Implementation of polarization in 3D Monte Carlo solver MYSTIC

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18 September 2008

ESAS-Light Progress Meeting 2

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Oberpfaffenhofen, Germany

Radiative transfer solver MYSTIC

Monte carlo code for the phYSically correct Tracing of photons In Cloudy atmospheres
Mayer [1999, 2000], *Emde and Mayer* [2007]

Implementation of polarization requires:

- 4 component Stokes vector instead of only intensity (weight vector)
- Extended optical properties data (phase matrix, extinction matrix, absorption vector)
- Rotation of Stokes vector in “scattering frame”

Description of polarisation - the Stokes components

Definition:

$$
\begin{aligned}
I &= \frac{1}{2}\sqrt{\frac{\epsilon}{\mu}}(E_\theta E_\theta^* + E_\phi E_\phi^*) \\
Q &= \frac{1}{2}\sqrt{\frac{\epsilon}{\mu}}(E_\theta E_\theta^* - E_\phi E_\phi^*) \\
U &= -\frac{1}{2}\sqrt{\frac{\epsilon}{\mu}}(E_\theta E_\phi^* + E_\phi E_\theta^*) \\
V &= i\frac{1}{2}\sqrt{\frac{\epsilon}{\mu}}(E_\phi E_\theta^* - E_\theta E_\phi^*)
\end{aligned}
$$

Degree of polarization:

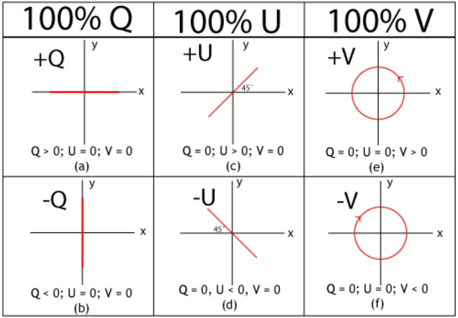
$$p = \frac{\sqrt{Q^2 + U^2 + V^2}}{I}$$

Completely polarized radiation:

$$Q^2 + U^2 + V^2 = I^2 \Rightarrow p = 1$$

For unpolarized radiation:

$$Q = U = V = 0 \Rightarrow p = 0$$



source: Wikipedia

Coordinate systems

- Model coordinate system (x,y,z)
  - z - altitude, vertical coordinate
  - x,y - horizontal coordinates

- Scattering frame $(\mathbf{n}^{\mathbf{inc}}, \mathbf{n}^{\mathbf{sca}}, \mathbf{n}^{\mathbf{inc}} \times \mathbf{n}^{\mathbf{sca}})$
  - Optical properties of spherical or randomly oriented can be represented as a function of scattering angle only.

Scattering phase matrix

- Definition:

$$\mathbf{I}^{\mathbf{sca}}(r\mathbf{n}^{\mathbf{sca}}) = \frac{1}{r^2}\mathbf{P}(\mathbf{n}^{\mathbf{sca}}, \mathbf{n}^{\mathbf{inc}})\mathbf{I}^{\mathbf{inc}}$$

- *Randomly oriented particles:*

$$\mathbf{P}(\Theta) = \begin{bmatrix} P_{11}(\Theta) & P_{12}(\Theta) & 0 & 0 \\ P_{12}(\Theta) & P_{22}(\Theta) & 0 & 0 \\ 0 & 0 & P_{33}(\Theta) & P_{34}(\Theta) \\ 0 & 0 & -P_{34}(\Theta) & P_{44}(\Theta) \end{bmatrix}$$

  phase matrix depends only on scattering angle in “scattering frame”

- *Arbitrarily oriented particles:*

  all phase matrix elements can be different and depend on incident and scattered direction (4 angles)

Extinction matrix

- Definition:

$$\mathbf{I}(r\mathbf{n}^{\mathbf{inc}})\Delta S = \mathbf{I}^{\mathbf{inc}}\Delta S - \mathbf{K}(\mathbf{n}^{\mathbf{inc}})\mathbf{I}^{\mathbf{inc}} + O(r^{-2})$$

- *Randomly oriented particles:*

$$\mathbf{K} = \begin{bmatrix} C_{ext} & 0 & 0 & 0 \\ 0 & C_{ext} & 0 & 0 \\ 0 & 0 & C_{ext} & 0 \\ 0 & 0 & 0 & C_{ext} \end{bmatrix}$$

- *Arbitrarily oriented particles:*

  all extinction matrix elements can be different and depend on incident and scattered direction (4 angles)

Stokes emission vector

- Definition:

$$W^e = \frac{1}{r^2}\mathbf{a}(\mathbf{r}, T, \omega)B(T, \omega)\Delta S \Delta\omega$$

- Calculation:

$$a_i^p(\mathbf{r}, T, \omega) = K_{i1}(\mathbf{r}, \omega) - \int_{4\pi} \mathrm{d}\mathbf{r}' P_{i1}(\mathbf{r}, \mathbf{r}', \omega), \quad i = 1 \cdots 4$$

- *Randomly oriented particles:*

$$\mathbf{a} = \begin{bmatrix} C_{abs} \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Optical cross sections

- extinction cross section:

$$C_{ext} = \frac{1}{I^{inc}}[K_{11}(\mathbf{n^{inc}})I^{inc} + K_{12}(\mathbf{n^{inc}})Q^{inc} + K_{13}(\mathbf{n^{inc}})U^{inc} + K_{14}(\mathbf{n^{inc}})V^{inc}]$$

- Scattering cross section:

$$C_{sca} = \frac{1}{I^{inc}} \int_{4\pi} \mathrm{d}\mathbf{n^{sca}}[P_{11}(\mathbf{n^{sca}}, \mathbf{n^{inc}})I^{inc} + P_{12}(\mathbf{n^{sca}}, \mathbf{n^{inc}})Q^{inc} + P_{13}(\mathbf{n^{sca}}, \mathbf{n^{inc}})U^{inc} + P_{14}(\mathbf{n^{sca}}, \mathbf{n^{inc}})V^{inc}]$$

- Absorption cross section:

$$C_{abs} = C_{ext} - C_{sca}$$

- Singe scattering albedo:

$$\omega_0 = \frac{C_{sca}}{C_{ext}} \leq 1$$

- Phase function:

$$p(\mathbf{n^{sca}}, \mathbf{n^{inc}}) = \frac{4\pi}{C_{sca} I^{inc}}[P_{11}(\mathbf{n^{sca}}, \mathbf{n^{inc}})I^{inc} + P_{12}(\mathbf{n^{sca}}, \mathbf{n^{inc}})Q^{inc} + P_{13}(\mathbf{n^{sca}}, \mathbf{n^{inc}})U^{inc} + P_{14}(\mathbf{n^{sca}}, \mathbf{n^{inc}})V^{inc}]$$

Vector radiative transfer equation

$$\frac{\mathrm{d}\mathbf{I}}{\mathrm{d}s}(\mathbf{n},\lambda) = -\langle \mathbf{K}(\mathbf{n},\lambda)\rangle \mathbf{I}(\mathbf{n},\lambda) + \langle \mathbf{a}(\mathbf{n},\lambda)\rangle B(\lambda, T) + \int_{4\pi} \mathrm{d}\mathbf{n}' \langle \mathbf{Z}(\mathbf{n},\mathbf{n}',\lambda)\rangle \mathbf{I}(\mathbf{n}',\lambda)$$

- Phase matrix in “model” frame (x,y,z):

$$\langle \mathbf{Z}\rangle = \mathbf{L}(-\sigma_2)\langle \mathbf{P}\rangle \mathbf{L}(\pi - \sigma_1)$$

- Stokes rotation matrix:

$$\mathbf{L}(\alpha) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(2\alpha) & -\sin(2\alpha) & 0 \\ 0 & \sin(2\alpha) & \cos(2\alpha) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Initialize photon (Solar radiative transfer)

- Initial direction $\mathbf{n_0}$ given by sun position
- Initial photon weight vector

$$\mathbf{w} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

corresponds to Stokes vector unpolarized extraterrestrial radiation

- Alternatively polarization (plane in which wave propagates) could be initialized randomly to each photon.

Sampling the pathlength

- Transmission:

$$P(\tau) = T = \exp(-\int_0^s \beta_{\text{ext}} s' ds') = \exp(-\tau)$$

  Probability that photon travels distance τ without interactions.

- Extinction coefficient: $\beta_{\text{ext}} = \sum N_p \cdot C_{\text{ext},p}$

- For randomly oriented particles no difference to scalar radiative transfer

Scattering (randomly oriented particles)

- Sample random number $r \in [0, 2\pi]$ for ϕ_i (isotropic for randomly oriented particles
- Scattering frame of first scattering event:

$$(\mathbf{n_0}, \mathbf{n}_{\phi\mathbf{1}}, \mathbf{n}_{\perp\mathbf{1}} = \mathbf{n_0} \times \mathbf{n}_{\phi\mathbf{1}})$$

- Rotate Stokes vector using

$$\mathbf{L}(\alpha) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(2\alpha) & -\sin(2\alpha) & 0 \\ 0 & \sin(2\alpha) & \cos(2\alpha) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\alpha_1 = \arccos(\mathbf{n}_{\perp\mathbf{1}} \cdot \mathbf{n_z})$$

- i^{th} scattering event:

$$\alpha_i = \arccos(\mathbf{n}_{\perp\mathbf{i}} \cdot \mathbf{n}_{\perp\mathbf{i-1}})$$

$$\mathbf{n}_{\perp\mathbf{i}} = \mathbf{n_{i-1}} \times \mathbf{n}_{\phi\mathbf{i}}$$

Scattering (randomly oriented particles)

- Calculate cross sections for all particle types and molecules

$$\beta_{sca,p} = \frac{2\pi N_p}{I^{inc}} \int_{2\pi} \mathrm{d}\Theta [P_{11,p}(\Theta) I^{inc} + P_{12,p}(\Theta) Q^{inc}]$$

- use random number $r \in [0, 1]$ to decide whether the photon interacts with a cloud droplet/particle, aerosol or molecule, e.g.

$$r \leq \frac{\beta_{\mathrm{sca,l}}}{\sum \beta_{\mathrm{sca,p}}}$$

- Calculate phase function:

$$p(\mathbf{n^{sca}}, \mathbf{n^{inc}}) = \frac{4\pi}{C_{sca} I^{inc}} [P_{11}(\Theta) I^{inc} + P_{12}(\Theta) Q^{inc}]$$

- Calculate scattered Stokes vector

$$\mathbf{I_i^{sca}} = \mathbf{P}(\Theta_i) \mathbf{I_i^{inc}} \tag{1}$$

Scattering (randomly oriented particles)

- Count the photon at the end of it journey, e.g. when it reaches the sensor
  - Rotate Stokes vector back to model frame (x,y,z)
- Sum up weight vectors of all photons $\Rightarrow$ polarized transmittance
- Multiply result with extraterrestrial irradiance $\Rightarrow$ polarized radiance

Scattering (arbitrarily oriented particles)

- phase matrix can only be calculated in the model coordinate frame (x, y, z)
- sample both angles Θ and ϕ using phase function
- no rotation of Stokes vector required
- *practical difficulty:*
  phase matrix depends on four angles (incoming and scattered directions), on wavelength and on effective radius
  $\Rightarrow$ requires a huge amount of computational memory
- The same applies for the extinction matrix and the absorption vector.

- First step: Only *randomly oriented particles* will be included

Calculate optical properties

- spherical particles, *Mie code* by Wiscombe, 1980
  - water droplets and some aerosols
  - database will be generated and included in *libRadtran*
  - can also be used by RT solver *polradtran*

- aspherical particles
  - T-matrix method for rotationally symmetric particles ($x \approx 1$, Mishchenko)
  - geometrical optics ($x \gg 1$, Macke)
  - discrete dipole approximation ($x < 15$, Draine & Flateau)
  - test and select tools that could be included in *libRadtran*

Validation

- Compare to *polRadtran* solver (Evans and Stephens, 1991) that is well validated
- Compare to benchmark results by Collins et al., 1972
- (Polarized UV-radiance measurements by M. Blumthaler)