}) = \frac{\Lambda}{4\pi} \sum_{k=0}^{K} (2k+1) \sum_{q=-k}^k \tilde{P}_r^k(\mu) \int e^{i(q \varphi - \varphi')} \tilde{X}_{\hat{\mathbf{i}}} \tilde{P}_r^k(\mu') \tilde{L}_r(\tau, \hat{\mathbf{i}}) d\varphi + \tilde{\Lambda}(\tau, \hat{\mathbf{i}}), \quad (14)$$

The scattering integral contains complex values though the whole expression (13) is real. With the symmetry of the introduced functions $\tilde{P}_r^k(\mu) = \tilde{P}_r^k(\mu*), \quad \tilde{P}_r^k(\mu) = -\tilde{P}_r^{-k}(\mu)$ one can eliminate the imaginary part [6] in the equation (13). The obtained expression is correct for all scattering matrices. However, in case of the aerosol block-diagonal matrix it could be simplified [6] more. One could present the solution of problem (3) in the form [6]:

$$L_r(\tau, \hat{\mathbf{i}}) = \sum_{m=0}^{M} (2 - \delta_{m,1}) \left[ \phi_r(m \varphi) L_{a,m}^r(\tau, \mu) + \phi_r(m \varphi) \tilde{L}_{a,m}^r(\tau, \mu) \right], \quad (15)$$

that reduces VRTE to the following form
\[
\frac{d \tilde{L}_m^\mu(\tau,\mu)}{d\tau} + \tilde{L}_m^\mu(\tau,\mu) = \frac{\Lambda}{2} \sum_{k=0}^{K} (2k+1) \tilde{\Pi}_k^\mu(\mu) \tilde{\chi}_k \int_{-1}^{1} \tilde{\Pi}_k^\mu(\mu') \tilde{L}_m^\mu(\tau,\mu') d\mu' + \tilde{\Delta}(\tau,\mu) , \quad c = 1, 2 ,
\]

where \( M \) is the term number in the Fourier series on the azimuth, \( m \in 0, M \),

\[
\tilde{\Pi}_k^\mu(\mu) = \begin{bmatrix} Q_k^\mu(\mu) & 0 & 0 & 0 \\ 0 & R_k^\mu(\mu) - T_k^\mu(\mu) & 0 \\ 0 & -T_k^\mu(\mu) & R_k^\mu(\mu) & 0 \\ 0 & 0 & 0 & Q_k^\mu(\mu) \end{bmatrix}, \quad \phi_1(\phi) = \text{diag}(\cos\phi, \cos\phi, \sin\phi, \sin\phi), \\
\phi_2(\phi) = \text{diag}(-\sin\phi, -\sin\phi, \cos\phi, \cos\phi),
\]

\[
R_k^\mu(\mu) = 0.5 i^n \left( P_{m,2}^k(\mu) + P_{m,-2}^k(\mu) \right), \quad T_k^\mu(\mu) = 0.5 i^n \left( P_{m,2}^k(\mu) - P_{m,-2}^k(\mu) \right), \quad Q_k^\mu(\mu) = \frac{(k-m)^1}{\sqrt{(k+m)^1}} P_{m}^n(\mu). \quad (17)
\]

In order to get the solution of the obtained equation using DOM, we present the integrals entering into the equation (15) taking into account the slab symmetry in the double Gaussian quadrature form. Accordingly we have the system of ordinary differential equations for the fixed \( m \) and \( c \) (therefore we omit them in the equation)

\[
\mu^2 \frac{d}{d\tau} \tilde{L}_m^\mu(\tau) + \tilde{L}_m^\mu(\tau) = \frac{\Lambda}{4} \sum_{j=1}^{N/2} \sum_{k=0}^{K} (2k+1) \tilde{\Pi}_k^\mu(\mu_j) \tilde{\chi}_k \left( \tilde{\Pi}_k^\mu(\mu_j') \tilde{L}_m^\mu(\tau) + \tilde{\Pi}_k^\mu(\mu_j') \tilde{L}_m^\mu(\tau) \right) + \tilde{\Delta}_m^\mu(\tau), \quad (18)
\]

where \( \tilde{L}_m^\mu(\tau) \equiv \tilde{L}_m^\mu(\tau,\mu_j^+), \quad \tilde{\Delta}_m^\mu(\tau) \equiv \tilde{\Delta}_m^\mu(\tau,\mu_j^+), \quad \mu_j^\pm = 0.5(\zeta_j \pm 1), \quad \zeta_j, w_j \) are the zeroes and weights of the Gaussian quadrature of the \( N/2 \) order.

Now we can introduce the following matrices and vectors

\[
\tilde{L} = \begin{bmatrix} \tilde{L}_+^\mu(\tau) \\ \tilde{L}_-^\mu(\tau) \end{bmatrix} , \quad \tilde{\Delta} = \begin{bmatrix} \tilde{\Delta}_+^\mu(\tau) \\ \tilde{\Delta}_-^\mu(\tau) \end{bmatrix} , \quad \tilde{\Pi} = \text{diag}(\mu_j^+, -\mu_j^+) , \quad \tilde{W} = \frac{\Lambda}{4} \text{diag}(w_j, w_j),
\]

\[
\tilde{\Delta} = \begin{bmatrix} \sum_{j=1}^{N/2} (2k+1) \tilde{\Pi}_k^\mu(\mu_j) \tilde{\chi}_k \tilde{\Pi}_k^\mu(\mu_j') \end{bmatrix} , \quad (19)
\]

\[
\tilde{L}_\pm(\tau) = \begin{bmatrix} I(\tau,\mu_j^\pm), Q(\tau,\mu_j^\pm), U(\tau,\mu_j^\pm), V(\tau,\mu_j^\pm), \ldots, I(\tau,\mu_{N/2}^+, Q(\tau,\mu_{N/2}^+), U(\tau,\mu_{N/2}^+), V(\tau,\mu_{N/2}^+) \end{bmatrix}^T.
\]

Other arrays are arranged in the same way.

Since the regular part is a smooth function of angle, all the matrices are finite. This allows rewriting the system (18) in the matrix form

\[
\frac{d \tilde{L}(\tau)}{d\tau} = -\tilde{B} \tilde{L}(\tau) + \tilde{M}^{-1} \tilde{\Delta}(\tau), \quad \tilde{B} \equiv \tilde{M}^{-1} (\tilde{I} - \tilde{\Delta} \tilde{W}).
\]

(21)

3. Solution regular part

The solution of the obtained equation system has the analytic view [4, 7] in the matrix form

\[
- \tilde{L}(0) + \int_{0}^{\tau} e^{\tilde{B} \tau} \tilde{L}(\tau_0) = \int_{0}^{\tau} e^{\tilde{B} \tau} \tilde{M}^{-1} \tilde{\Delta}(\tau,\mu_0) d\tau .
\]

(22)

This expression (22) is equivalent to the solution representation that is the sum of the general solution of homogeneous equation and the particular solution of the inhomogeneous one [8]. A matrix representation is more convenient for the analytic transformation and implementation of solutions for the computer. The solution of the homogeneous equation

\[
\tilde{L}(\tau_0) = e^{-\tilde{B} \tau_0} \tilde{L}(0) \equiv \tilde{F}(\tau_0) \tilde{L}(0) : \quad \frac{d \tilde{F}(\tau)}{d\tau} = -\tilde{B} \tilde{F}(\tau),
\]

(23)

connects the radiation at the slab lower boundary with an expression on the top and is called the prop-
The problem of the solution (22) is connected with negative and positive exponents in the expression that leads to fast worsening of the system matrix conditions. In order to eliminate this effect, we used the scale transformation \([4]\). The matrix exponent is represented in the form \([4]\)

\[
e^{B_{\tau}} = \tilde{U}e^{\tau_{e}}\tilde{U}^{-1},
\]

where \(\tilde{U}\) is the matrix of eigenvectors of the matrix \(B\) and \(\tau = \text{diag}(\tau_{+}, \tau_{-})\) is the diagonal matrix of eigenvalues sorted by ascending ordering so that \(\tau_{-} = -\tau_{+}\).

Consequently, the equation (22) can be rewritten as

\[
-\begin{bmatrix}
\tilde{u}_{11} & \tilde{u}_{12} \\
\text{e}^{-\tau_{+}\cdot\tilde{u}_{21}} & \text{e}^{-\tau_{-}\cdot\tilde{u}_{22}}
\end{bmatrix}
\begin{bmatrix}
\tilde{L}_{+}(0) \\
\tilde{L}_{-}(0)
\end{bmatrix}
+\begin{bmatrix}
e^{\tau_{+}\cdot\tilde{u}_{11}} & e^{\tau_{-}\cdot\tilde{u}_{12}} \\
\tilde{u}_{21} & \tilde{u}_{22}
\end{bmatrix}
\begin{bmatrix}
\tilde{L}_{+}(\tau_{0}) \\
\tilde{L}_{-}(\tau_{0})
\end{bmatrix}
= \begin{bmatrix}
\tilde{j}_{-} \\
\tilde{j}_{+}
\end{bmatrix},
\]

where \(\tilde{j} \equiv \begin{bmatrix}
\tilde{j}_{-} \\
\tilde{j}_{+}
\end{bmatrix} = S_{\delta} \int_{0}^{\tau_{+}} e^{\tau_{+}\cdot\tilde{u}_{11}}\tilde{M}^{-1}\Delta(\tau, \mu_{0})d\tau, \tilde{u}_{-} \equiv \begin{bmatrix}
\tilde{u}_{11} \\
\tilde{u}_{12} \\
\tilde{u}_{21} \\
\tilde{u}_{22}
\end{bmatrix}.

Note that expression (25) contains the exponent only with the positive power. Expressing in equation (25) the emerging radiation \(\tilde{L}_{+}(0), \tilde{L}_{-}(\tau_{0})\) from a layer through the incident radiation \(\tilde{L}_{+}(0), \tilde{L}_{-}(\tau_{0})\) we find a smooth regular part of the solution in the form of the so-called scatterers \([7]\):

\[
\begin{bmatrix}
\tilde{L}_{-}(\tau_{0}) \\
\tilde{L}_{+}(\tau_{0})
\end{bmatrix}
= \begin{bmatrix}
\tilde{F} & \tilde{R} \\
\tilde{F} & \tilde{T}
\end{bmatrix}
\begin{bmatrix}
\tilde{L}_{+}(0) \\
\tilde{L}_{-}(0)
\end{bmatrix}
\]

\[
= \begin{bmatrix}
\tilde{H} & \tilde{F} \\
\tilde{H} & \tilde{T}
\end{bmatrix}
\begin{bmatrix}
\tilde{u}_{11} & -e^{\tau_{+}\cdot\tilde{u}_{12}} \\
e^{-\tau_{+}\cdot\tilde{u}_{21}} & -\tilde{u}_{22} \\
\end{bmatrix}
\]

\[
= \begin{bmatrix}
\tilde{u}_{11} & -e^{\tau_{+}\cdot\tilde{u}_{12}} \\
e^{-\tau_{+}\cdot\tilde{u}_{21}} & -\tilde{u}_{22} \\
\end{bmatrix}^{-1}.
\]

The obtained system (26) is the desired solution that makes definition of the radiance distribution of the reflected and transmitted radiations possible. Note that the expression (26) is the rigorous analytical solution of the boundary value problem for VRTE discretized by DOM. The transfer from VRTE (1) to the equation system (26) is possible due to the singularity elimination (2) and to the change of the scattering integral (discretization) by the Gaussian quadrature (18).

The solution obtained in the form of scatterers (26) has a functional type and allows entering a photometric concept of the layer radiance factor by the reflection or transmission. This immediately gives the possibility to formulate a matrix-operator method to replace the two adjacent layers by the equivalent one described by the expression identical to (32), but with effective parameters \([3]\). Consequently, the solution in the form of scatterers possesses the property of invariance.

Equation (26) can be reorganized in a form similar to the propagator (23):

\[
\tilde{L}(\tau_{0}) = \begin{bmatrix}
\tilde{T} - \tilde{R} & \tilde{T}^{-1} \tilde{R} \\
-\tilde{T}^{-1} \tilde{R} & \tilde{T}
\end{bmatrix}
\begin{bmatrix}
\tilde{L}_{+}(0) \\
\tilde{L}_{-}(0)
\end{bmatrix}
+ \tilde{F}.
\]

This kind of transformation has been called the “star product” \([7]\). Since one knows the differential equation (23) for the propagator, one is able to get the one-point problem with initial conditions of the matrix Riccati equation for the matrix elements of the scatterers \([7]\), e.g. the reflection:

\[
\frac{d\tilde{R}_{+}}{d\tau} = \tilde{b}_{+} + \tilde{b}_{+} \tilde{R}_{+} + \tilde{R}_{-} \tilde{b}_{+} + \tilde{R}_{-} \tilde{b}_{+} \tilde{R}_{-}; \quad \frac{d\tilde{R}_{-}}{d\tau} = -\tilde{b}_{+} + \tilde{b}_{+} \tilde{R}_{-} - \tilde{R}_{+} \tilde{b}_{+} - \tilde{R}_{+} \tilde{b}_{+} \tilde{R}_{-}; \quad \tilde{B} \equiv \begin{bmatrix}
\tilde{b}_{1} \\
\tilde{b}_{2}
\end{bmatrix},
\]

and similarly for the transmission \(\tilde{T}\).

It is easy to see that (28) is an equivalent to the equations of Ambartsumyan-Chandrasekhar \([8]\), derived from the principle of invariant embedding. Thus, after eliminating the solution anisotropic part and the equation discretization we reach a unique analytical solution in the matrix form (26). In this sense the method of successive orders of scattering is an iterative method for finding the inverse matrix \(\tilde{A}\) in (26), and the Monte Carlo is a stochastic method.
Implementing the suggested solution (26) as the algorithm includes the calculation of the following components: zeroes and weights of the quadrature formula for the VRTE discretization (18), source function (4), eigenvectors and values of the system matrix (24), and products of matrices in (26).

The practical implementation of the indicated algorithm depends mainly on the size of matrices in (26). Note that (26) is obtained for the regular part, therefore, its size is determined mostly not by the medium optical parameters and the boundary conditions, but by the elimination of the solution anisotropic part. In general, $M \approx N = K$. However, in case of correct elimination of the anisotropic part solution, i.e. the smooth regular part is near to the isotropic angular distribution, it is possible that $M \ll N \ll K$. This improves considerably the algorithm performance.

4. Solution anisotropic part elimination

Now let’s analyse and compare all the main known methods of the anisotropic part elimination from the point of view of matrix size $M$ and $N$ reduction and the enhancement of calculation efficiency of the solution (26).

4.1. Elimination of direct non-scattering radiation

For the first time Eddington proposed the elimination of the anisotropic part by subtracting the direct non-scattered radiation on the basis of the Bouguer law, Milne developed the theory and it was fully crystallized in the works of Chandrasekhar [8]. Thus, the expression for the direct non-scattered radiation in the plane of reference coincided with the plane of incidence is given by:

$$
\tilde{L}_0(\tau, \mu, \varphi) = \tilde{L}_0(\tau, \mu, \varphi) = e^{-\tau \mu_0} \tilde{R}(\varphi) \tilde{L}_0 \delta(\hat{i} - \hat{i}_0), \quad \tilde{L}_0^0 = E_0 \left[ p \cos \varphi_0, \ p \sin \varphi_0, \ q \right]^\top,
$$

where $\tilde{L}_0$ is the vector of Stokes parameters of incident radiation, $E_0$ is the normal to beam irradiance, $p, q$ are degrees of linear and circular polarization of the beam, and $\varphi_0$ is the azimuth of polarization.

In this case the source function in the equation for the regular part takes the form

$$
\tilde{\Lambda}(\tau, \hat{i}) = \frac{\Lambda}{4\pi} e^{-\tau \mu_0} \tilde{R}(\varphi) \tilde{x}(\hat{i}, \hat{i}_0).
$$

Under these conditions the radiation scattered into small angles slightly differs from the direct radiation, and this method becomes inefficient. Strongly anisotropic scattering leads to a significant increase in the number of terms in the expansion of the scattering matrix in a series of generalized spherical functions $K$, which correspondingly increases the size of matrices $N$ and $M$ in the solution (26).

4.2. Delta-M method

Some works were done to solve the anisotropy problem. Various algorithms based on the truncation of scattering phase function were used. Delta-M method is the most efficient among them; it could be generalized in the vector case [9]. As in the scalar one the scattering phase function is represented as a sum of a delta-function and a smooth part

$$
\tilde{x}(\hat{i}, \hat{i}) = 4\pi f \tilde{I} \delta(\hat{i} - \hat{i}) + (1 - f) \tilde{x}^* (\hat{i}, \hat{i})
$$

Here $f$ is a part of anisotropy scattering; $\tilde{I}$ is an identity matrix.

Equation (31) for Greek matrix (11) can be written down as

$$
\tilde{x}_k = f \tilde{I} + (1 - f) \tilde{x}^*_k, \quad \tilde{x}^*_k = (\tilde{x}_k - f \tilde{I})/(1 - f).
$$

This phase matrix transformation leads to the scale transformation of optical depth and single scattering albedo

$$
\tau' = (1 - \Lambda f) \tau, \quad \Lambda' = \Lambda (1 - f)/(1 - \Lambda f).
$$

Thus, delta-M method could decrease $K$ significantly. However such an approach distorts initial boundary problem and leads to the error in a small sighting angle (intrinsically we do not consider the coarsest fraction of aerosol) or to oscillations in the angular radiance distribution.
4.3. TMS and IMS-methods

To eliminate the problems in VRTE solution mentioned above, Nakajima and Tanaka [10] returned to the idea of determination of the anisotropic part in the solution on the base of approximate analytical presentation of angular distribution of Stokes parameters for the first and second order of scattering:

\[ \hat{L}(\tau, \hat{I}) = \hat{L}_0(\tau, \hat{I}) + \hat{L}_1(\tau, \hat{I}) + \hat{L}_2(\tau, \hat{I}) + \hat{L}_3(\tau, \hat{I}). \] (34)

Here the first two orders satisfy the equations:

\[ \mu \frac{\partial \hat{L}_1(\tau, \hat{I})}{\partial \tau} + \hat{L}_1(\tau, \hat{I}) = \frac{\Lambda}{4\pi} e^{\nu \mu} \tilde{R}(\nu) \hat{L}_0(\hat{I}_0, \hat{I}), \] (35)

\[ \mu \frac{\partial \hat{L}_2(\tau, \hat{I})}{\partial \tau} + \hat{L}_2(\tau, \hat{I}) = \frac{\Lambda}{4\pi} \int \tilde{R}(\chi) \hat{L}_0(\hat{I}, \hat{I}') \hat{L}_1(\chi, \hat{I}') d\hat{I}'. \] (36)

Equations (35) and (36) are solved analytically. However the solution of equation (36) is a triple integral, and the run-time of its calculations can exceed the run-time of the initial problem solution (26). For this reason an approximation describing Stokes parameters distribution near the incident direction is generally used. The most efficient way is to use the small angle approximation, where the dispersion of scattered and non-scattered rays is not taken into account. This approximation is equivalent to the change of \( \mu \) in (35), (36) by \( \mu_0 \). The most known codes using both delta-M and TMS methods are DISORT [11] in the scalar case and Pstar [12] in the vector one.

4.4. Small angle modification of spherical harmonic method

It could be shown that the natural evolution of TMS-method is the inclusion in \( \hat{L}_a(\tau, \hat{I}) \) of all orders of scattering at small angle approximation [6]. This approach is described in [6] on the basis of small angle modification of spherical harmonics method (MSH).

In this case the anisotropic part of angular distribution of Stokes parameters in CP-representation is expanded with spherical functions with reference to the incident direction \( \hat{I}_0 \):

\[ \hat{L}_a(\tau, \hat{I}) = \sum_{m=-\infty}^{\infty} \sum_{k=0}^{\infty} \frac{2k+1}{4\pi} \tilde{Y}_m^k(\nu) \tilde{f}_m^k(\tau) \exp(i m \psi), \] (37)

here \( \nu = (\hat{I}, \hat{I}_0) \), \( \psi \) is azimuth \( \hat{I} \) in the system toward \( \hat{I}_0 \).

For the strong anisotropic angular distribution its spectrum is a smooth function of harmonic index \( k \). For this reason we can get the differential equation [6] for expansion coefficients

\[ \mu_0 \frac{\partial \tilde{f}_m(\tau,k)}{\partial \tau} + (\hat{I} - \hat{\Lambda}_x) \tilde{f}_m(\tau,k) = 0, \] (38)

the solution of which is simple

\[ \tilde{f}_m(\tau,k) = \exp\left\{-((\hat{I} - \hat{\Lambda}_x)\tau/\mu_0)\right\} \tilde{f}_m(0,k). \] (39)

After the conversion in the solution to SP-representation MSH [6] could be presented in the coordinate system about the normal to the layer boundary:

\[ \hat{L}_a(\tau, \hat{I}, \hat{I}_0) = \sum_{l=1,2}^2 \sum_{m=0}^\infty (2-\delta_{m,0}) \tilde{g}_l(\nu m \phi) \sum_{k=0}^{2k+1} \frac{2k+1}{4\pi} \tilde{\Pi}_m^k(\mu_0) \tilde{Z}_l(\tau) \tilde{\Pi}_m^k(\mu_0) \tilde{D}_l, \] (40)

where \( \tilde{D}_1 = \text{diag}(1 1 0 0) \), \( \tilde{D}_2 = \text{diag}(0 0 1 1) \), \( \tilde{Z}_l(\tau) = \exp\left\{-((\hat{I} - \hat{\Lambda}_x)\tau/\mu_0)\right\} \).

By substituting expression (40) in (4), and after some transformations [6] we get an expression for the source function

\[ \mu_0 \tilde{\Lambda}_m^k(\tau, \mu_0) = \sum_{l=1,2}^2 \sum_{m=0}^{2k+1} (\tilde{\Pi}_m^k(\mu_0) \tilde{D}_l, \tilde{I}_0) \tilde{g}_l(\nu m \phi) \sum_{k=0}^{2k+1} \frac{2k+1}{4\pi} \tilde{\Pi}_m^k(\mu_0) \tilde{Z}_l(\tau) \tilde{\Pi}_m^k(\mu_0) \tilde{D}_l, \tilde{I}_0, \] (41)

\[ + \tilde{\Lambda}_m^{k+1}(\tau, \mu_0) \tilde{D}_l, \tilde{I}_0, \tilde{Z}_{k+1}^l(\tau) \tilde{\Pi}_m^{k+1}(\mu_0) - \tilde{\Pi}_m^k(\mu_0) \tilde{D}_l, \tilde{I}_0, \tilde{Z}_k(\tau) \tilde{\Pi}_m^k(\mu_0) \tilde{D}_l, \tilde{I}_0, \]
where \( \hat{a}_k = I - \Lambda \chi_k \),

\[
\left[ \hat{A}_{m,s}^k \right] = \frac{1}{k} \sqrt{(k^2 - m^2)(k^2 - s^2)} \delta_{m,s}.
\]

This approach makes the regular part of the solution almost an isotropic function. So \( M \) can be small, and \( N \) does not practically depend on \( K \). We implemented this method of the solution anisotropic part elimination as two codes: MDOM in the scalar case and MVDOM in the vector one. Both codes are realized by languages FORTRAN as well as Matlab [13].

5. Numerical implementation

First of all we note that the numerical implementation of the solution (26) is based on solving the basic problems of linear algebra. There are some libraries where the necessary subroutines are collected: LAPACK, IMSL, NAG etc. Math Kernel Library (MKL) is a package that is specially optimized for Intel processors (MKL has versions both for Windows and Linux systems). Great advantages result from the use of the supporting multicore and multiprocessor systems and automatic parallelization. This feature can increase computing speed significantly. It has vector implementations of element operations (e.g. square root from elements of an array) in a parallel mode. Special mathematical program packages like Matlab, Maple, Mathematica use MKL by playing the role of library cover.

A perspective way to accelerate the code is a general-purpose graphics processing units (GPUs). Compute Unified Device Architecture (CUDA) is the computing engine in nVIDIA GPUs. It gives access to the instruction set of computing elements of video card. Standard LAPACK routines can be accelerated by CUDA as well. Instead of reprogramming LAPACK subroutines, it is advisable to apply the special library CULA. Also MATLAB 2010b supports nVIDIA CUDA-capable GPUs, and no knowledge and experience in CUDA is required to use GPU-computing features.

The significant acceleration and saving the memory can be reached by using sparse matrices. The basic idea is the following: while working with matrix that has a lot of zero elements, it is wise to store only non-zero elements and the additional information that can be used to restore the indices of nonzero elements or indices themselves. There are some formats to store the sparse matrices: compressed sparse row (CSR) format, compressed sparse column format (CSC), and Coordinate Format. The choice of format depends on type of operation; for instance, CSC format is convenient when using sparse matrix since its elements are arranged by each column. The use of sparse matrices can be efficient for computing the anisotropic part (49) and dealing with a modified source function.

6. Results and discussions

We analyzed the effect of different hardware-software resources for the efficiency of implementation of solution (26) with the anisotropic part elimination on a basis of MSH by example of codes MDOM and MVDOM. The comparison of run-time for different modes of compiling and computing is represented in Table 1 for two tests (test1: \( N = 101, K=500, M=32 \); test 2: \( N = 101, K=1000, M=32 \)). The tests were run on system Ubuntu 10.04, Intel Core 2 Duo 3GHz, 2 Gb RAM, Intel Fortran Compiler 11.1 with MKL 10.2. Two compilers gfortran and ifort, optimization and sparse matrix technique were used.

Note that MKL uses all available computing cores of the system (2 cores in this case) and provides the results in half of the time. The sparse matrix technique used for computing the anisotropic part reduces run-time significantly. Due to sparse matrices, the two-dimensional arrays are reduced to one-dimensional array. Thus, the run-time is proportional to \( K \) instead of \( K^2 \).

We increased acceleration by about 20% due to the matrix multiplication on nVIDIA GeForce 480 GTX GPU. GPU computations provide advantages only for big size arrays, otherwise CPU computing is more preferable. The profiler tool shows that the calculation of eigenvectors and values take the half of the run-time. Unfortunately, the subroutines for these problems have not been implemented for Matlab GPU tool. The sizes of matrices are significantly reduced due to the solution anisotropic part elimination by MSH. In practice, \( N \) is less than 300. However in the case computations of spectra the parallelization of wavelength loop also can be implemented within CUDA technology. It is a possible way to use CUDA advantages, but not for a single wavelength problem.
### Table 1. Comparison of calculating time for two tests.

| Features                                      | Run-time I, sec | Run-time II, sec |
|-----------------------------------------------|-----------------|------------------|
| gfortran+LAPACK                               | 240             | 530              |
| gfortran+LAPACK + optimization                | 230             | 505              |
| ifort+LAPACK                                  | 210             | 490              |
| ifort+MKL                                     | 115             | 250              |
| ifort+MKL+optimization                        | 105             | 230              |
| ifort+MKL+optimization + sparse matrix        | 33              | 44               |
| Matlab 2010b                                  | 27              | 45               |
| Matlab 2010b + CUDA                           | 22              | 33               |

Now let’s consider the effectiveness of different methods of the solution anisotropic part elimination by the numerical comparison of the radiance angular distribution calculation for the same task by different codes: DISORT and MDOM in the scalar case and Pstar and MVDOM in the vector one. It is worth mentioning that the speed of DISORT calculation can be significantly increased by using the sparse matrix algorithm in subroutine ZEROIT, which zeros a given matrix. In this case the speed for quite smooth phase functions ($g<0.9$) of MDOM and DISORT is of the same order. For the phase function Henyey-Greenstein $g=0.98$, the MSH method of anisotropic part elimination appears to be better. Figure 1 provides the numerical comparison of the reflectance calculations for the medium scattering anisotropy, and figure 2 for the strong anisotropy.

![Figure 1](image1.png)  
**Figure 1.** Comparison of MDOM and DISORT in the case of medium scattering anisotropy.

![Figure 2](image2.png)  
**Figure 2.** Comparison of MDOM and DISORT in the case of strong scattering anisotropy.

Note that even an average degree of scattering anisotropy mandatory requires the use of TMS method. Isolation of the solution singularities on the basis of MSH operates independently from the degree of scattering anisotropy. The running time in the first case is approximately the same $t \sim 0.5$ sec, but it differs greatly in the second case: MDOM $t \sim 2$ seconds, and DISORT $t \sim 14$ sec.

Quite similar results were obtained in the vector case. We compared Pstar and MVDOM in the cases of the phase matrix for log-normal distribution with parameters $r_0=5$, $s=0.4$, $\Lambda=0.99$; and geometry of the observation scheme with $\theta_0=45^\circ$, $\tau_0=1.0$, $\varphi=30^\circ$. Figure 3 shows a comparison of...
calculations of the angular distribution of polarization transmitted by slab, and figure 4 provides a comparison of the reflected radiation.

![Figure 3.](image1) ![Figure 4.](image2)

For the best fit, we used the parameters: \( N = 71 \), \( K = 171 \), \( M = 20 \) in the code MVDOM and 30 streams in the code Pstar. The comparison of results showed the perfect coincidence at the computer accuracy level, but the computation time was 11 seconds for MVDOM and for the program Pstar more than 180 seconds.

7. Conclusions
The discretized VRTE for a slab has a unique analytic solution in the matrix form. The high level of optimization of linear algebra packages permits a single algorithm implementation on a computer for this solution. Various implementations differ in the method of the solution anisotropic part elimination. Taking into account our algorithm analysis, the analytical anisotropy elimination on the basis of MSH is supposedly a more precise algorithm than TMS. At the algorithm implementation it is necessary to use the algorithm of sparse matrices, and when using the Intel processor the application of MKL library is very essential.

References
[1] Kokhanovsky AA, Budak VP, Cornet C, Duan M, Emde C, Katsev IL, Klyukov DA, Korkin SV, C-Labonnote L, Mayer B, Min Q, Nakajima T, Ota Y, Priakhch AS, Rozanov VV, Yokota T, Zege EP 2010 *J. Quant. Spectrosc. Radiat. Transf.* **111** 1931.
[2] Doicu A and Trautmann T 2009 *J. Quant. Spectrosc. Radiat. Transf.* **110** 159
[3] Budak VP, Klyuykov DA, and Korkin SV 2011 *J. Quant. Spectrosc. Radiat. Transf.* **112** 1141.
[4] Karp AH, Greenstadt J, and Fillmore JA 1980 *J. Quant. Spectrosc. Radiat. Transf.* **24** 391.
[5] Kuščer I and Ribarič M 1959 *Opt Acta* **6** 42.
[6] Budak VP and Korkin SV 2008 *J. Quant. Spectrosc. Radiat. Transf.* **109** 220.
[7] Flatau PJ and Stephens GL 1988 *J. Geophys. Res.* **93** 11037.
[8] Chandrasekhar S 1950 *Radiative transfer* (London: Oxford University Press)
[9] Wiscombe WJ 1977 *J. Atmos. Sci.* **34** 1408.
[10] Nakajima T and Tanaka M 1988 *J. Quant. Spectrosc. Radiat. Transf.* **40** 51.
[11] ftp://climate1.gsfc.nasa.gov/wiscombe/Multiple_Scatt
[12] http://www.ccsr.u-tokyo.ac.jp/~clastr/
[13] http://www.svet-mpei.org