

Relevance of Radiative Transfer Approximation for Forward Model and Inversion Scheme for Retrieval of Optically Active Water Constituents

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Superficial aquatic environments (oceans, lakes, rivers...) contain a great diversity of particulate and dissolved materials.

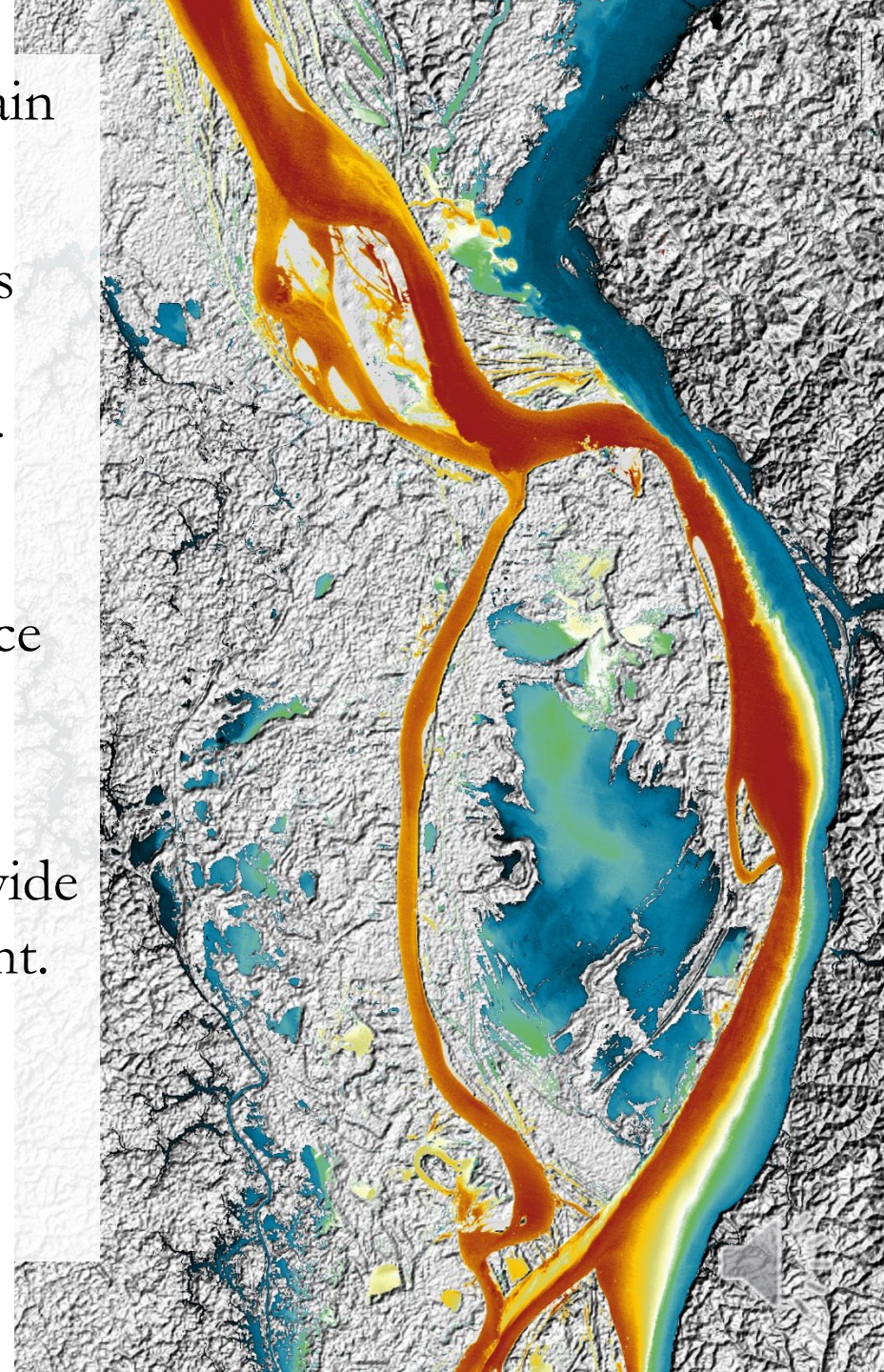
Water-leaving radiance \leftrightarrow optically active water constituents (OAWC).

Inherent optical properties (IOPs) dependent on the nature of the particles in suspension (i.e., microalgae, sediments).

The relationship between remotely measurable water reflectance and the IOPs is still to be better elucidated in turbid and very turbid waters.

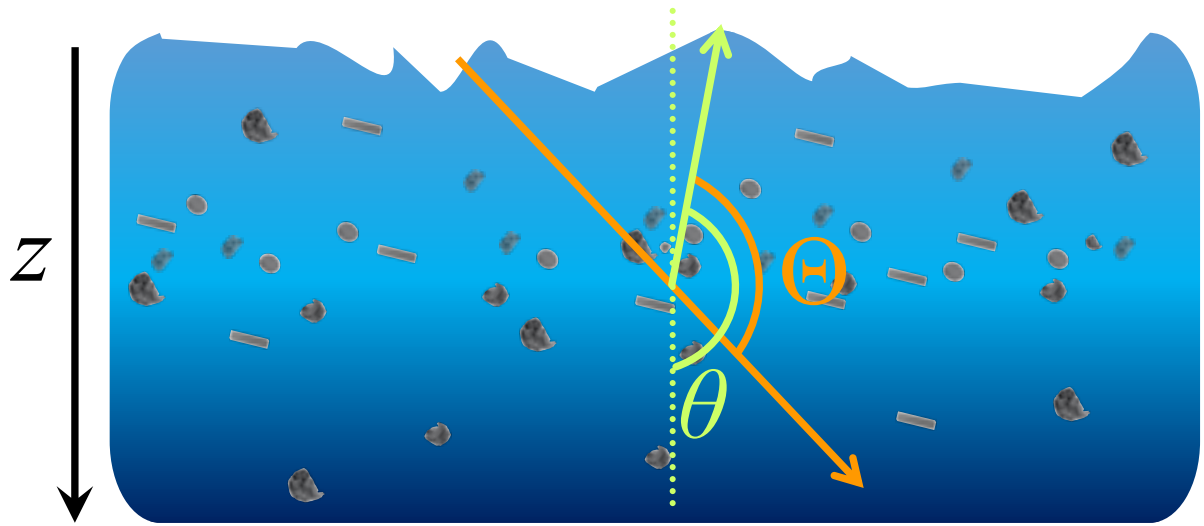
Reassessment of the IOPs-reflectance forward model over a wide range of water turbidity, accounting for the polarization of light.

Based on this forward model, a specific python package (InvRrs) was developed to retrieve hyperspectral or multispectral IOPs from field or satellite sensors.



Posing the radiometric problem: polarization impacts

Radiative Transfer Equation* (RTE)



$$\cos \theta \frac{dI(z, \theta)}{dz} = -c(z)I(z, \theta) + \int_0^\pi VSF(z, \Theta) I(z, \Theta) \sin \Theta d\Theta$$

$$c = a + b$$

\swarrow \nwarrow
 absorption + scattering

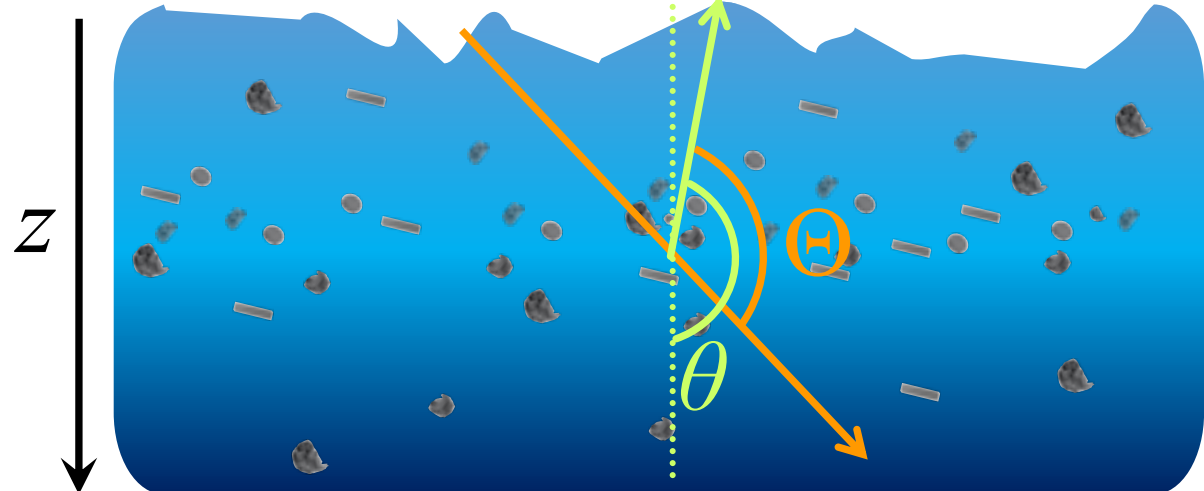
$$b = 2\pi \int_0^\pi VSF(\Theta) \sin \Theta d\Theta$$

Backscattering coefficient

$$b_b = 2\pi \int_{\pi/2}^\pi VSF(\Theta) \sin \Theta d\Theta$$

Posing the radiometric problem: polarization impacts

Vector Radiative Transfer Equation* (VRTE:
with polarization)



Stokes Vector

$$\mathbf{I} = \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix}$$

Mueller Matrix

$$\mathbf{M} = \begin{pmatrix} m_{11} & \dots & m_{14} \\ \vdots & \ddots & \vdots \\ m_{41} & \dots & m_{44} \end{pmatrix}$$

$$\cos \theta \frac{d\mathbf{I}(z, \theta)}{dz} = -c(z)\mathbf{I}(z, \theta) + \int_0^\pi \mathbf{M}(z, \Theta)\mathbf{I}(z, \Theta)\sin \Theta d\Theta$$

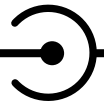
$$\cos \theta \frac{d\mathbf{I}(z, \theta)}{dz} = -c(z)\mathbf{I}(z, \theta) + \mathbf{S}$$

Source function to be documented

Posing the radiometric problem: polarization impacts

Mixture

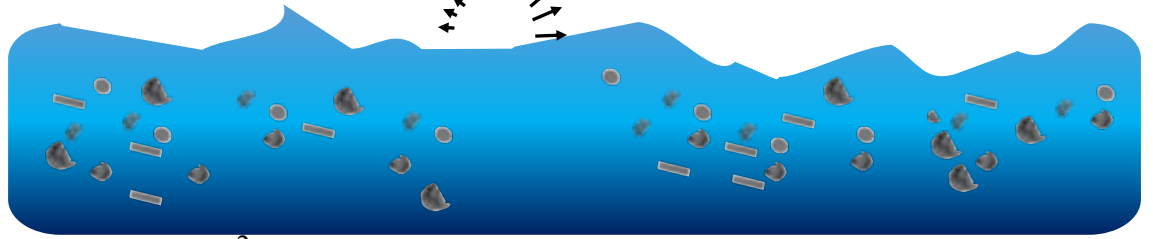
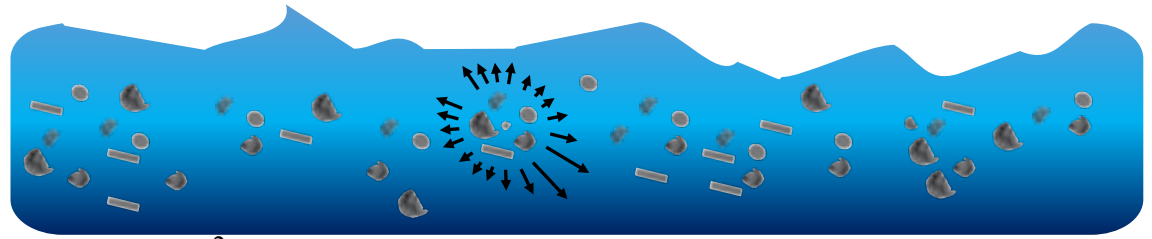
Absorption & scattering



Reflection & transmission

Water-leaving radiance (L_w)

Surface radiance (L_{surf})



$$S = \int_0^{2\pi} d\varphi' \int_0^{\pi} d\theta' \mathbf{M}(z, \theta, \varphi, \theta', \varphi') \mathbf{I}(z, \theta', \varphi')$$

$$S = \int_0^{2\pi} d\varphi' \int_0^{\pi} d\theta' \mathbf{BRDF}(z, \theta, \varphi, \theta', \varphi') \mathbf{I}(z, \theta', \varphi')$$

Need to document angularly and spectrally:

Scattering matrix **M**

Reflection matrix **BRDF**

→ Forward model → Remote sensing exploitation



Background

Quasi-single scattering approximation (QSSA):

$$r_{rs}^{QSSA}(\mu_s, \phi_s, \mu_v, \phi_v) = \frac{b_b}{a + b_b} \frac{P(\mu_s, \phi_s, \mu_v, \phi_v)}{\tilde{b}_b} \frac{1}{\mu_s - \mu_v},$$

And other parameterization of the radiative transfer

$$r_{rs}(\mu_s, \phi_s, \mu_v, \phi_v) = f\left(\frac{b_b}{a + b_b}, \mu_s, \mu_v, \Delta\phi\right),$$

or

$$R_{rs}(\mu_s, \phi_s, \mu_v, \phi_v) = f\left(\frac{b_b}{a + b_b}, \mu_s, \mu_v, \Delta\phi\right),$$

or

$$R_{rs}(\mu_s, \phi_s, \mu_v, \phi_v) = f\left(\frac{b_b}{a}, \mu_s, \mu_v, \Delta\phi\right) \dots$$

But those relation are theoretically wrong for multiple scattering (turbid waters)...

r_{rs} : remote sensing reflectance
below water surface (sr^{-1})

R_{rs} : remote sensing reflectance
above water surface (sr^{-1})

a : absorption coefficient (m^{-1})

b_b : scattering coefficient (m^{-1})

\tilde{b}_b : backscattering ratio

P : phase function (sr^{-1})

μ_s : cosine of source angle

μ_v : cosine of view angle

ϕ_s : source azimuth

ϕ_v : view azimuth

$\Delta\phi$: relative azimuth



Forward model

Single particle scattering
(Mie, T-matrix, DDA...)

IOPs

Cross sections,
Mueller matrix:
 $C(m,\lambda)$, $\mathbf{M}(m,\lambda)$

Radiative transfer for coupled air-water system:

*OSOAA code: aerosol, surface roughness,
OAWC concentration...*

Stokes parameters

$(R_{rs}$ and polarization terms)
water components for various viewing geometries

Inverse model

Retrievals

Absorption and backscattering coefficient, concentration of OAWC, size group and refractive index

Hyperspectral or multispectral Radiometric measurements

For given viewing geometry

Non-linear optimization
(Levendberg-Marquardt,...)

**Radiative transfer for coupled
air-water system:**

*OSOAA code: aerosol, surface roughness,
sediment, microalgae, cdom concentration...*

*

Forward simulation: Simulated Rrs

Increasing concentration →

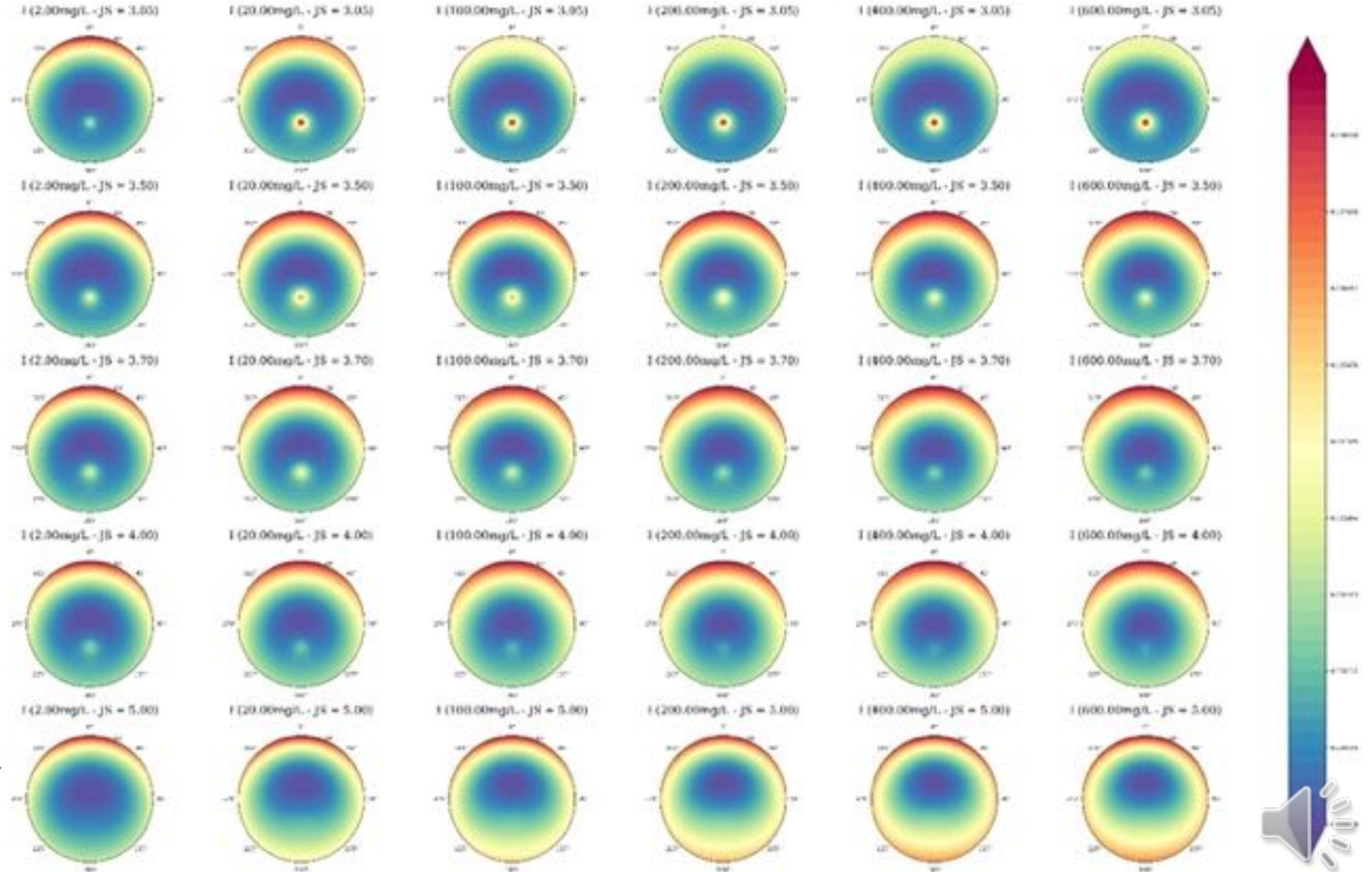
*All the computations were performed in
multiproc mode (Number of CPU = 40)

Sun glint
area

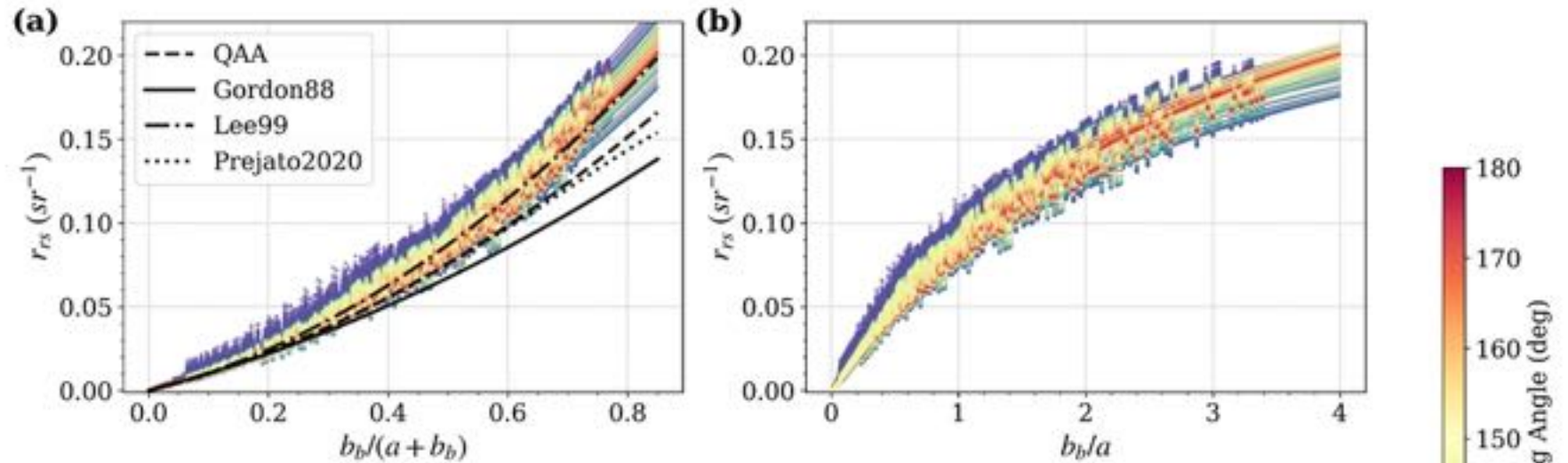
Azimuth

View
Angle

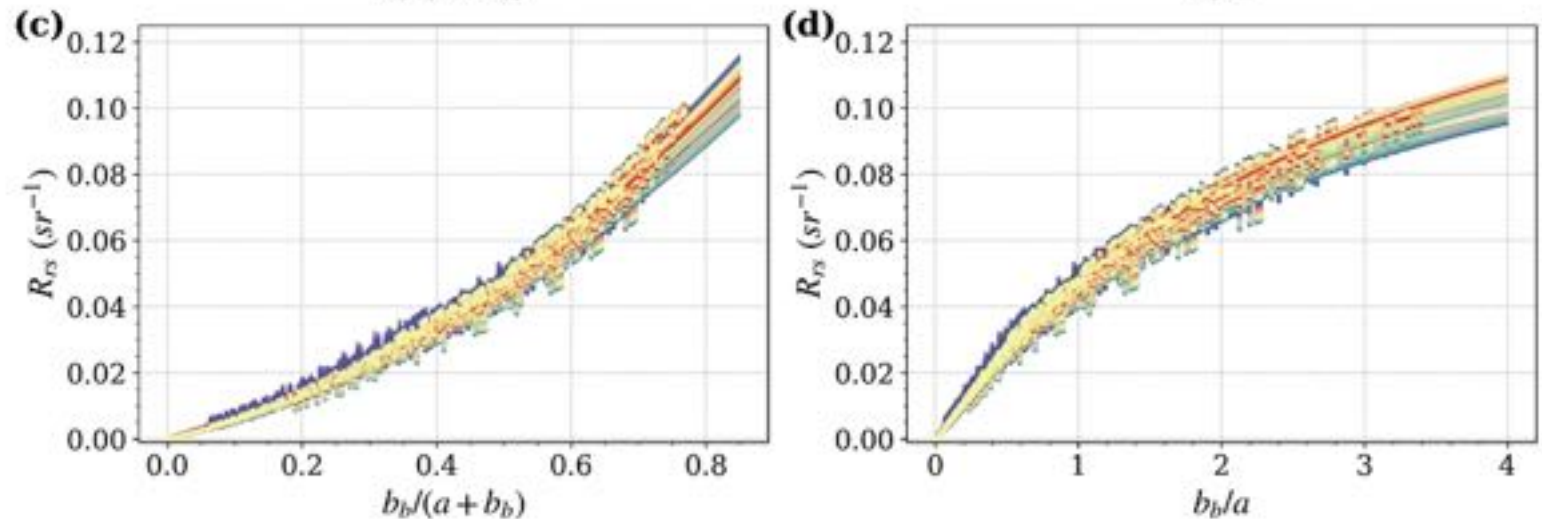
Decreasing particle size ↓



Below-surface level



Above-surface level



Polynomial order > 2
might lead to
mismatch

→ Better to use
monotonic functions

$$R_{rs} = \sum_{i=1}^{N=2} B_i x^i, \text{ with } x = \frac{b_b}{a+b_b}$$

N-order polynomials

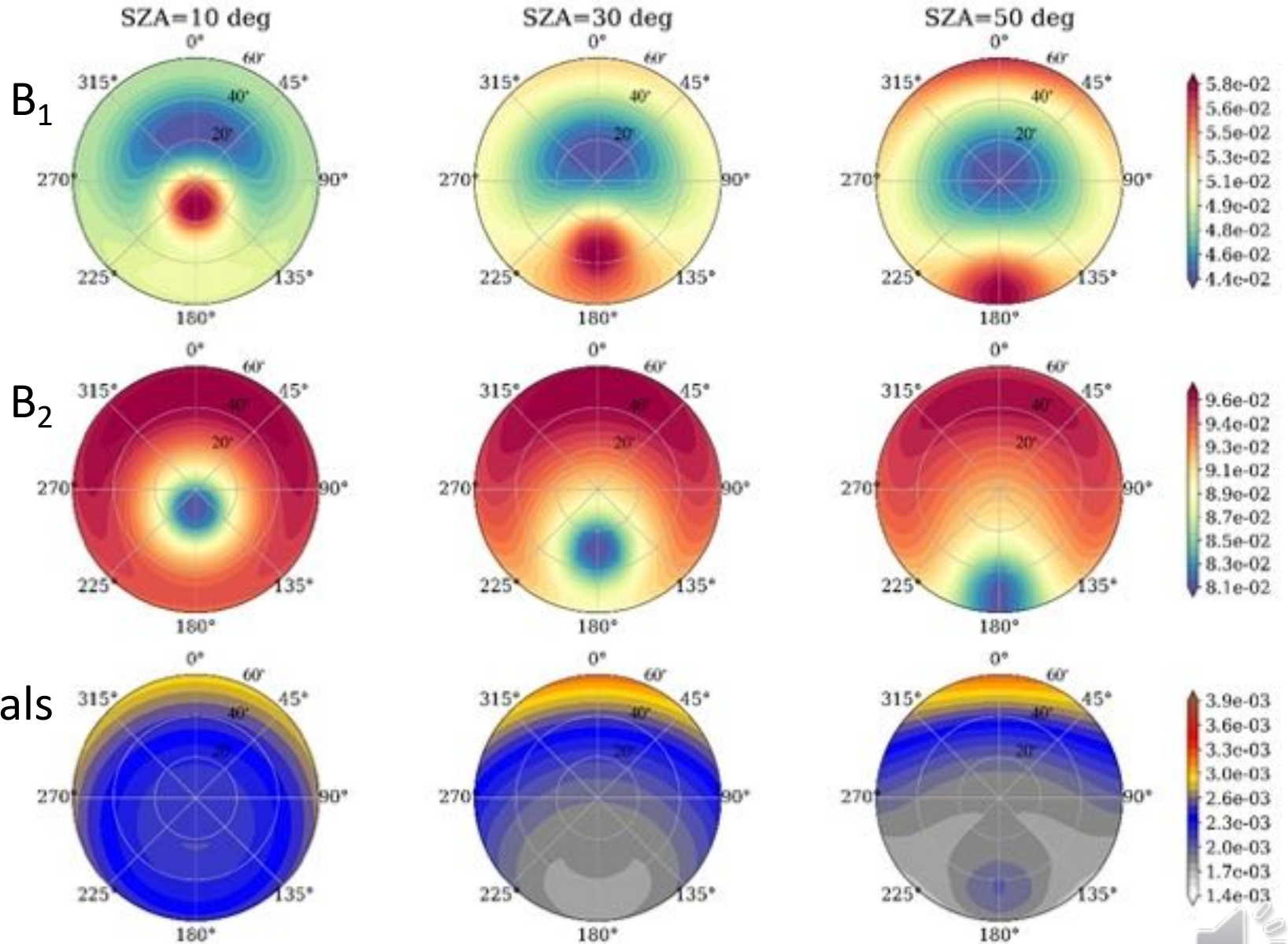
$$R_{rs} = \frac{B_1 x}{B_0 + x}, \text{ with } x = \frac{b_b}{a}$$

Michaelis-Menten equation



Above water surface

$$R_{rs} = \sum_{i=1}^{N=2} B_i x^i, \text{ with } x = \frac{b_b}{a + b_b}$$



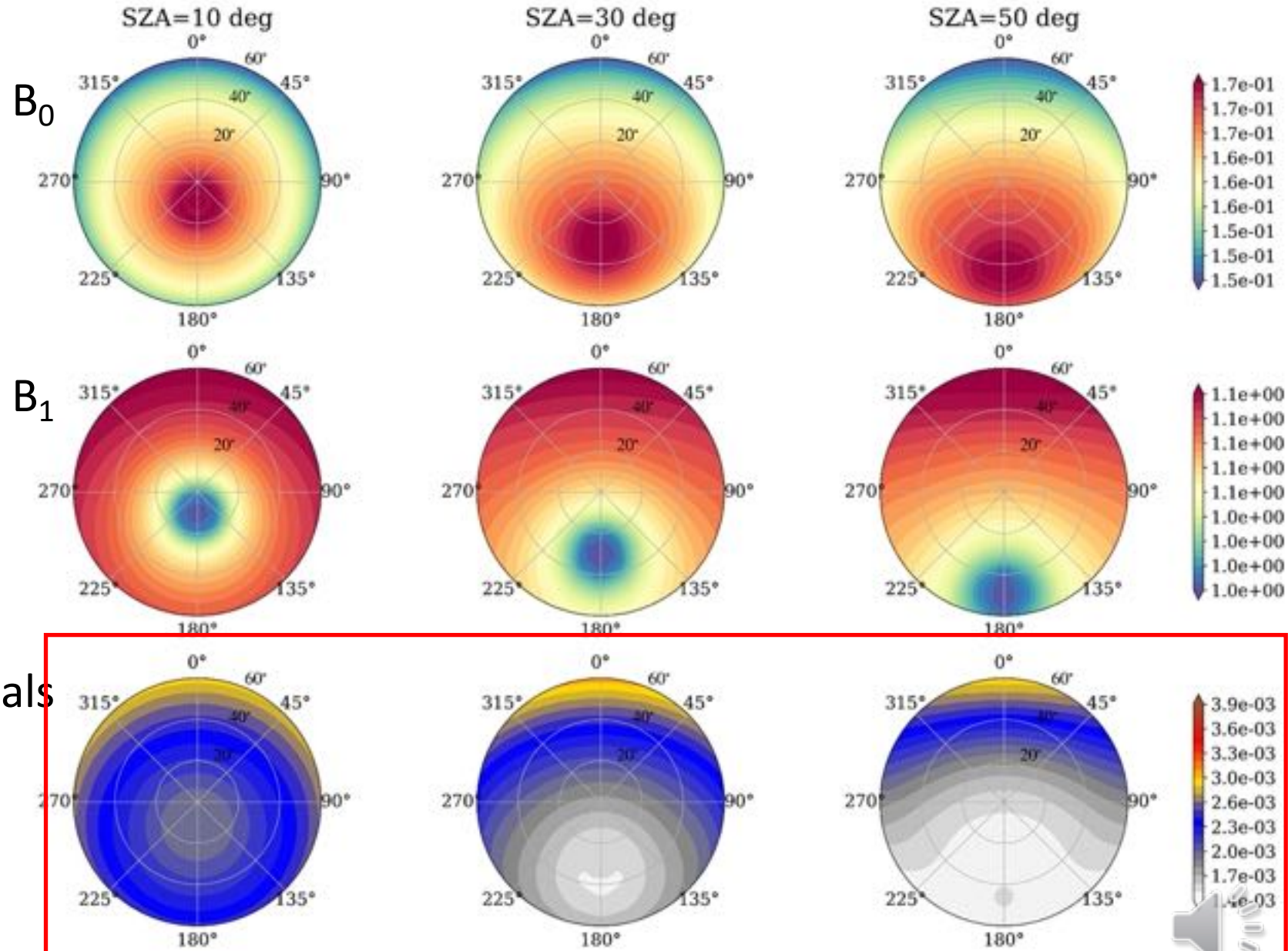
Above water surface

$$R_{rs} = \frac{B_1 x}{B_0 + x}, \text{ with } x = \frac{b_b}{a}$$

Directly handle
transmission through
the rough water-air
interface

All parameters are
available through
netcdf LUT files

Residuals



InvRrs python package



Notebooks



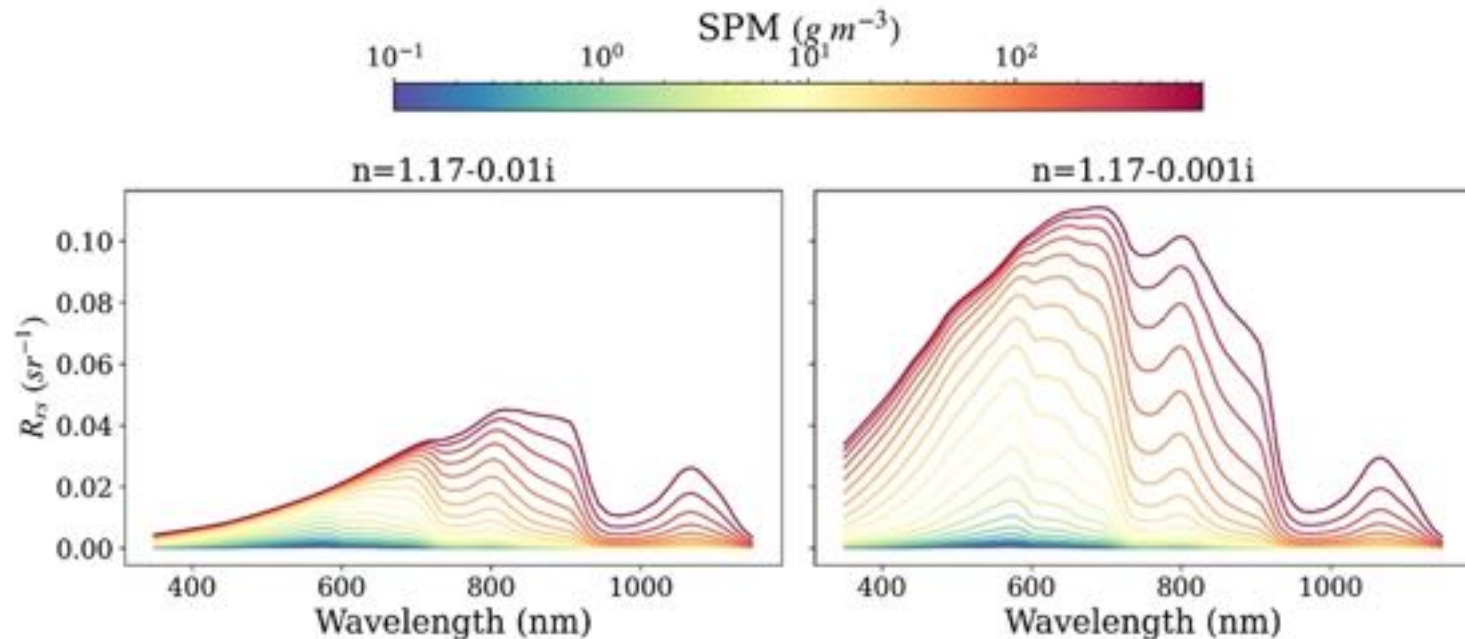
```
invrrs_examples.ipynb
Python 3
*chl, a_bg_ref, S_bg, spm_norm*
for spm_norm in np.logspace(-2, 2.5, 25):
    model.forward_model([20, 1, 0.015, 0.5 * spm_norm, 0.45 * spm_norm, 0.05 * spm_norm, 1.15, -0.0005, 0.018], output='Rrs').plot(
        color=cmmap(norm(spm_norm * 2)), ax=axs[0])
    model.forward_model([20, 1, 0.015, 0.5 * spm_norm, 0.45 * spm_norm, 0.05 * spm_norm, 1.25, -0.0007, S_ni], output='Rrs').plot(
        color=cmmap(norm(spm_norm * 2)), ax=axs[1])

cb = fig.colorbar(sm, ax=axs, shrink=0.6, aspect=30, pad=0.15, location='top')
cb.set_label('SPM $(g m^{-3})$', fontsize=22)
axs[0].set_title('n=1.15-0.0005i')
axs[1].set_title('n=1.25-0.0007i')

axs[0].set_xlabel('Wavelength (nm)')
axs[1].set_xlabel('Wavelength (nm)')
axs[0].set_ylabel('$R_{rs} (sr^{-1})$')

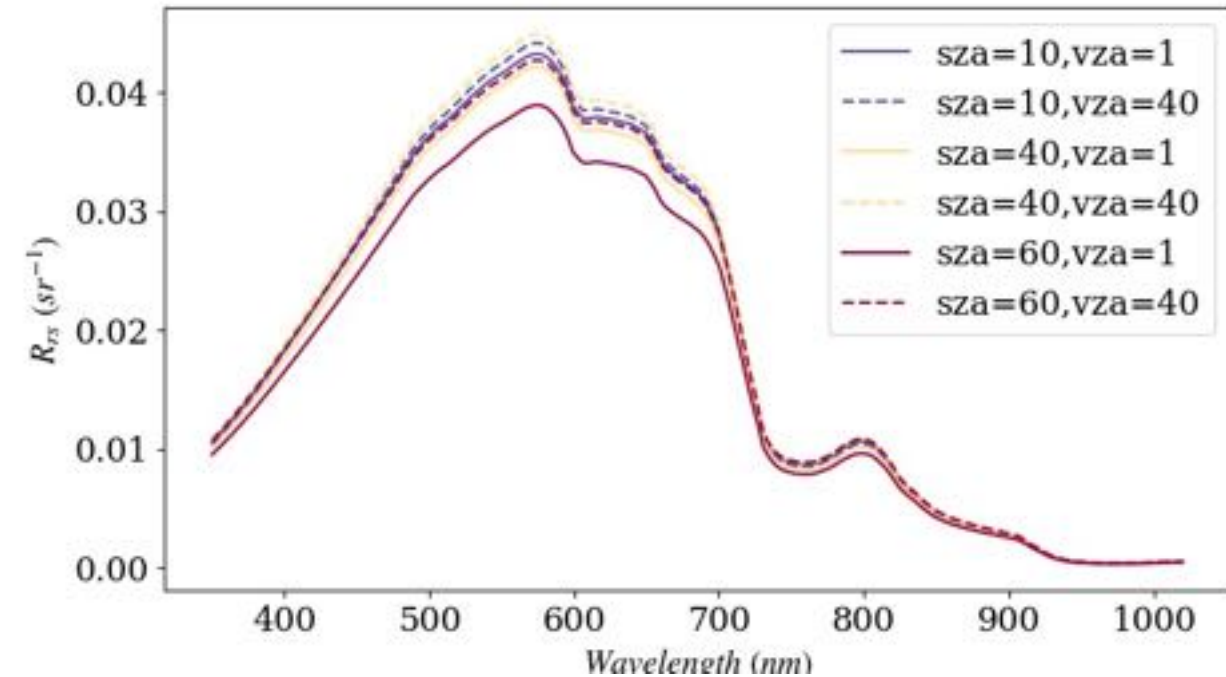
plt.show()
```

SPM: concentration of
Suspended Particulate
Matter

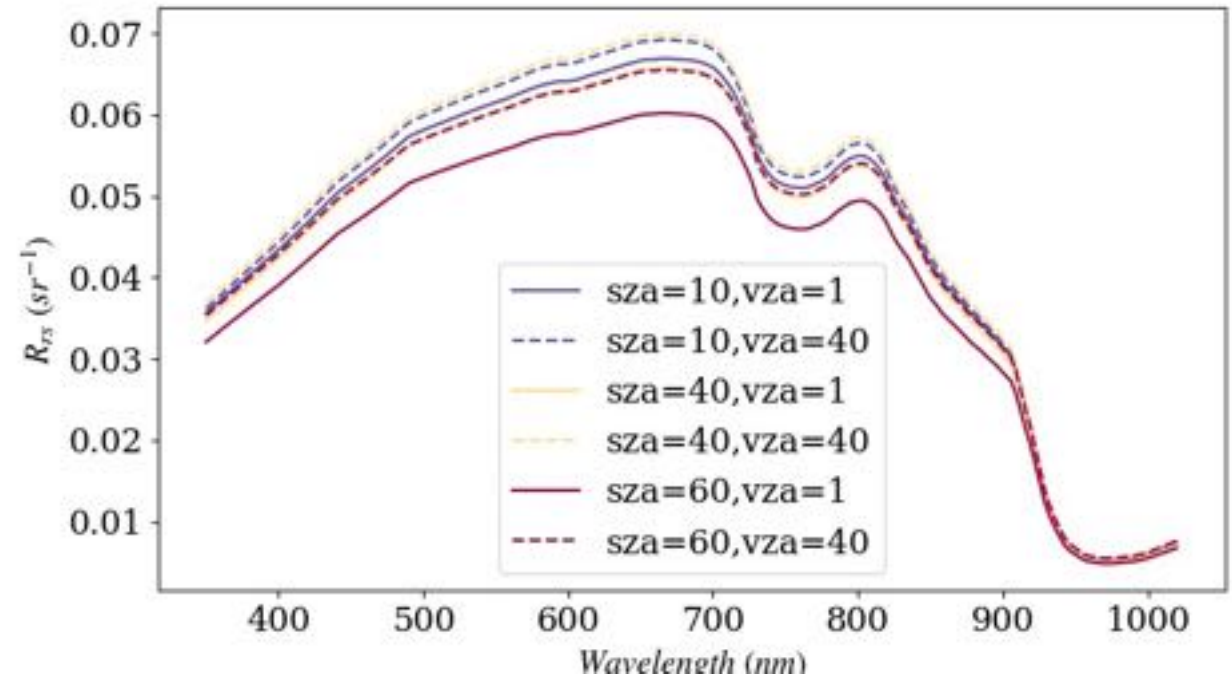


Water-column “BRDF” impacts

Chl=2, SPM=36.4, aCDOM=0.5



Chl=2, SPM=520.0, aCDOM=0.5



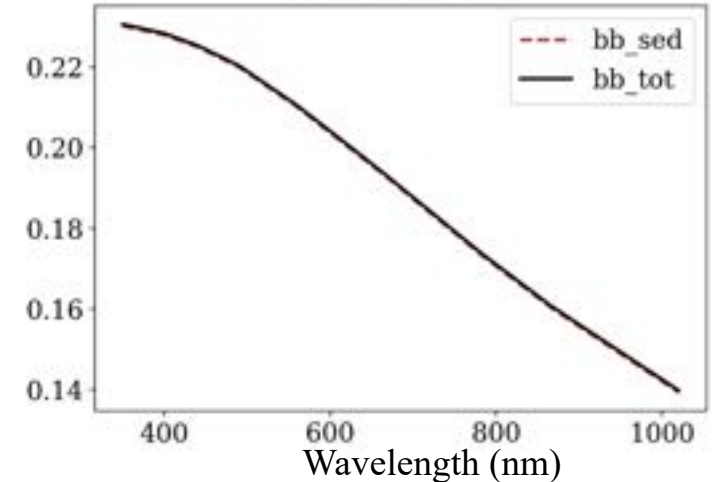
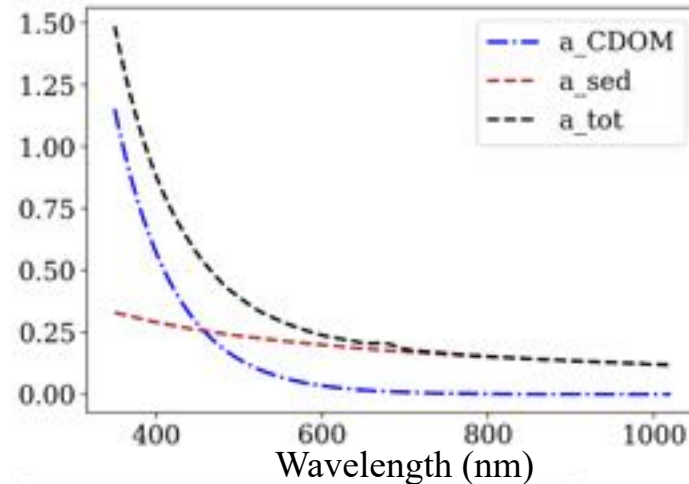
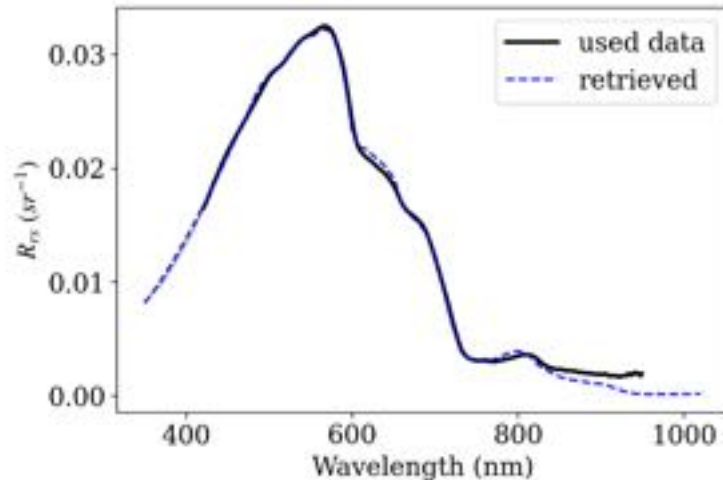
Inversion algorithm outcomes

Retrievals

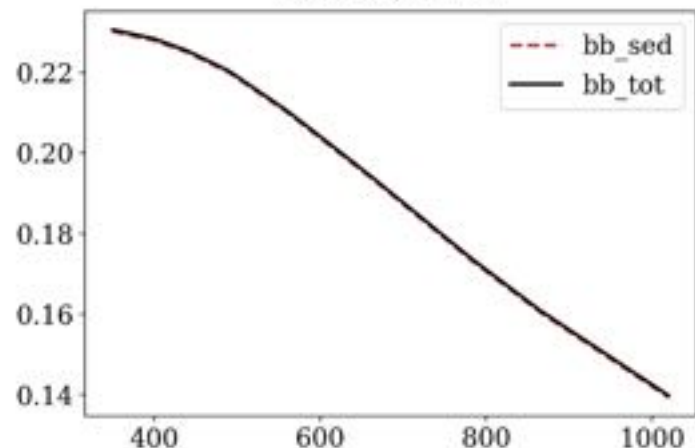
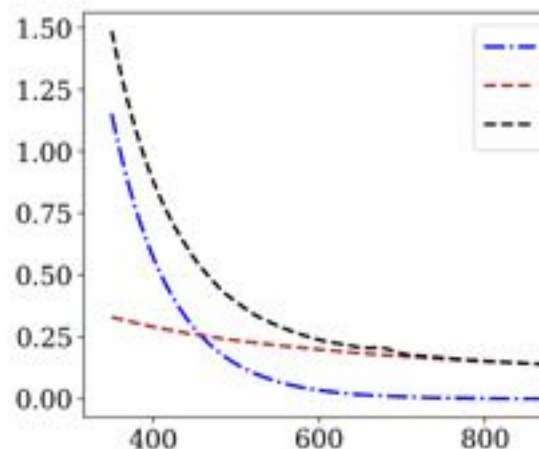
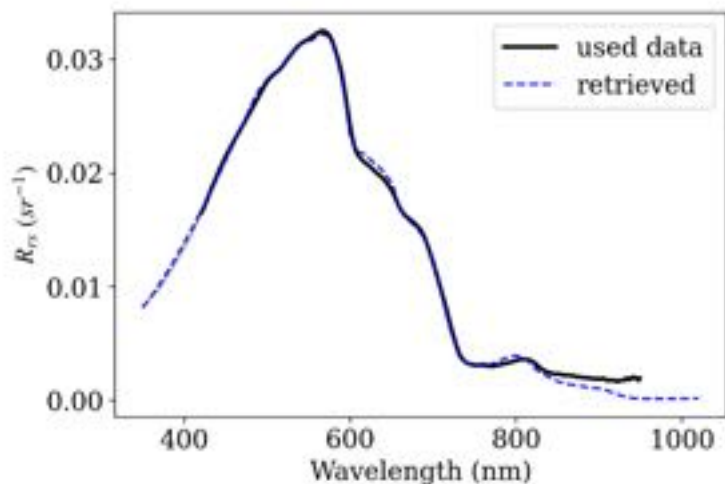
Absorption and backscattering coefficient, concentration of OAWC, size group and refractive index

Hyperspectral or multispectral Radiometric measurements
For given viewing geometry

Non-linear optimization
(Levendberg-Marquardt,...)



Station V7, SPM= 13.793
retrieved:12.258765748179737



```

[[Retrieved variables]]
chl: 1.16561159 +/- 0.57871577 (49.65%) (init = 3)
a_bg_ref: 0.32683997 +/- 0.09607264 (29.39%) (init = 0.5)
S_bg: 0.01400000 +/- 0.00182126 (13.01%) (init = 0.017)
spm_norm: 4.62594934 +/- 5.58481767 (120.73%) (init = 1)
fine_prop: 0.10000000 +/- 0.21262846 (212.63%) (init = 0.6)
nr: 1.20000000 +/- 0.09140867 (7.62%) (init = 1.18)
ni_ref: -0.00120298 +/- 0.00156230 (129.87%) (init = -0.00)
S_ni: -5.0744e-06 +/- 0.00124901 (24614.10%) (init = 0.0)
[[Correlations]] (unreported correlations are < 0.100)
C(spm_norm, nr) = -0.997
C(spm_norm, fine_prop) = -0.985
C(spm_norm, ni_ref) = 0.982
C(fine_prop, ni_ref) = -0.976
C(nr, ni_ref) = -0.971
C(fine_prop, nr) = 0.971
C(S_bg, S_ni) = 0.957
C(a_bg_ref, S_ni) = -0.888
C(a_bg_ref, S_bg) = -0.861
C(chl, a_bg_ref) = -0.689
C(chl, S_bg) = 0.571
C(a_bg_ref, ni_ref) = 0.554
C(chl, S_ni) = 0.527
C(chl, ni_ref) = -0.427
C(a_bg_ref, spm_norm) = 0.395
C(a_bg_ref, fine_prop) = -0.389
C(a_bg_ref, nr) = -0.368
C(chl, fine_prop) = 0.335
C(chl, nr) = -0.331

```

[[Retrieved variables]]

```

chl: 1.16561159 +/- 0.57871577 (49.65%) (init = 3)
a_bg_ref: 0.32683997 +/- 0.09607264 (29.39%) (init = 0.5)
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S_ni: -5.0744e-06 +/- 0.00124901 (24614.10%) (init = 0.001)

```

[[Correlations]] (unreported correlations are < 0.100)

```

C(spm_norm, nr) = -0.997
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C(chl, ni_ref) = -0.427
C(a_bg_ref, spm_norm) = 0.395
C(a_bg_ref, fine_prop) = -0.389
C(a_bg_ref, nr) = -0.368
C(chl, fine_prop) = 0.335
C(chl, spm_norm) = -0.331

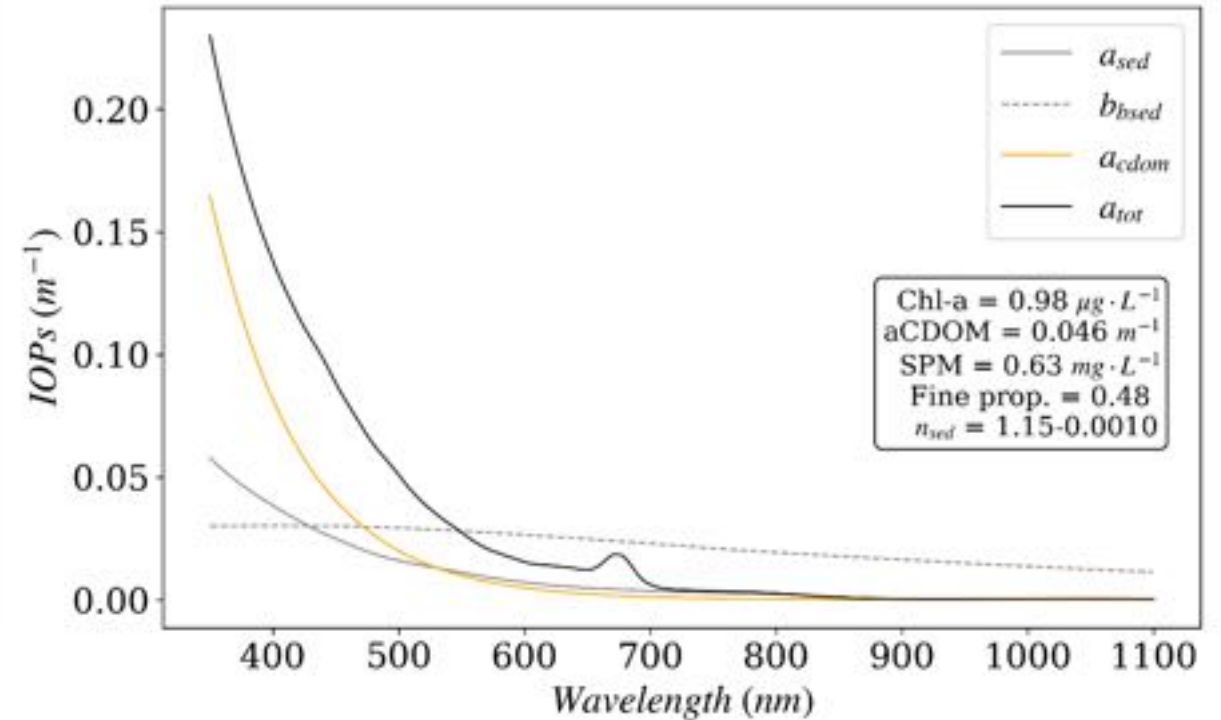
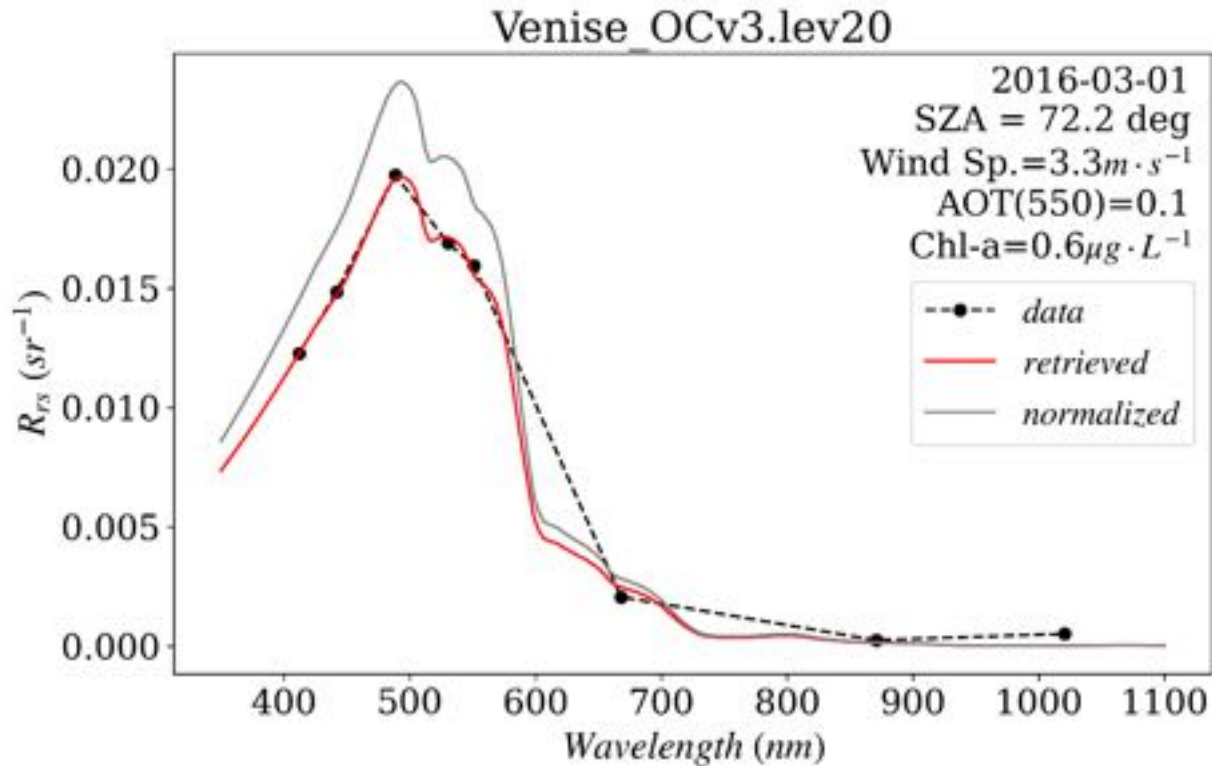
```



Application of InvRrs to AERONET-OC database

Retrieved: $R_{rs} = \text{InvRrs}(\theta_s, \theta_v, \Delta\varphi)$

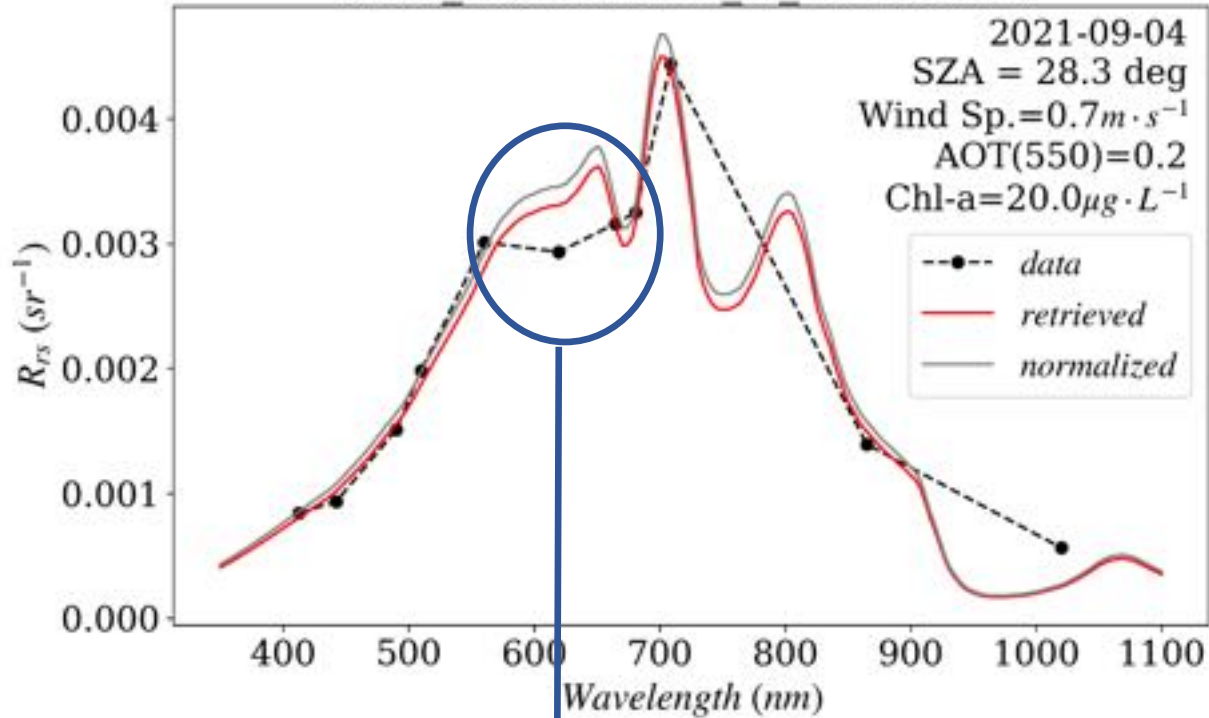
Normalized: $R_{rs} = \text{InvRrs}(\theta_s = 0, \theta_v = 0)$



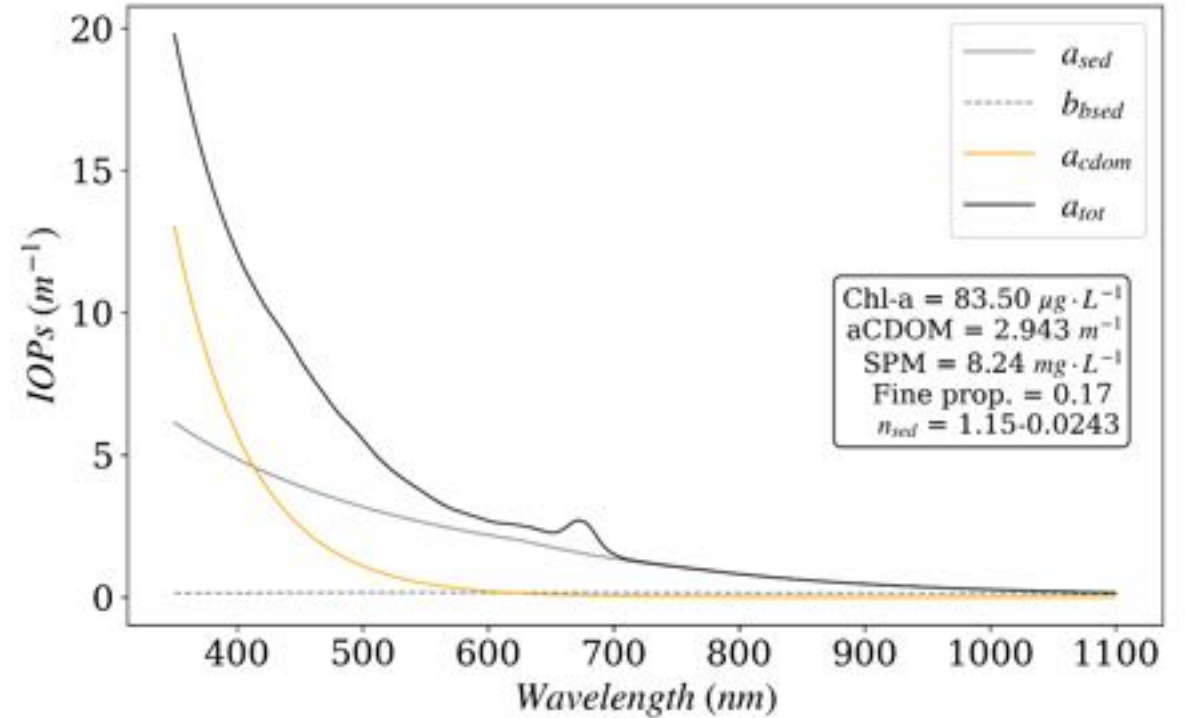
Application of InvRrs to AERONET-OC database

Lake Okeechobee known to be prone to Cyanobacteria bloom

Lake_Okeechobee_N_OCv3.lev20



Spectral range of
Phycocyanin absorption

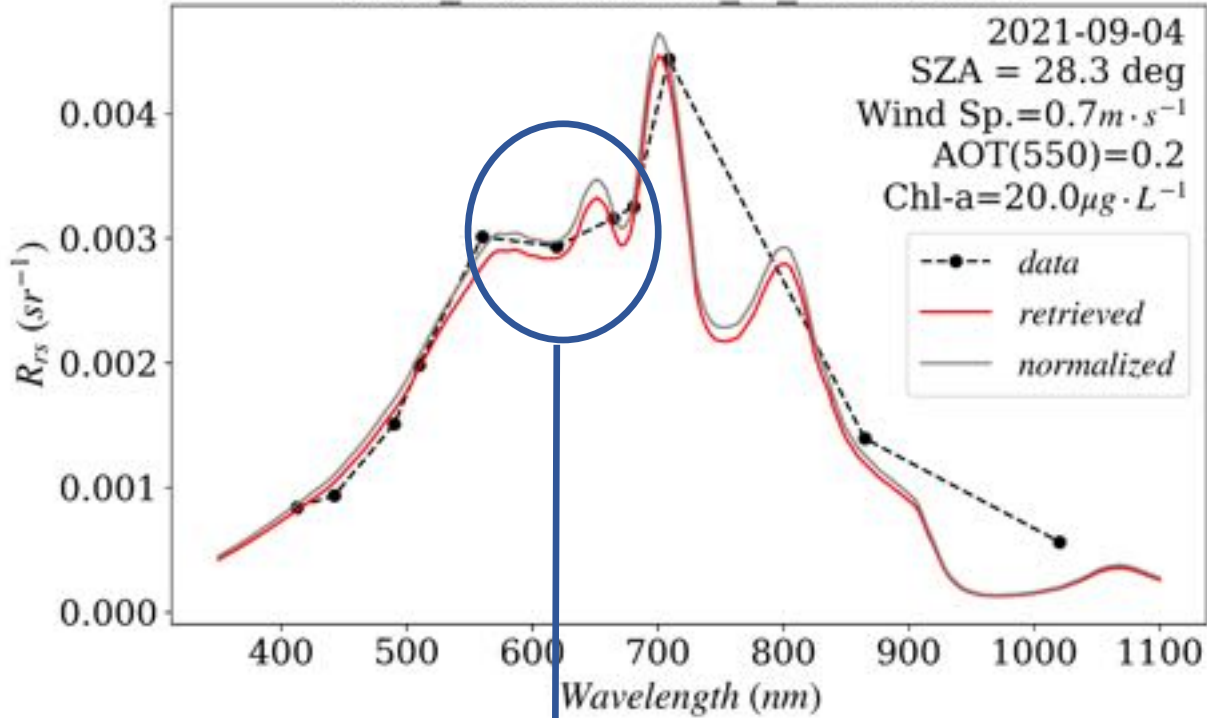


Application of InvRrs to AERONET-OC database

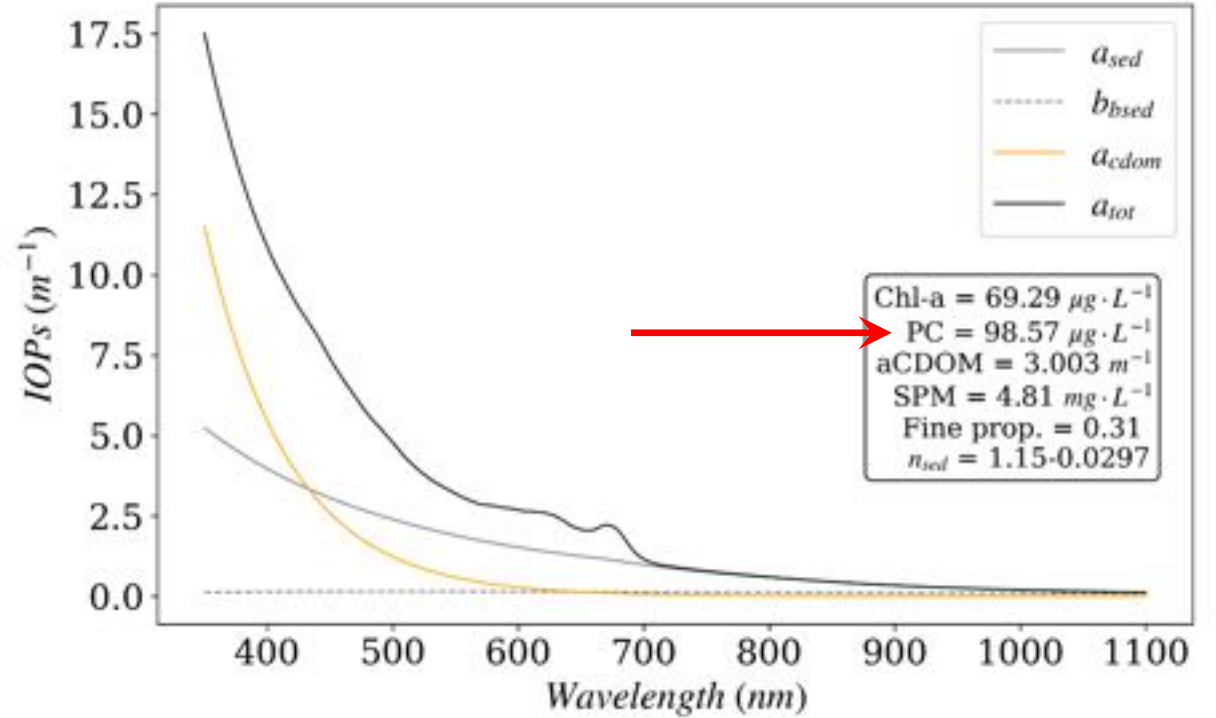
Lake Okeechobee known to be prone to Cyanobacteria bloom

Addition of Phycocyanin (PC) Specific absorption in InvRrs

Lake_Okeechobee_N_OCv3.lev20



Spectral range of
Phycocyanin absorption



Need to be continued...

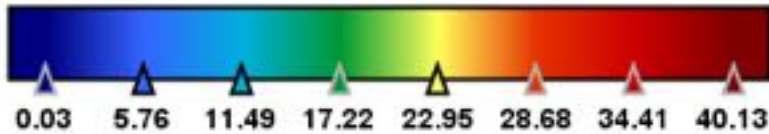


satellite applications -- Going beyond first order...

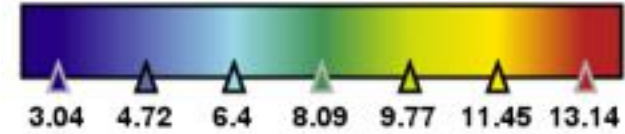
S2A, 30PYT, 20200521

GRS processed + L3 algo

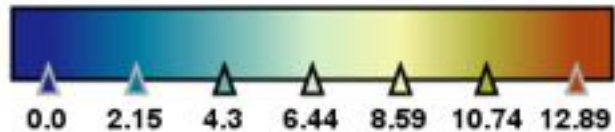
Chlorophyll-a (mg m^{-3})



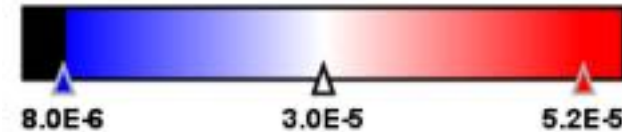
Absorption 440nm (m^{-1})



Backscattering 440nm (m^{-1})



Residual/goodness of fit



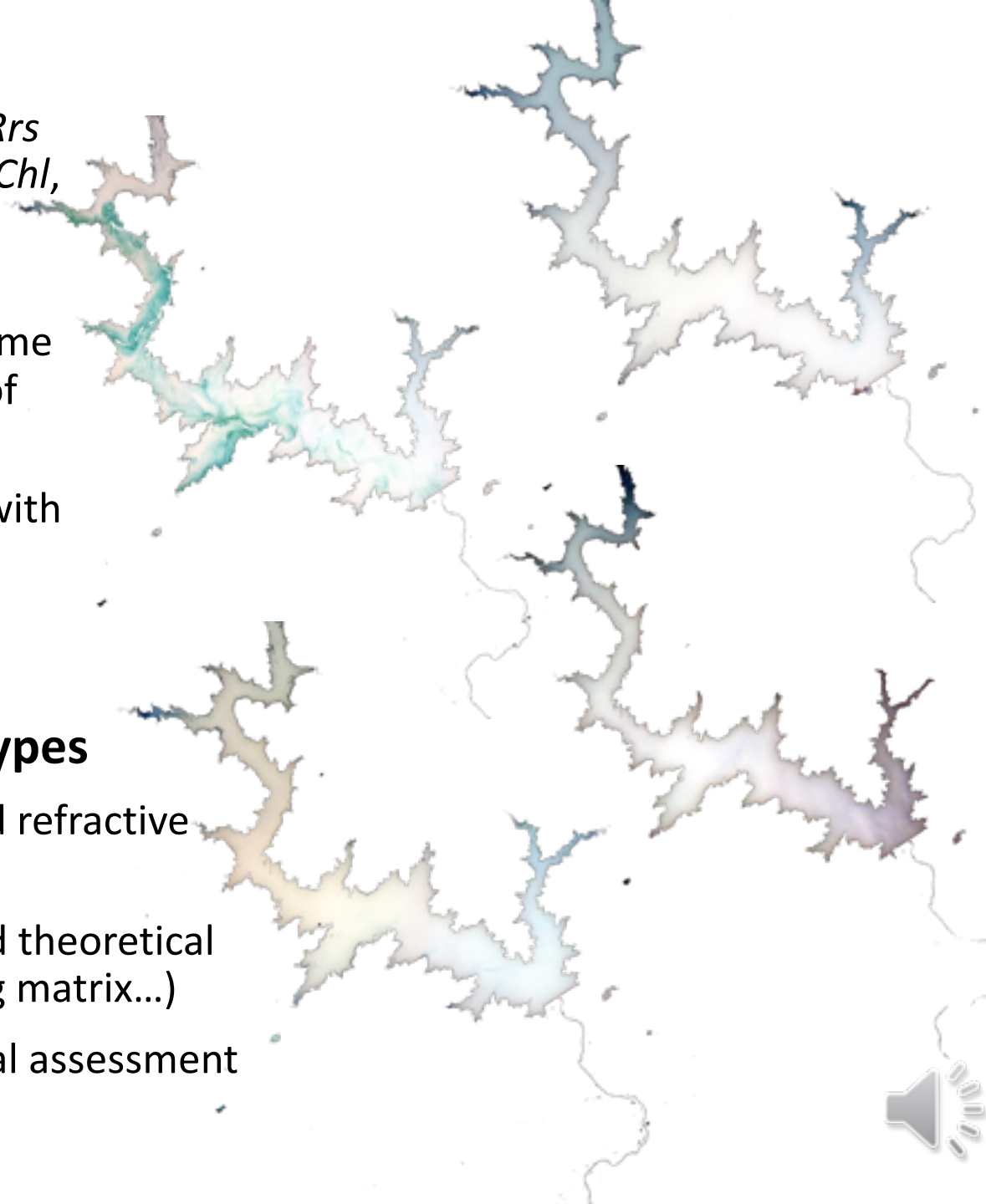
Summary

- A forward/inversion algorithm has been developed (*InvRrs* package) with easy function to build up your on model (*Chl*, algae species, sediment mineralogy (two, three modes, spectral complex refractive index)
- Recommended to use the above-water reflectance scheme that includes all the multiple reflections/transmissions of the air-water interface.
- Multispectral or hyperspectral field or satellite sensors with direct band width integration

Future works:

Algae or Cyanobacteria species, mineralogical types

- Based on spherical particles: need to include shapes and refractive index distribution, orientation, inner structure
- Need of more understanding between lab. exp. data and theoretical modeling (need accurate measurement of the scattering matrix...)
- Need of a lot more data from the field with mineralogical assessment



OBS2CO  cnes

A CNES-Hysope-2 processing chain
for water color and quality

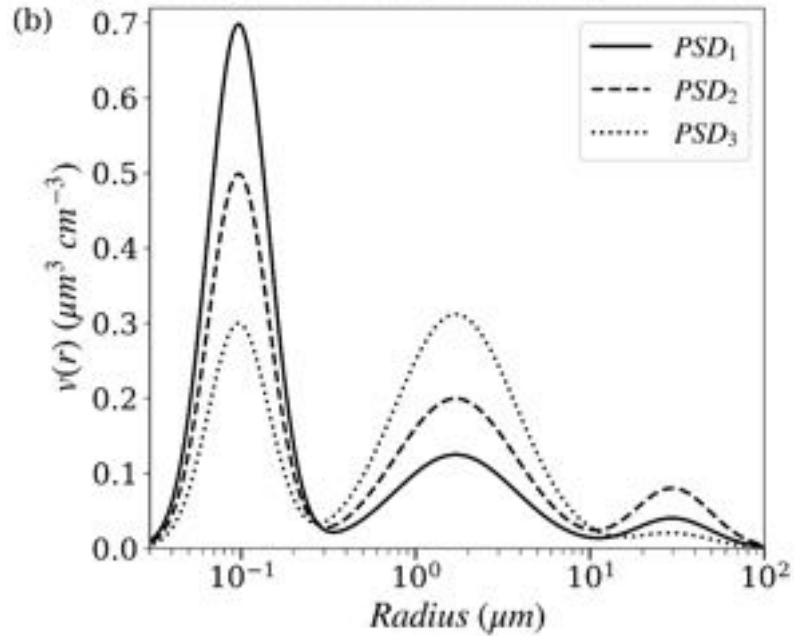


Thank you



Sediment modeling

Multimodal size distribution

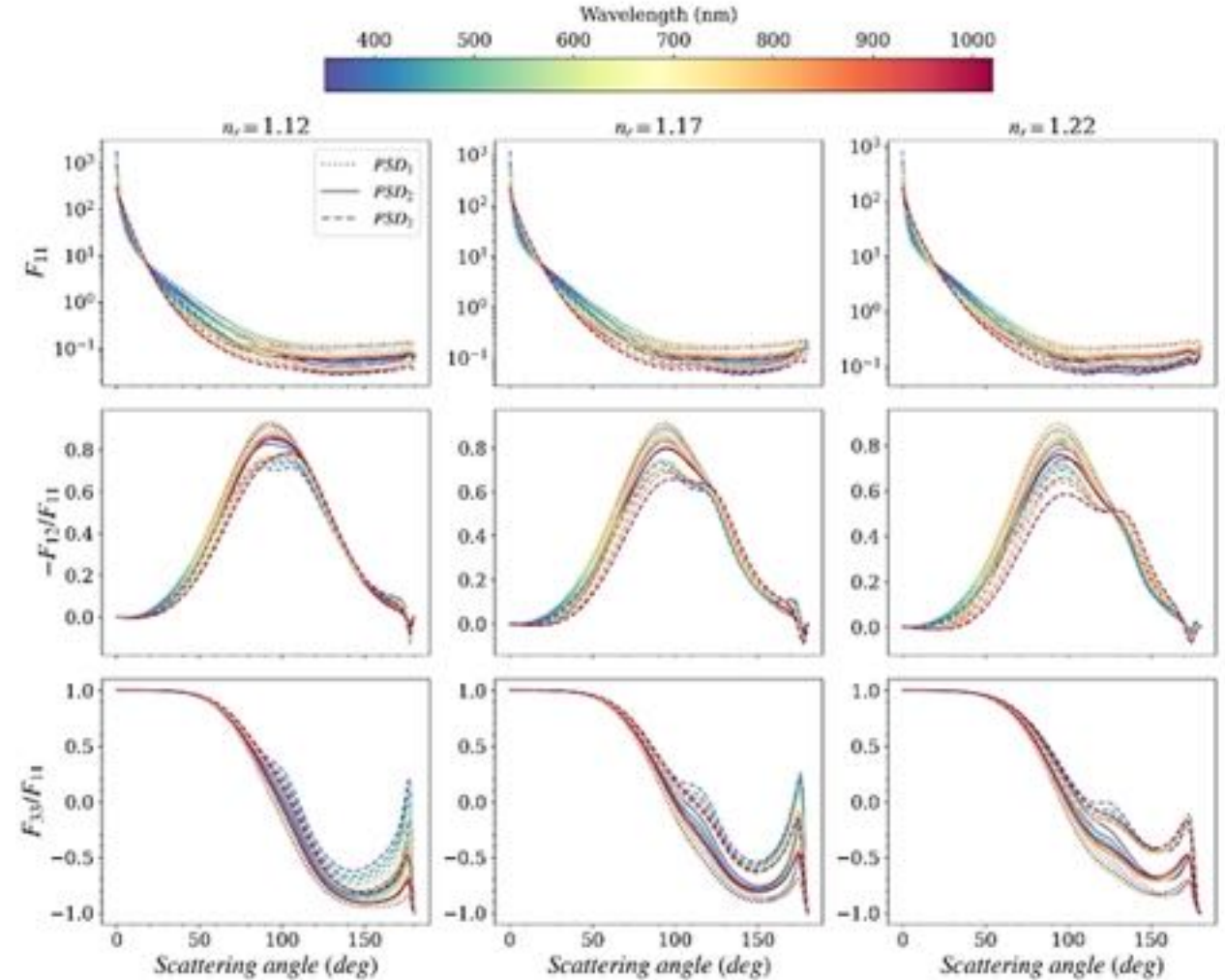


Complex refractive index and spectral variation:

$$m = n + ik$$

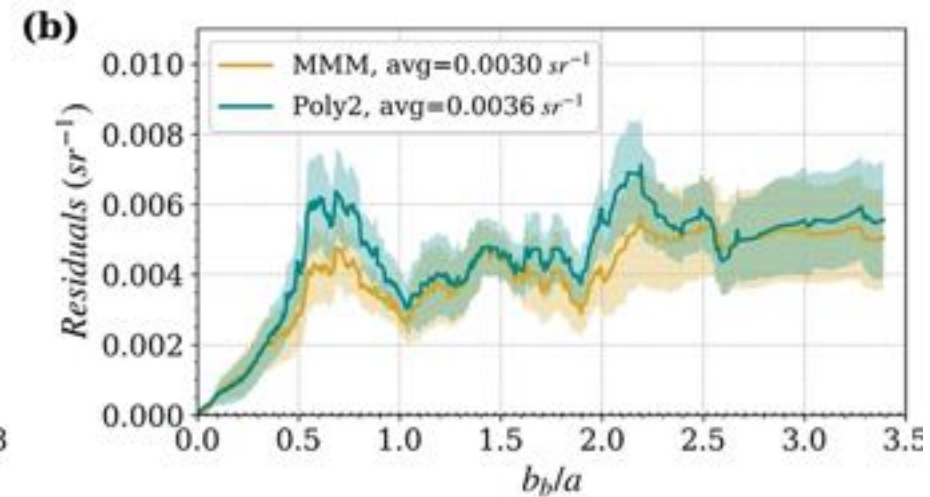
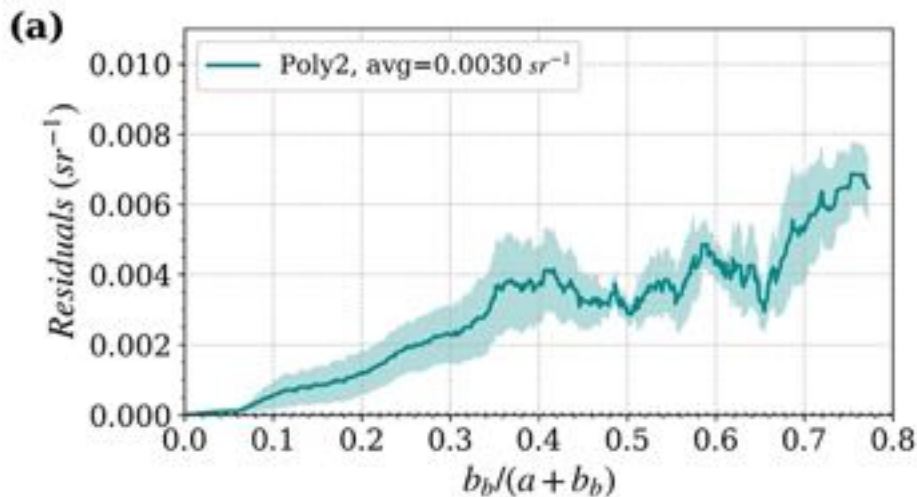
$$k(\lambda) = k(\lambda_{ref}) \exp(-S(\lambda - \lambda_{ref}))$$

Assumption: spherical particles for scattering matrices

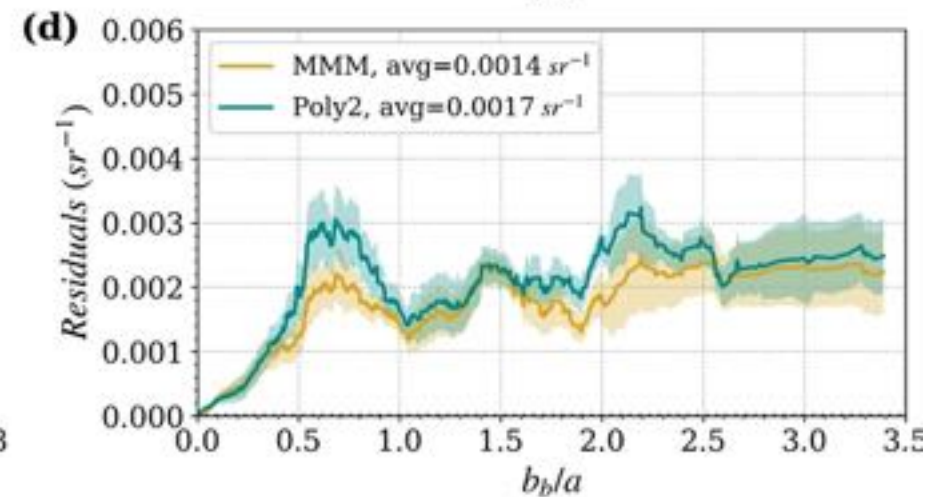
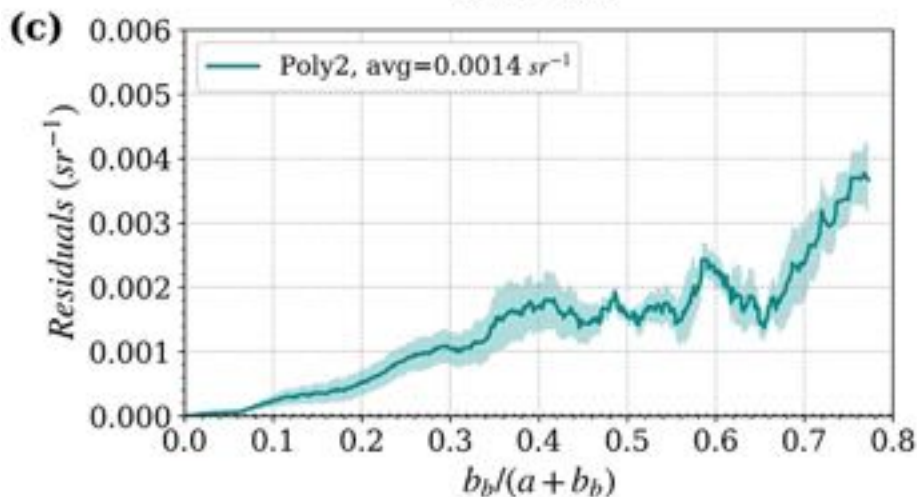


Goodness of fit: overall residuals

Below-surface level



Above-surface level



$$R_{rs} = \sum_{i=1}^{N=2} B_i x^i, \text{ with } x = \frac{b_b}{a+b_b}$$

N-order polynomials

$$R_{rs} = \frac{B_1 x}{B_0 + x}, \text{ with } x = \frac{b_b}{a}$$

Michaelis-Menten equation

