# Point by point response to the reviewers

#### of the manuscript entitled Two-decade satellite monitoring of surface phytoplankton

#### functional types in the Atlantic Ocean

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Text in black – Comments from the reviewers Text in blue – Authors' response

Remarks:

- Line numbers indicating major changes made in the track-changes file are highlighted throughout the answers. While converting the track-changes file to .pdf version we have noticed that the line numbering was somehow changed, therefore we updated them in this response file. Note that the highlighted line numbers are now different from the previously uploaded author comments to each reviewer (AC1, AC2 & AC3), however, the responses and answers are not affected.
- In situ data used for validation has been submitted to PANGAEA. It is now however in the proof-reading stage and will be soon freely available via the doi link below. Xi, Hongyan; Peeken, Ilka; Gomes, Mara; Brotas, Vanda; Tilstone, Gavin H; Brewin, Robert J W; Dall'Olmo, Giorgio; Murawski, Sandra; Wiegmann, Sonja; Bracher, Astrid (2023): Phytoplankton pigment concentrations and phytoplankton groups measured on water samples collected from various expeditions in the Atlantic Ocean from 71°S to 84°N. PANGAEA, https://doi.pangaea.de/10.1594/PANGAEA.954738

# **Reviewer 1**

Review of "Two-decade satellite monitoring of surface phytoplankton functional types in the Atlantic Ocean" by Hongyan Xi et al.

# **General comment:**

The paper submitted by Hongyan Xi et al. focuses on PFTs in the Atlantic Ocean as seen by satellite in the last two decades. The paper is well written and easy to be read and represents a useful analysis and report to understand what is the Atlantic Ocean ecosystem status.

Overall, I have some specific comments that are preferable be included in the revised version of the manuscript. Especially, some sections need to be extended with more information: for instance, some more details about the EOFs technique in the section of time-series analysis, or the definition of the statistical indexes used to evaluate the satellite products in respect to the in-situ dataset. Two key points are: extend the discussion of the results found in the validation test of satellite vs. in situ data, specifically for what concern the statistics; and the inclusion xof a significance test (e.g. p-value) to better interpret the trends found in the different regions.

However, on my opinion, the paper needs only minor corrections before the publication. This is a useful work for the ocean colour community from both scientific (the understanding of the PFTs changes in the Atlantic Ocean ecosystem) and technical (e.g. products validation, long-term time-series) perspectives.

We thank very much the reviewer for the positive feedback and constructive comments on this manuscript. We have considered carefully all the suggestions to improve the manuscript. Before we address each of the comments individually, we would like to preface with a brief response to the above general comment.

Firstly, we would like to clarify that the EOF technique was not used in the time series analysis but is used in the satellite PFT estimation approach that was proposed and detailed in Xi et al. (2020, 2021). The CMEMS global PFT products used in this study are generated based on the EOF-PFT approach therefore we only mentioned it briefly while describing CMEMS PFT products in the manuscript. Secondly, the discussion on the validation results and statistics has been updated and extended. Lastly, more details about the time series analysis have been added. However, we would like to point out that this manuscript was submitted as a contribution to an upcoming Ocean State Report, for which specific requirements in paper length and number of tables/figures have to be followed. The current paper length is just at this limit; therefore, we extended/added the necessary discussion/information in the manuscript as concise as possible, but more details are provided in the individual responses below.

# Specific comment:

Section 2.1

I would include a table with the wavelengths/bands of the different sensor here used and that have been controlled. I would add a Figure that pointed out the life cycle of each sensor and the overlap of the different mission. Such a information give to the reader a clear, easy details about the last 20 years of satellite sensors and mission.

We agree with the reviewer that such information would give clearer details on the past/current satellite missions. We did not include the detailed wavelengths/bands of different sensors because of the length limit for such a report and also because they are detailed in our previous work (Xi et al. 2020; 2021). The period of PFT products from each sensor or sensor combinations has also been provided both in section 2.1 and Table1 in the manuscript (no figure was added for brevity).

However, in response to the reviewer we have still prepared the table and the figure (see below), as the review reports and responses are eventually also publicly available online for all readers.



Figure R1. Lifespans of ocean colour sensor (combinations) where Rrs products were acquired.

Table R1:	Wavebands	of	satellite	sensor	(combinations)	involved	in	the	PFT	estimation	n
approach.											

Sensors involved	Center wavebands used in the EOF-PFT approach (nm)						
SeaWiFS/MODIS/MERIS merged <sup>a</sup>	412 443 490 510 531 547 555 670 678						
MODIS/VIIRS merged	412 443 490 531 547 551 555 670 678						
Sentinel 3A OLCI	400 412 443 490 510 555 <sup>b</sup> 560 620 665 674 681						
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<sup>a</sup> SeaWiFS terminated in December 2010, therefore from Jan 2011 to April 2012 only MODIS/MERIS merged data were available.

<sup>b</sup> There is no band at 555 nm for OLCI itself, but the GlobColour Team provides also the 555 nm band through an inter-spectral conversion from 560 nm (details see ACRI-ST GlobColour Team et al., 2017)

# Section 2.3

Please extend the section with more details about the method you have applied (i.e. EOFs). Currently, it is not mentioned in the section about the time-series analysis.

The EOF-based approach is actually the theoretical basis of the CMEMS PFT products algorithm that were used in this study. Details about the algorithm are provided in Xi et al. (2020; 2021). Since this study focuses mainly on the PFT long term observations and time series extracted from the satellite operational PFT products but not on the EOF-based approach itself, we only cited the references but did not include the details in the manuscript.

Regarding the time series analysis, the reviewer was right that more information should be included. We have extended Section 2.3 by adding brief descriptions regarding the computations of the 20-year trend, phenology indicators and anomaly of 2021.

Text added in the revised manuscript (**section 2.3 Lines 131-138**): "We investigate the trends in the PFTs for the last 20 years using linear regression in the format of Y=SX+I, where Y is the monthly PFT Chla of either per-pixel or the regional log-based mean, X is the time on monthly basis, S is the slope of the regression and I is the intercept. Only trends with statistically significant correlations of the regression (p<0.05) are shown. Indicators of PFT phenology and the anomaly of 2021 (the last year of the considered time period) are also extracted in order to identify potential changes/shifts in PFTs. Abundance maxima time, as one of the phenology indicators, is identified for each pixel by finding the month when the maximum PFT Chla occurred during the year. Anomaly in percentage is determined by computing the relative difference between the PFT state of 2021 and the average state of the last two decades (i.e., climatology)."

# Section 3.1

Lines 134: you mentioned that the same correction approach is then applied on Sentinel-3A OLCI derived PFTs. Please add some details about how it works for OLCI.

We have added more information about the correction on the OLCI derived PFTs.

**Lines 146-152** "The same is applied to the Sentinel 3A OLCI derived PFTs by comparing them to the corrected MODIS/VIIRS derived PFTs for the overlapped period April – December 2016, so that all PFT data from both MODIS/VIIRS and OLCI are now referenced to SeaWiFS/MODIS/MERIS derived PFTs. Though R<sup>2</sup> is slightly weaker (R<sup>2</sup> between 0.77 and 0.83) compared to that from the MODIS/VIIRS versus SeaWiFS/MODIS/MERIS derived PFTs (R<sup>2</sup> between 0.82 and 0.98), OLCI derived PFTs still showed overall good correlations to the corrected MODIS/VIIRS data with regression slopes between 0.83 and 1.03 despite that prokaryote Chla retrievals from OLCI data are in general higher."

Figure R2 shows scatterplots and regression relationships between the two products. However, due to the paper length limit, we decided not to include the figure in the revised manuscript.



Figure R2: Scatterplots of monthly PFTs derived from OLCI Rrs and corrected MODIS/VIIRS merged Rrs data for the overlapping period April – December 2016. The 1:1 line is shown in black and the linear regression line (using type II regression with per-pixel uncertainty) in red. R<sup>2</sup>, slopes and offsets determined in log-10 scale are also presented.

Lines 139: Please add some more details about the type of errors reported in the table 1. How is defined the MDPD? and the RMSD? What means a MDPD of 89.6%? It indicates a good agreement between satellite and in-situ data or vice versa. Which is the unit of median uncertainty, it is expressed in %.

We agree with the reviewer that the statistics should be described in more detail, therefore we have updated the caption of the statistics table (Table 2) with more details

**Lines 494-500** "Table 2. Statistical validation results of satellite derived PFT Chla (after intermission correction) as a function of in situ PFT Chla using least square fit in logarithmic scale. N: number of matchups; R<sup>2</sup>: coefficient of determination; MDPD: median percent difference; RMSD: root-mean-square difference; definition equations of these terms were referred to Xi et al. 2020. Note that Slope, Intercept and R were calculated based on logarithmic scale. Median uncertainties calculated based on satellite per-pixel PFT uncertainty (equivalent to relative error in %) are also shown in the last column."

Regarding the statistics indicating how good the agreement between the satellite and in-situ data is, please see our response below to the next relevant comment.

The authors need to better describe the results found here, since this is the first step behind the successive important and impactful time-series analysis: for instance, an R coefficient of 0.6 is equal to an R2 of 0.36 that implies not a strong correlation between in-situ and satellite-

derived PFT. This is consistent or a better results in respect to the previous works and literature?

During the "under-review" stage we have obtained more in situ data for the validation also with a more thorough matchup extraction, therefore, we have been able to extend the matchup data set and update the statistics in Table 2. We have added Figure R3 in this response document to show the scatterplots between the inter-sensor corrected satellite PFTs versus the in situ PFT data. This figure is not included in the revised documents as Table 2 summarizes adequately the statistics.

The discussion regarding the validation has been also updated in Section 3.1 and the Discussion (Section 4).

**Section 3.1 Lines 153-159**: "Validation was carried out by comparing the collocated satellite PFTs with the in situ PFTs using the extracted matchup data. Statistical results of the validation in Table 2 show in general acceptable agreement between the in situ and satellite derived PFTs. Median percent differences (MDPD) are consistent with the median satellite PFT uncertainties (relative error in %) estimated through Monte Carlo simulation and error propagation in Xi et al. (2021), and for dinoflagellates, notably lower. Higher MDPD is found for prokaryotes due to a systematic overestimation of the picophytoplankton in the retrieval algorithms for all the three sets of satellite OC sensors, however, no significant bias of satellite prokaryote products is detected between different sensors, therefore the overestimation should have minor influence on the time series data of prokaryotes."

**Section 4 Lines 250-258**: "Validation using in situ data shows no significant biases of PFTs derived from different sensors, indicating that the inter-mission offset was effectively corrected. Chla of different PFTs are more upscaled retrievals compared to bulk satellite OC products such as total chlorophyll a, coloured dissolved organic matter (CDOM) and absorption properties. Especially, it is still challenging to retrieve accurately prokaryotic phytoplankton because in the open ocean these are dominating in the low Chla areas for which the satellite signals are weaker. Therefore higher uncertainties exist in these products (e.g., Brewin et al. 2017; Losa et al. 2017; Xi et al. 2021) as compared to uncertainties for other PFTs (see Table 2). In summary, our statistical results of PFT validation are comparable to the evaluations of satellite PFT products derived from different approaches, according to the Quality Information Documents (QUID) that have been published on CMEMS (Garnesson et al., 2022; Pardo et al., 2022)."

# Table 2 has been updated (Lines 494-500):

Table 2: Statistical validation results of satellite derived PFT Chla (after inter-mission correction) as a function of in situ PFT Chla using least square fit in logarithmic scale. N: number of matchups; R<sup>2</sup>: coefficient of determination; MDPD: median percent difference; RMSD: root-mean-square difference; definition equations of these terms were referred to Xi et al. 2020. Note that Slope, Intercept and R were calculated based on logarithmic scale. Median uncertainties calculated based on satellite per-pixel PFT uncertainty (equivalent to relative error in %) are also shown in the last column.

	Ν	Slope	Intercept	R <sup>2</sup>	MDPD (%)	RMSD (mg m <sup>-3</sup> )	Median satellite PFT uncertainty (%)
Diatoms	192	0.71	-0.27	0.76	60.5	0.30	57.3
Haptophytes	191	0.95	-0.007	0.41	58.9	0.18	41.5
Prokaryotes	187	0.71	0.12	0.36	185	0.06	86.5
Dinoflagellates	144	1.07	0.04	0.66	59.1	0.07	74.3



Figure R3: Scatterplots of matched satellite derived PFT Chla after inter-mission correction versus in situ PFT Chla including statistical results.

# Section 3.3.

Discussion of trend (increasing/decreasing) needs to be also coupled to a statistical significance test as the p-value. This coefficient could give to the reader a tool to understand the inter-annual variability and if it has a statistical significance in the last 20 years.

We would like to clarify that only areas with significant trends (p<0.05) were shown in the per-pixel trend maps and were discussed in the manuscript. We have mentioned the significant level in section 2 (section 2.3 Lines 131-138) and also in the figure captions. For the overall trends of the four PFTs shown in Figure 3b, significant trend was found for prokaryotes only and the slope and p-value were indicated.

For Figure 4 trendlines with slopes and correlation coefficients are now shown in the time series plots for provinces with significant trends (p<0.05) only. These trends in different provinces correspond well to the previous descriptions in the results (Section 3.3 Lines 202-212).



Figure 4: Time series of diatom Chla (unit: mg m<sup>-3</sup>) in 11 Longhurst provinces in the Atlantic Ocean with bathymetric information based on ETOPO1 bathymetry (Amante & Eakins, 2009). Provinces according to Longhurst (2007) are: NADR for North Atlantic Drift Province, NWCS for Northwest Atlantic Shelves Province, NASW for North Atlantic Subtropical Gyral Province (West), NASE for North Atlantic Subtropical Gyral Province (East), NATR for North Atlantic Tropical Gyral Province, CNRY for Canary Current Coastal Province, WTRA for Western Tropical Atlantic Province, ETRA for Eastern Tropical Atlantic Province, SATL for South Atlantic Gyral Province, SSTC for South Subtropical Convergence Province, SANT for Subantarctic Water Ring Province, respectively. Trendlines with slopes (unit: Chla mg m<sup>-3</sup> month<sup>-1</sup>) and correlation coefficients are shown for provinces with significant trends (p<0.05).

#### Section 3.4

How did you compute the abundance maxima time? How it is defined? Please add more details about the computation in the Section 2.3 (time-series analysis).

As monthly data were used in this study, the abundance maxima for the year of 2021 was identified by finding the month for each pixel when the maximal PFT Chla occurred during the year.

More details (but have also to be concise due to length limit) on time series analysis have been added in **section 2.3 Lines 131-138**: "We investigate the trends in the PFTs for the last 20 years using linear regression in the format of Y=SX+I, where Y is the monthly PFT Chla of either per-pixel or the regional log-based mean, X is the time on monthly basis, S is the slope of the regression and I is the intercept. Only trends with statistically significant correlations of the regression (p<0.05) are shown. Knowledge of PFT phenology and anomaly of 2021 (the last year of the considered time period) are also gained through to help identify potential changes/shifts in the PFTs. Abundance maxima time, as one of the phenology indicators, is identified for each pixel by finding the month when the maximal PFT Chla occurred during the

year. Anomaly in percentage is determined by computing the relative difference between the PFT state of 2021 and the average state of the last two decades (i.e., climatology)."

# **Technical Corrections (some examples):**

Lines 35-38: please rephrase the sentence.

The sentence was rephrased to "Climate induced changes causing temperature rise, ocean acidification and ocean deoxygenation, stress the ocean's contemporary biogeochemical cycles and ecosystems, thereby impact the phytoplankton communities (Gruber, 2011; 2021; Bindoff et al. 2019)." (Lines 36-38)

Line 42: I'd remove "as a whole" à you can leave the sentence as: "phytoplankton biomass does not provide a full description of the complex nature of phytoplankton community and function".

# Removed as suggested.

Line 44: please rephrase the sentence "Phytoplankton composition structure varies across ocean biomes and different phytoplankton groups influence marine ecosystem and biogeochemical processes differently (Bracher et al., 2017) à I would change in "Phytoplankton composition varies across ocean biomes and the different phytoplankton groups influence marine ecosystem and biogeochemical processes differently (Bracher et al., 2017)"

# Revised as suggested.

Line 51: I would remove "as well", it is not necessary here.

#### Removed as suggested.

Lines 72-74: I do not understand to what referred such sentence, from "Previously" to "measured pigments".

This sentence referred to the previous studies of Xi et al. (2020; 2021) and the algorithms developed therein. We moved the citations right after this sentence for a better clarification.

Line 78: chlorophyll a can be modified in Chla since you have defined in the first part of the paragraph.

#### Removed as suggested.

Line 80: maybe a refuse of something, maybe you can change in in this work.

Thanks for the comment. By "refuse" we suppose the reviewer means data fusion? So far we would only focus on merging the PFT data sets from different sensors for a consistent long-term data set to enable trustworthy time series analysis of the phytoplankton groups on either global or regional scales.

# References

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Pardo, S., Jackson, T., Netting, J., Calton, B., & Howey, B. (2022). QUID for OC TAC Products Atlantic and Arctic Observation Products. Issue 2.0, Ref: CMEMS-OC-QUID-009-111 to114-121to124, Date: 16 June 2022.

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# **Reviewer 2**

Review of "Two-decade satellite monitoring of surface phytoplankton functional types in the Atlantic Ocean"

Hongyan Xi, Marine Bretagnon, Svetlana N. Losa, Vanda Brotas, Mara Gomes, Ilka Peeken, Antoine Mangin, Astrid Bracher

# General comments

Using long-time series of satellite-derived PFT products, Xi et al. investigate the two-decade trends, climatology, phenology, and anomaly of PFT in the whole Atlantic Ocean and its different biogeochemical provinces. Firstly, based on their previous studies (Xi et al., 2020, 2021), the authors obtain PFT Chla products (mainly four phytoplankton groups) using three different sets of ocean color data, covering from 2002 to 2021. Through the independent validation and the inter-comparison of among three sets of ocean color data within overlapping time periods, they then identify the systematic differences caused by different data sources, set up the SeaWiFS/MODIS/MERIS-derived products as reference, and correct the other two PFT datasets, to generate a consistent long-time series PFT products over the last two decades. Finally, the trends and variations of PFTs in the Atlantic Ocean and its biogeochemical provinces are analyzed.

In general, the manuscript is well written and logically organized, with clear purposes and conclusions. The findings of this work provide a preliminary distribution and variation of four PFTs in the Atlantic Ocean, and potential contribution of understanding how these phytoplankton groups respond to climate changes. However, there are some issues to be addressed before it can be considered for publication. Please see below for some major and specific comments.

We thank very much the reviewer for the constructive comments on this manuscript which we have carefully considered in our revision. We would also like to point out that this manuscript was submitted as a contribution to an upcoming Ocean State Report, for which specific requirements in paper length and number of tables/figures have to be followed. The current paper length is just at this limit; therefore, we extended/added the necessary discussion/information in the manuscript as concise as possible, but more details are provided in the individual responses below.

# Major comments

1. In this study, when generating the consistent PFT products from different OC data sources, systematic differences among three sources are adjusted based on the relationships between Chla of PFTs derived from each OC data, as shown in section 2.1 and Figure 1. Since the Chla of PFTs are derived from Rrs, i.e., secondary products, why not consider correcting inter-mission bias of the Rrs first, then derive PFTs using the corrected Rrs? In this circumstance, for each of the other two OC datasets, only one correction with respect to Rrs is required, rather than four corrections for different phytoplankton groups. Have you compared the differences of PFT products between these two procedures?

The reviewer's suggestion is very constructive and that would be a good idea when one could adjust the biases at the very beginning on the input data. However, that normally requires extensive data sets and thorough analyses to support the correction for each available band. In fact, the Rrs products (from merged sensors or OLCI) used for PFT estimation are provided in the frame of the EU funded GlobColour project, which aims for continuous data sets of merged L3 Ocean Colour products (https://www.globcolour.info/). One of the goals of GlobColour is merging outputs from different sensors that ensures data continuity, improves spatial and temporal coverage and reduces data noise. Systematic differences of Rrs from GlobColour have been already adjusted among different sensors after a series of in situ data validation, uncertainty assessment, and different merging approaches (Maritorena et al. 2010). We don't think we could do a better bias correction of the Rrs than the GlobColour team who has put much effort in achieving it. So far, OLCI Rrs data have not been merged to other sensors (e.g., MODIS and VIIRS) yet, but the two OLCI Rrs data sets from Sentinel 3A and 3B have been merged – however, current CMEMS PFT products are still based on S3A OLCI data only.

There are actually a few reasons that cause the differences of PFTs from different periods: 1) the Rrs data with different bands (Table R1) are used for each period to involve as many bands as possible to improve the PFT estimation performance of the PFT approached based on EOF analysis; 2) PFT estimation models were assessed and finally established based on best algorithm performance separately for the three types of sensor (combinations), in which specific data sets (both in situ and satellite data) within the specific period have been used for model development (examples can be found in Xi et al. 2020 where both merged and OLCI Rrs were used); 3) Model input data for the three sets of sensor(s) are not only different in time, but also different in data size, and geolocations. Promisingly, despite these influencing factors the PFT retrievals from the three sets of data are still highly comparable both in magnitudes and spatial distribution pattern, we therefore would like to take the advantage to explore further the long term PFT observations.

Table R1: Wavebands of satellite sensor (combinations) involved in the PFT estimation approach.

Sensors involved	Center wavebands used in the EOF-PFT approach (nm)
SeaWiFS/MODIS/MERIS merged <sup>a</sup>	412 443 490 510 531 547 555 670 678
MODIS/VIIRS merged	412 443 490 531 547 551 555 670 678
Sentinel 3A OLCI	400 412 443 490 510 555 <sup>b</sup> 560 620 665 674 681

<sup>a</sup> SeaWiFS terminated in December 2010, therefore from Jan 2011 to April 2012 only MODIS/MERIS merged data were available.

<sup>b</sup> There is no band at 555 nm for OLCI itself, but the GlobColour Team provides also the 555 nm band through an inter-spectral conversion from 560 nm (details see ACRI-ST GlobColour Team et al., 2017)

 As mentioned in the discussion, 20-year observation may not be enough for a robust trend analysis. I was wondering why PFT results derived from SeaWiFS between 1997 and 2002 are not included in this study? If they are included, the length could be extended to ~25 years.

Indeed, if we could include the single SeaWiFS sensor it would be ~25 years observation. The PFT products were however derived based on satellite remote

sensing reflectance (Rrs) data at **9 (for merged OC sensors) or 11 (for OLCI sensor) bands in the visible region (400-700 nm)** using the EOF-PFT approach developed in Xi et al. (2020) and a retuned version in Xi et al. (2021); Rrs from single SeaWiFS sensor contains only six bands which were not sufficient to get reliable PFT estimations through EOF trainings. It also the reasoning why for different sensor life times different band combinations were needed to be chosen for the EOF-PFT approach. Therefore, the SeaWiFS-only period (1997-2001) was not included.

3. Some parts of section Data and Method are lack of details, including: (1) the quality control of pigment data from Aiken et al. (2009); (2) diagnostic pigment analysis; (3) the correct functions among different OC data sources; (4) the sources/website of Longhurst's geographic classification system; (5) per-pixel uncertainties of PFT products derived from Rrs data; and (6) the calculation of the anomaly of PFTs for year 2021. Please consider including more details here, such as the description, equations, or detailed information from the references cited here (e.g., the number of equations/figures in previous works).

We did not describe much in detail some of the points listed by the reviewer due to the strict length limit of such a paper contributed to the upcoming Copernicus Ocean State Report (OSR7) and also due to that the details could be found in the literature cited in the manuscript.

The quality control procedure (point 1) of pigment data proposed Aiken et al. (2009, Section 2.3 therein) has been widely used by many other peers (Also in Xi et al. 2020, 2021 and reference provided in section 2.2). Therefore, details are not included. We have listed the procedure here in the response only (not in the manuscript): According to Aiken et al. (2009), only pigment data are considered if the following conditions are satisfied: "(a) The difference of TChla and AP (accessary pigments) concentration should be less than 30% of the TPig (total pigment) concentration. (b) Regression between TChla and AP should have a slope within the range 0.7-1.4 and must explain more than 90% of total variance ( $R^2$ >0.9). (c) The cruise data were accepted only if the number of samples passing the qualifying criteria were more than 85% of the total observations for a particular cruise". Point 2 regarding the diagnostic pigment analysis (DPA), has been also detailed in both Xi et al. (2020 and 2021) following different updates from previous studies listed in the manuscript (e.g., Vidussi et al., 2001; Brewin et al. 2015, etc.)

Point 3: The correction functions have been added to Figure 1.

Point 4: we have added the reference in the manuscript (Line 128) for the shapefile sources of the Longhurst provinces <u>https://www.marineregions.org/sources.php#longhurst</u> Reference: Flanders Marine Institute (2009). Longhurst Provinces. Available online at <u>https://www.marineregions.org/</u>. Consulted on 21 March 2022. Point 5: A major part of the Xi et al. (2021) publication contributes to the methodology and detailed implementation of the per-pixel uncertainty assessment of PFTs to the satellite PFT products. We apologize for not including much information here in the manuscript due to the length limit. The uncertainty is used rather as hidden supporting information (in inter-mission PFT type II regressions as shown in Figure 1 and as median satellite PFT uncertainty in Table 2), therefore we did not extend it too much. To clarify it briefly in the manuscript, we have added a sentence in section 2.1 when describing the CMEMS PFT products (**Lines 103-104**): "Sections 2.3 and 3.3 in Xi et al (2021) may be referred to for a detailed description of the per-pixel uncertainty assessment of the PFT products."

Point 6: We briefly added the anomaly calculation in **section 2.3 (Lines 137-138)**: "Anomaly in percentage is determined by computing the relative difference between the PFT state of 2021 and the average state of the last two decades (i.e., climatology)." Also in the caption of updated Figure 6 the definition of anomaly used in this study has been described.

#### Specific comments

1. Line 89. Swich the order of Table 1 and Table 2. It seems that the Table 2 comes out firstly in the manuscript.

Thanks for pointing it out. They have been switched.

2. Lines 142-144. This sentence is not clear. Please rewrite it.

This sentence was rephrased (Lines 155-156): "Median percent differences (MDPD) are consistent with the median satellite PFT uncertainties (relative error in %) estimated through Monte Carlo simulation and error propagation analysis in Xi et al. (2021), and for dinoflagellates, notably lower."

3. Lines 174 and 251. A decline of prokaryotes from 2013 onwards are observed in the study. Is there any possibility that the decline is related to the removal of MERIS data at this time? As argued in van Oostende et al. (2022), MERIS is able to observe more pixels near the coast and at high latitude, where Chla is higher. It may out of the scope of this study, but the coverage variability among different satellite missions should be taken into consideration in analyzing long-time series studies. van Oostende, M., Hieronymi, M., Krasemann, H., Baschek, B., & Röttgers, R. (2022). Correction of intermission inconsistencies in merged ocean colour satellite data. Frontiers in Remote Sensing, 3(July), 1–17. <u>https://doi.org/10.3389/frsen.2022.882418</u>

We have considered this possibility as well. However, we assume (added in **Section 4 Lines 279-285**), "the retreat of MERIS in 2012 should not influence very much on the prokaryote data set for the following reasoning: firstly, such a decline was not found in other PFTs; secondly, MERIS observed more pixels in the coast and high latitude, we however focus on the open ocean and have excluded the coastal regions with bathymetry <200 m, and this study covers the Atlantic Ocean between 50°N to 50°S. The main reason might be the relatively lower retrieval accuracy of prokaryotes compared to other PFTs as discussed above on the validation. Our previous work showed that all of the retrieval models for the three sets of sensor(s) have poorer performance for prokaryotic phytoplankton than for other PFT retrievals, this may cause weaker consistency of prokaryotes for the two decade period even after intermission correction."

We also strongly agree with the reviewer that it is worthwhile considering the coverage variability among different satellite missions when we look at the time series on the global scales and different waters, therefore we have added this statement in the discussion (**Section 4 Lines 285-287**): "Nevertheless, coverage variability among different satellite missions should be taken into consideration in analyzing long-time series studies as the ability of the sensors to observe certain waters may differ (van Oostende et al. 2022)."

4. Line 177. Slight increasing trend of haptophytes on the...

Revised as suggested.

 Figure 1. Since the SeaWiFS/MODIS/MERIS mission is used as the reference and the MODIS/VIIRS (or OLCI) is corrected to SeaWiFS/MODIS/MERIS, the x-axis should be MODIS/VIIRS and the y-axis should be SeaWiFS/MODIS/MERIS? Also, the equations should be changed accordingly.

Thanks for the careful checking. Indeed MODIS/VIIRS is corrected to SeaWiFS/MODIS/MERIS, the calculations made in the manuscript are all correct. To avoid confusion, we have switched the x and y-axis and updated the equations as suggested in the revised Figure 1.



Figure 1: Scatterplots of monthly PFTs derived from SeaWiFS/MODIS/MERIS merged and MODIS/VIIRS merged Rrs data for the overlapping period January-April 2012. (a) diatoms, (b) haptophytes, (c) prokaryotes, and (d) dinoflagellates. The 1:1 line is shown in black and the linear regression line (using type II regression with per-pixel uncertainty) in red. R<sup>2</sup>, slopes and offsets determined in log-10 scale are also presented.

6. Figure 3. Please change the colormap of the figures (c)-(f) here. It is not clear whether the white color in the figures represents the slope very close to 0 but significant (p<0.05) or the slope not significant (p>0.05).

Thanks for the comment. The color palette we used was with the white color in the middle to indicate zero change, however the reviewer was right that it could cause the confusion that it is difficult to differentiate between the areas with significant small changes (p<0.05) and the areas with p>0.05. Another reviewer also suggested to use a different color palette. In response to the comments from both reviewers, we have now updated the maps also with a colorblind friendly colormap in the revised manuscript (Figure 3c-f).



Figure 3: (a) Annual cycle of the four PFTs of diatoms, haptophytes, prokaryotes and dinoflagellates in the Atlantic Ocean (-50°S to 50°N, 60°W to 10°E), (b) 20-year time series from 2002 to 2021, and (c) per-pixel slope based on monthly Chla products of diatoms, (d) haptophytes, (e) prokaryotes and (f) dinoflagellates from 2002 to 2021 (where p<0.05 were shown, slope unit: Chla mg m<sup>-3</sup> month<sup>-1</sup>).

7. Figure 4. Consider changing the limits of y-axis for some provinces, such as the NATR, WTRA. Maybe it is worth adding the trend line in these time-series plots if there is a significant trend?

Limits in y-axis for a few provinces were adjusted in Figure 4. Trendlines with slopes and correlation coefficients are also shown in the time series plots for provinces with significant trends (p<0.05). These trends in different provinces correspond well to the descriptions in the results.



Figure 4: Time series of diatom Chla (unit: mg m<sup>-3</sup>) in 11 Longhurst provinces in the Atlantic Ocean with bathymetric information based on ETOPO1 bathymetry (Amante & Eakins, 2009). Provinces according to Longhurst (2007) are: NADR for North Atlantic Drift Province, NWCS for Northwest Atlantic Shelves Province, NASW for North Atlantic Subtropical Gyral Province (West), NASE for North Atlantic Subtropical Gyral Province (East), NATR for North Atlantic Tropical Gyral Province, CNRY for Canary Current Coastal Province, WTRA for Western Tropical Atlantic Province, ETRA for Eastern Tropical Atlantic Province, SATL for South Atlantic Gyral Province, SSTC for South Subtropical Convergence Province, SANT for Subantarctic Water Ring Province, respectively. Trendlines with slopes (unit: Chla mg m<sup>-3</sup> month<sup>-1</sup>) and correlation coefficients are shown for provinces with significant trends (p<0.05).

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# **Reviewer 3**

# RC3: 'Comment on sp-2022-6', Sorin Constantin

As general comments, I would say that this study is well written, tackles an important subject and would definitely be of interest to a large audience. I have only minor suggestions that will hopefully help the authors to clarify some details, especially in the methodology section.

We thank very much the reviewer for the positive feedback and comments on this study. We have considered carefully the suggestions to improve the manuscript. We would also like to point out that this manuscript was submitted as a contribution to an upcoming Ocean State Report, for which specific requirements in paper length and number of tables/figures have to be followed. The current paper length is just at this limit; therefore, we extended/added the necessary discussion/information in the manuscript as concise as possible, but more details are provided in the individual responses below.

Line 48: "Bracher et al., 2022" cannot be found in the final reference list. Either it's missing from there, or it should be 2020 instead of 2022 in the text.

Thanks for pointing out the missing reference (listed below). We have added it in the reference list.

Bracher, A., Brewin, R.J.W., Ciotti, A.M., Clementson, L.A., Hirata, T., Kostadinov, T., Mouw, C.B., & Organelli, E., (2022). Applications of satellite remote sensing technology to the analysis of phytoplankton community structure on large scales. In L.A. Clementson, R.S. Eriksen, & A. Willis (Eds.), Advances in Phytoplankton Ecology, pp. 217-244. Elsevier. doi: 10.1016/B978-0-12-822861-6.00015-7

L89: Why Table 2 and not Table 1, since it's the first one to be mentioned? Also, the CMEMS product mentioned here (OCEANCOLOUR\_GLO\_CHL\_L4\_REP\_OBSERVATIONS\_009\_082) seems to be no longer available in the catalogue. I assume there were some changes and the new product containing these datasets is OCEANCOLOUR\_GLO\_BGC\_L4\_MY\_009\_104. Can you please verify?

We have now switched Table 1 and Table 2 to be in the right order.

We apologize for the unavailability of the data sets. In the last months there was an upgrade from CMEMS and the naming of many products was affected. Indeed, the new product is OCEANCOLOUR\_GLO\_BGC\_L4\_MY\_009\_104. We have updated Table 1 with the correct product name and links.

L123: "Time series analysis is done both, per-pixel [...]" – not sure if the comma is needed here.

# The comma was removed.

Section 3.1 – since you are showing scatterplots of monthly PFTs derived from SeaWiFS/MODIS/MERIS merged and MODIS/VIIRS merged Rrs data (figure 1), I think it might

be useful (and more consistent, I would add) to show also such scatterplots between corrected MODIS/VIIRS and Sentinel 3A (as you mention in lines 133-134).

Thanks for the comment. This point was also raised by Reviewer 1. Due to length limit of such a report contribution, we did not include similar plots in the first manuscript. We have now added more information about the correction on the OLCI derived PFTs **(Lines 146-152)**: "The same is applied to the Sentinel 3A OLCI derived PFTs by comparing them to the corrected MODIS/VIIRS derived PFTs for the overlapped period April – December 2016, so that all PFT data from both MODIS/VIIRS and OLCI are now referenced to SeaWiFS/MODIS/MERIS derived PFTs. Though R<sup>2</sup> is slightly weaker (R<sup>2</sup> from 0.77 to 0.83) compared to that from the MODIS/VIIRS versus SeaWiFS/MODIS/MERIS derived PFTs (R<sup>2</sup> from 0.82 to 0.98), OLCI derived PFTs still showed overall good correlations to the corrected MODIS/VIIRS data with regression slopes between 0.83 and 1.03 despite that prokaryote Chla retrievals from OLCI data are in general higher."

Figure R2 shows scatterplots and regression relationships between the two products, however due to the paper length limit we decided not to include the figure in the revised manuscript.



Figure R2: Scatterplots of monthly PFTs derived from OLCI Rrs and corrected MODIS/VIIRS merged Rrs data for the overlapping period April – December 2016. The 1:1 line is shown in black and the linear regression line (using type II regression with per-pixel uncertainty) in red. R<sup>2</sup>, slopes and offsets determined in log-10 scale are also presented.

L137: I think it can be useful if you briefly explain what this "match-up criterion" is about. For more details readers can always go to the cited publication, but couple of words would make

things clearer. Also, can you specify the time range for these match-ups (e.g. "match-ups corresponding to years 2015 and 2016")?

Brief sentences have been added to the text about the matchup extraction criterion (**Lines 120-123**): "For each in situ measurement a matchup of  $3\times3$  pixels around the in situ location on the same day was extracted. Averaged data based on  $3\times3$  pixels were computed following the matchup protocol as in Xi et al. (2020, 2021), including only matchups containing at least 50% of the valid pixels with a coefficient of variation (CV) of the valid pixel values lower than 0.15."

The time range of these matchups is from 2009 to 2019, which is the spanning period of our in situ data set described in **section 2.2** (Lines 113-116): "To evaluate the satellite PFT products, we use in situ HPLC pigment data from past expeditions between 2009 and 2019 covering the whole Atlantic polar to polar region (65°S to 80°N) which included nine expeditions from the North Atlantic to the Arctic Fram Strait (PS74, PSS76, PS78, PS80, PS85, PS93, PS99, PS106, PS107, PS121) and four expeditions in the trans-Atlantic Ocean (PS113, PS120, AMT28 and AMT29)."

L139-140: "Slope is always below one indicating that satellite retrievals show overestimation in low concentrations but underestimation in high concentrations." - A slope below one does not, by itself, infer information on both under and overestimation. The value of the intercept is required, as well. So, it might be useful if you insert these values into current Table 1 or you show the distribution of points as scatterplots. Also, it is not completely clear if the slopes are computed taking into consideration the in situ derived PFT as a function of satellite PFT and not vice-versa. I assume the first option is true, but is not completely clear.

During the "under-review" stage we have obtained more in situ PFT data for the validation also with a more thorough matchup extraction, therefore, we have been able to extend the matchup data set and update the statistics in Table 2. The new validation is much more reliable and statistics has become overall better. We have added Figure R2 in this response document to show the scatterplots between the inter-sensor corrected satellite PFTs versus the in situ PFT data. This figure is not included in the revised manuscript as Table 2 summarizes adequately the statistics. It is also indicated in the caption of Table 2 that the statistical parameters are computed based on satellite derived PFT Chla (after inter-mission correction) as a function of in situ PFT Chla using least square fit.

The discussion regarding the validation statistics has also been updated in Section 3.1 and the Discussion (Section 4).

**Section 3.1 Lines 153-159**: "Validation was carried out by comparing the collocated satellite PFTs with the in situ PFTs using the extracted matchup data. Statistical results of the validation in Table 2 show in general acceptable agreement between the in situ and satellite derived PFTs. Median percent differences (MDPD) are consistent with the median satellite PFT uncertainties (relative error in %) estimated through Monte Carlo simulation and error propagation in Xi et al. (2021), and for dinoflagellates, notably lower. Higher MDPD is found for prokaryotes due to a systematic overestimation of the picophytoplankton in the retrieval algorithms for all the three sets of satellite OC sensors, however, no significant bias of satellite

prokaryote products is detected between different sensors, therefore the overestimation should have minor influence on the time series data of prokaryotes."

**Section 4 Lines 250-258**: "Validation using in situ data shows no significant biases of PFTs derived from different sensors, indicating that the inter-mission offset was effectively corrected. Chla of different PFTs are more upscaled retrievals compared to bulk satellite OC products such as total chlorophyll a, coloured dissolved organic matter (CDOM) and absorption properties. Especially, it is still challenging to retrieve accurately prokaryotic phytoplankton because in the open ocean these are dominating in the low Chla areas for which the satellite signals are weaker. Therefore, higher uncertainties exist in these products (e.g., Brewin et al. 2017; Losa et al. 2017; Xi et al. 2021) as compared to uncertainties for other PFTs (see Table 2). In summary, our statistical results of PFT validation are comparable to the evaluations of satellite PFT products derived from different approaches, according to the Quality Information Documents (QUID) that have been published on CMEMS (Garnesson et al., 2022; Pardo et al., 2022)."

# Table 2 has been updated (Lines 494-500):

Table 2: Statistical validation results of satellite derived PFT Chla (after inter-mission correction) as a function of in situ PFT Chla using least square fit in logarithmic scale. N: number of matchups; R<sup>2</sup>: coefficient of determination; MDPD: median percent difference; RMSD: root-mean-square difference; definition equations of these terms were referred to Xi et al. 2020. Note that Slope, Intercept and R were calculated based on logarithmic scale. Median uncertainties calculated based on satellite per-pixel PFT uncertainty (equivalent to relative error in %) are also shown in the last column.

	Ν	Slope	Intercept	R <sup>2</sup>	MDPD (%)	RMSD (mg m <sup>-3</sup> )	Median satellite PFT uncertainty (%)
Diatoms	192	0.71	-0.27	0.76	60.5	0.30	57.3
Haptophytes	191	0.95	-0.007	0.41	58.9	0.18	41.5
Prokaryotes	187	0.71	0.12	0.36	185	0.06	86.5
Dinoflagellates	144	1.07	0.04	0.66	59.1	0.07	74.3



Figure R2: Scatterplots of the satellite derived PFT Chla after inter-mission correction versus in situ PFT Chla.

L143: "[...] are consistent with, the median satellite [...]" – probably the comma is not required.

#### It was removed.

L180: "Per-pixel time series in Fig. 3c shows that significant increase is found only in the west coast of Africa (CNRY)" – shouldn't it be decrease?

# We apologize for the typo. The reviewer was correct that it should be "...significant decrease is found...". We have modified it in the text.

L222: "Dinoflagellates show a stable state in 2021 among the four PFTs with only a very slight increase of Chla in the north Atlantic Ocean." - To what extent this observed stable state is due to the overall low Chla concentration of dinoflagellates? The PFT anomalies shown in figure 6 are given using mg m-3 as units. Would the same stable state be observed if the anomalies are shown as percentages, for example?

Thanks for the constructive comment. Indeed, the anomaly could be further normalized by the climatology to enhance the visibility of small absolute changes. Therefore we have redefined the anomaly **in Section 2.3 Lines 137-138** "Anomaly in percentage is determined by computing the relative difference between the PFT state of 2021 and the average state of the last two decades (i.e., climatology)." Figure 6 has been modified with the maps of anomaly in percentage. This has altered some detailed patterns as small absolute changes especially

in the gyres are now magnified, hence, the abstract and Section 3.4 regarding the description of the anomaly have been updated correspondingly. Dinoflagellates however still show a relatively stable state.

Accordingly, we have updated the **abstract Lines 21-24**: "The PFT anomaly (in percentage) of 2021 compared to the 20-year mean reveals mostly a slight decrease in diatoms and a prominent increase in haptophytes in most areas of the high latitudes. Both diatoms and prokaryotes show a mild decrease along coastlines and an increase in the gyres, while prokaryotes show a clear decrease in the mid- to low latitudes and an increase in the western African coast (CNRY and GUIN) and southwest corner of NATR", and also Section 3.4 Lines 231-242: "Anomalies in percentage of the four PFTs in 2021 compared to the average state of the last two decades are shown in Fig. 6. Diatom anomaly presents changes mainly in high latitudes, gyres and some coastal regions (such as CNRY). The anomaly shows mostly lower diatom Chla in high latitudes except for NWCS and the southeastern part of NADR where diatom Chla is increased. Opposed to that, diatom Chla of 2021 in the gyres is generally higher (~ 30%) compared to the 20-year average state. Note that changes are shown in percentage instead of the absolute values to enhance the visibility of small absolute changes, which in the gyres can be very sensitive, as diatom Chla is extremely low there (< 0.01 mg  $m^{-3}$ ). Haptophyte anomaly presents changes in similar regions with diatoms but reversely in high latitudes, especially in the Southern Ocean, where a more prominent increase and also larger coverage are observed. Increase of haptophytes in the area north of the equator in WTRA is more significant than diatoms. Different from diatoms and haptophytes, prokaryotes reveal a very slight decrease in 2021 mostly in low latitudes within 20°N-20°S, with higher prokaryote Chla in the west coast of Africa especially CNRY, whereas only mild increase (< 20%) is found in high latitudes. Dinoflagellates show the most stable state in 2021 among the four PFTs with only a slight increase of Chla in the north Atlantic Ocean above 40°N and a small decrease in CNRY."



Figure 6: PFT anomaly in percentage [%] of 2021 compared to the 20-year mean for (a) diatoms, (b) haptophytes, (c) prokaryotes and (d) dinoflagellates. Anomaly in percentage is defined as (PFT<sub>2021</sub> – climatology)/climatology\*100. Black lines indicate boundaries of Longhurst provinces as in Fig. 4.

Fig. 3 c-f: did you try a different colour palette? One that would allow to spot even the smaller changes? Maybe you could try a version where the interval is set to [-3; 3] instead of [-5; 5]. Just an idea.

The color palette we used was with the white color in the middle to indicate zero change, however it could also cause the confusion as pointed out by another reviewer, that it is difficult to differentiate between the areas with significant small changes (p<0.05) and the areas with p>0.05. In response to both related comments from two reviewers, we have now used a different color palette in the revised manuscript.

It actually does not make much difference using a narrower interval such as [-3; 3] instead of [-5; 5] because the bigger changes (with the slope such as ~4  $\times 10^{-5}$ ) in coastal areas are an order of 2 higher in magnitude than those very small changes (such as ~3  $\times 10^{-7}$  only) mainly in the mid- to low latitudes. We have slightly adjusted the interval for different PFTs with the updated color palette (Figure 3 c-f).



Figure 3: (a) Annual cycle of the four PFTs of diatoms, haptophytes, prokaryotes and dinoflagellates in the Atlantic Ocean (-50°S to 50°N, 60°W to 10°E), (b) 20-year time series from 2002 to 2021, and (c) per-pixel slope based on monthly Chla products of diatoms, (d) haptophytes, (e) prokaryotes and (f) dinoflagellates from 2002 to 2021 (where p<0.05 were shown, slope unit: mg m<sup>-3</sup> month<sup>-1</sup>).

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