Global chlorophyll a concentrations of **phytoplankton functional types** with detailed **uncertainty assessment** using multi-sensor ocean color and sea surface temperature products – **EOF-PFT algorithm v2**

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Motivation

- Within the frame of a collaborative **project OLCI-PFT (2018-2020)**
  https://www.awi.de/en/science/climate-sciences/physical-oceanography/main-research-focus/ocean-optics/projects/olci-pft.html
- **Project Goal:**
  Globally retrieving multiple phytoplankton functional types (PFTs) from multisensor ocean color products and Sentinel-3 OLCI data
- **Long-term consistent PFT monitoring on both global and regional scales**
- **Support more accurate ecosystem modelling**

Objectives of the current study

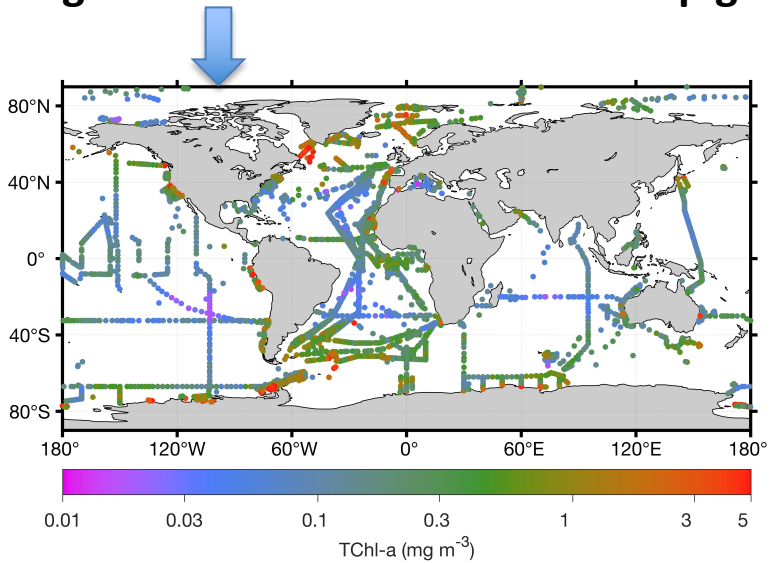
I. Improve the previously developed **algorithm for retrieving phytoplankton functional types (PFT)** (EOF-PFT v1 → v2)

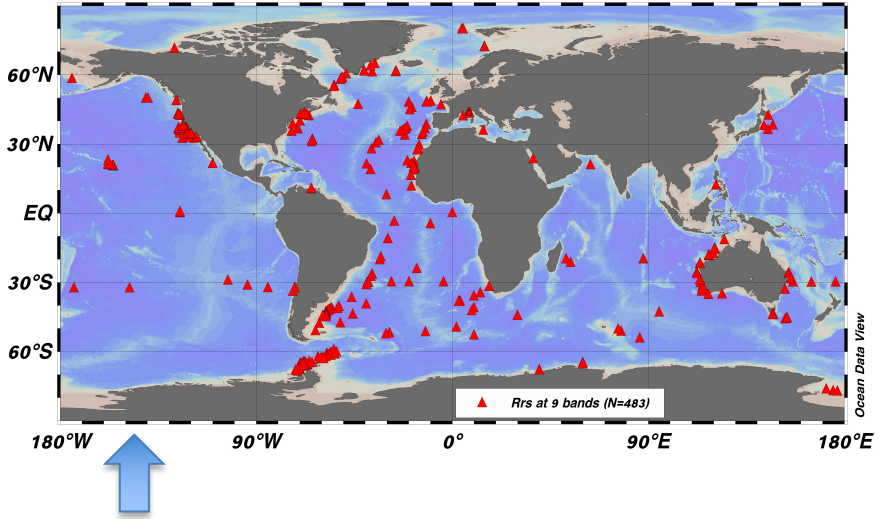
II. Provide **per-pixel uncertainty** for the satellite PFT products

III. Extend EOF-PFT approach to different ocean color sensors to **obtain continuous PFT observations from space**

Data sets

- **global database** of in situ HPLC **pigments for PFT** (N>17,000)

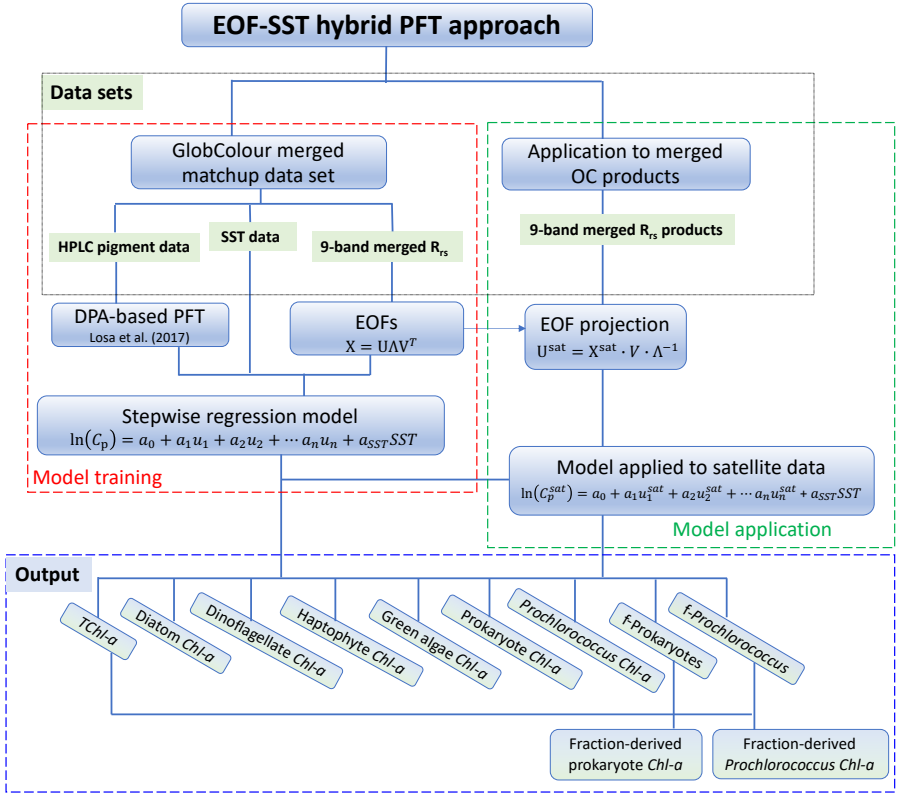




- Matchups between **satellite reflectance (Rrs), in situ PFT data, and sea surface temperature (SST)**
- **Merged OC** products SeaWiFS-MODIS-MERIS (2002-2012), MODIS-VIIRS (2012-present), and **OLCI** data (2016-present), CMEMS OSTIA SST products

Algorithm

- Re-tuned PFT Algorithm EOF-PFT v2.0



Flowchart of EOF-PFT v2.0 based on SeaW-MOD-MER merged products

Input data for model establishment:

Collocated

- In situ phytoplankton functional types (PFT) data
- Satellite Remote sensing reflectance (Rrs)
- Sea surface temperature

Method

- Empirical orthogonal function (EOF) analysis in Rrs
- Regression model for PFT:
  In situ PFT as a function of EOFs derived from Rrs and SST

Input data for application to satellites

- Satellite Rrs products (global)
- Satellite SST products (global)

Final Output

- Total chlorophyll concentration (TChl-a, total biomass)
- 6 different PFTs: diatoms, haptophytes etc.
- 2 fractions of picophytoplankton

Uncertainty sources and error propagation

The final PFT retrieval model:

$$y(\boldsymbol{a}, \boldsymbol{u}(R_{rs}), SST) = \ln(C_P^{sat}) = a_o + a_1 u_1^{sat} + a_2 u_2^{sat} + \cdots a_n u_n^{sat} + a_{SST} SST$$

Model parameters

EOF scores derived from satellite Rrs

$\boldsymbol{a}$, $\boldsymbol{u}$, and SST in Eq. (3) are not correlated with each other, the uncertainty of the PFT is presented as:

$$\sigma_y = \sqrt{\sigma_{y(Rrs)}^2 + \sigma_{y(a)}^2 + \sigma_{y(SST)}^2} = \sqrt{\sum_{i=1}^{N} \left(\frac{\partial y}{\partial Rrs_i}\right)^2 \sigma_{Rrs_i}^2 + \sum_{i=0}^{n} \left(\frac{\partial y}{\partial a_i}\right)^2 \sigma_{a_i}^2 + \left(\frac{\partial y}{\partial SST}\right)^2 \sigma_{SST}^2}$$

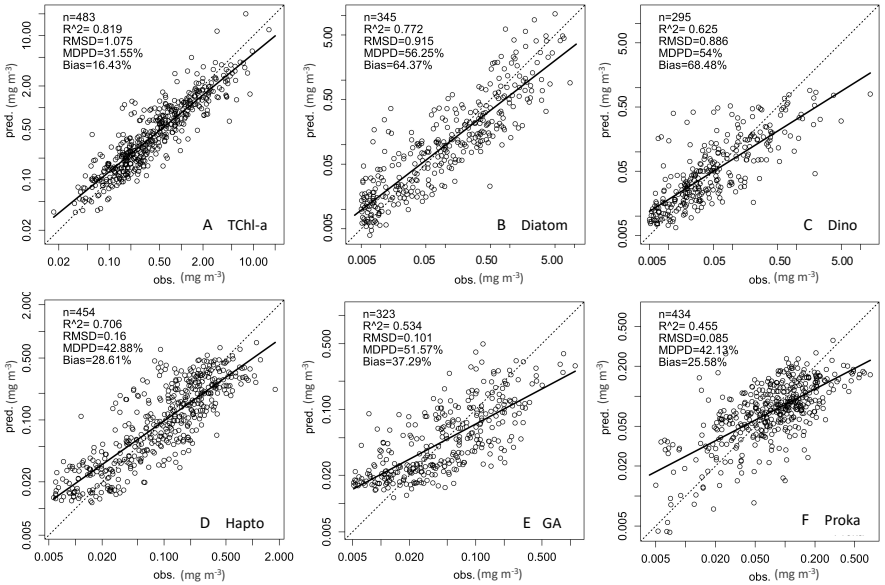
$$\sigma_{y(a)}^2 + \sigma_{y(SST)}^2 = \sum_{i=0}^{N} \left(\frac{\partial y}{\partial a_i}\right)^2 \sigma_{a_i}^2 + \left(\frac{\partial (y)}{\partial a_{sst}}\right)^2 \sigma_{a_{sst}}^2 + \left(\frac{\partial (y)}{\partial SST}\right)^2 \sigma_{SST}^2$$

$\sigma_{y(Rrs)}$ is not as straightforward as the other two uncertainty sources due to nonlinear transformation from the Rrs spectra.
Monto Carlo simulation is performed.

Results

Statistical results of EOF-PFT v2.0 versus v1.0

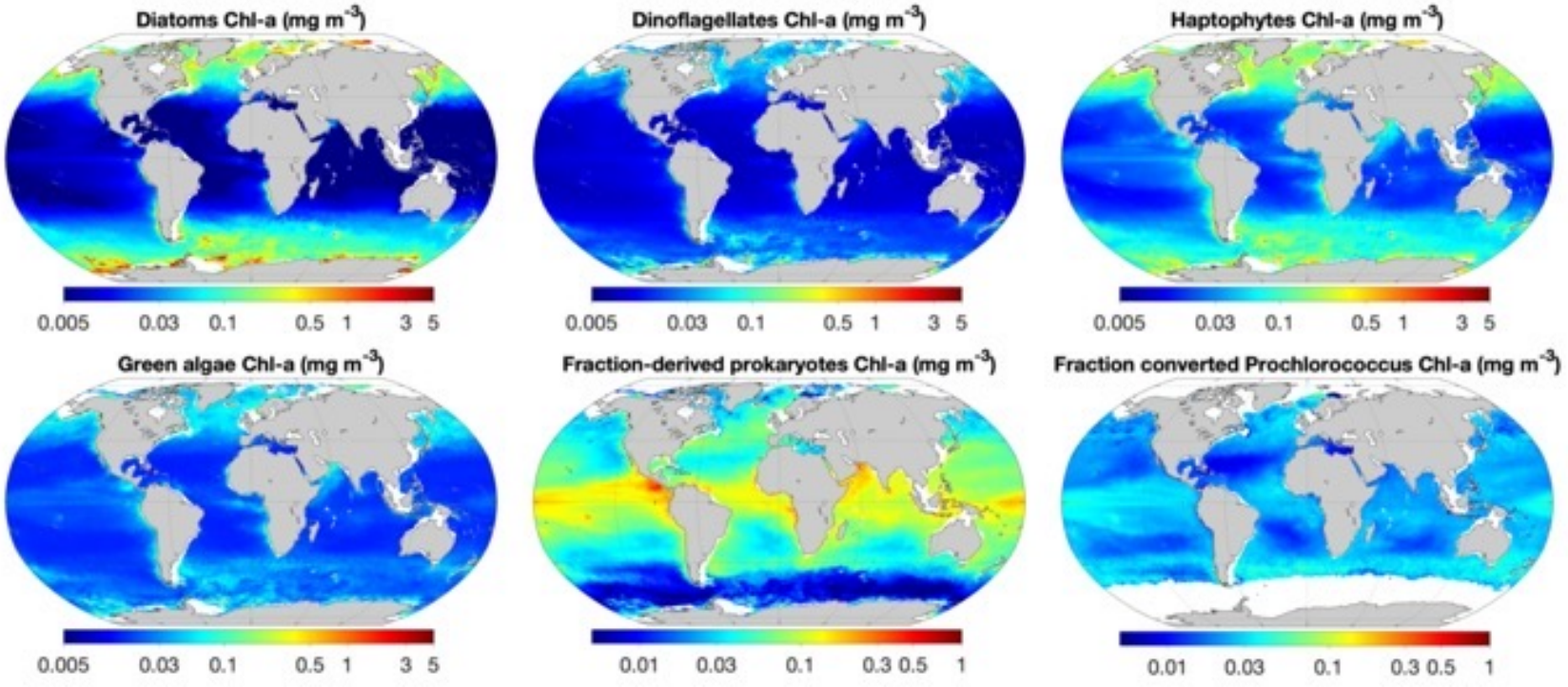
	N	MDPD (%)	RMSD (mg m^{-3})	R^2	MDPDcv (%)	RMSDcv (mg m^{-3})	R^2cv
EOF-SST hybrid model	EOF-PFT v2.0						
TChl-a	483	**31.55**	**1.08**	**0.82**	**31.51**	**1.14**	**0.81**
Diatoms	345	**56.25**	**0.92**	**0.77**	**57.71**	**0.98**	**0.76**
Dinoflagellates	295	**54.00**	**0.89**	**0.62**	**54.68**	**0.71**	**0.60**
Haptophytes	454	**42.88**	**0.16**	**0.71**	**43.63**	**0.17**	**0.69**
Green algae	323	**51.57**	**0.10**	**0.53**	**52.96**	**0.11**	**0.51**
Prokaryotes	438	**43.79**	**0.09**	**0.42**	**45.44**	**0.09**	**0.38**
f-Prokaryotes	441	47.35	0.21*	0.70	47.72	0.21*	0.68
Fraction-derived prokaryotes	434	**42.13**	**0.09**	**0.46**			
Prochlorococcus	204	42.60	0.02	0.24	44.97	0.02	0.17
f-Prochlorococcus	210	41.52	0.09*	0.62	43.99	0.09*	0.57
Fraction-derived *Prochlorococcus*	198	39.90	0.02	0.24			
Original EOF-based algorithm	EOF-PFT v1.0						
TChl-a	394	37.41	1.24	0.76	37.08	1.27	0.75
Diatoms	306	73.70	1.21	0.65	74.74	1.29	0.63
Dinoflagellates	272	55.32	0.93	0.62	57.29	0.72	0.59
Haptophytes	387	47.16	0.22	0.64	48.62	0.24	0.61
Green algae	262	55.81	0.11	0.51	56.26	0.11	0.48
Prokaryotes	367	53.70	0.13	0.15	55.08	0.13	0.11
Prochlorococcus	142	39.65	0.02	0.24	42.68	0.02	0.18



Examples of regressions between observed (x-axis, obs.) and predicted (y-axis, pred.) PFT quantities using EOF-PFT v2.0

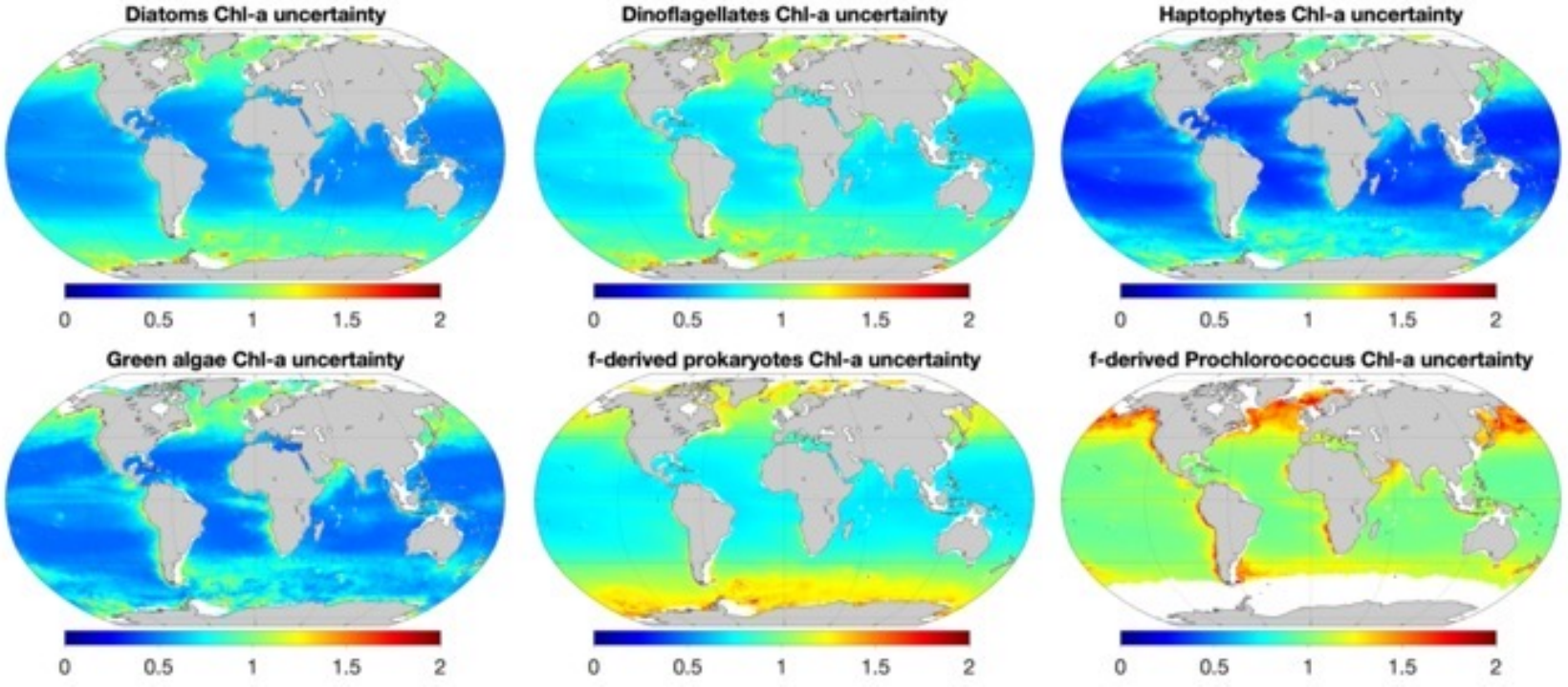
PFT products from EOF-PFT v2.0

Satellite-derived estimates of annual (2011) mean surface TChl-a and Chl-a concentrations of six PFTs

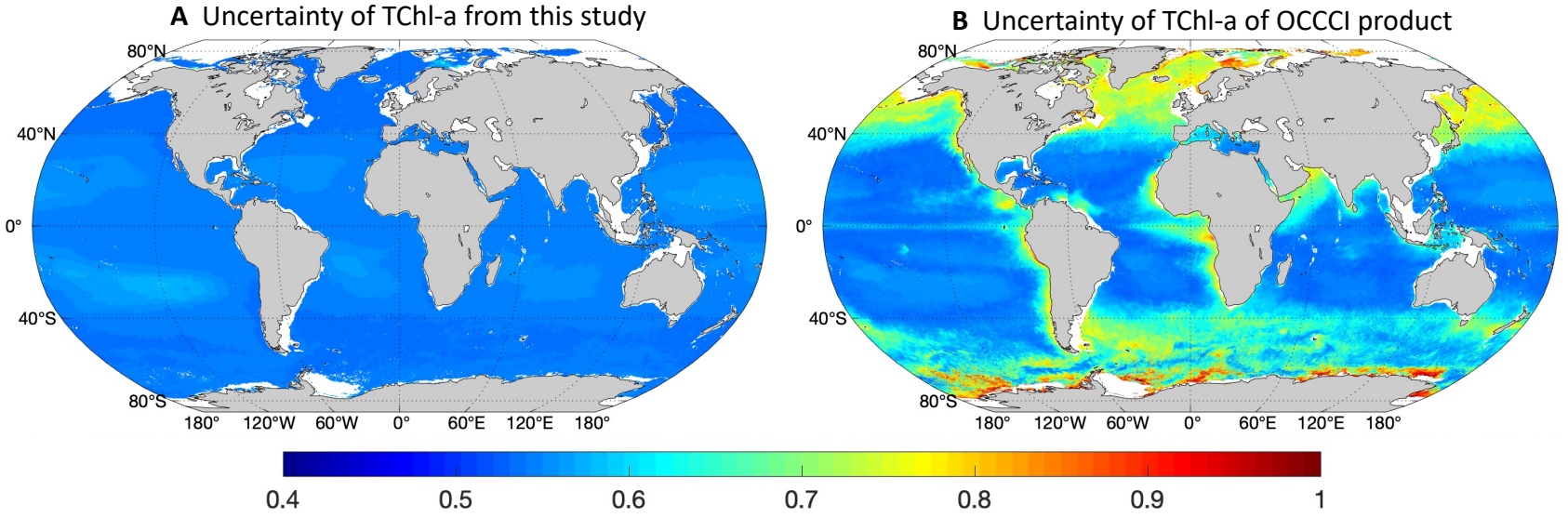


PFT uncertainty from EOF-PFT v2.0

Per-pixel uncertainty (in natural logarithmic scale) of the annual mean of 2011 for the satellite-derived PFT quantities from EOF-PFT v2.0



Uncertainty comparison



EOF-PFT v2.0: 52% – 58%

OC-CCI: 43% - 118%

- TChl-a uncertainty derived from EOF-PFT v2.0 is in general lower than the OC-CCI standard product
- First time the per-pixel PFT uncertainty description on a global scale

Extended versions v2.1 and v2.2

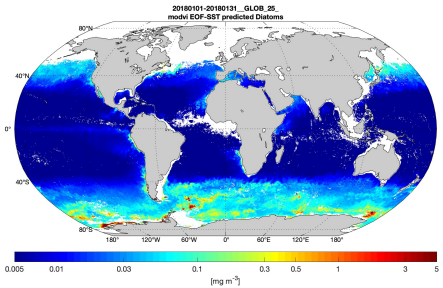
- EOF-PFT v2.1 for MOD-VIR merged products

- EOF-PFT v2.2 for OLCI products

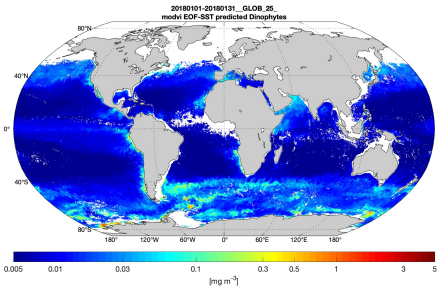
EOF-PFT v2.1

Application to MOD/VIIRS 201801

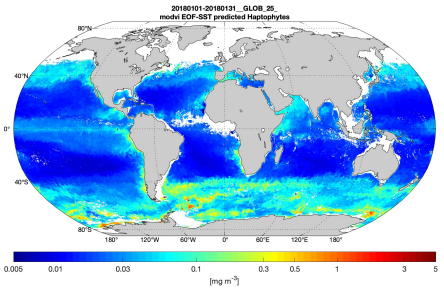
Diatom



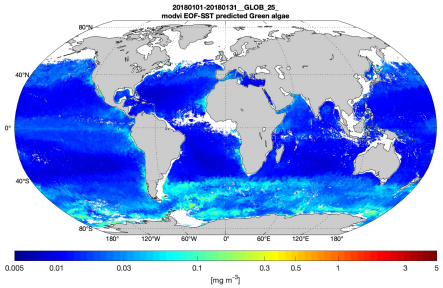
Dinoflagellates



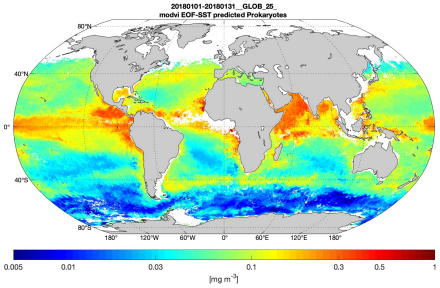
Haptophytes



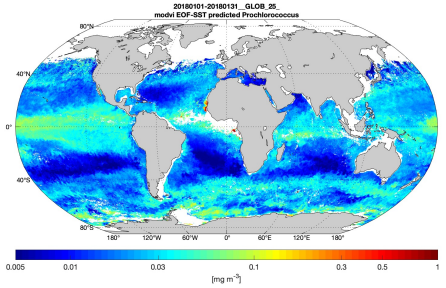
Green algae



Prokaryotes



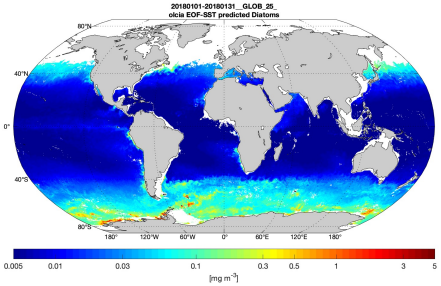
Prochlorococcus



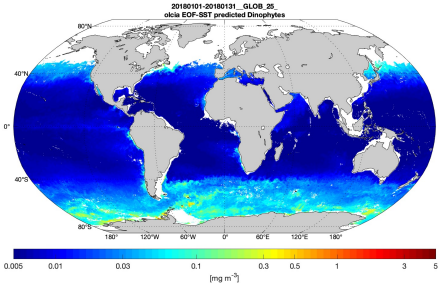
EOF-PFT v2.2

Application to OLCI 201801

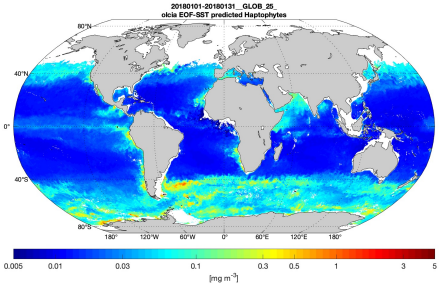
Diatom



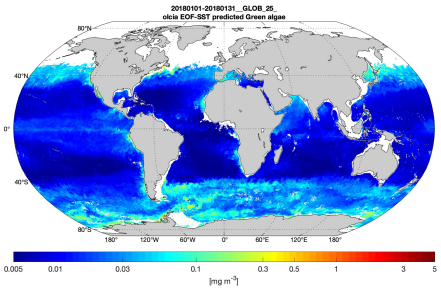
Dinoflagellates



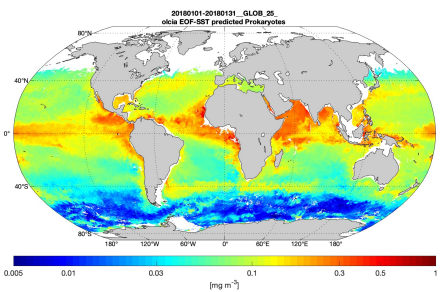
Haptophytes



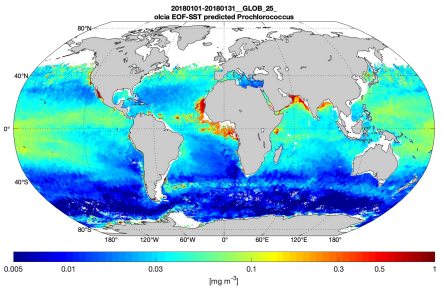
Green algae



Prokaryotes



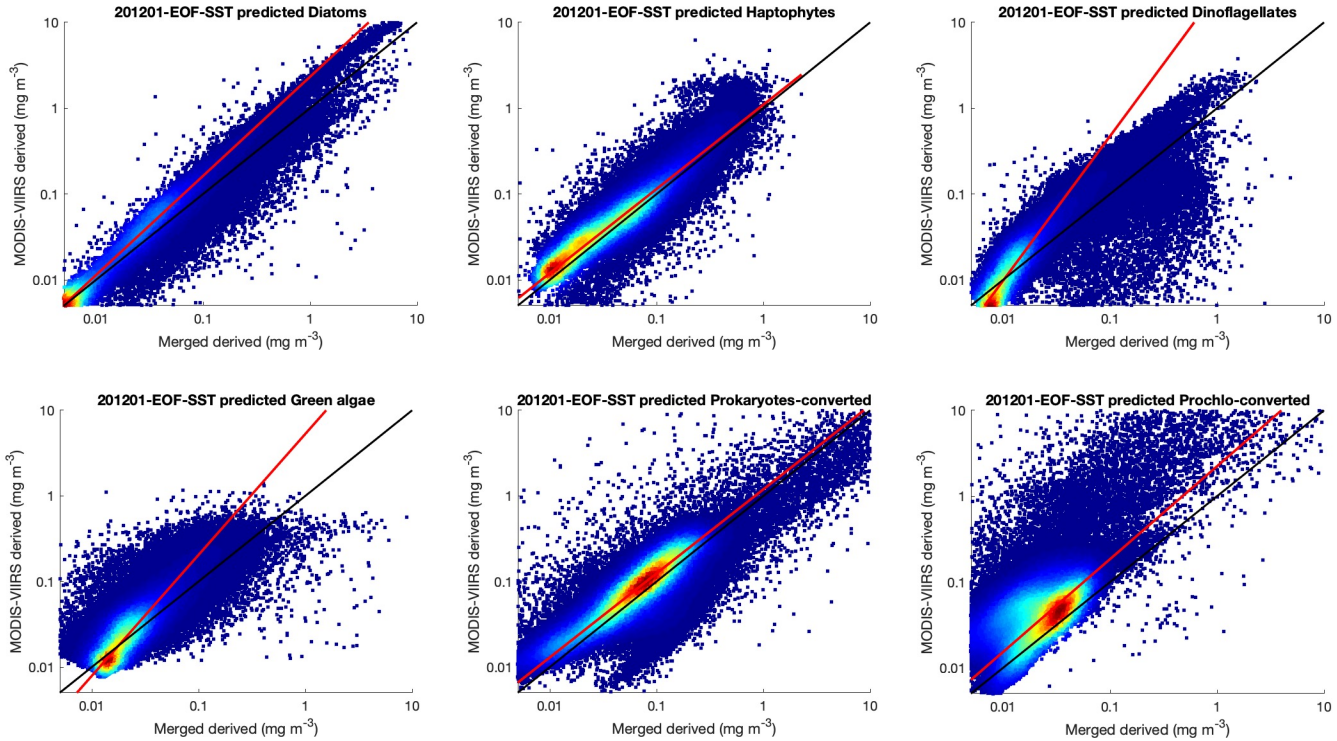
Prochlorococcus



Product consistency

EOF-PFT v2.0 versus 2.1

	Slope	Intercept	R^2
Diatoms	1.16	0.37	0.96
Dinoflagellates	1.68	1.36	0.82
Haptophytes	0.98	0.04	0.93
Green algae	1.41	0.72	0.78
Proka_converted	0.98	0.08	0.86
Prochlo-converted	1.08	0.35	0.41



Statistics of type II Regression with uncertainty accounted between **MOD/VIR** and **SeaW/MOD/MER** monthly PFTs for Jan 2012.

List of EOF-PFT algorithm versions

	EOF-PFT version	Date of development	Applicable sensor(s)	Input data	Product time frame	Remarks
EOF-based algorithm	**v1.0**	Dec 2019	SeaWiFS/MODIS/MERIS merged product	9-band merged R_{rs}	2002-2012	In situ data from Losa et al. (2017)
	v1.1	Jan 2019	MODIS/VIIRS merged product	9-band merged R_{rs}	2012-present	Losa et al. (2017) and own cruises
	v1.2	Jan 2019	Sentinel 3 OLCI-A product	11-band OLCI R_{rs}	2016-present	In situ data from own cruises
EOF-SST hybrid algorithm	**v2.0**	Mar 2020	SeaWiFS/MODIS/MERIS merged product	9-band merged R_{rs}, SST	2002-2012	Updated pigment data
	v2.1	May 2020	MODIS/VIIRS merged product	9-band merged R_{rs}, SST	2012-present	Updated pigment data
	v2.2	May 2020	Sentinel 3 OLCI-A product	11-band OLCI Rrs, SST	2016-present	Updated pigment data
SST-separated hybrid algorithm	**v3.0**	Jul 2020	SeaWiFS/MODIS/MERIS merged product	9-band merged R_{rs}, SST	2002-2012	Updated pigment data

Algorithm and Products Available online

- **Algorithm implemented into Coastal-TEP** : https://www.coastal-tep.eu/geobrowser/

- **Data products available** in **CMEMS** Under “Ocean Products” at https://marine.copernicus.eu/

  Updated version available online in May 2021

Summary and Outlook

- Improved satellite PFT products are provided using updated algorithms EOF-PFT v2
- Per-pixel uncertainty of the satellite PFT products is assessed in detail by accounting for errors from input data and model parameters
- Extendable to other ocean color satellite products

Outlook:

- **Continuous time series of global PFT – long term monitoring**
- **PFT shifting and trend** under the changing climate

For more detailed information please check on the publication by Xi et al. 2021: **https://doi.org/10.1029/2020JC017127**

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- NASA, ESA, EUMETSAT for the SeaWiFS, MODIS, MERIS and OLCI data
- GlobColour program for the L3 merged products
- CMEMS for the sea surface temperature products
- Ocean-Colour Climate Change Initiative (OC-CCI) program for global chlorophyll-a data products