

# On Modeling Elastic and Inelastic Polarized Radiation Transport in the Earth Atmosphere with Monte Carlo Methods

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# outline

## Introduction and Motivation

- Atmospheric Radiation Transport
- Remote Sensing
- Standard DOAS

## Monte Carlo RTM

- RTE Integral Form
- Monte Carlo Method
- Functionals

## Ring Effect Modelling

- RRS Modified RTE
- Path Generation
- Local Estimates
- Elastic Biasing
- Validation

## Synthesis: DOAS 2.0

- Variance Side Effects
- Conclusions
- Fin

## Postambel

- Theory
- Polarization
- Derivatives

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# Naming Optical Properties



- ▶ merely elastic **scattering** (s) on N<sub>2</sub>, O<sub>2</sub>, Ar molecules (Rayleigh) and on particles (Mie),  
**absorption** (a) on O<sub>3</sub>, H<sub>2</sub>O, CO<sub>2</sub> and CH<sub>4</sub>,  
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$$\vec{\omega} \cdot \vec{\nabla} R(\vec{r}, \vec{\omega}) = -\varepsilon_e(\vec{r}) R(\vec{r}, \vec{\omega}) + \frac{\varepsilon_s(\vec{r})}{4\pi} \int R(\vec{r}, \vec{\omega}') P(\vec{r}, \vec{\omega}') d\vec{\omega}' \quad (2)$$

# Airborne Spectroscopy



DLR Falcon



DLR Falcon on the ground



DLR HALO

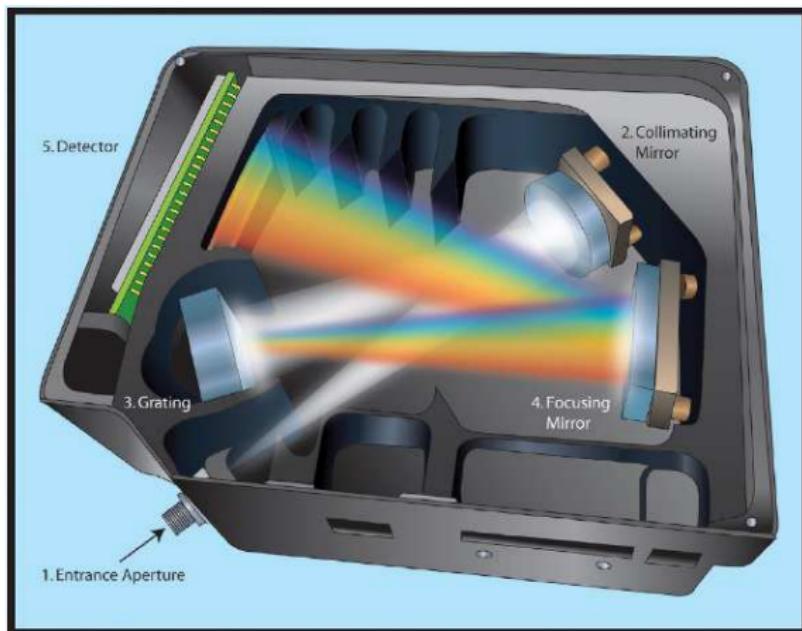


NASA GlobalHawk

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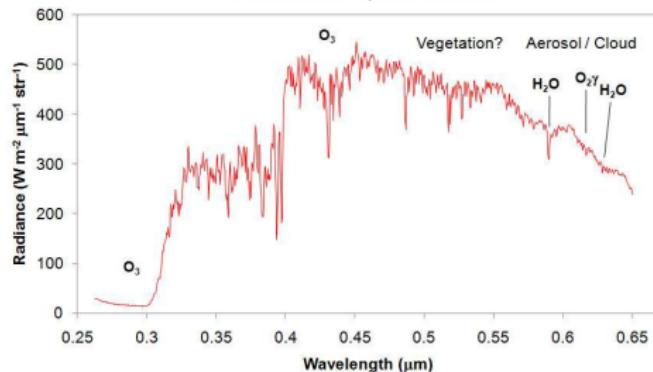


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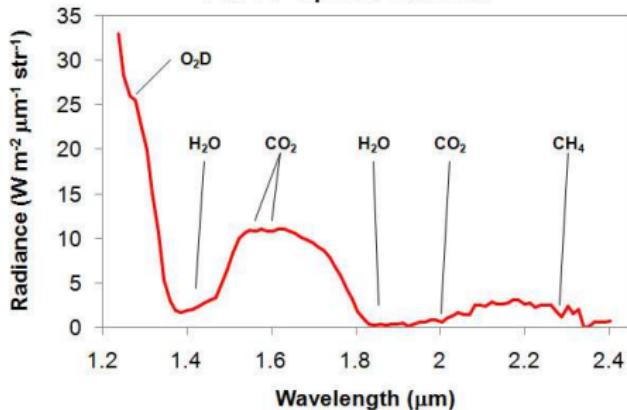


# Airborne Spectroscopy

UV/Visible Spectrometer

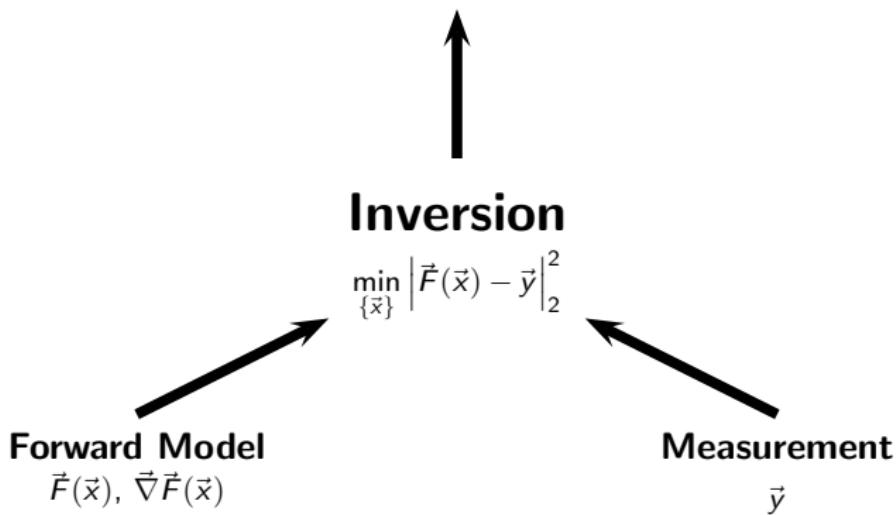


NIR1 Spectrometer

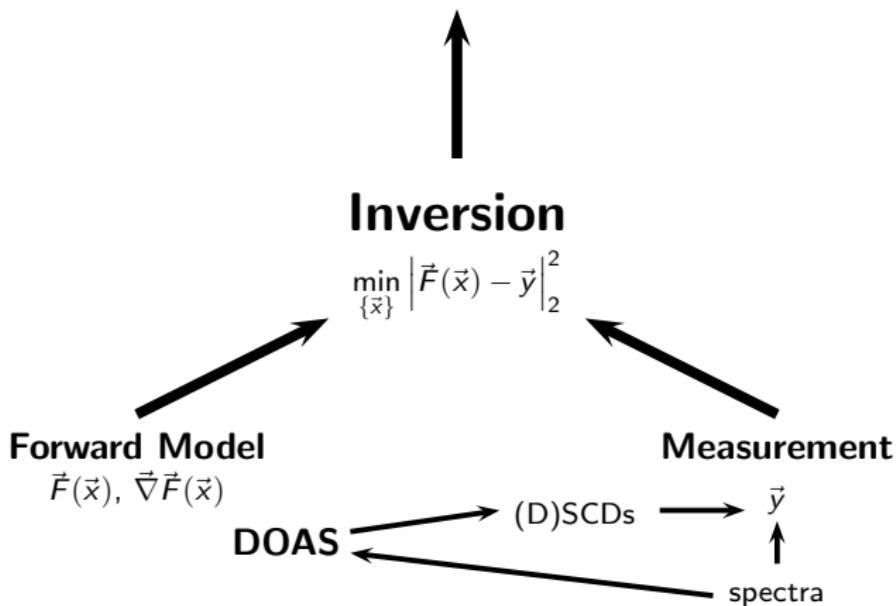


Source:  
NASA quicklook

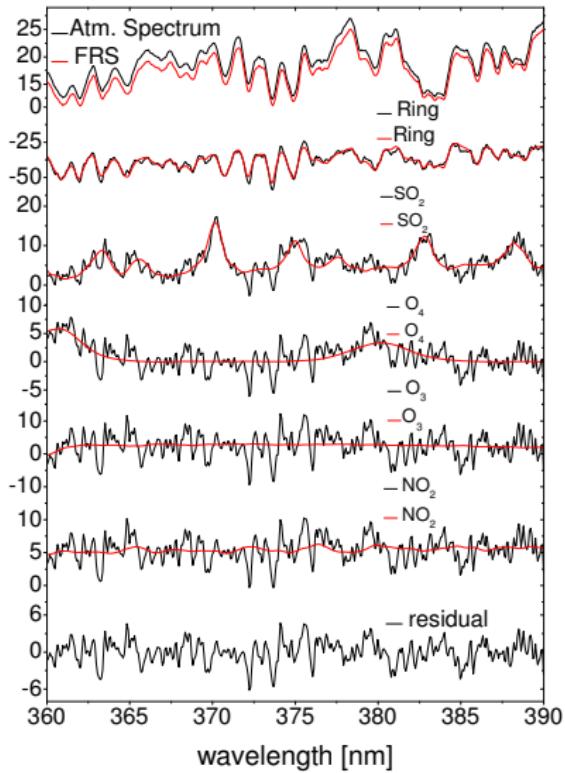
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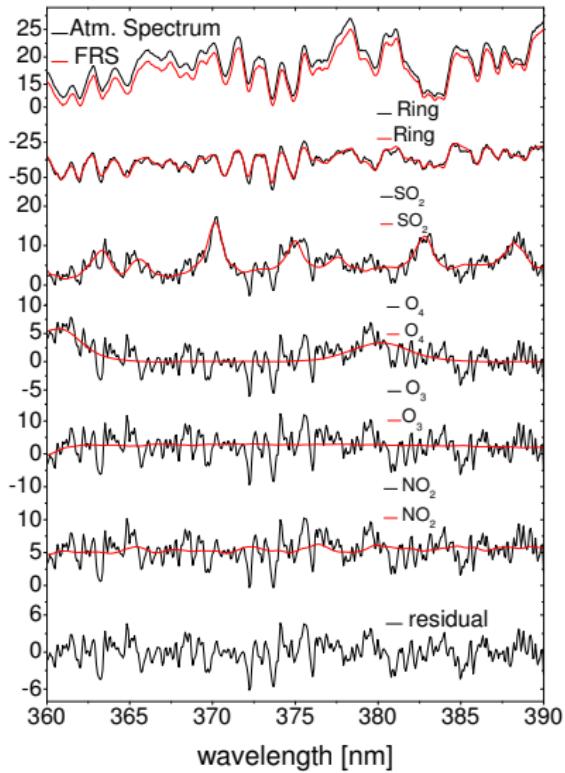


## Standard DOAS



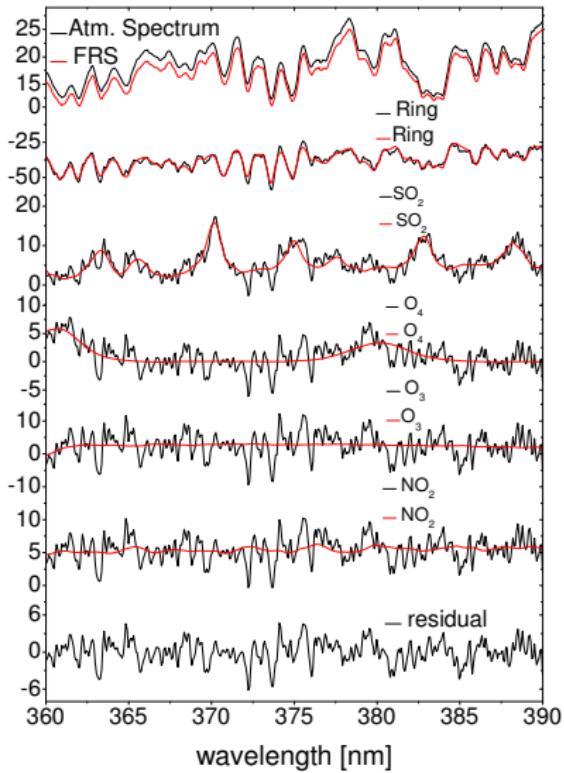
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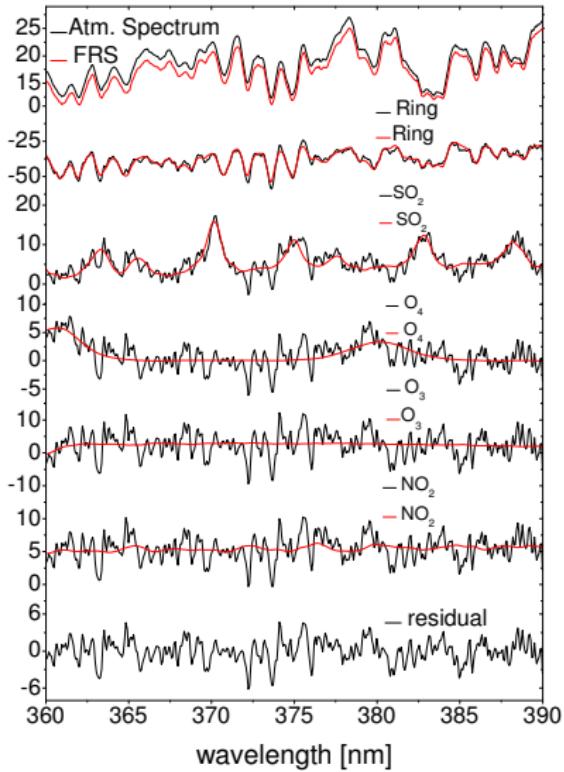
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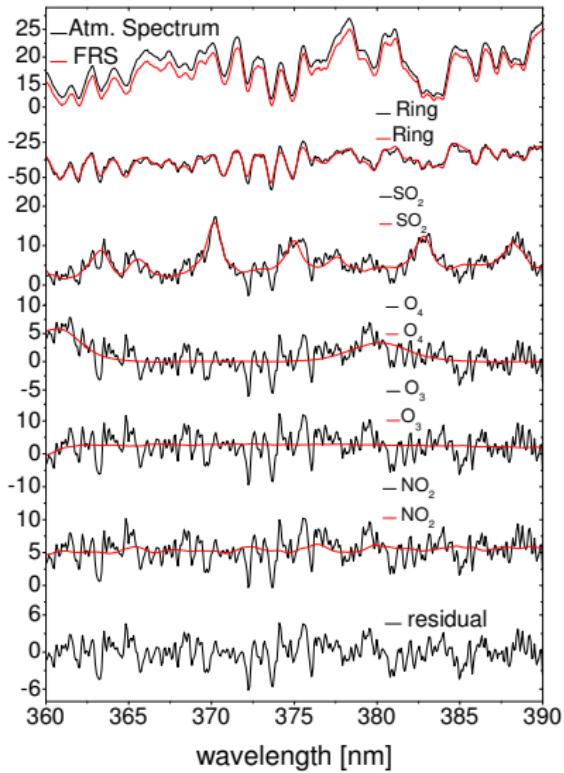
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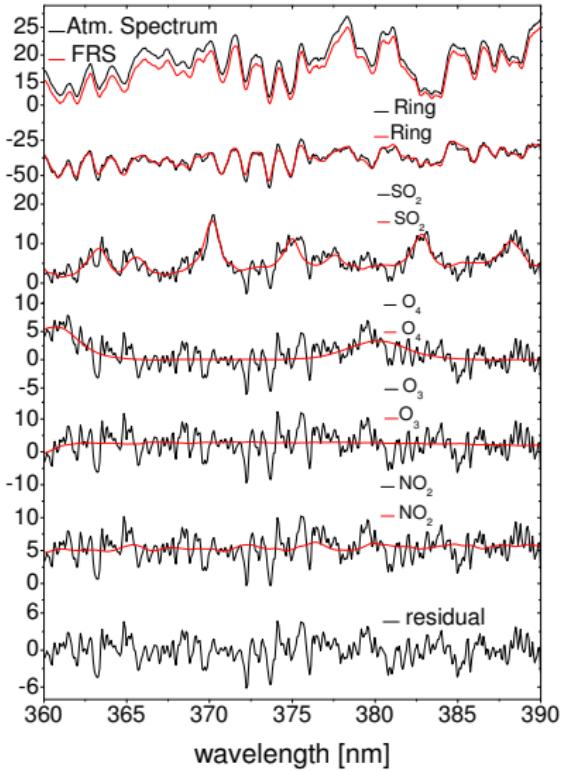
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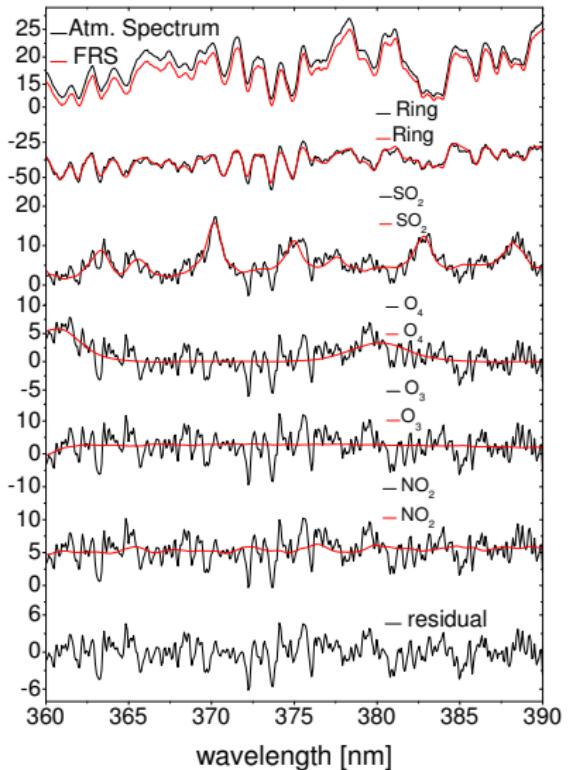
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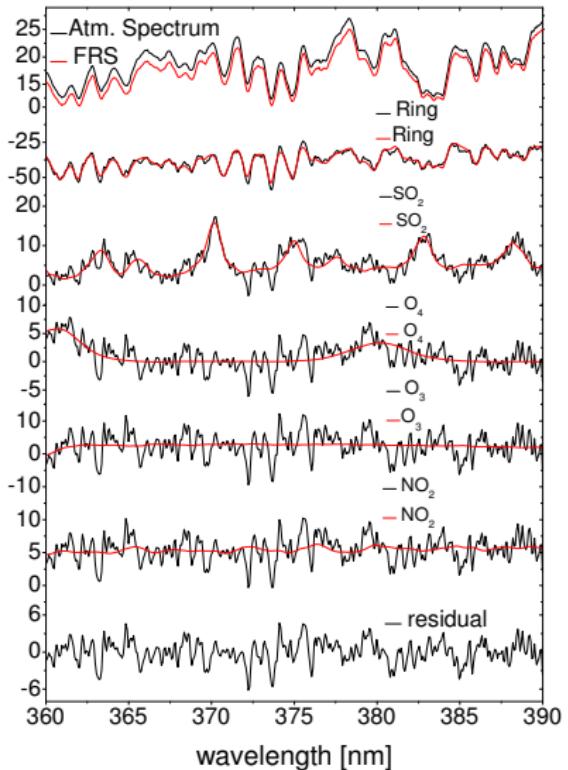
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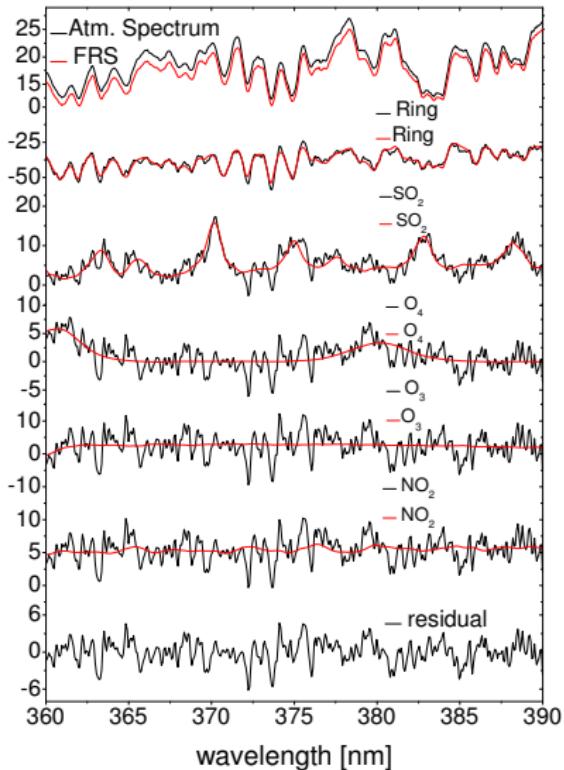
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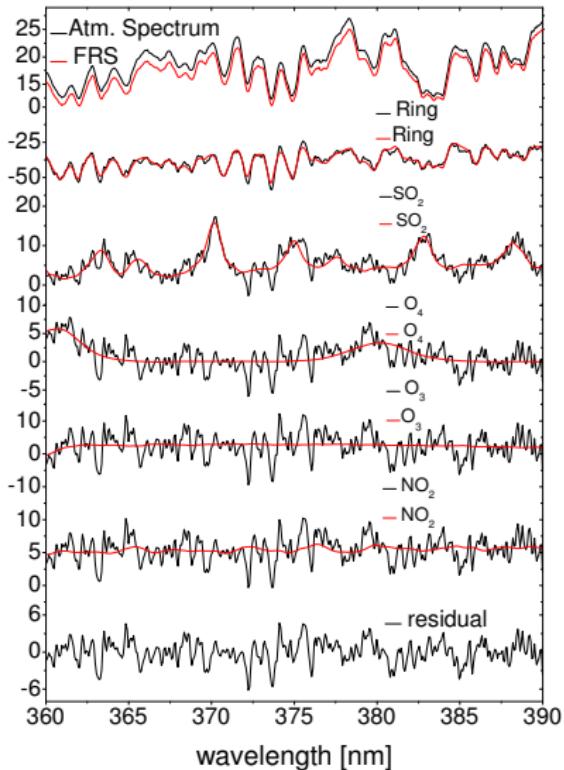
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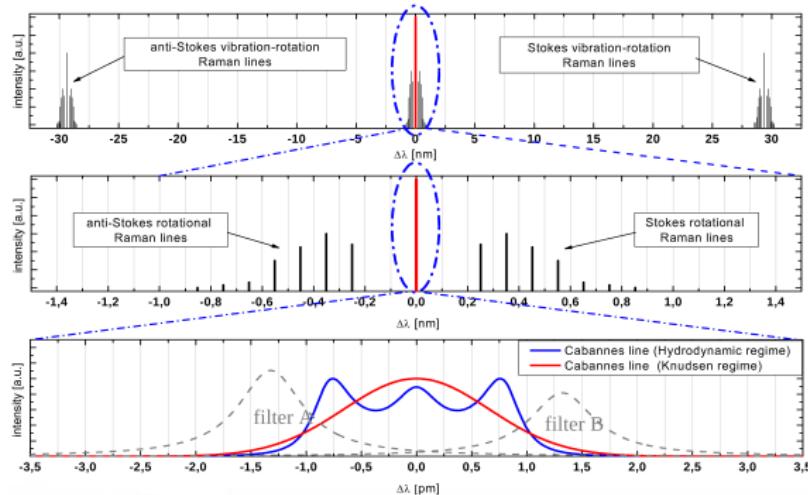


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- ▶ **Ring effect modelling error rest structures?**

# Rotational Raman Scattering - Ring Effect

Andrew Young on Rayleigh Scattering [Young, 1981]:

*Molecular scattering consists of Rayleigh scattering and vibrational Raman scattering. The Rayleigh scattering consists of rotational Raman lines and the central Cabannes line. The Cabannes line is composed of the Brillouin doublet and the central Gross or Landau-Placzek line. None of the above is completely coherent. The term "Rayleigh line" should never be used.*



**Figure:** Plot from: Oliver Reitebuch, Benjamin Witschas, Ofelia Vieitez, Eric-Jan van Duijn, Willem van de Water, Wim Ubachs: Rayleigh-Brillouin Scattering in N<sub>2</sub>, O<sub>2</sub>, and Air, 33rd Lidar Working Group, Destin (FL), 2-4 Feb 2010 Institut für Physik der Atmosphäre, DLR Oberpfaffenhofen. Details in the main text.

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# Scalar Elastic IRTE

$$f(\vec{r}, \vec{\omega}) = \int_G \int_{4\pi} k_p [(\vec{r}', \vec{\omega}') \rightarrow (\vec{r}, \vec{\omega})] f(\vec{r}', \vec{\omega}') \frac{\delta\left(\vec{\omega} - \frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|}\right)}{|\vec{r}-\vec{r}'|^2} d\vec{r}' d\vec{\omega}' + f_0(\vec{r}, \vec{\omega})$$

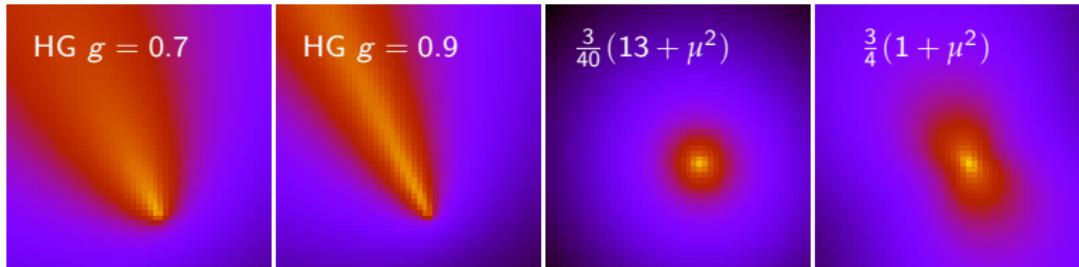
$f(\vec{r}, \vec{\omega}) := \varepsilon(\vec{r}) R(\vec{r}, \vec{\omega})$  collision density  $\left[ \frac{W}{m^3 sr} \right]$

$R(\vec{r}, \vec{\omega})$  radiance  $\left[ \frac{W}{m^2 sr} \right]$

$\varepsilon(\vec{r}), \varepsilon_s(\vec{r})$  total extinction, scattering coefficient  $\left[ \frac{1}{m} \right]$

$f_0(\vec{r}, \vec{\omega})$  initial collision density

$k_p [(\vec{r}', \vec{\omega}') \rightarrow (\vec{r}, \vec{\omega})]$  transition density



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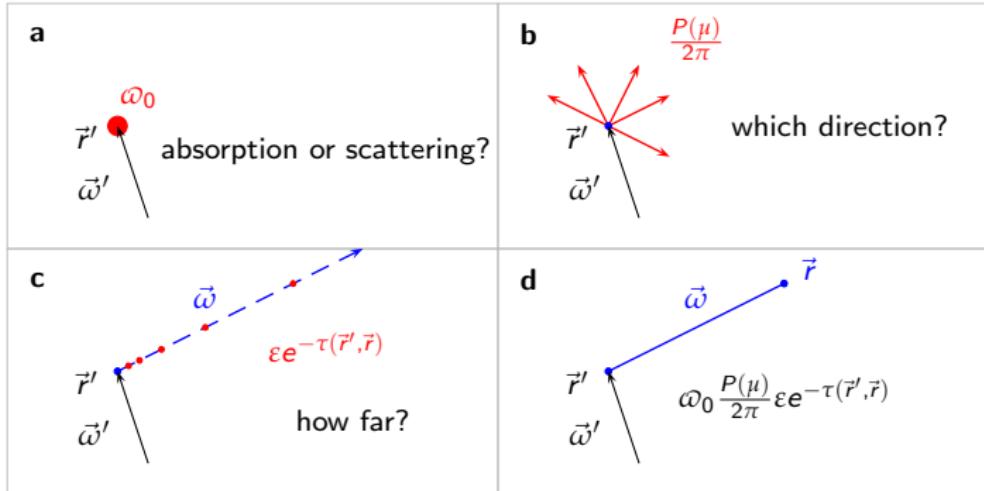
$$\tilde{f} = \lim_{N \rightarrow \infty} \underbrace{T \circ \cdots \circ T}_{N-5} \circ (K^5 f_0 + K^4 f_0 + K^3 f_0 + K^2 f_0 + K f_0 + f_0)$$

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# Scalar Elastic Monte Carlo



**Figure:** Schematic depictions scalar elastic path generation. In total, the procedure generates an event  $\vec{x}_{n+1} = (\vec{r}, \vec{\omega})$  from its predecessor  $\vec{x}_n$  represented here by  $\vec{r}'$  and  $\vec{\omega}'$ , i.e. simulates  $k^\dagger(\vec{x}_n \rightarrow \vec{x}_{n+1})$

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- ▶ raytracing: estimate K integrals with random numbers

## Patchy Cloud Scatter Events

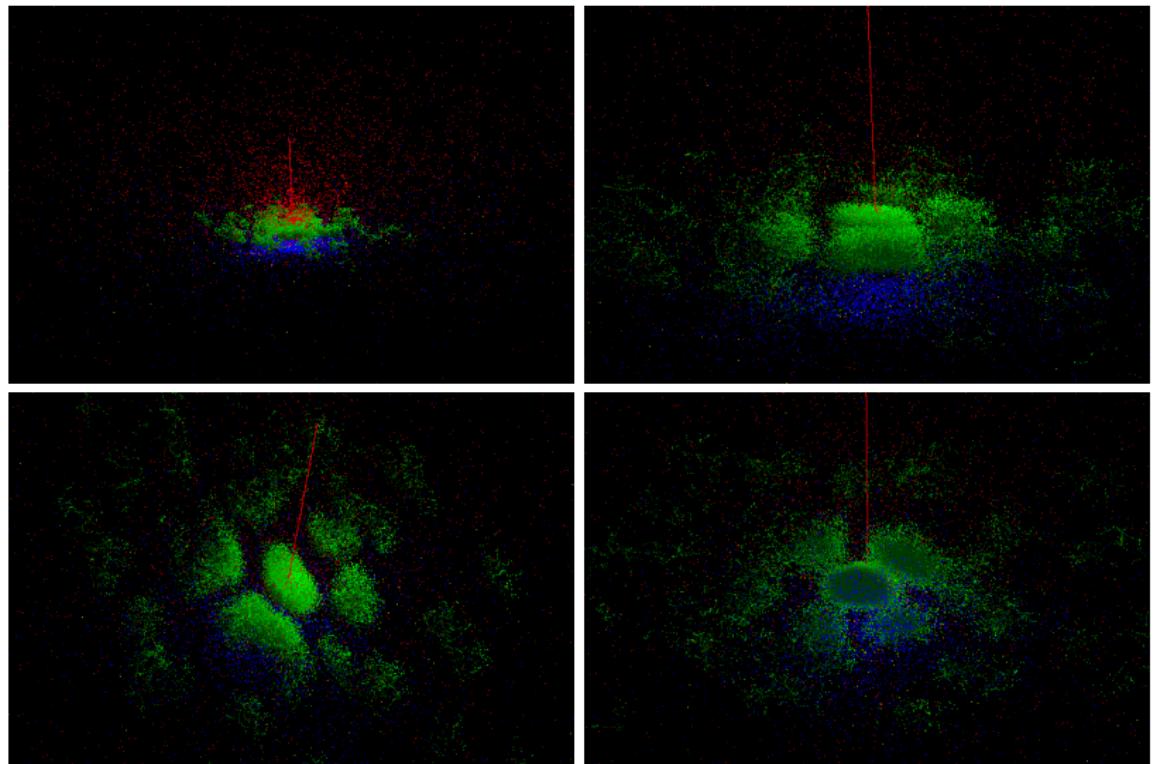


Figure: Scatter and absorption events: **Rayleigh**, **cloud particle**, **absorption** and **ground scattering**

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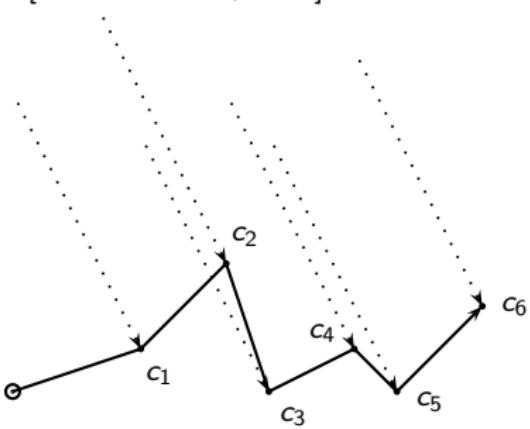
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- ▶ estimates of the intensity: local estimate method [Marchuk et al., 1976]

$$I \approx \sum_{n=0}^{\#\text{s.e.}} c_n \quad (4)$$

$$c_n = \frac{1}{4\pi} P(\vec{r}_n, \mu_n^*) \exp(-\tau_n^*) \quad (5)$$

$$\tau_n^* = \int_{\vec{r}_n}^{\text{Sun}} \varepsilon(\vec{r}(l)) dl \quad (6)$$



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$$\varepsilon_s(\lambda) = \varepsilon_{s,\text{el}}(\lambda) + \varepsilon_{\text{RRS,out}}(\lambda) \quad \varepsilon_e(\lambda) = \varepsilon_{e,\text{el}}(\lambda) + \varepsilon_{\text{RRS,out}}(\lambda) \quad (7)$$

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- ▶ add RRS source term:

$$\frac{1}{4\pi} \int \int_{4\pi} \varepsilon_{\text{RRS}}(\lambda' \rightarrow \lambda) P_{\text{RRS}}(\mu) R(\vec{\omega}', \lambda') d\vec{\omega}' d\lambda' \quad (8)$$

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$$\varepsilon_s(\lambda) = \varepsilon_{s,\text{el}}(\lambda) + \varepsilon_{\text{RRS,out}}(\lambda) \quad \varepsilon_e(\lambda) = \varepsilon_{e,\text{el}}(\lambda) + \varepsilon_{\text{RRS,out}}(\lambda) \quad (7)$$

- ▶ modify source term:

- ▶ add RRS source term:

$$\frac{1}{4\pi} \int \int_{4\pi} \varepsilon_{\text{RRS}}(\lambda' \rightarrow \lambda) P_{\text{RRS}}(\mu) R(\vec{\omega}', \lambda') d\vec{\omega}' d\lambda' \quad (8)$$

- ▶ rewrite elastic source term in integral form:

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- ▶ combine everything:

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where

$$P(\mu, \lambda' \rightarrow \lambda) = \frac{1}{\varepsilon_s(\lambda)} \left\{ \varepsilon_{s,\text{el}}(\lambda') P_{\text{el}}(\mu, \lambda') \delta(\lambda' - \lambda) + \varepsilon_{\text{RRS}}(\lambda' \rightarrow \lambda) P_{\text{RRS}}(\mu) \right\} \quad (11)$$

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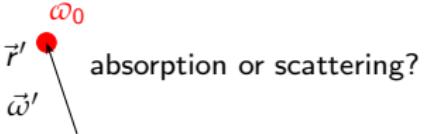
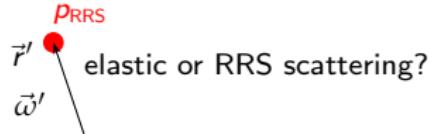
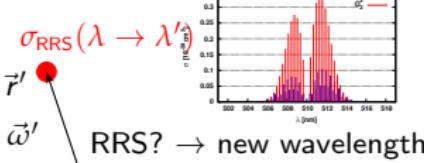
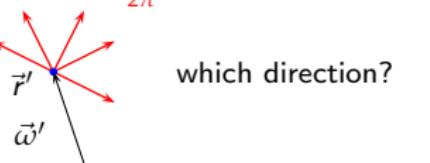
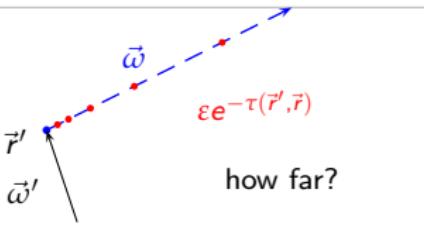
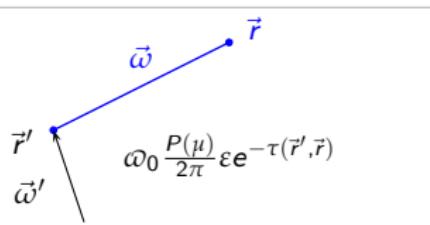
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- ▶ algebraic structure identical to elastic case → **similar path generation scheme**

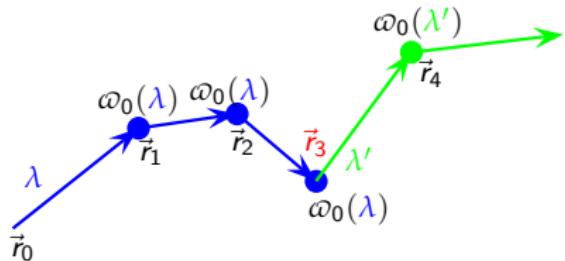
# Scalar Inelastic Path Generation

<b>a</b>  <p><math>\omega_0</math></p> <p><math>\vec{r}'</math></p> <p><math>\vec{\omega}'</math></p> <p>absorption or scattering?</p>	<b>a'</b>  <p><math>P_{RRS}</math></p> <p><math>\vec{r}'</math></p> <p><math>\vec{\omega}'</math></p> <p>elastic or RRS scattering?</p>
<b>a''</b>  <p><math>\sigma_{RRS}(\lambda \rightarrow \lambda')</math></p> <p><math>\vec{r}'</math></p> <p><math>\vec{\omega}'</math></p> <p>RRS? <math>\rightarrow</math> new wavelength</p>	<b>b</b>  <p><math>\frac{P(\mu)}{2\pi}</math></p> <p><math>\vec{r}'</math></p> <p><math>\vec{\omega}'</math></p> <p>which direction?</p>
<b>c</b>  <p><math>\vec{\omega}</math></p> <p><math>\varepsilon e^{-\tau(\vec{r}', \vec{r})}</math></p> <p><math>\vec{r}'</math></p> <p><math>\vec{\omega}'</math></p> <p>how far?</p>	<b>d</b>  <p><math>\vec{\omega}</math></p> <p><math>\omega_0 \frac{P(\mu)}{2\pi} \varepsilon e^{-\tau(\vec{r}', \vec{r})}</math></p> <p><math>\vec{r}'</math></p> <p><math>\vec{\omega}'</math></p>

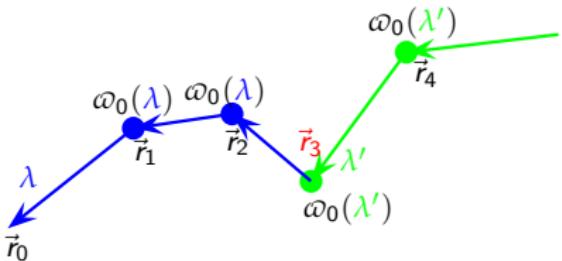
**Note:** only one random number used in a, a' and a''!

## Adjoint Correction Weights

path generation:

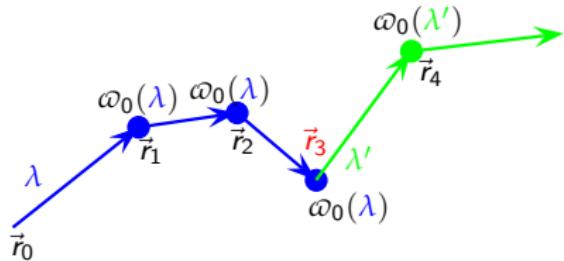


local estimation:

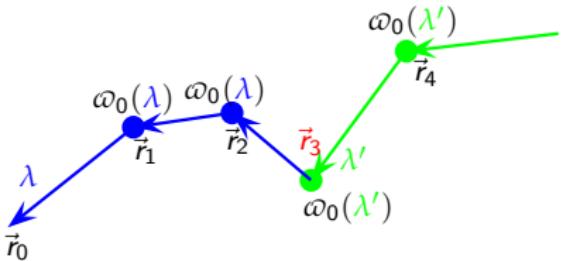


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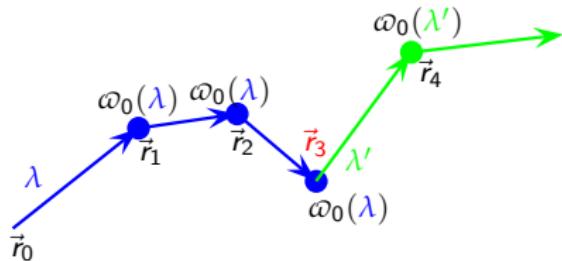
local estimation:



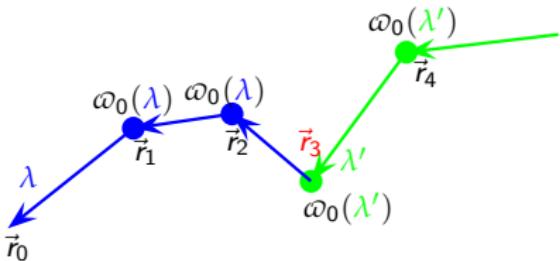
- ▶ physical interpretation of trajectories → adjoint correction weight

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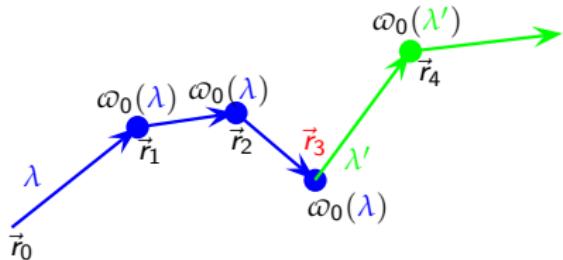


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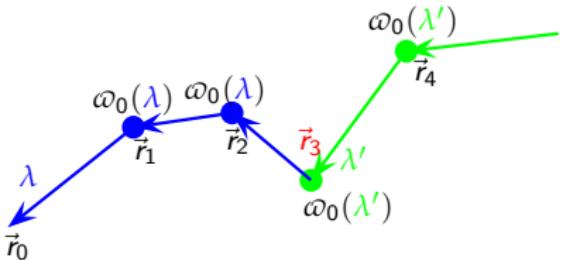
$$k_{\lambda \rightarrow \lambda'} = \varepsilon(\lambda) \omega_0(\lambda) p_{\text{RRS}}(\lambda) \frac{\varepsilon_{\text{RRS}}(\lambda' \rightarrow \lambda)}{\varepsilon_{\text{RRS,in}}(\lambda)} \quad \doteq \quad \frac{\varepsilon_{\text{RRS,out}}(\lambda)}{\varepsilon_{\text{RRS,in}}(\lambda)} \varepsilon_{\text{RRS}}(\lambda' \rightarrow \lambda) \quad (12)$$

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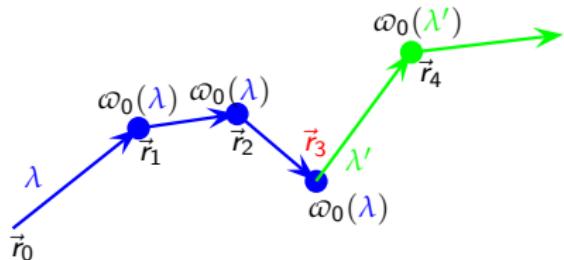
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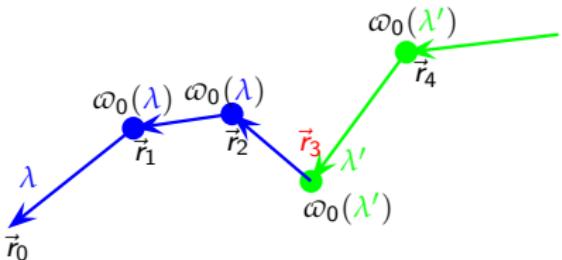
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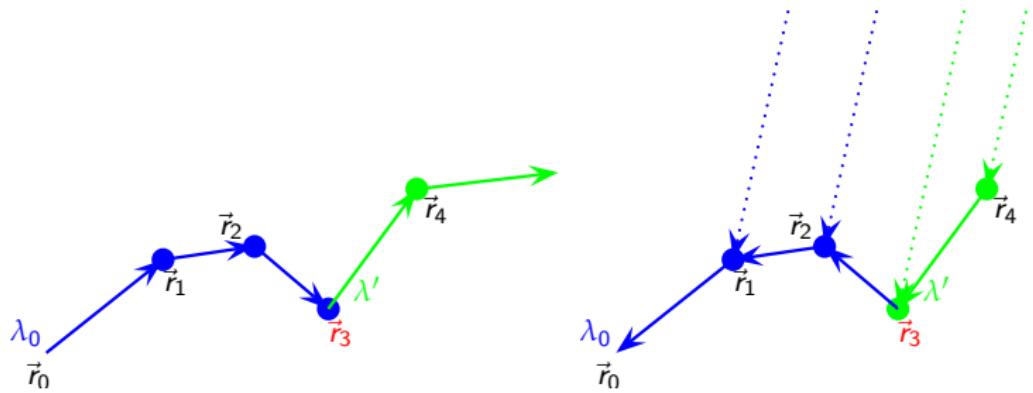
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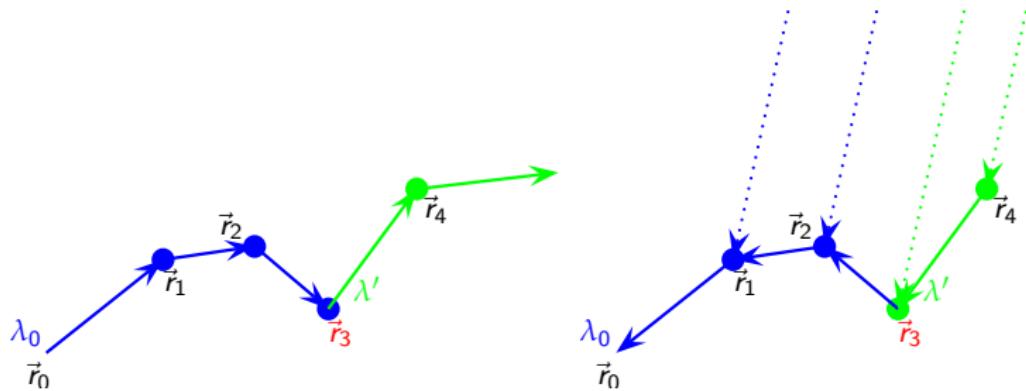
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## Local Estimates With Rotational Raman Scattering

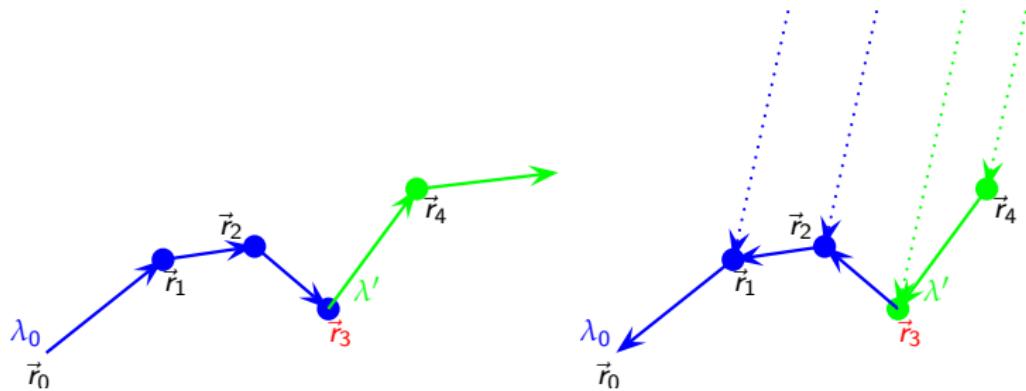


## Local Estimates With Rotational Raman Scattering



- ▶ local estimate  $c_{l.e.}$  calculation analog to elastic simulation scheme

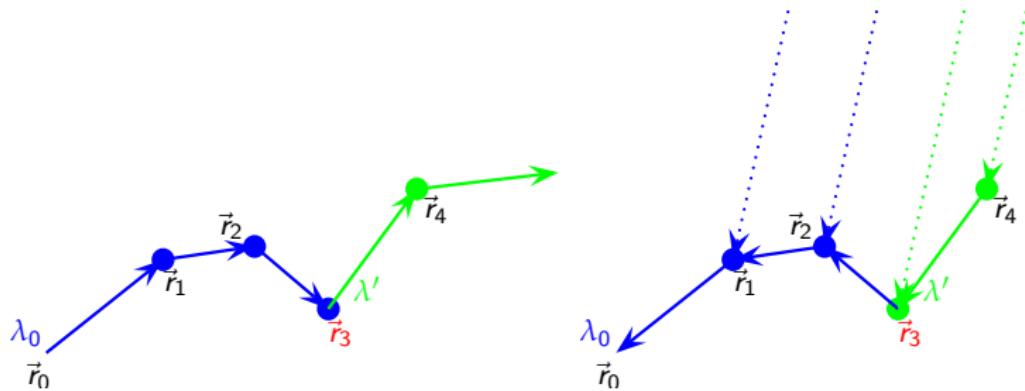
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$$c_{l.e.} = (1 - p_{RRS}(\lambda)) \frac{P_{el}(\mu^*, \lambda)}{4\pi} F(\lambda) + p_{RRS}(\lambda) w_{IS, RRS}(\lambda' \rightarrow \lambda) \frac{P_{RRS}(\mu^*)}{4\pi} F(\lambda') \quad (14)$$

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- ▶ total intensity estimate:

$$I \approx \sum_{n=1} \prod_{i=1}^{n-1} w_{IS, RRS}(\lambda_i \rightarrow \lambda_{i-1}) c_{l.e., n}(\lambda_{n-1}, \lambda_n) \quad (15)$$

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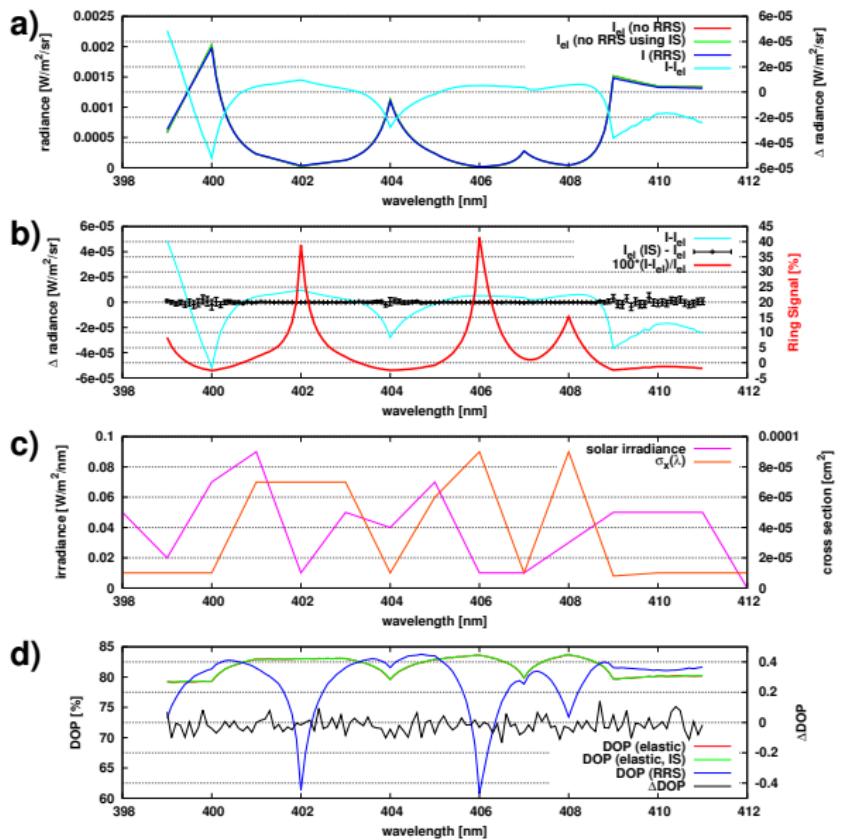
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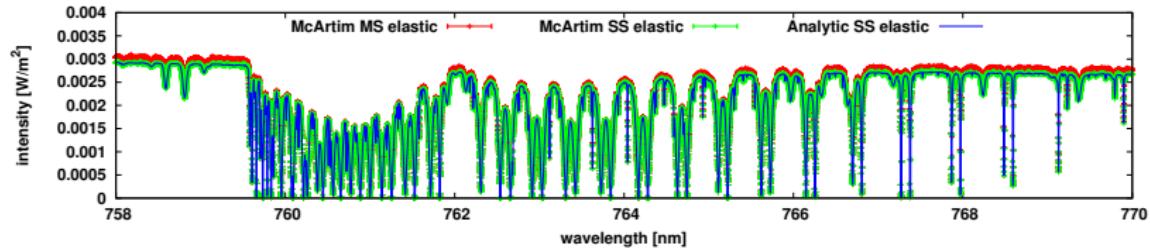
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# Test of Elastic Biasing

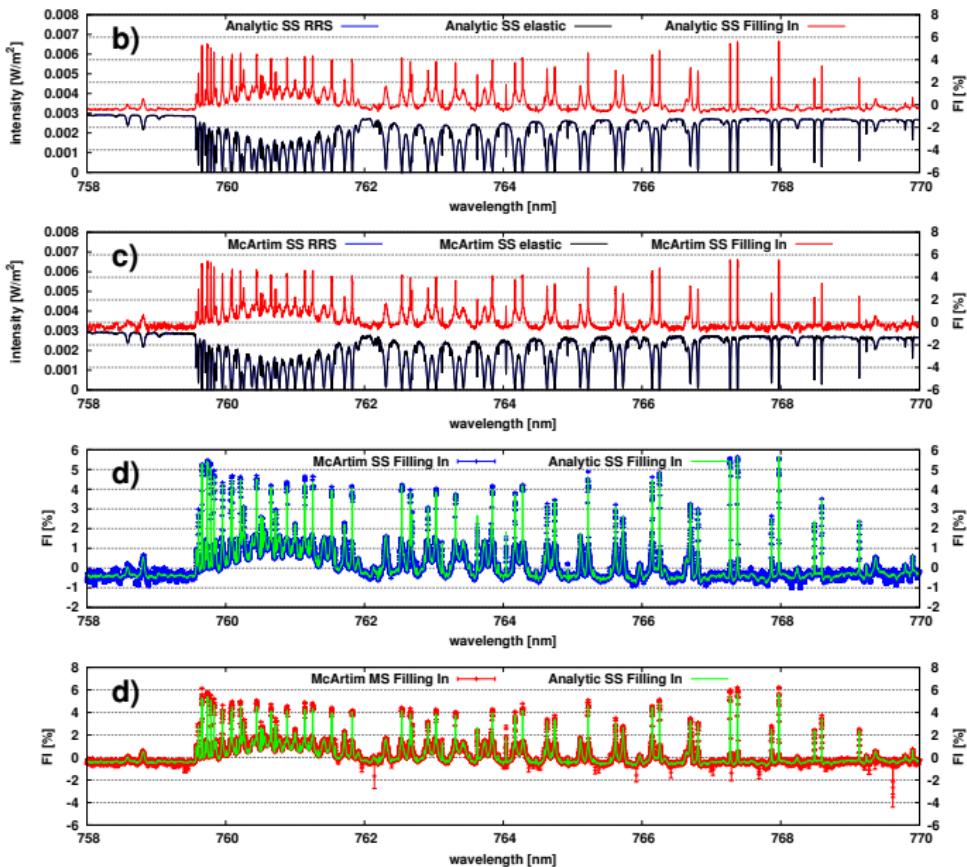


# Single Scattering Test I

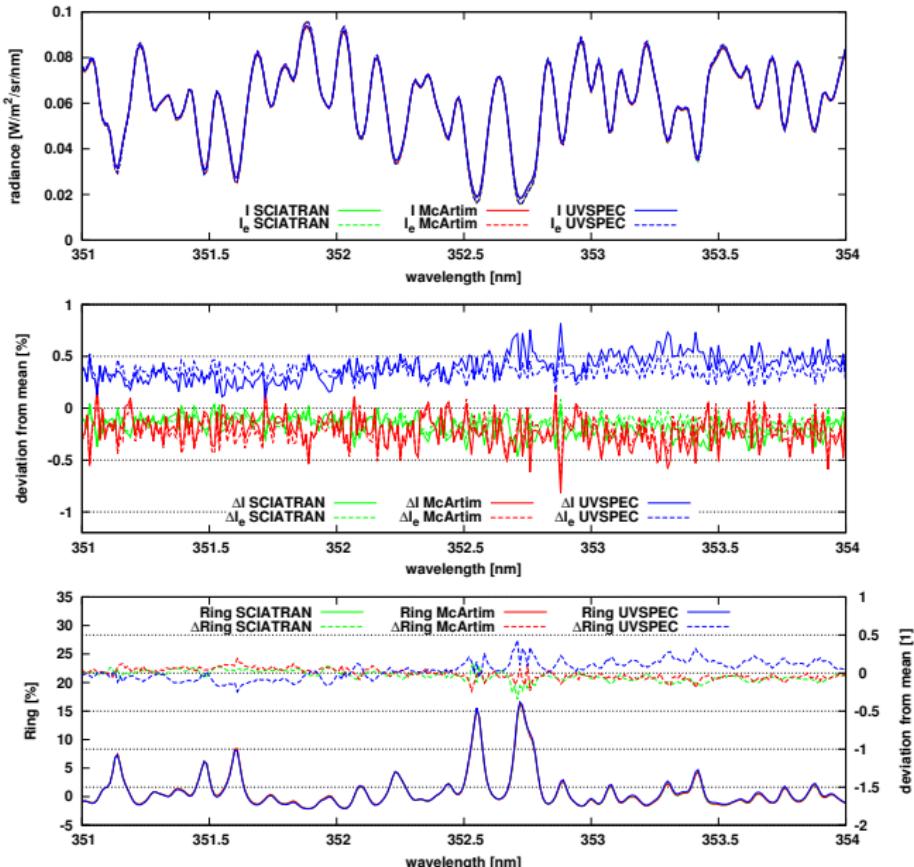


**Figure:** Simulated O<sub>2</sub> A band spectrum for a satellite nadir geometry with 45° SZA and  $\delta$ -FOV. The surface albedo is zero and no aerosols or clouds are present. The red curve shows the (multiple scattering) RTE solution, green is the result from the single scattering approximation (Neumann series truncation) and the blue line shows the result of the analytic single scattering model.

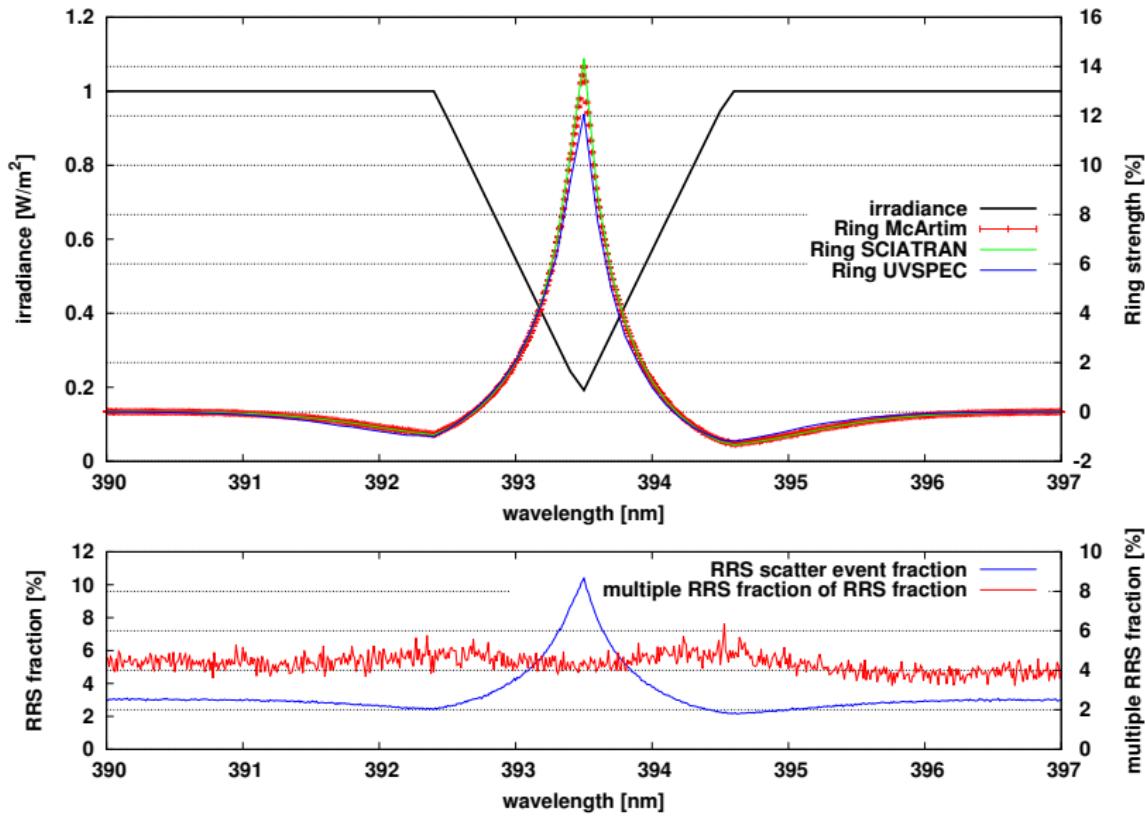
# Single Scattering Test II



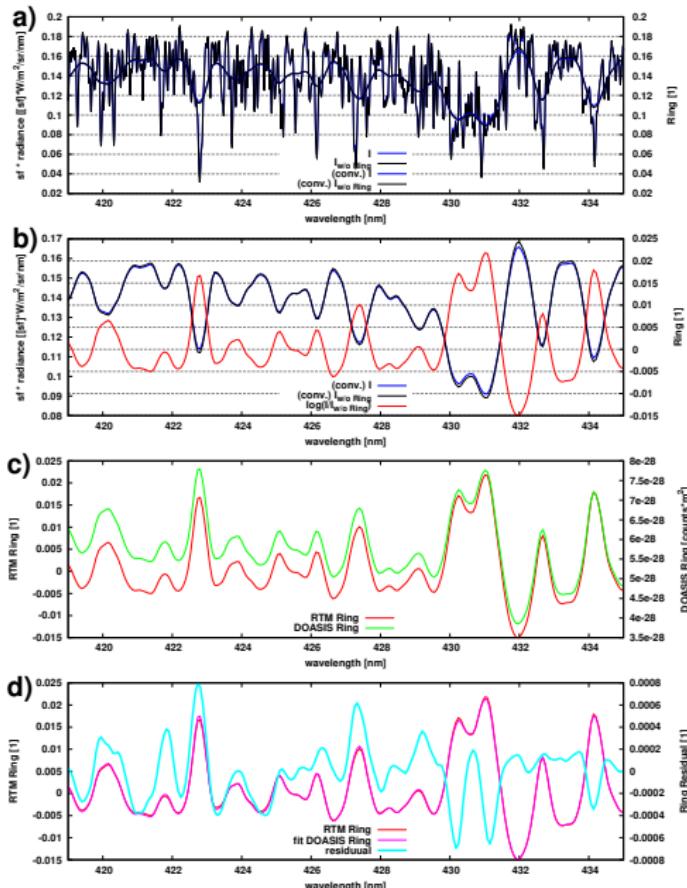
# Multiple Scattering I



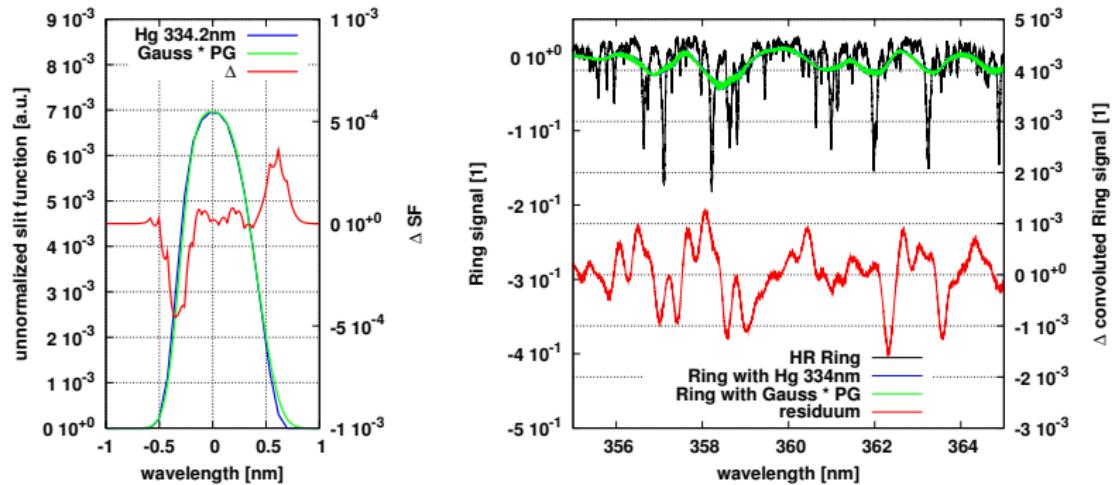
## Multiple Scattering II



# DOASIS and the Ring



# Influence of the Line Shape



**Figure:** The effect of choosing the wrong slit function for DOAS modeling. **Left panel:** a mercury lamp emission line as it is observed on a typical spectrometer (green) and a Gaussian fit to its shape (blue). The **right panel** shows a high resolution Shefov-Ring spectrum (black) as it would be measured with the slit functions shown in the left panel (same colors) and the corresponding DOAS fit residuum (red) of relative strength of  $2.5 \cdot 10^{-3}$  peak-to-peak.

# outline

small outline inbetween

## Introduction and Motivation

- Atmospheric Radiation Transport
- Remote Sensing
- Standard DOAS

## Monte Carlo RTM

- RTE Integral Form
- Monte Carlo Method
- Functionals

## Ring Effect Modelling

- RRS Modified RTE
- Path Generation
- Local Estimates
- Elastic Biasing
- Validation

## Synthesis: DOAS 2.0

- Variance Side Effects
- Conclusions
- Fin

## Postambel

- Theory
- Polarization
- Derivatives

## Removal of the Ring Effect and Absorption I

- ▶ remove absorption and Ring effect from spectra

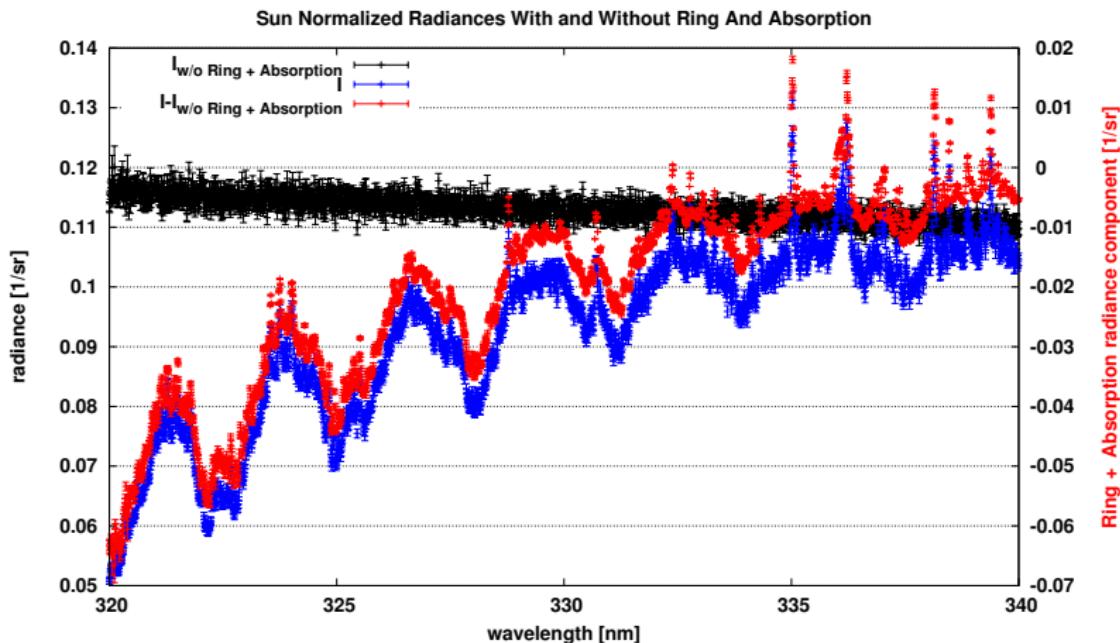
$$w_{\text{elb},n}^* = \exp(\tau_{\text{abs},n}) w_{\text{elb},n} \quad (16)$$

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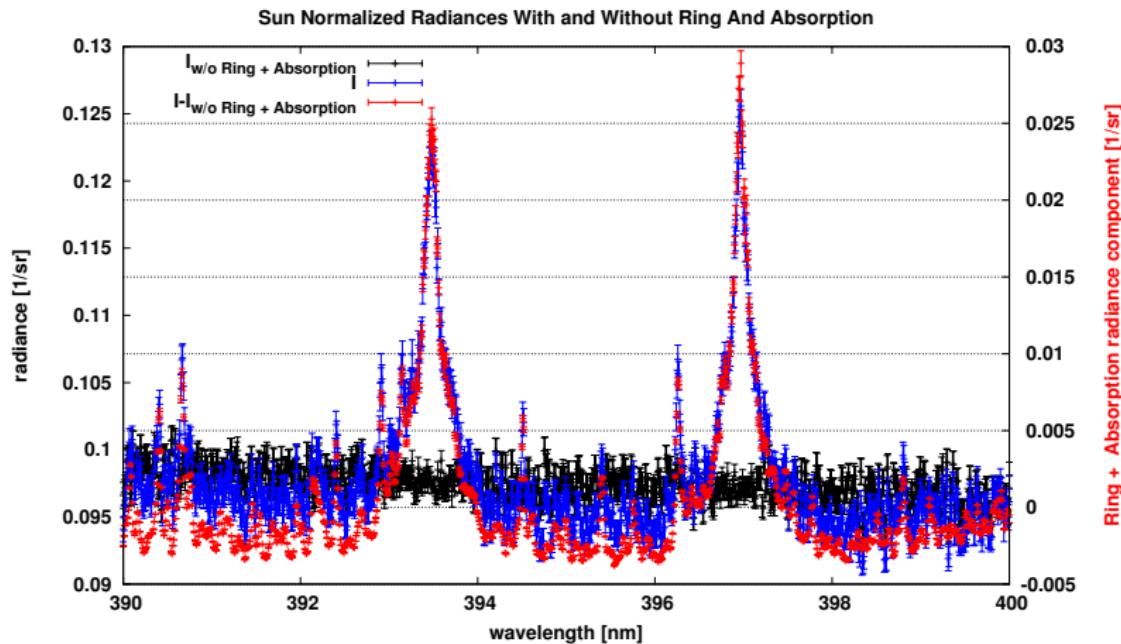
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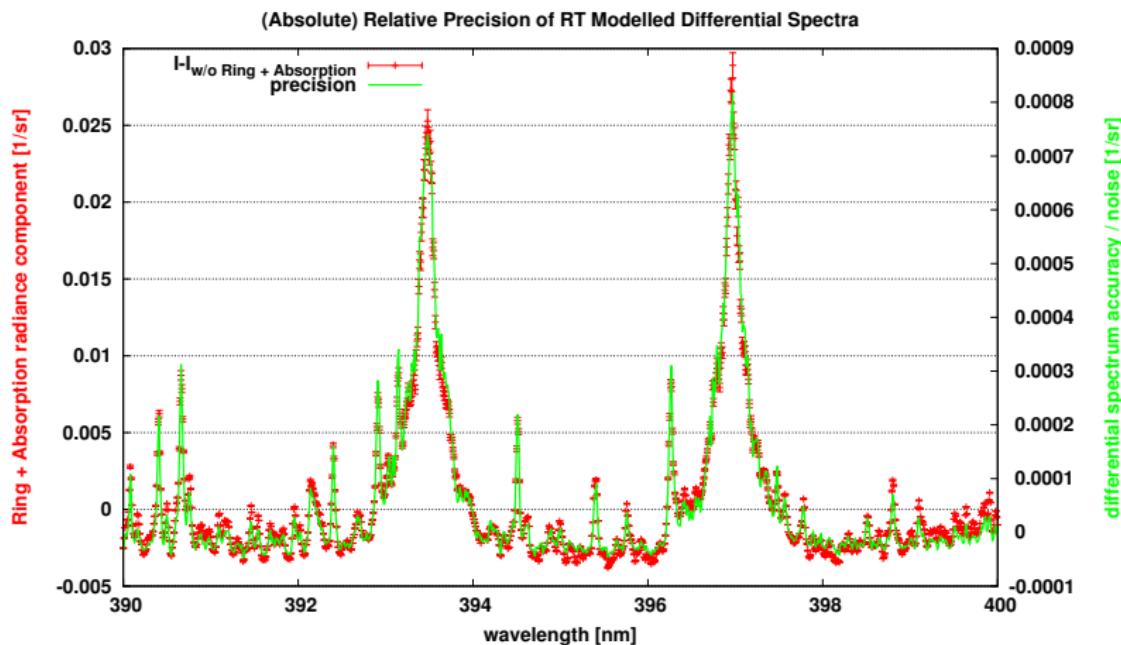
- leads to



# Removal of the Ring Effect and Absorption II



# Removal of the Ring Effect and Absorption III



# Conclusions

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## Summary

- ▶ basis: scalar elastic 3D Monte Carlo RTM
- ▶ importance sampling technique: estimation of more complicated RTE functionals
- ▶ this thesis:
  - ▶ intensity derivatives from logarithmic derivatives of the transport kernel
  - ▶ polarized (vector) intensities from product of Stokes scattering matrices
  - ▶ filling in / ring structure from elastic biasing

## Spectroscopy and Remote Sensing

- ▶ advanced instrument characterisation required (slit function)
- ▶ steps towards absolute calibration
- ▶ more sensors, more simultaneous measurements (observation points)

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Thank you Uni Leipzig, IUP Heidelberg, MPI Chemie Mainz!

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# outline

small outline inbetween

## Introduction and Motivation

- Atmospheric Radiation Transport
- Remote Sensing
- Standard DOAS

## Monte Carlo RTM

- RTE Integral Form
- Monte Carlo Method
- Functionals

## Ring Effect Modelling

- RRS Modified RTE
- Path Generation
- Local Estimates
- Elastic Biasing
- Validation

## Synthesis: DOAS 2.0

- Variance Side Effects
- Conclusions
- Fin

## Postambel

- Theory
- Polarization
- Derivatives

# Importance Sampling

- ▶ principle:

Integral	Estimate
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- i.e.: differences in the kernels are corrected by the weight product

# Elastic Biasing Theory I

- ▶ section of backward trajectory:

$$\cdots \rightarrow \begin{pmatrix} \vec{r}_{n-1} \\ \vec{\omega}_{n-1} \\ \lambda_{n-1} \end{pmatrix} \rightarrow \begin{pmatrix} \vec{r}_n \\ \vec{\omega}_n \\ \lambda_n \end{pmatrix} \rightarrow \cdots \quad (20)$$

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## Elastic Biasing Theory II

- ▶ resulting “elastic biasing” importance sampling weight

$$w_{IS,el,n} = \frac{k_{el^*, \vec{r}_n \rightarrow \vec{r}_{n-1}}}{k_{el} + RRS, \vec{r}_{n-1} \rightarrow \vec{r}_n} \quad (24)$$

$$= \exp(-\Delta\tau_{0,n}) \cdot \frac{\varepsilon_{s,el^*}(\vec{r}_n, \lambda_0) P_{el^*}(\vec{r}_n, \mu_n, \lambda_0)}{\varepsilon_s(\vec{r}_n, \lambda_{n-1}) P(\vec{r}_n, \mu_n, \lambda_{n-1})} \quad (25)$$

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$$w_{elb,n} = \prod_{i=1}^{n-1} w_{IS,el,i} = e^{-\Delta\tau_{0,n,\text{total}}} \cdot \prod_{i=1}^{n-1} \left[ \begin{cases} \frac{[\varepsilon_{s,el^*} P_{el^*}(\mu_i)](\lambda_0)}{[\varepsilon_{s,el} P_{el}(\mu_i)](\lambda_{i-1})} & \text{elastic event} \\ \frac{[\varepsilon_{s,el^*} P_{el^*}(\mu_i)](\lambda_0)}{[\varepsilon_{RRS} P_{RRS}(\mu_i)](\lambda_{i-1})} & \text{else} \end{cases} \right] (\vec{r}_i) \quad (27)$$

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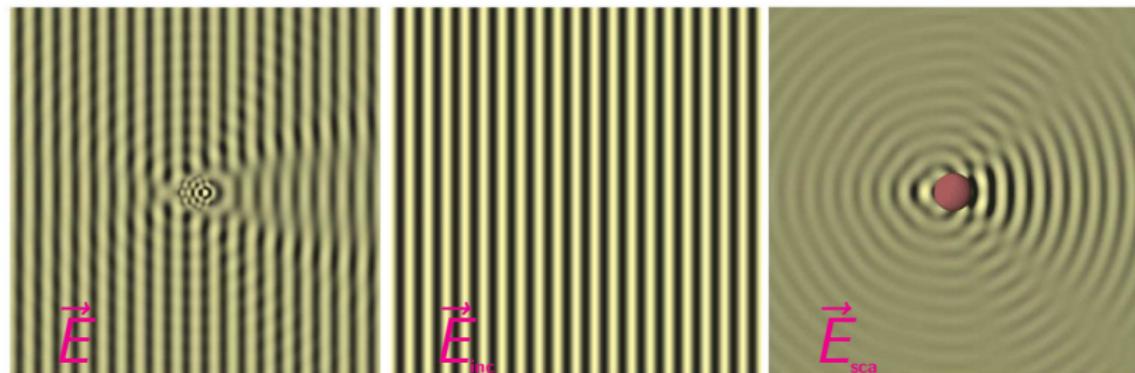
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- ▶ modified local estimate:

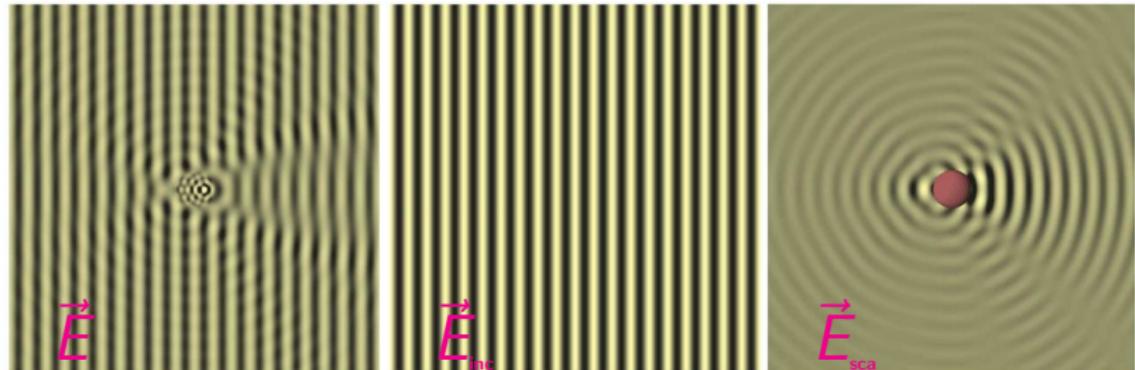
$$c_{\text{elastic I.e., } n} = w_{elb,n} \cdot e^{-\tau_{el^*, \vec{r} \rightarrow \vec{r}_{\text{Sun}}}(\lambda_0)} P_{el^*}(\vec{r}_n, \mu_n^*, \lambda_0). \quad (29)$$

## Photon Spin / Wave Polarization I



**Figure:** The total, incident and scattered field in a scattering process. The incident wave is a linearly polarized plane wave. The refractive index of the particle (red ball) is considerably larger causing a fine ripple structure in the internal field in  $\vec{E}$ . Figure taken and modified from [Mishchenko, 2009].

# Photon Spin / Wave Polarization I

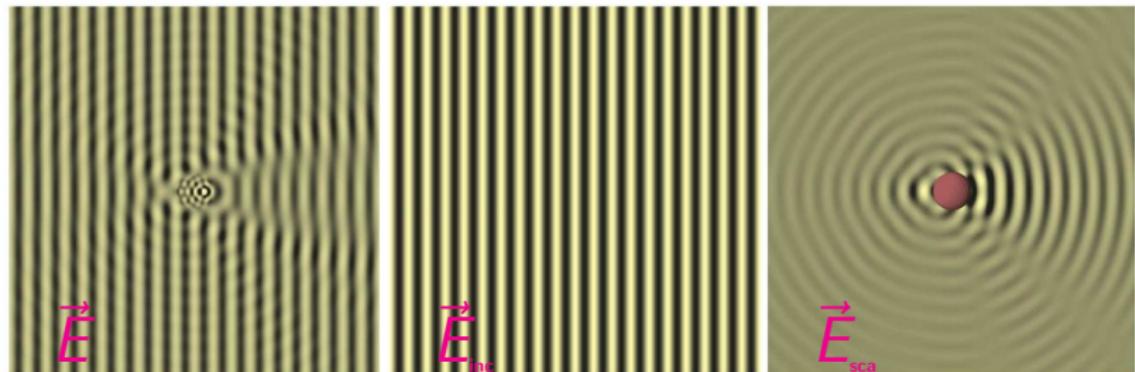


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- ▶ incident single photon / wave

$$\vec{E} = (E_{0x} \vec{e}_x + E_{0y} \vec{e}_y) e^{i(kz - \omega t)} \quad \text{with} \quad E_{0x} = |E_{0x}| e^{i\varphi} \quad \text{and} \quad E_{0y} = |E_{0y}| e^{i(\varphi + \delta)} \quad (30)$$

# Photon Spin / Wave Polarization I



**Figure:** The total, incident and scattered field in a scattering process. The incident wave is a linearly polarized plane wave. The refractive index of the particle (red ball) is considerably larger causing a fine ripple structure in the internal field in  $\vec{E}$ . Figure taken and modified from [Mishchenko, 2009].

- ▶ incident single photon / wave

$$\vec{E} = (E_{0x} \vec{e}_x + E_{0y} \vec{e}_y) e^{i(kz - \omega t)} \quad \text{with} \quad E_{0x} = |E_{0x}| e^{i\varphi} \quad \text{and} \quad E_{0y} = |E_{0y}| e^{i(\varphi + \delta)} \quad (30)$$

- ▶ total electric field in presence of a scatter object

$$\vec{E}_{\text{inc}} = \vec{E}_{\text{inc}} + \vec{E}_{\text{sca}}. \quad (31)$$

## Photon Spin / Wave Polarization II

- ▶ scattering amplitudes  $S_i$ :

$$\begin{pmatrix} E_{\parallel \text{sca}} \\ E_{\perp \text{sca}} \end{pmatrix} = \frac{ie^{ik(r-z)}}{kr} \begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix} \begin{pmatrix} E_{\parallel \text{inc}} \\ E_{\perp \text{inc}} \end{pmatrix} \quad (32)$$

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- ▶ Stokes: description of fields with real numbers

$$\begin{pmatrix} F \\ Q \\ U \\ V \end{pmatrix} = \frac{k}{2\omega\mu} \begin{pmatrix} E_{0x}E_{0x}^* + E_{0y}E_{0y}^* \\ E_{0x}E_{0x}^* - E_{0y}E_{0y}^* \\ E_{0x}E_{0y}^* + E_{0y}E_{0x}^* \\ i(E_{0x}E_{0y}^* - E_{0y}E_{0x}^*) \end{pmatrix} = \frac{k}{2\omega\mu} \begin{pmatrix} |E_{0x}|^2 + |E_{0y}|^2 \\ |E_{0x}|^2 - |E_{0y}|^2 \\ 2|E_{0x}||E_{0y}|\cos(\delta) \\ 2|E_{0x}||E_{0y}|\sin(\delta) \end{pmatrix}. \quad (33)$$

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- scattering in Stokes' language:

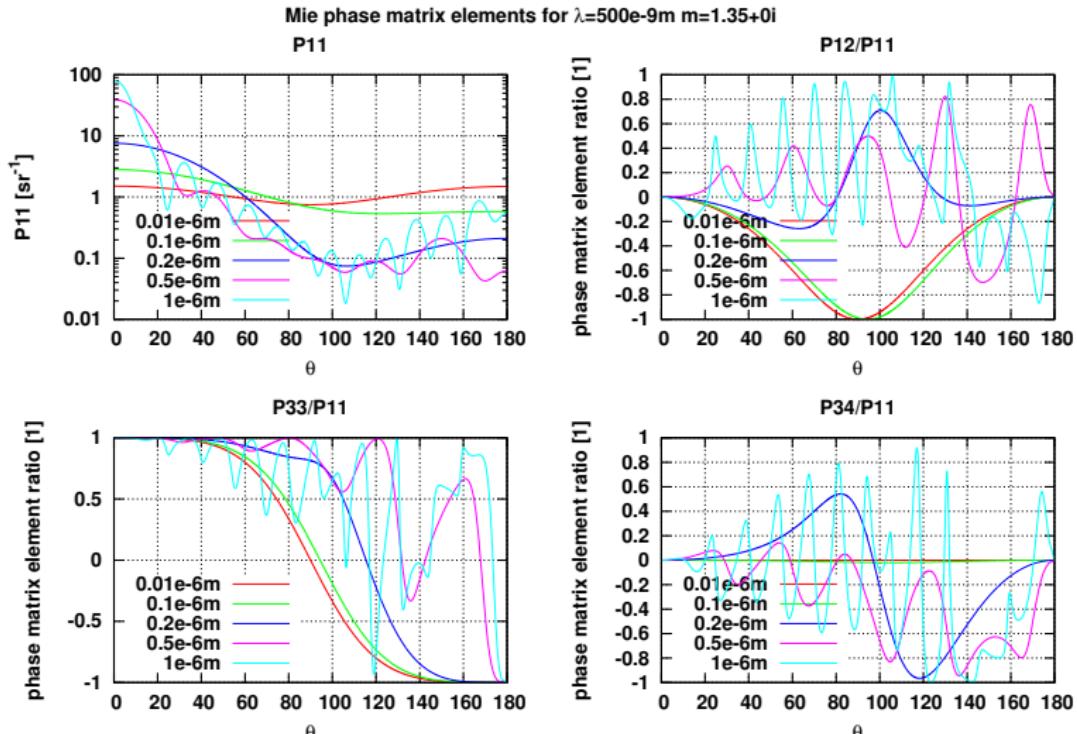
$$\begin{pmatrix} F_{\text{sca}} \\ Q_{\text{sca}} \\ U_{\text{sca}} \\ V_{\text{sca}} \end{pmatrix} = \frac{1}{k^2 r^2} \mathbf{Z}(\vec{\omega}_{\text{inc}}, \vec{\omega}_{\text{sca}}) \begin{pmatrix} F_{\text{inc}} \\ Q_{\text{inc}} \\ U_{\text{inc}} \\ V_{\text{inc}} \end{pmatrix} \quad (34)$$

with

$$\mathbf{Z}(\vec{\omega}_{\text{inc}}, \vec{\omega}_{\text{sca}}) = \mathbf{L}(\alpha_{\text{sca}}) \begin{pmatrix} P_{11}(\mu_s) & P_{12}(\mu_s) & 0 & 0 \\ P_{21}(\mu_s) & P_{22}(\mu_s) & 0 & 0 \\ 0 & 0 & P_{33}(\mu_s) & P_{34}(\mu_s) \\ 0 & 0 & P_{43}(\mu_s) & P_{44}(\mu_s) \end{pmatrix} \mathbf{L}(\alpha_{\text{inc}}) \quad (35)$$

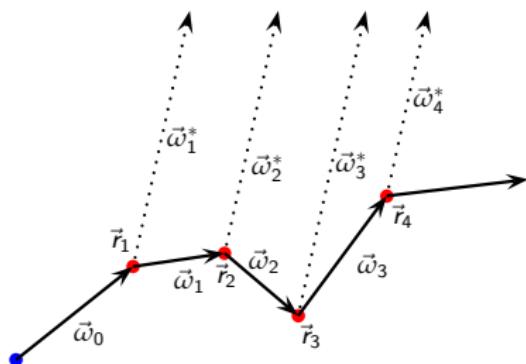
where  $\mu_s = \vec{\omega}_{\text{inc}} \cdot \vec{\omega}_{\text{sca}}$  and  $\mathbf{L}(\alpha)$  are so called Stokes rotations.

## Phase Matrix Example



**Figure:** Example of water droplet phase matrix elements as a function of the scatter angle obtained from Gustav Mie's theory.

## Transport of the Polarization State

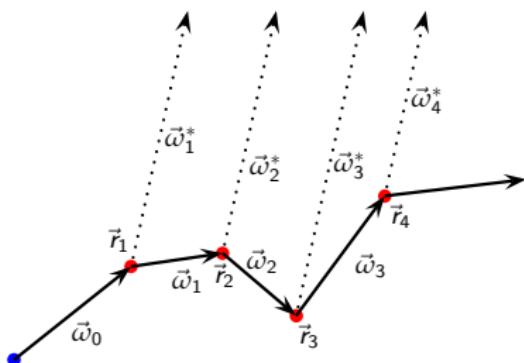


- importance sampling: polarized intensity functional from scalar intensity functional:

$$\vec{I} = \frac{1}{\varepsilon} \sum_{n=0}^{\infty} (\vec{\Psi}, \mathbf{K}^{\dagger n} \vec{\varphi}) \quad (36)$$

(39)

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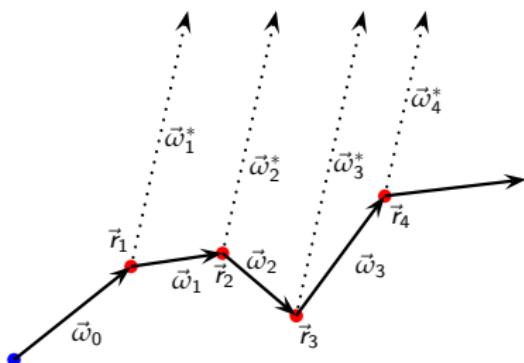
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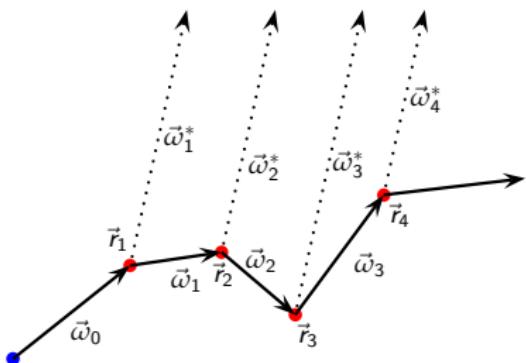
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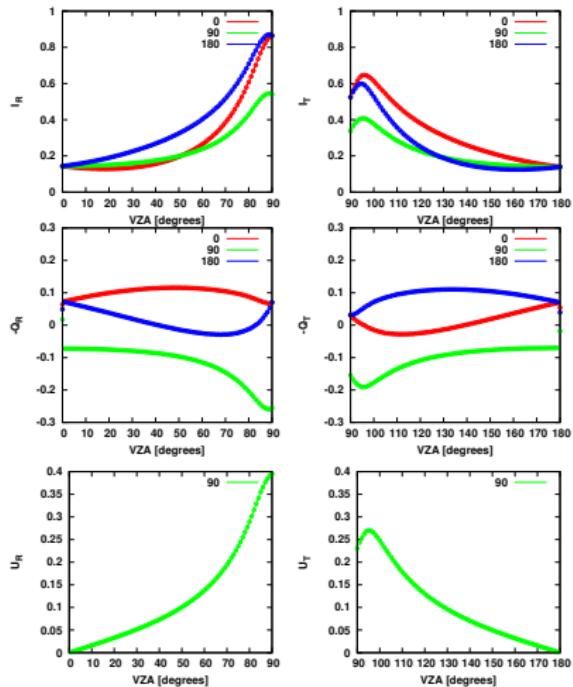
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$$\frac{k^\dagger(\vec{x}_{n-1} \rightarrow \vec{x}_n)}{k^\dagger(\vec{x}_{n-1} \rightarrow \vec{x}_n)} \cdots \frac{k^\dagger(\vec{x}_0 \rightarrow \vec{x}_1)}{k^\dagger(\vec{x}_0 \rightarrow \vec{x}_1)} \vec{\varphi}(\vec{x}_0) d\vec{x}_0 \dots d\vec{x}_n \quad (38)$$

$$\stackrel{\text{LE}}{\approx} \# \text{s.e.} \prod_{n=0}^{n-1} \frac{\mathbf{Z}^T(\vec{r}_n, \vec{\omega}_{n-1}, \vec{\omega}_n)}{P_{11}(\vec{r}_n, \vec{\omega}_{n-1}, \vec{\omega}_n)} \mathbf{Z}^T(\vec{r}_n, \vec{\omega}_{n-1}, \vec{\omega}_n^*) \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \exp(-\tau_n^*) \quad (39)$$

# Validation Of The Polarization Simulation I



**Figure:** Shown are reflected (left column) and transmitted (right column) Stokes vector intensity components for a one layered plane parallel pure molecular (Rayleigh) atmosphere over a black ground. Solid lines: SCIA TRAN model, points and errorbars: McArtim. Reproduction of Fig. 2 from [Kokhanovsky et al., 2010] with McArtim results.

## Validation Of The Polarization Simulation II

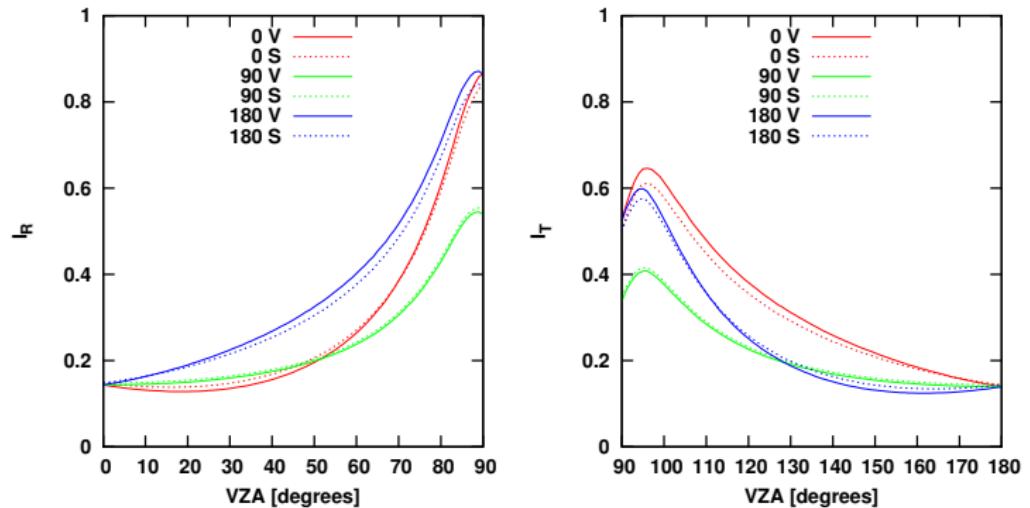


Figure: Comparison of scalar and vector intensities.

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- ▶ validation by self consistence test (next slide):

1. calculate  $I(\xi)$  and  $D_\xi I(\xi)$  for a range  $[\xi_A, \xi_B]$
2. fit  $h(\xi)$  to  $I(\xi)$  and compare  $D_\xi h(\xi)$  with  $D_\xi I(\xi)$

# Validation of Derivatives

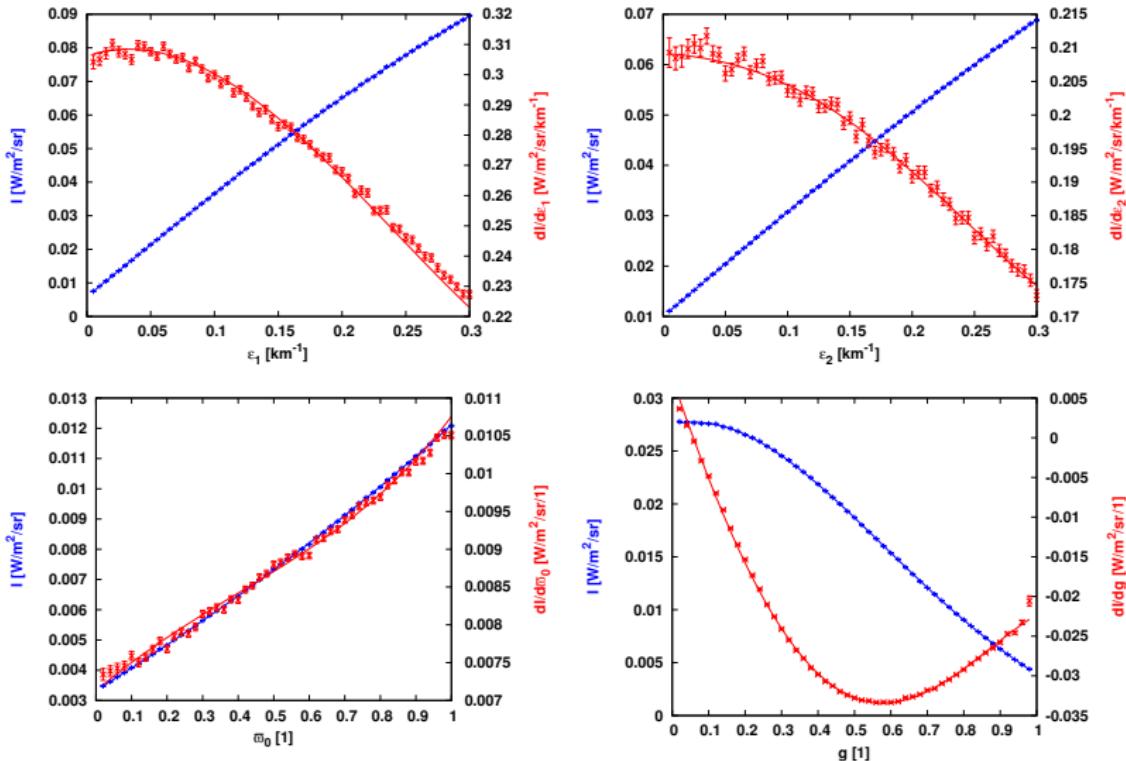


Figure: Validation of 1<sup>st</sup> order scalar intensity derivatives

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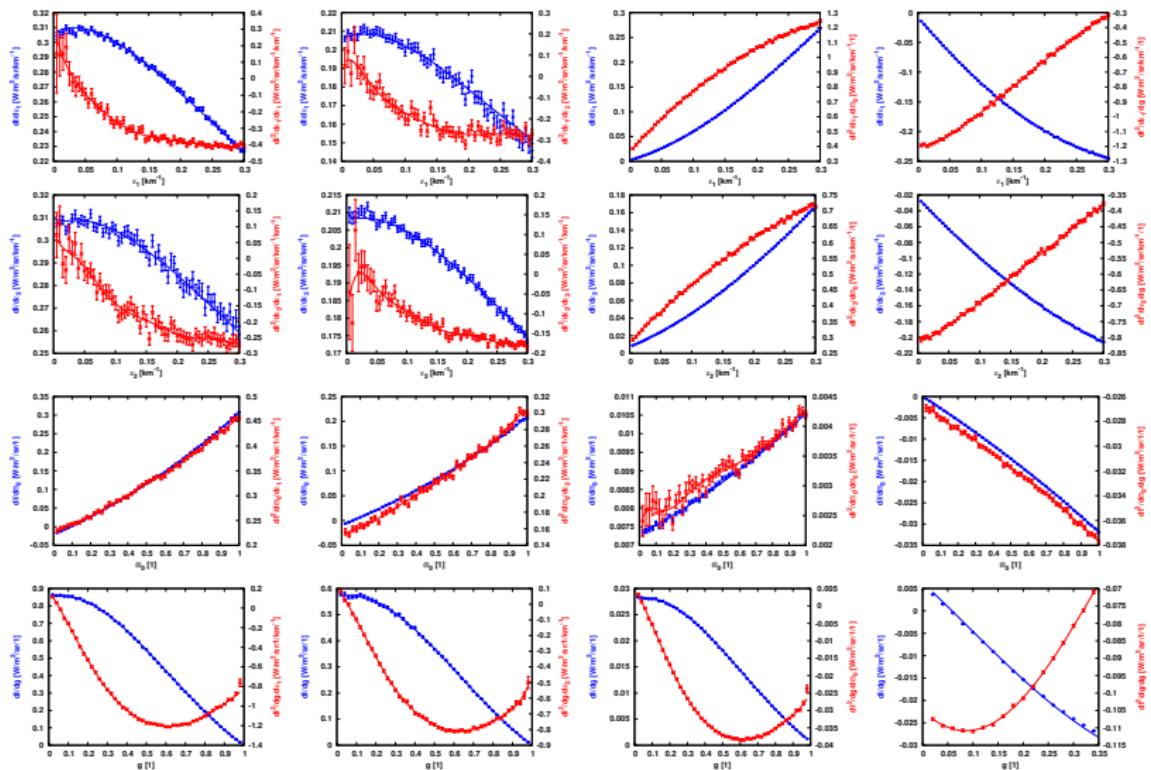


Figure: Validation of 2<sup>nd</sup> order scalar intensity derivatives