

Scientific Roadmap for Phytoplankton Diversity from Ocean Color

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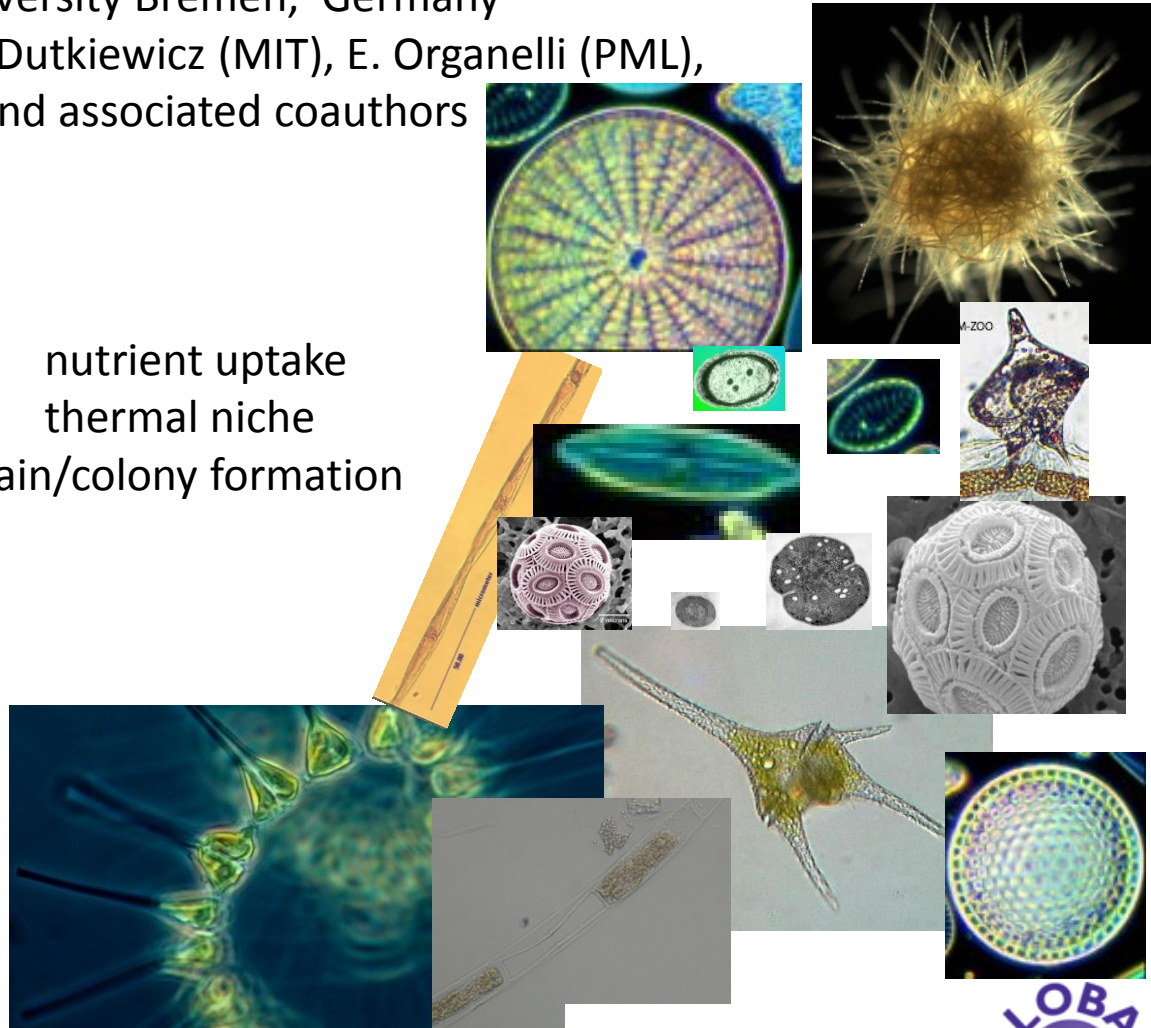
Contributions: A. Chase (UMaine), S. Dutkiewicz (MIT), E. Organelli (PML), J. Uitz (LOV), A. Wolanin (AWI/HZG) and associated coauthors

Phytoplankton differ in terms of:

size biogeochemical function nutrient uptake
accessory pigments morphology thermal niche
predation protection/avoidance chain/colony formation
symbiosis
....

Phytoplankton diversity matters:

- As base of foodweb
- For carbon cycling
- For resilience of ecosystem



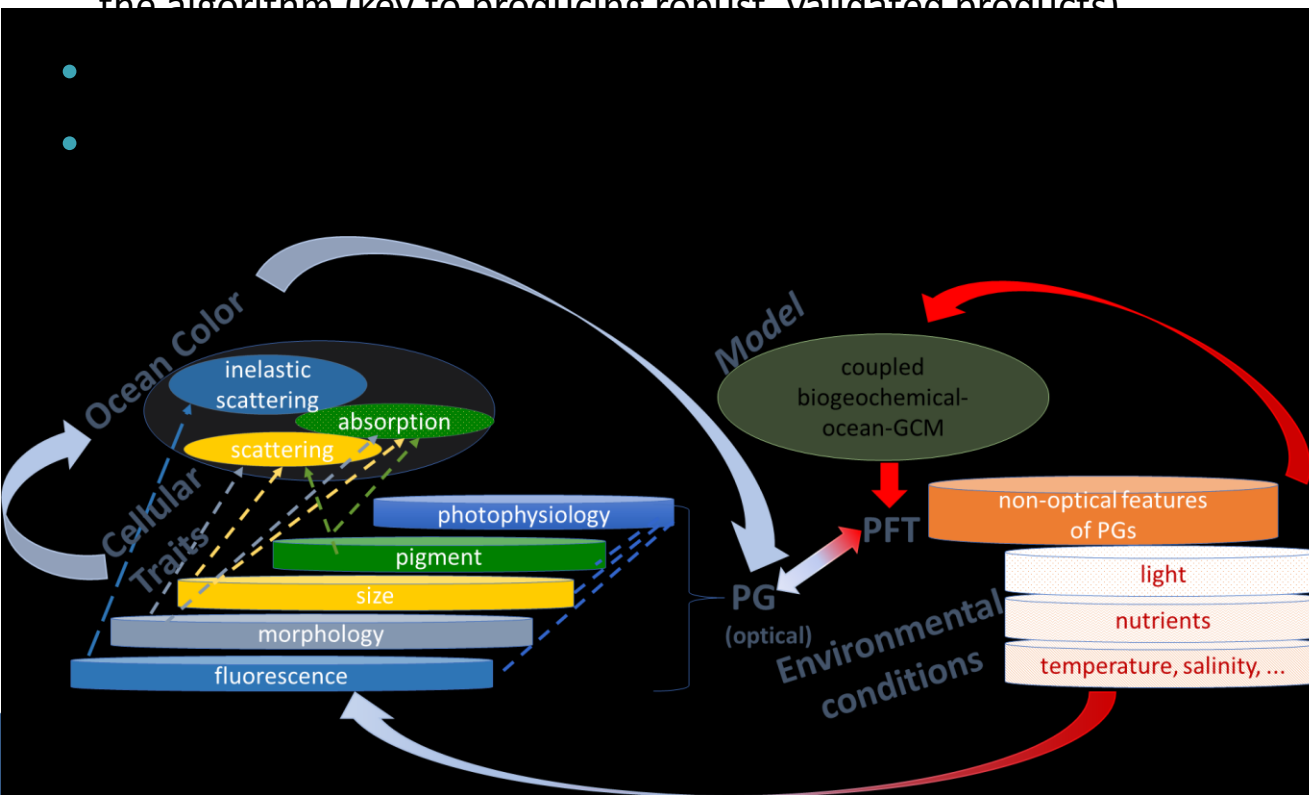
Scientific Roadmap for Phytoplankton Diversity from OC

Bracher & 20 more PFT-experts worldwide (2017) *Frontier in Marine Science* 4: 55

Developing algorithms on phytoplankton diversity (PFTs) from OC very active research for > decade.

Scientific roadmap identified user needs, summarizes the current state and pinpoints major gaps in long-term objectives to deliver space-derived phytoplankton diversity data (PFT) that meets the user requirements. Specific way forwards are to:

- Improve match between what can be produced/what is actually needed by users
- Improve methodology for quantifying systematically errors associated with PFT products at each step of the algorithm (key to producing robust, validated products)



from development & validation)

optical approach to PFTs

compared to multi-spectral



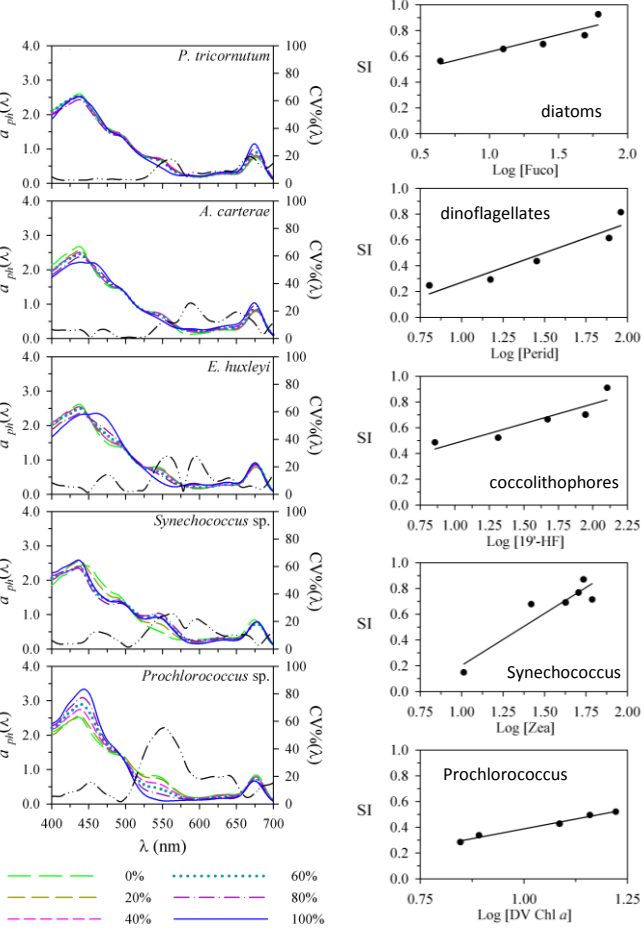
On the discrimination of multiple phytoplankton groups from light absorption spectra of assemblages with mixed taxonomic composition and variable light conditions

EMANUELE ORGANELLI,^{1,2,*} CATERINA NUCCIO,¹ LUIGI LAZZARA,¹ JULIA UITZ,³ ANNICK BRICAUD,³ AND LUCA MASSI¹

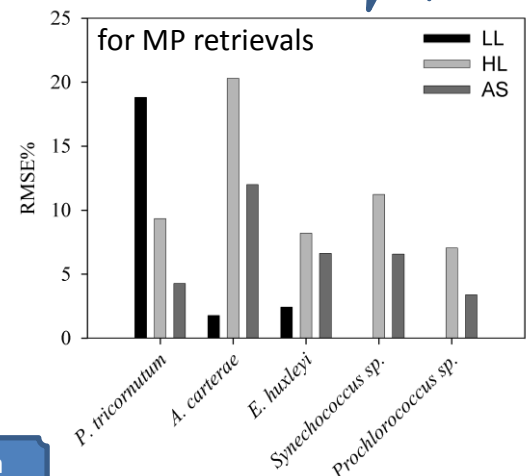
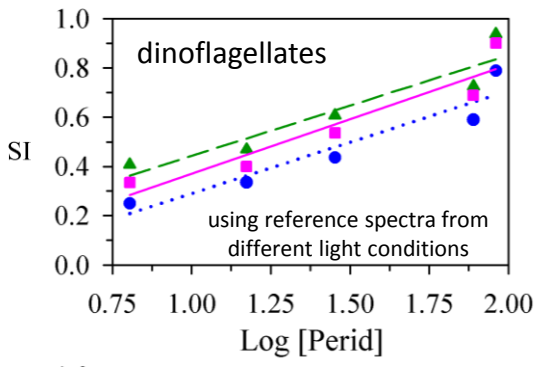
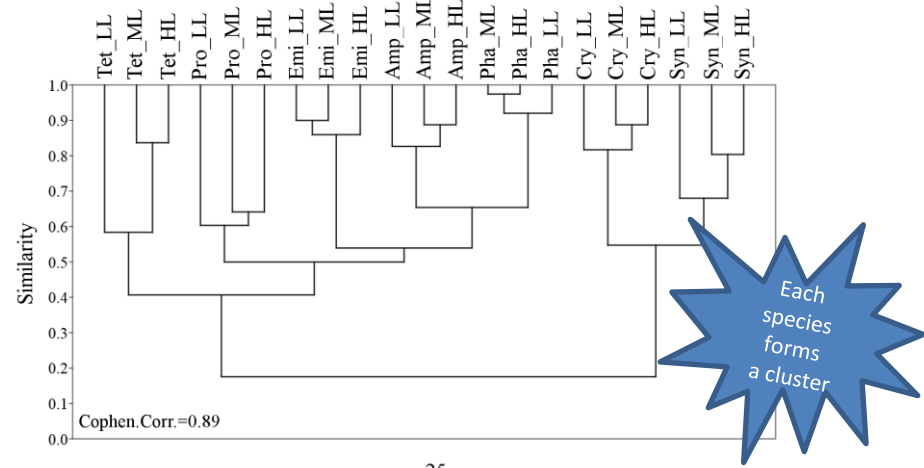
Use of the fourth-derivative spectra of phytoplankton light absorption coefficients (400-700 nm, 1 nm resolution) to:

- 1) investigate uncertainties and limits for phytoplankton group discrimination from assemblages with mixed taxonomic composition;
- 2) evaluate the extent to which modifications of the absorption spectral features due to variable light conditions affect the optical discrimination of phytoplankton.

5 algal groups can be quantified from the bulk light absorption spectrum (if group contribution > 20% in terms of TChl a)



Intra-specific plasticity of light absorption spectra due to changes in light conditions does not significantly affect optical classification and discrimination of phytoplankton (RMSE < 21% for retrieval of Marker Pigment concentrations)



SI indicates similarity with respect to reference spectra

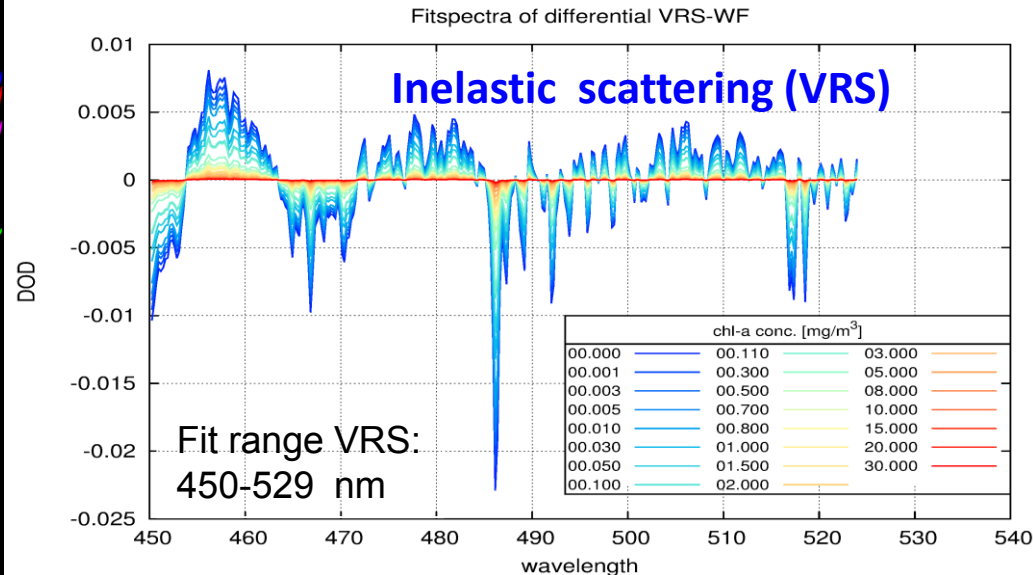
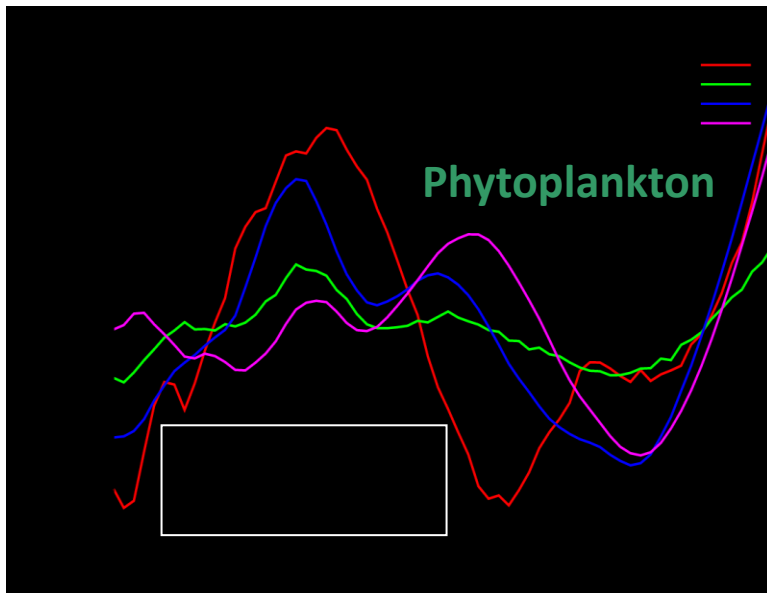
- Differential Optical Absorption Spectroscopy applied to Phytoplankton and to oceanic inelastic processes: based on Beer-Lambert-Law, aims to fulfill following minimization

$$I(\lambda) = I_0(\lambda) \cdot e^{-\tau(\lambda)} \Rightarrow \tau(\lambda) = \ln \left(\frac{I_0(\lambda)}{I(\lambda)} \right)$$

$$\left\| \tau(\lambda) - \sum_{k=1}^K S_k \sigma_k(\lambda) - \sum_{j=1}^J S_j a_j(\lambda) - S_{VRS} \nu(\lambda) - S_{int}(\lambda) - \sum_{i=0}^I x_i \lambda^i \right\| \Rightarrow \min.$$

Atmosphere Phytoplankton Inelastic scattering (VRS), water Polynom

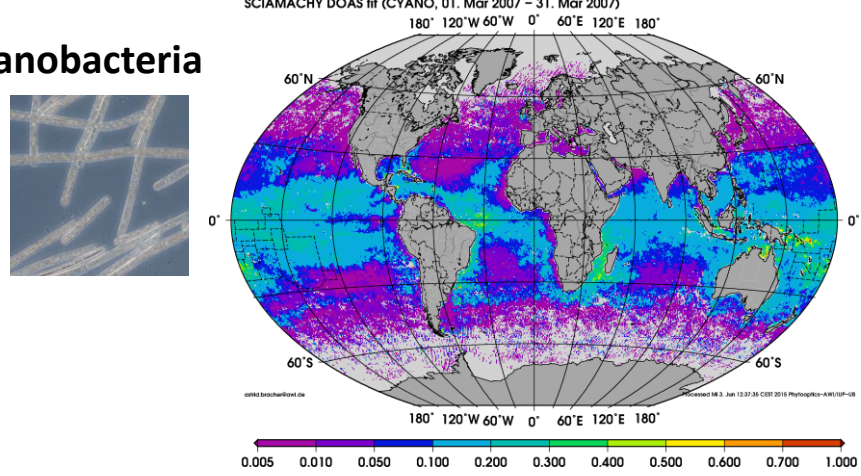
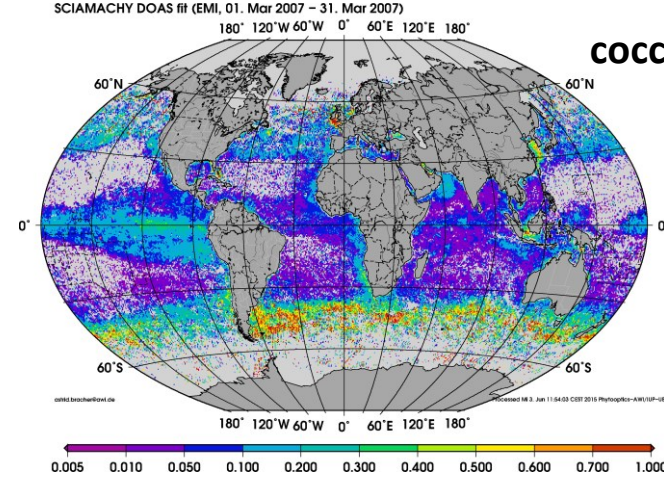
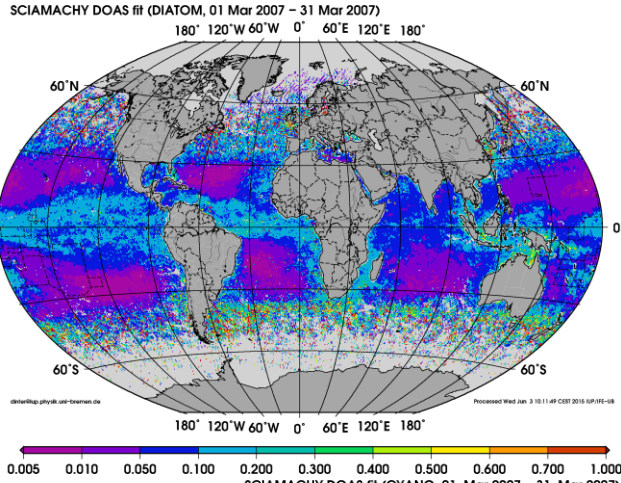
- Satellite earthshine and solar spectra (e.g, SCIAMACHY/ENVISAT)
- Measured absorption spectra of all relevant absorbers
- Low frequency changes (Mie/Rayleigh sc., ...) approximated with low order polynomial



PhytoDOAS applied to hyperspectral (<1 nm)

SCIAMACHY/ENVISAT (Bracher et al. Biogeosc. 2009, Sadeghi et al. Ocean Science 2012)

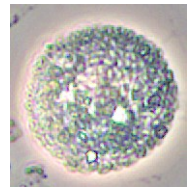
Monthly Chl-a Concentration (mg m^{-3}) – March 2007



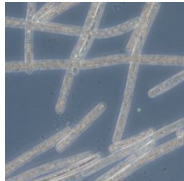
diatoms



coccolithophores



cyanobacteria



Longterm data set: SCIAMACHY (2002-2012)

<https://doi.pangaea.de/10.1594/PANGAEA.870486>

SCIAMACHY Drawback:

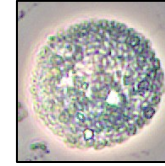
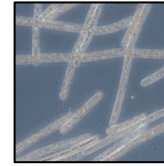
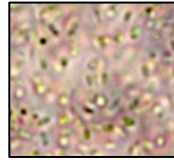
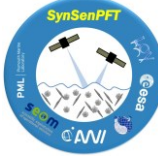
- spatial resolution ~60 km x 30 km
- 6 day, open ocean only
- Only top of atmosphere data available: difficult data handling

Application to current sensor OMI (2004 until today): **IOCS-Poster Oelker et al.**

Merging with multispectral: SynSenPFT 4 km, daily - **IOCS-Poster Losa et al.**

Spectral Band Requirements for PFT Retrievals

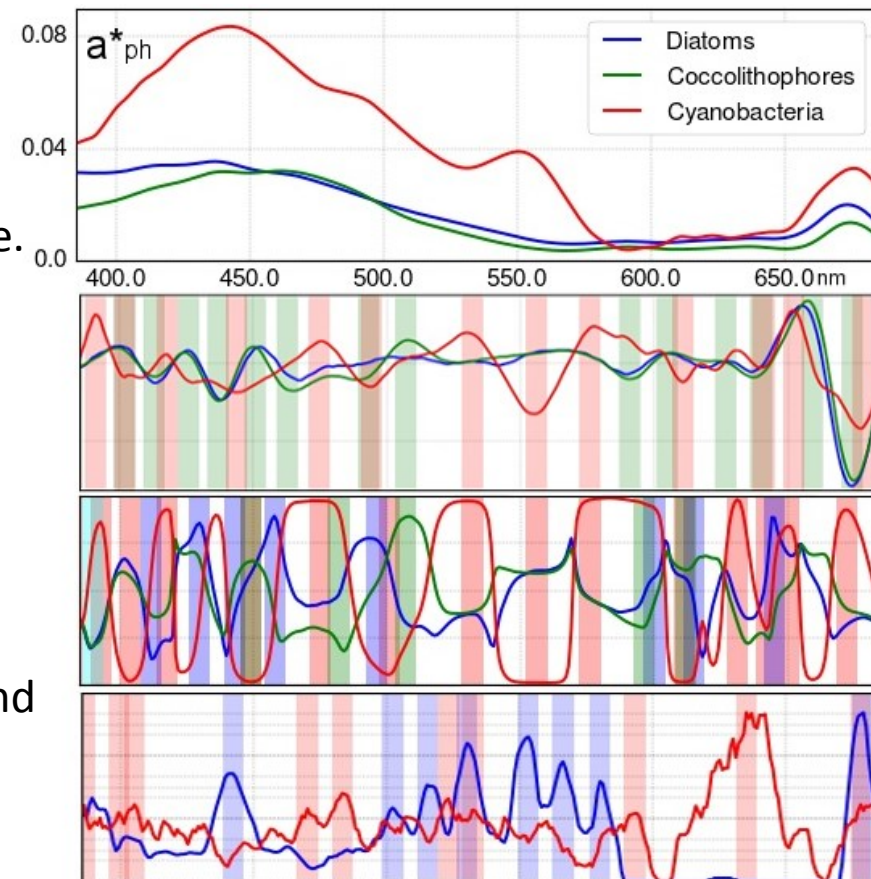
Wolanin, Soppa, Bracher (2016). Remote Sensing 8: 871



Retrieving diatom, coccolithophore & cyanobacteria chl-a with GIOP applied to simulated RRS & abs. data (>100 000,, 6 PFT mixtures): selected bands, continuous data, OC sensors

Major results

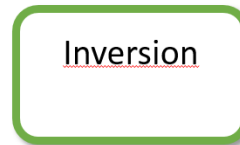
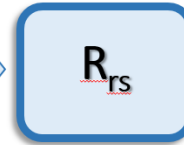
1. Hyperspectral data at 5 nm resolution: best results for discriminating multiple PFTs :
2. Small reduction of bands improves performance.
3. No specific band setting best for all PFTs.
4. MERIS best for diatoms & cyanos, SeaWiFS for coccos.
5. Adding 380, 500, 530 nm bands to OLCI may enable optical retrievals of this 3 PFTs.
6. Choice of band settings depends on
 - internal variability of the dataset investigated
 - different PFTs drive different spectral changes and hence lead to a different choice of bands.



Exploit inversion to get PFT from R_{rs} data: hyperspectral and multispectral with more bands

$A_{\phi, Dia} \cdot a_{\phi, Dia}^*(\lambda)$	$A_{\phi, Dia} \cdot b_{b\phi, Dia}^*(\lambda)$
$A_{\phi, Coc} \cdot a_{\phi, Coc}^*(\lambda)$	$A_{\phi, Coc} \cdot b_{b\phi, Coc}^*(\lambda)$
$A_{\phi, Cya} \cdot a_{\phi, Cya}^*(\lambda)$	$A_{\phi, Cya} \cdot b_{b\phi, Cya}^*(\lambda)$
$a_{dg(443\text{ nm})} \cdot a_{dg}^*(\lambda)$	$B_{bd} \cdot b_{bd}^*(\lambda)$
$a_w(\lambda)$	$b_{bw}(\lambda)$

*forward
modelling*

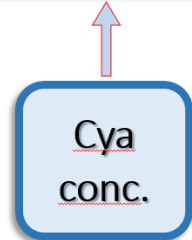
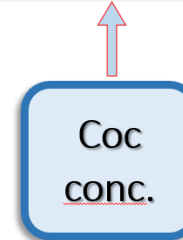
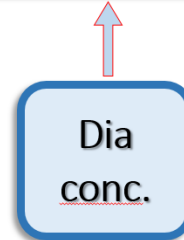


IOPs

$$a_{dg}(\lambda) = a_{dg}(443\text{ nm}) \cdot a_{dg}^*(\lambda)$$

$$b_{bp}(\lambda) = B_{bp} \cdot b_{bp}^*(\lambda)$$

$$a_{\phi}(\lambda) = A_{\phi, Dia} a_{\phi, Dia}(\lambda) + A_{\phi, Coc} a_{\phi, Coc}(\lambda) + A_{\phi, Cya} a_{\phi, Cya}(\lambda)$$



Inversion methods to build on:
Moisan et al. 2013, Chase et al. 2013 & **IOCS poster**, Organelli et al. 2013, Zhan et al. 2013; Evers-King et al. 2014, Werdell et al. 2014, Xi et al. 2015 & **IOCS poster**, Wolanin et al. 2016...

- Optimize inversion (RTM, ORM) of PFT by improved parametrizations of IOPs (mainly scattering!)
- Test PFT inversions for various hyper-spectral sensor settings (HICO, SCIAMACHY, OMI, TROPOMI, EnMAP, PACE)
- Test PFT inversions on OLCI data with 3-4 bands added (e.g. Operation Change Request for S3-B commissioning phase)

Scientific roadmap for long time series PFT data from OC

Bracher & 20 more PFT-experts worldwide (2017) *Frontier in Marine Science* 4: 55

Gap	Status	Medium-term action	Long-term action
Satellite Sensors	<p><u>Multispectral</u> sensors with limited PFT information</p> <p>Limited exploitation of <u>hyperspectral</u>:</p> <ul style="list-style-type: none"> - SCIAMACHY PFT data but <u>low coverage/resolution</u> - <u>AC failed</u> to derive hyperspectral Lw, RRS data (HICO) 	<p><u>Develop AC</u> for hyperspectral sensors</p> <p>Adapt <u>hyperspectral PFT algorithms to current</u> hyperspectral satellite data</p> <p>Develop <u>synergistic</u> hyper& multispectral PFT products</p>	<p>Exploit <u>adding bands</u> to multispectral (OLCI,...)</p> <p><u>Merge</u> all sensors' PFT data for long term coverage</p> <p><u>Launch</u> hyperspectral OC sensors (PACE, ...)</p>
Uncertainties	<p><u>Deficient theoretical background</u> for inversions?</p> <p>RTM lack PFT-info (esp. bb)</p> <p><u>No appropriate in-situ</u> HPLC-not really PFT, other PFT data require integration</p> <p>Spectral IOPs (esp. bb) limited</p>	<p><u>Optimize inversion (RTM)</u></p> <p><u>Round-Robins</u>: PFT data format, method & QC</p> <p><u>Exploit all in-situ</u> PFT, auton. techniques, hyper AOP&IOP</p> <p><u>Use complementary data</u> to constrain algorithms</p>	<p><u>Framework for clear traceability of errors</u></p> <p>Curate existing data sets</p> <p>Ensure complete PFT, hyperspectral IOP & AOP acquisition</p>