Polarized Radiative Transfer in a Multi-Layer Medium Subject to Fresnel Boundary and Interface Conditions

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Objective

- To develop a discrete-ordinates solution for polarized radiative transfer driven by a uniform beam of parallel rays that is incident obliquely on a multi-layer medium
- The index of refraction is taken to be layer-dependent, so Fresnel boundary and interface conditions are required in the formulation
- A general form of the phase matrix is considered (also layer-dependent)

Applications

- Modeling of the atmosphere-ocean system
- Biomedical optics
- Remote sensing
The Radiative Transfer Equation (RTE)

For each of the layers $k = 1, 2, \ldots, K$:

$$\mu \frac{\partial}{\partial \tau} I_k(\tau, \mu, \phi) + I_k(\tau, \mu, \phi) = \frac{\varpi_k}{4\pi} \int_{-1}^{1} \int_{0}^{2\pi} P_k(\mu, \mu', \phi - \phi') I_k(\tau, \mu', \phi') \, d\phi' \, d\mu' \quad (1)$$

$\tau \in (a_{k-1}, a_k)$: optical variable that defines the position in layer $k$

$\mu \in [-1, 1]$: cosine of the polar angle $\theta$

$\phi \in [0, 2\pi]$: azimuthal angle

$\varpi_k$: single-scattering albedo for layer $k$

$P_k(\mu, \mu', \phi - \phi')$: phase matrix for layer $k$

The Stokes vector $I(\tau, \mu, \phi)$ has the four Stokes parameters as components:

$$I(\tau, \mu, \phi) = \left( \begin{array}{c} I(\tau, \mu, \phi) \\ Q(\tau, \mu, \phi) \\ U(\tau, \mu, \phi) \\ V(\tau, \mu, \phi) \end{array} \right) \quad (2)$$
The Phase Matrix

We consider a general form for the phase matrix (Siewert, 1982):

\[
P_k(\mu, \mu', \phi - \phi') = \frac{1}{2} \sum_{m=0}^{L} (2 - \delta_{0,m})[C_k^m(\mu, \mu') \cos m(\phi - \phi') + S_k^m(\mu, \mu') \sin m(\phi - \phi')],
\]

where

\[
C_k^m(\mu, \mu') = A_k^m(\mu, \mu') + DA_k^m(\mu, \mu')D
\]

and

\[
S_k^m(\mu, \mu') = A_k^m(\mu, \mu')D - DA_k^m(\mu, \mu').
\]

In these expressions, \(D = \text{diag}\{1, 1, -1, -1\}\) and

\[
A_k^m(\mu, \mu') = \sum_{l=m}^{L} P_l^m(\mu)B_lP_l^m(\mu'),
\]

where

\[
B_l = \begin{pmatrix}
\beta_l & \gamma_l & 0 & 0 \\
\gamma_l & \alpha_l & 0 & 0 \\
0 & 0 & \zeta_l & -\epsilon_l \\
0 & 0 & \epsilon_l & \delta_l
\end{pmatrix}
\]

and

\[
P_l^m(\mu) = \begin{pmatrix}
P_l^m(\mu) & 0 & 0 & 0 \\
0 & R_l^m(\mu) & -T_l^m(\mu) & 0 \\
0 & -T_l^m(\mu) & R_l^m(\mu) & 0 \\
0 & 0 & 0 & P_l^m(\mu)
\end{pmatrix}.
\]

\{\alpha_l, \beta_l, \gamma_l, \delta_l, \epsilon_l, \zeta_l\}: Greek constants

\(P_l^m(\mu)\): normalized version of the associated Legendre function of the first kind

\(R_l^m(\mu)\) and \(T_l^m(\mu)\): given in terms of the generalized spherical functions \(P_{m,-2}(\mu)\) and \(P_{m,2}(\mu)\)
Fresnel Boundary and Interface Conditions

Consider a beam of parallel rays described by the Stokes parameters

\[ F = \begin{pmatrix} F_I \\ F_Q \\ F_U \\ F_V \end{pmatrix} \]  \hspace{1cm} (7)

traveling in an external medium \( \tau < a_0 \) characterized by an index of refraction \( n_0 \) towards the surface located at \( \tau = a_0 \) along a direction defined by \( (\mu_0, \phi_0) \).

The boundary condition for the first layer is

\[ I_1(a_0, \mu, \phi) = X(n_{1,0}, \mu)I_1(a_0, -\mu, \phi) + Y(n_{1,0}, \mu)F \delta[f(n_{1,0}, \mu) - \mu_0] \delta(\phi - \phi_0), \]  \hspace{1cm} (8)

for \( \mu \in (0, 1] \) and \( \phi \in [0, 2\pi] \).

General definitions:

\[ n_{k,k'} = n_k/n_{k'} \]  \hspace{1cm} (9)

\[ f(n, \mu) = [1 - n^2(1 - \mu^2)]^{1/2} \]  \hspace{1cm} (10)

\( X(n_{k,k'}, \mu) \) is the reflection matrix by layer \( k' \) for radiation coming from layer \( k \).

\( Y(n_{k,k'}, \mu) \) is the transmission matrix for radiation from layer \( k' \) to layer \( k \).
Fresnel Boundary and Interface Conditions (cont.)

The reflection and transmission matrices:

\[ X(n, \mu) = \begin{cases} \mathbf{G}(n, \mu), & n \leq 1, \\ \mathbf{G}(n, \mu)H[\mu - \mu_c(n)] + \mathbf{\Gamma}(n, \mu)\{1 - H[\mu - \mu_c(n)]\}, & n \geq 1, \end{cases} \]  \hspace{1cm} (11a)

\[ Y(n, \mu) = \begin{cases} \mathbf{D}(n, \mu), & n \leq 1, \\ \mathbf{D}(n, \mu)H[\mu - \mu_c(n)], & n \geq 1. \end{cases} \]  \hspace{1cm} (11b)

where \( H(x) \) is the Heaviside function and \( \mu_c(n) = (1 - 1/n^2)^{1/2} \) is the cosine of the critical angle,

\[ \mathbf{G}(n, \mu) = \frac{1}{2} \begin{pmatrix} \frac{\mu - n f(n, \mu)}{\mu + n f(n, \mu)} \frac{\mu - n f(n, \mu)}{\mu + n f(n, \mu)} \frac{\mu - n f(n, \mu)}{\mu + n f(n, \mu)} \frac{n \mu f(n, \mu)}{n \mu f(n, \mu)} \\ \frac{n \mu f(n, \mu)}{n \mu f(n, \mu)} \frac{\mu - n f(n, \mu)}{\mu + n f(n, \mu)} \frac{n \mu f(n, \mu)}{n \mu f(n, \mu)} \frac{\mu - n f(n, \mu)}{\mu + n f(n, \mu)} \\ \frac{\mu - n f(n, \mu)}{\mu + n f(n, \mu)} \frac{\mu - n f(n, \mu)}{\mu + n f(n, \mu)} \frac{\mu - n f(n, \mu)}{\mu + n f(n, \mu)} \frac{n \mu f(n, \mu)}{n \mu f(n, \mu)} \\ 0 \end{pmatrix} \]  \hspace{1cm} (12)

\[ \mathbf{\Gamma}(n, \mu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 \frac{2(1 - \mu^2)^2}{1 - (1 + 1/n^2)\mu^2} - 1 & -2\mu(1 - \mu^2)[\mu^2(n - \mu^2)^{1/2}] & 0 \\ 0 & 0 \frac{2\mu(1 - \mu^2)[\mu^2(n - \mu^2)^{1/2}]}{1 - (1 + 1/n^2)\mu^2} & \frac{2(1 - \mu^2)^2}{1 - (1 + 1/n^2)\mu^2} - 1 \end{pmatrix} \]  \hspace{1cm} (13)
Fresnel Boundary and Interface Conditions (cont.)

\[
\mathbf{D}(n, \mu) = 2n^3 \mu f(n, \mu) \begin{pmatrix}
\frac{1}{[\mu+nf(n,\mu)]^2} & \frac{1}{\mu+nf(n,\mu)} & \frac{1}{[\mu+nf(n,\mu)]^2} & \frac{1}{\mu+nf(n,\mu)} & 0 & 0 \\
\frac{1}{[\mu+nf(n,\mu)]^2} & \frac{1}{\mu+nf(n,\mu)} & \frac{1}{[\mu+nf(n,\mu)]^2} & \frac{1}{\mu+nf(n,\mu)} & 0 & 0 \\
0 & 0 & \frac{2}{[\mu+nf(n,\mu)]^2} & \frac{2}{\mu+nf(n,\mu)} & 0 & 0 \\
0 & 0 & 0 & \frac{2}{[\mu+nf(n,\mu)]^2} & \frac{2}{\mu+nf(n,\mu)} & 0 \\
\end{pmatrix}
\]

(14)

At the interfaces, the conditions couple adjacent layers:

\[
\mathbf{I}_k(a_k, -\mu, \phi) = \mathbf{X}(n_{k,k+1}, \mu)\mathbf{I}_k(a_k, \mu, \phi) + \mathbf{Y}(n_{k,k+1}, \mu)\mathbf{I}_{k+1}[a_k, -f(n_{k,k+1}, \mu), \phi]
\]

(15a)

and

\[
\mathbf{I}_{k+1}(a_k, \mu, \phi) = \mathbf{X}(n_{k+1,k}, \mu)\mathbf{I}_{k+1}(a_k, -\mu, \phi) + \mathbf{Y}(n_{k+1,k}, \mu)\mathbf{I}_k[a_k, f(n_{k+1,k}, \mu), \phi],
\]

(15b)

for \( \mu \in (0, 1] \) and \( \phi \in [0, 2\pi] \), and \( k = 1, 2, \ldots, K - 1 \).

At the surface of the last layer (\( \tau = a_K \)), we assume that there is no radiation coming from an external medium (\( \tau > a_K \)) with index of refraction \( n_{K+1} \) and so we get

\[
\mathbf{I}_K(a_K, -\mu, \phi) = \mathbf{X}(n_{K,K+1}, \mu)\mathbf{I}_K(a_K, \mu, \phi), \quad \text{for } \mu \in (0, 1] \text{ and } \phi \in [0, 2\pi].
\]

(16)

The difficulty caused by the polar angle shift in the transmission terms is overcome by what we call “pre-processing of the interface conditions”.

Pre-processing involves algebraic manipulations of the boundary/interface conditions and the RTE. See details for the scalar case in Garcia, Siewert, and Yacout (2008).
Pre-Processed Fresnel Boundary and Interface Conditions

\[ I_k(a_{k-1}, \mu, \phi) - Z_k^-(\mu)I_k(a_{k-1}, -\mu, \phi) = F_k \delta(\mu - \mu_k)\delta(\phi - \phi_0) + W_k^- (\mu, \phi) \]  
(17a)

and

\[ I_k(a_k, -\mu, \phi) - Z_k^+(\mu)I_k(a_k, \mu, \phi) = W_k^+ (\mu, \phi), \]  
(17b)

for \( \mu \in (0, 1], \phi \in [0, 2\pi], \) and \( k = 1, 2, \ldots, K. \)

The 4 \times 4 matrices \( Z_k^\pm(\mu) \) and the 4-vectors \( F_k \) and \( W_k^\pm(\mu, \phi) \) are defined by recurrence along the layers.

Equations (17) for a given layer are coupled by way of \( W_k^\pm(\mu, \phi) \), which depend on the Stokes vectors in the other layers.

Decomposition into Scattered and Unscattered Problems

\[ I_k(\tau, \mu, \phi) = I_k^{(0)}(\tau, \mu, \phi) + I_k^{(*)}(\tau, \mu, \phi) \]  
(18)

The unscattered Stokes vector is given, for \( \mu \in (0, 1] \), by

\[ I_k^{(0)}(\tau, \mu, \phi) = S_k^+ e^{-(\tau - a_{k-1})/\mu} \delta(\mu - \mu_k)\delta(\phi - \phi_0) \]  
(19a)

and

\[ I_k^{(0)}(\tau, -\mu, \phi) = S_k^- e^{-(a_k - \tau)/\mu} \delta(\mu - \mu_k)\delta(\phi - \phi_0), \]  
(19b)

where the 4-vectors \( S_k^\pm \) are defined by recurrence along the layers.
Decomposition into Scattered and Unscattered Problems (cont.)

The scattered Stokes vector must satisfy, for layers \( k = 1, 2, \ldots, K \),

\[
\frac{\partial}{\partial \tau} I_k^{(*)}(\tau, \mu, \phi) + I_k^{(*)}(\tau, \mu, \phi) = \frac{\omega_k}{4\pi} \int_{-1}^{1} \int_{0}^{2\pi} P_k(\mu, \mu', \phi - \phi') I_k^{(*)}(\tau, \mu', \phi') \, d\phi' \, d\mu' \\
+ \frac{\omega_k}{4\pi} P_k(\mu, \mu_k, \phi - \phi_0) S_k^+ e^{-(\tau - a_{k-1})/\mu_k} + \frac{\omega_k}{4\pi} P_k(\mu, -\mu_k, \phi - \phi_0) S_k^- e^{-(a_k - \tau)/\mu_k},
\]

for \( \tau \in (a_{k-1}, a_k) \), \( \mu \in [-1, 1] \) and \( \phi \in [0, 2\pi] \), subject to

\[
I_k^{(*)}(a_{k-1}, \mu, \phi) - Z_k^-(\mu) I_k^{(*)}(a_{k-1}, -\mu, \phi) = W_k^- (\mu, \phi)
\]

and

\[
I_k^{(*)}(a_k, -\mu, \phi) - Z_k^+(\mu) I_k^{(*)}(a_k, \mu, \phi) = W_k^+ (\mu, \phi),
\]

for \( \mu \in (0, 1] \) and \( \phi \in [0, 2\pi] \).

- The \( \phi \)-dependence of the scattered problem can be treated with a Fourier decomposition in terms of sines and cosines
- In principle, the source terms that come from the unscattered solution introduce the need for particular solutions but we were able to circumvent this
**Fourier Decomposition of the Scattered Problem**

Noting that the phase matrix can also be expressed as

\[
P(\mu, \mu', \phi - \phi') = \sum_{m=0}^{L} \sum_{\alpha=1}^{2} \Phi_{\alpha}^{m}(\phi - \phi') A_{\alpha}^{m}(\mu, \mu') D_{\alpha}
\]  

(22)

where \( D_{1} = \text{diag}\{1, 1, 0, 0\}, \ D_{2} = \text{diag}\{0, 0, 1, 1\}, \)

\[
\Phi_{1}^{m}(\phi) = (2 - \delta_{0,m}) \text{diag}\{\cos m\phi, \cos m\phi, \sin m\phi, \sin m\phi\}
\]  

(23a)

and

\[
\Phi_{2}^{m}(\phi) = (2 - \delta_{0,m}) \text{diag}\{-\sin m\phi, -\sin m\phi, \cos m\phi, \cos m\phi\},
\]  

(23b)

we propose, for \( \mu \in (0, 1] \),

\[
I_{k}^{(\tau, \mu, \phi)} = \frac{1}{2\pi} \sum_{m=0}^{L} \sum_{\alpha=1}^{2} \Phi_{\alpha}^{m}(\phi - \phi_{0})\left[I_{k,\alpha}^{m}(\tau, \mu) - D_{\alpha} S_{k}^{\pm} e^{-\left(\tau - a_{k-1}\right)/\mu_{k}}\delta(\mu - \mu_{k})\right]
\]  

(24a)

and

\[
I_{k}^{(\tau, -\mu, \phi)} = \frac{1}{2\pi} \sum_{m=0}^{L} \sum_{\alpha=1}^{2} \Phi_{\alpha}^{m}(\phi - \phi_{0})\left[I_{k,\alpha}^{m}(\tau, -\mu) - D_{\alpha} S_{k}^{-} e^{-\left(a_{k-1} - \tau\right)/\mu_{k}}\delta(\mu - \mu_{k})\right].
\]  

(24b)

We get \(2(L + 1)\) azimuthally-independent problems for each layer.
Fourier Decomposition of the Scattered Problem (cont.)

For \( m = 0, 1, \ldots, L \) and \( \alpha = 1 \) and \( 2 \), we get

\[
\mu \frac{\partial}{\partial \tau} I_{k,\alpha}^m(\tau, \mu) + I_{k,\alpha}^m(\tau, \mu) = \frac{\nu_k}{2} \int_{-1}^{1} A_k^m(\mu, \mu') I_{k,\alpha}^m(\tau, \mu') d\mu',
\]

for \( \tau \in (a_{k-1}, a_k) \) and \( \mu \in [-1, 1] \), subject to

\[
I_{k,\alpha}^m(a_{k-1}, \mu) - Z_k^- (\mu) = D_\alpha F_k \delta(\mu - \mu_k) + W_{k,m,\alpha}^-(\mu),
\]

and

\[
I_{k,\alpha}^m(a_k, -\mu) - Z_k^+ (\mu) = W_{k,m,\alpha}^+(\mu),
\]

for \( \mu \in (0, 1] \). Here, the quantities

\[
W_{k,m,\alpha}^\pm (\mu) = \frac{1}{2} (1 + \delta_{0,m}) \int_0^{2\pi} \Phi^m_\alpha (\phi - \phi_0) W_{k,m,\alpha}^\pm (\mu, \phi) d\phi
\]

couple the problems for all layers and are defined (and computed) by recurrence along the layers. The Dirac delta \( \delta(\mu - \mu_k) \) in Eq. (26a) is approximated by the rectangular nascent delta

\[
\delta_\epsilon(\mu - \mu_k) = \left\{ \begin{array}{ll}
(\mu_{\text{max}} - \mu_{\text{min}})^{-1}, & \mu_{\text{min}} \leq \mu \leq \mu_{\text{max}}, \\
0, & \text{otherwise},
\end{array} \right.
\]

where

\[
\mu_{\text{min}} = \max\{0, \mu_k - \epsilon/2\} \quad \text{and} \quad \mu_{\text{max}} = \min\{\mu_k + \epsilon/2, 1\}
\]

and \( \epsilon \) is the “narrowness” parameter.
The ADO solution

To define the quadrature to be used with the ADO method, we:

1. Split the integration interval $[-1, 1]$ into two half-range intervals $[-1, 0)$ and $(0, 1]$

2. Subdivide the interval $(0, 1]$ into smaller sub-intervals to avoid discontinuities in the derivative of Stokes vector w.r.t. $\mu$ at the interfaces. For layer $k$, the break points that define these sub-intervals are given by the critical cosines that obey certain conditions (Garcia, 2009)

3. Add $\mu_{\min}$ and $\mu_{\max}$ to the set of break-points

4. Use a shifted Gauss-Legendre quadrature in each sub-interval. A very low order quadrature (e.g., 2) is sufficient in the interval of support of $\delta(\mu - \mu_k)$

5. Reflect the nodes and weights used in $(0,1]$ about 0 to define the quadrature in $[-1,0)$

The composite quadrature so obtained is layer-dependent and so its order is denoted as $N_k$.

ADO solution in layer $k$ for $\pm \mu_n, n = 1, 2, \ldots, N_k$:

$$I_{k,\alpha}^m(\tau, \pm \mu_n) = \sum_{j=1}^{4N_k} A_{k,j}^{\alpha,m} \Phi_k^m(\nu_j, \pm \mu_n) e^{-(\tau-a_k-1)/\nu_j} + B_{k,j}^{\alpha,m} \Phi_k^m(\nu_j, \mp \mu_n) e^{-(a_k-\tau)/\nu_j},$$

where the separation constants $\pm \nu_j$ and the elementary solutions $\Phi_k^m(\nu_j, \pm \mu_n)$ come from the solution of an eigensystem of order $4N_k$ (Siewert, 2000).
The ADO solution (cont.)

The unknown coefficients $A_{\alpha,m}^{\alpha,m}$ and $B_{\alpha,m}^{\alpha,m}$ are determined by using the ADO solution in the boundary/interface conditions for $\mu = \mu_n, n = 1, 2, \ldots, N_k$.

For each pair of $(m, \alpha)$, we get a linear system of order $8N_k$ for layer $k$:

$$
\sum_{j=1}^{4N_k} A_{\alpha,m}^{\alpha,m} \left[ \Phi_k^m(\nu_j, \mu_n) - Z_k^- (\mu_n) D \Phi_k^m(\nu_j, -\mu_n) \right] + \sum_{j=1}^{4N_k} B_{\alpha,m}^{\alpha,m} \left[ \Phi_k^m(\nu_j, -\mu_n) - Z_k^- (\mu_n) D \Phi_k^m(\nu_j, \mu_n) \right] e^{-\frac{(a_k-a_{k-1})}{\nu_j}} = D_\alpha F_k \delta_\epsilon (\mu_n - \mu_0) + W_{k,m,\alpha}^- (\mu_n) \quad (31a)
$$

and

$$
\sum_{j=1}^{4N_k} A_{\alpha,m}^{\alpha,m} \left[ D \Phi_k^m(\nu_j, -\mu_n) - Z_k^+ (\mu_n) \Phi_k^m(\nu_j, \mu_n) \right] e^{-\frac{(a_k-a_{k-1})}{\nu_j}} + \sum_{j=1}^{4N_k} B_{\alpha,m}^{\alpha,m} \left[ D \Phi_k^m(\nu_j, \mu_n) - Z_k^+ (\mu_n) \Phi_k^m(\nu_j, -\mu_n) \right] = W_{k,m,\alpha}^+ (\mu_n) \quad (31b)
$$

As the functions $W_{k,m,\alpha}^\pm (\mu_n)$ couple the linear systems for all the layers, solutions are found by iteration (sweeps along the layers).
Post-Processing of the ADO Solution

- Used to get a solution valid for any $\mu$, not just at the ordinates.

- Why is this important?
  1. Layers have different ordinates.
  2. Good for computational efficiency, as it allows the use of smaller quadrature orders when $m \to L$.

Numerical Results

- There is no work in the literature with numerical results in tabular form

- Difficulty in finding realistic phase matrices for media other than atmospheres

- Synthetic 3-layer system

- Stokes vector converged to 5 figures