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ENHANCING BGC-ARGO CHLOROPHYLL-A DATA QUALITY AND UNIFORMITY USING MACHINE LEARNING

R. Sauzède, C. Schmechtig, P.R. Renosh, J. Uitz & H. Claustre

Ocean Predict 24
19th of November 2024

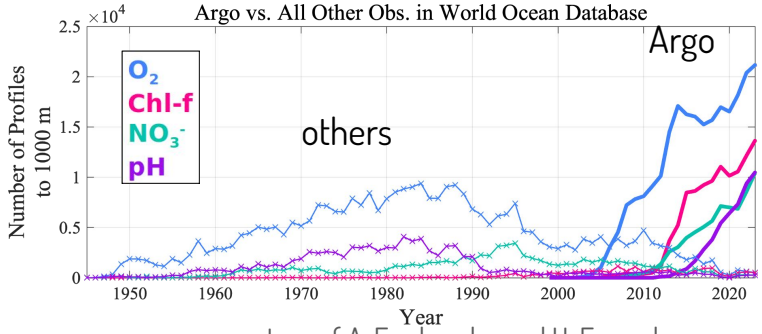
Autonomous platforms are delivering high-quality biogeochemical observations with impressive spatial distribution and seasonal resolution → BGC-Argo has become a key data source for operational oceanography.

~ 315,000 profiles of O2

(+ ~27,000 / year)

~ 145,000 profiles of Chla + POC

(+ ~17,000 / year)



courtesy of A. Fassbender and H. Frenzel

biogeochemical Argo

Claustre et al., 2020

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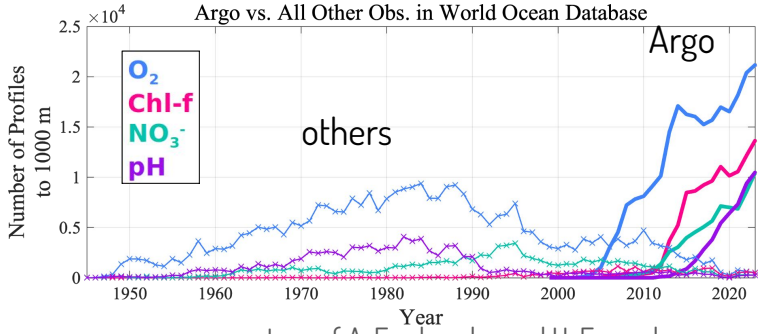

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biogeochemical Argo

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BGC-Argo floats measure bio-optical proxies of biogeochemical quantities.

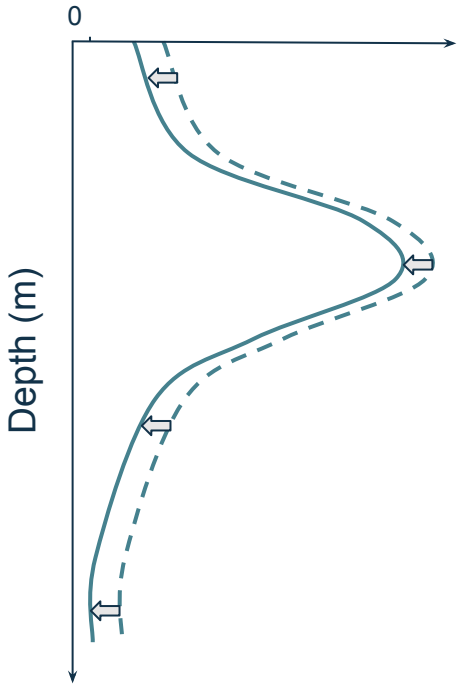
→ BGC-Argo fluorescence (FChla) has to be converted into Chlorophyll-a concentration (Chla)

$$FChla = E\, a^{*}\, \Phi f\, [Chla]$$

- ➔ E is the excitation irradiance (mole quanta $m^{-2}\, s^{-1}$): assumed to be **constant**
- ➔ a* is the Chla-specific absorption coefficient [m^2 (mg Chl a)$^{-1}$]: **related to physiology, species composition, package effect**
- ➔ Φf, the fluorescence yield [mole quanta emitted (mole quanta absorbed)$^{-1}$]: related to **physiology**

→ The FChla/[Chla] ratio is a function of **physiological constraints** and **community composition**

Calibration of Fluorescence (FChla) to Chlorophyll-a Concentration (Chla)



To be converted in Chla concentration, FChla correction needs to consider of:

1. **Dark correction** (sensor-specific correction)
   - Adjusted in Real-Time mode (RT): use of the median of the minimum values of the first 5 profiles sufficiently deep
   - Delayed mode (DM): use the median of the minimum values across the entire time series

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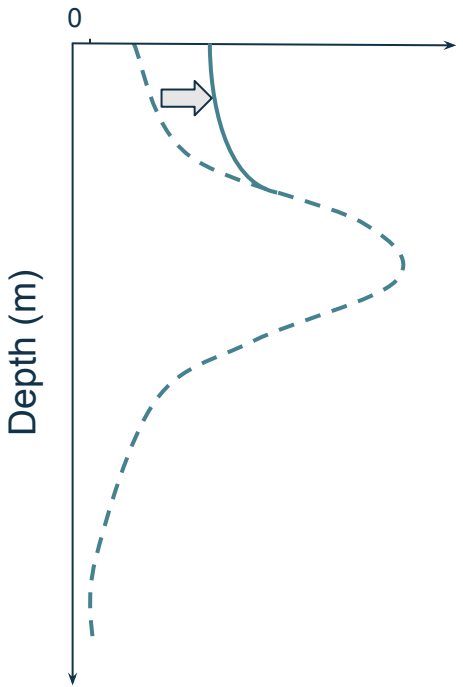

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   - RT: Xing et al. (2012) based on Mixed Layer Depth (MLD)
   - DM: Terrats et al. (2020) based on MLD and light (PAR)

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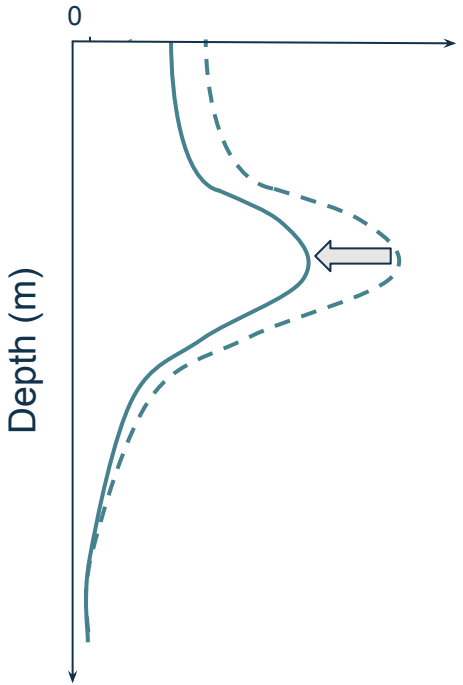

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3. **Physiological ratio correction**
   - RT: Roesler et al. (2017) → global ratio of 2
   - DM: Xing et al. (2011) → uses the light from radiometer or machine learning (Renosh et al., 2023)

Correction of Chla in DM

- New dataset of Chlorophyll-a, **semi-automatically** adjusted to DM
- Schmechtig et al., 2024: available on SEANOE with DOI
- Snapshot based on Argo data from **January 2024**


SEANOE SEA SCIENTIFIC OPEN DATA PUBLICATION

Search Dataset Bookmarks

DOI 10.17882/102324

Collection of BGC-Argo single synthetic profile files with improved post processed Chlorophyll-A at the global scale

DATE 2024

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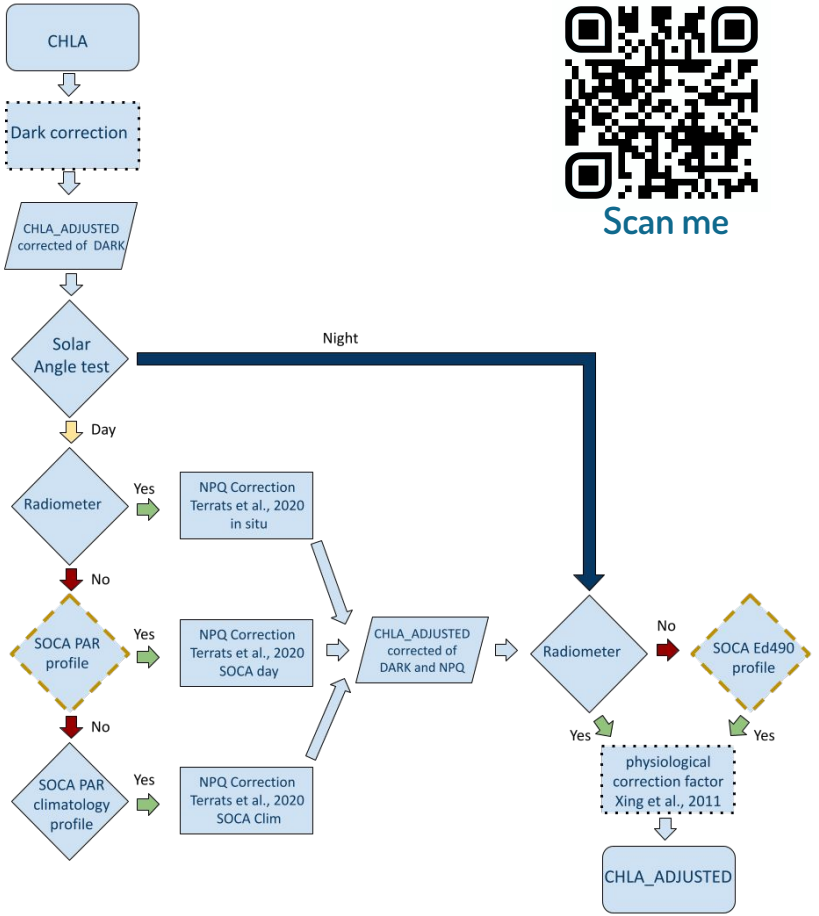
On January 9, 2024, (http://doi.org/10.17882/42182#107470), in the Argo data stream, very few Chlorophyll-A (Chla) profiles are available in Delayed Mode (DM). For SOCA2024 (Sauzede et al., 2016) development, we have applied a specific post-processing that acts similarly to a DM adjustment to improve Chla accuracy, but unlike DM data, data produced are not fully scrutinized. This post-processing procedure aims to apply three main corrections:

1) the median of the minima for dark correction;

2) the Non-Photochemical Quenching (NPQ) correction from Terrats et al. (2020), adapted from Xing et al. (2018), based on both Photosynthetically Available Radiation (PAR) and b_{bp} measurements;

DOWNLOAD DATA

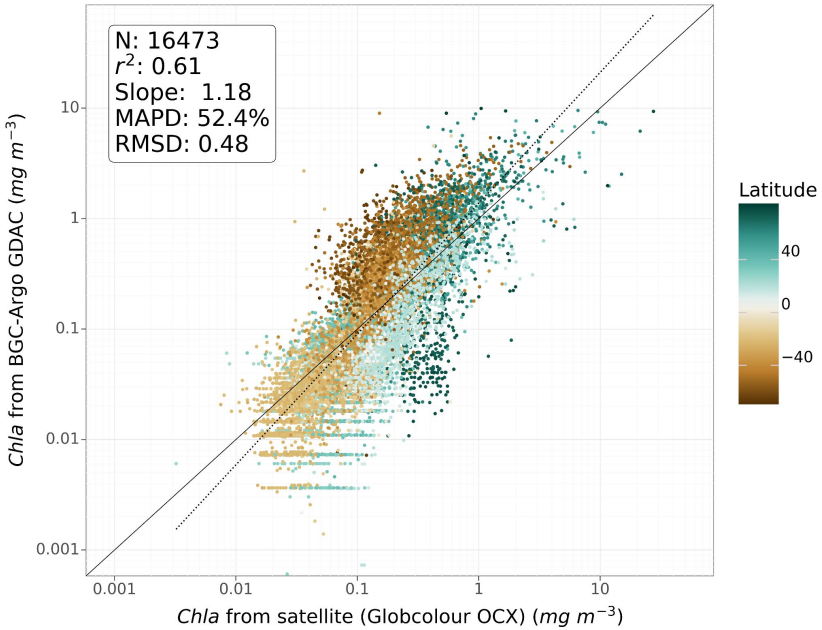
BGC Argo float
© Antoine Poteau



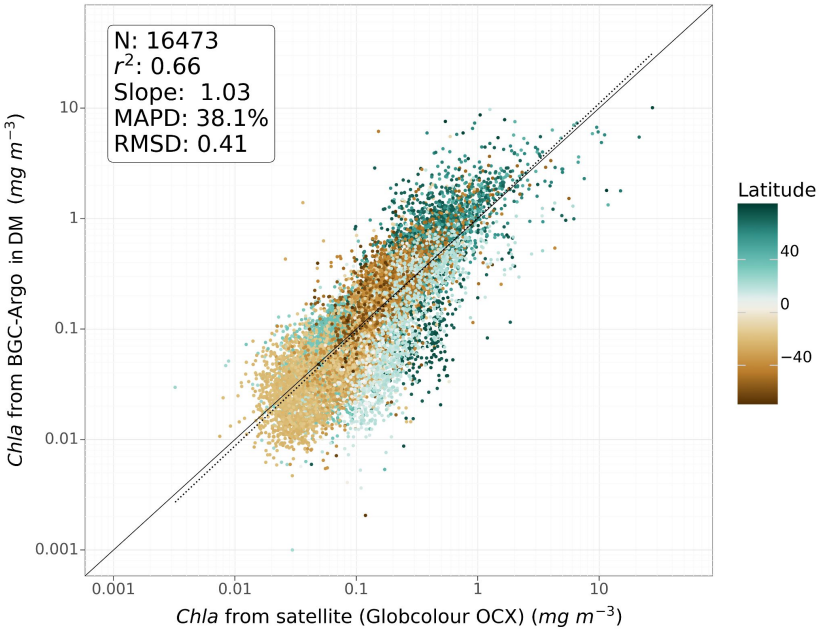
Scan me

DM and RT correction – comparison with satellite ocean color Chla

RT CHLA_ADJUSTED



DM CHLA_ADJUSTED



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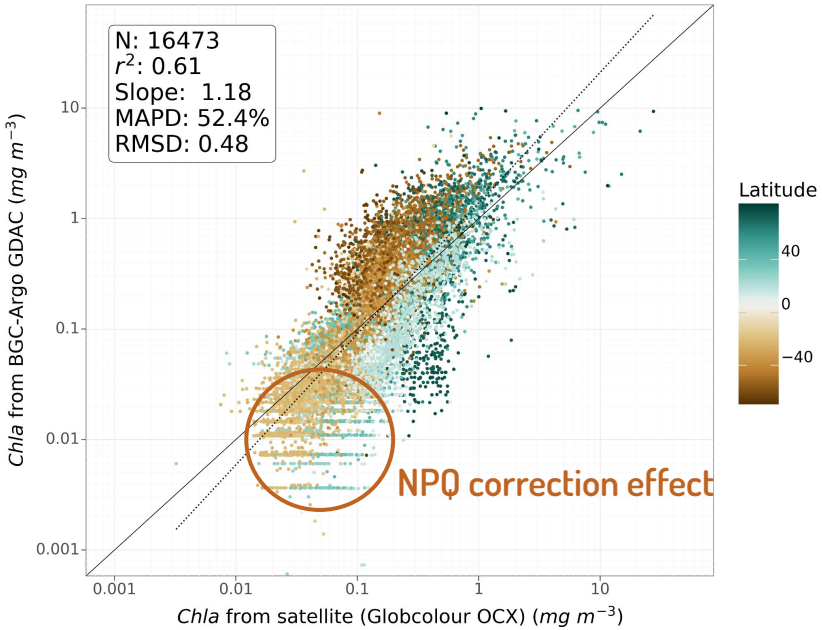

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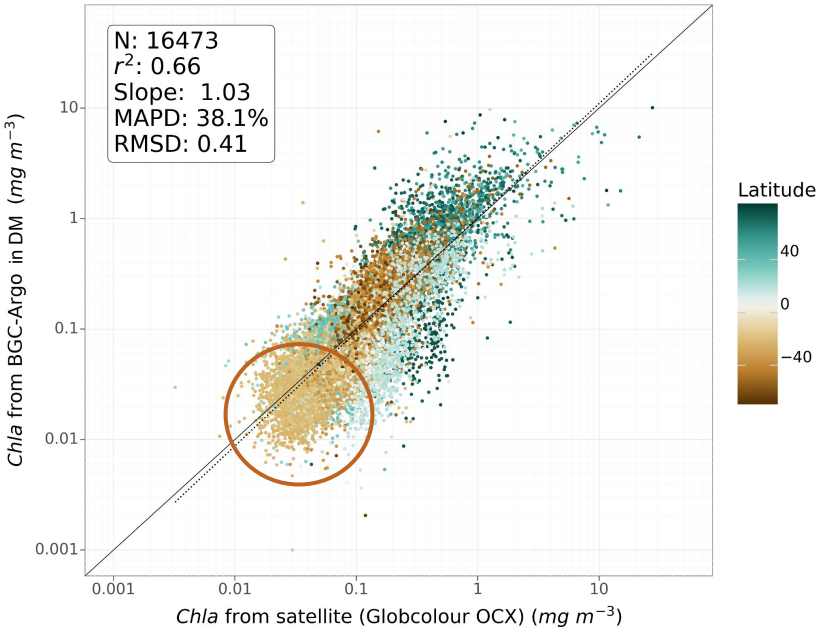

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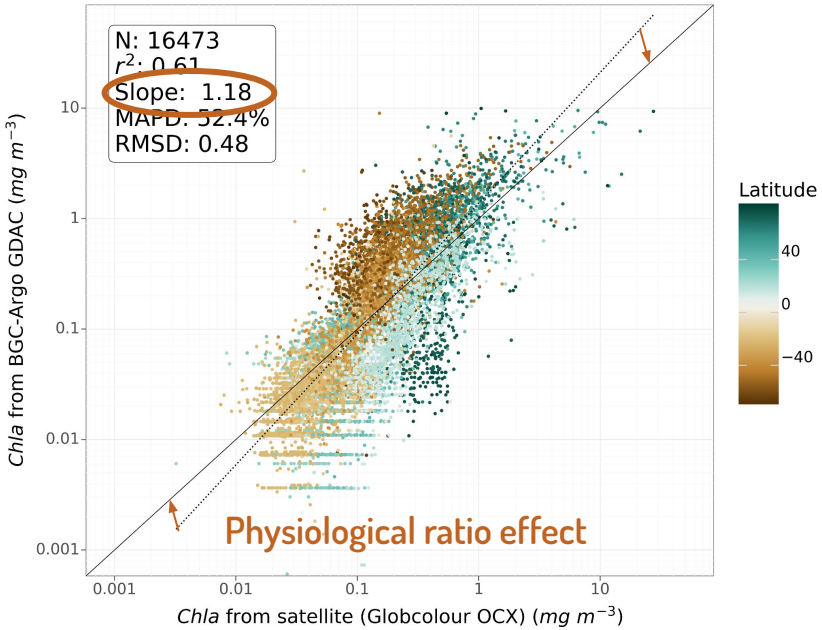

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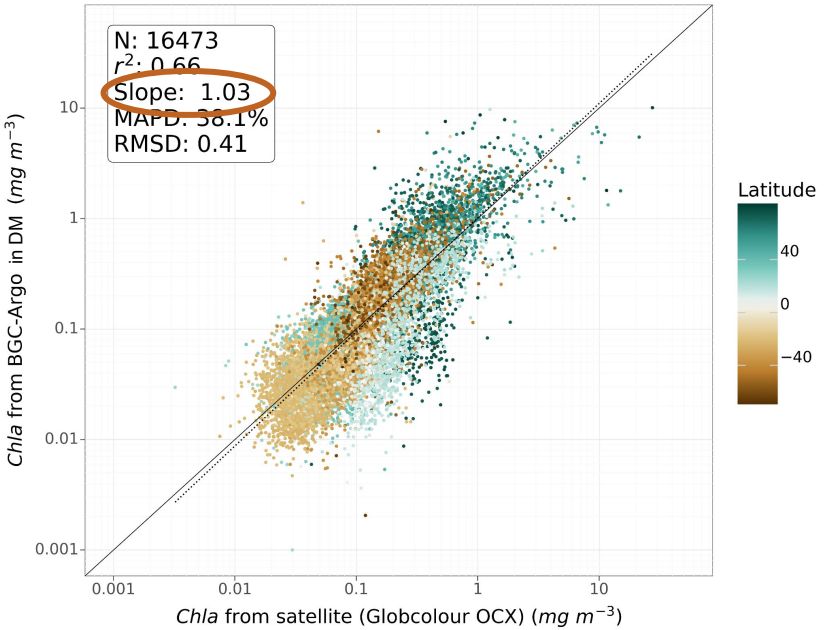
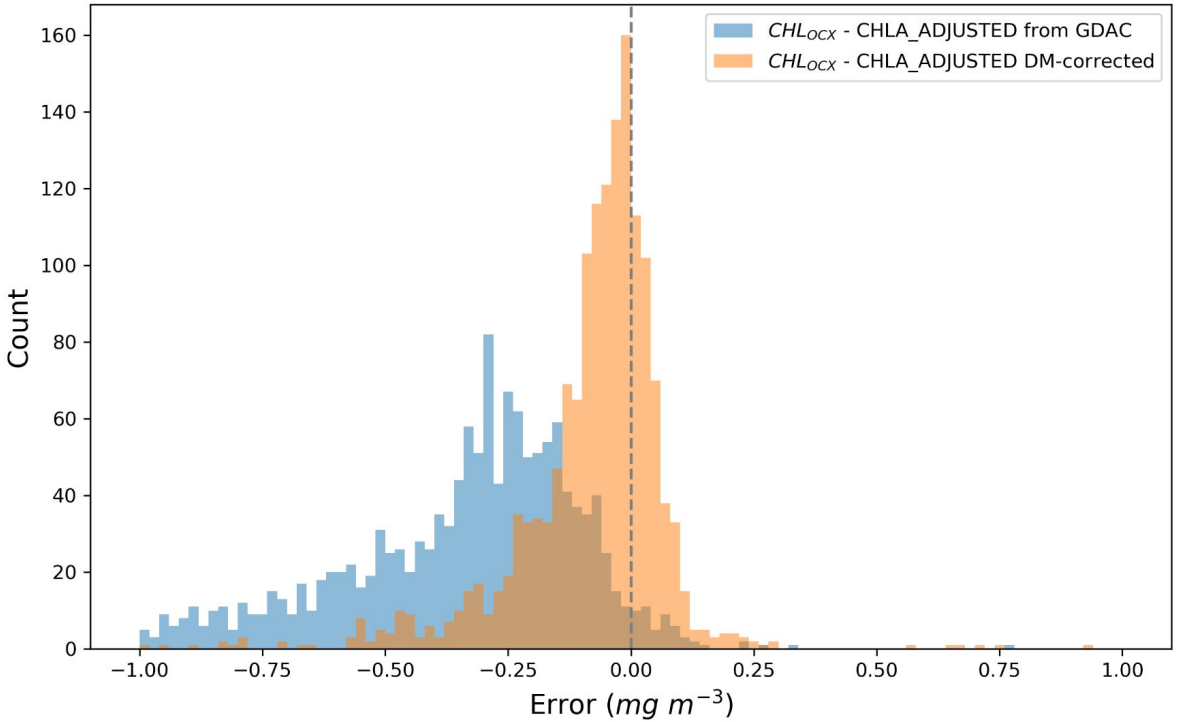


DM and RT correction – comparison with satellite ocean color Chla

Southern Ocean (>45°S)

Float-specific corrections to the physiological ratio between FChla and Chla help correct the overestimation of BGC-Argo Chla in the Southern Ocean.



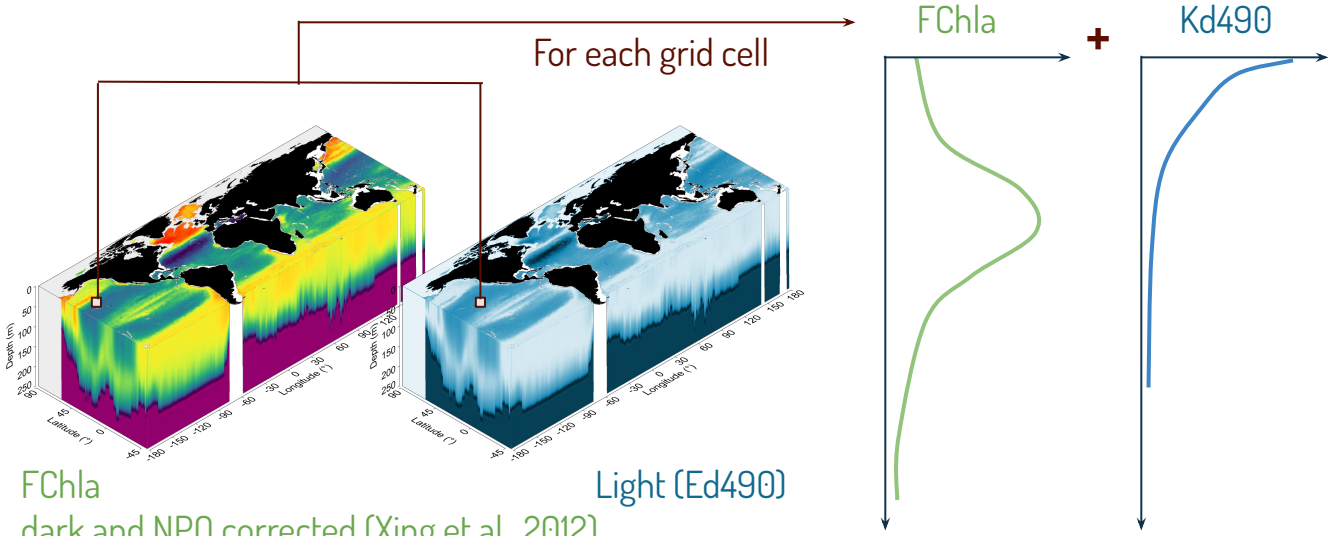
Improving the RT CHLA correction using Machine learning

SOCA: Neural network-based global gridded 3D products of **Chla and POC** (Sauzède et al. 2016, Sauzède et al., in prep.) + **SOCA-light** (Renosh et al., 2023)

Thanks to 3D SOCA products : **new climatologies of Chla (BGC-Argo CHLA_ADJUSTED) and LIGHT (e.g. Ed490)**

SCAN ME

SOCA Chla and POC products available from Copernicus



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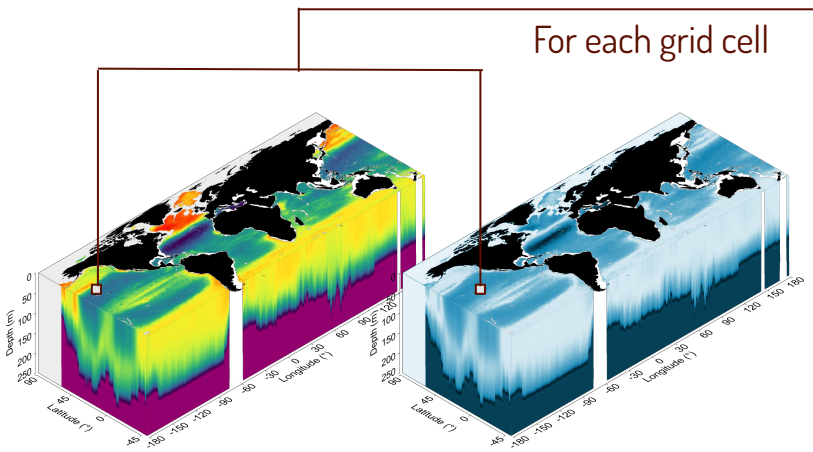
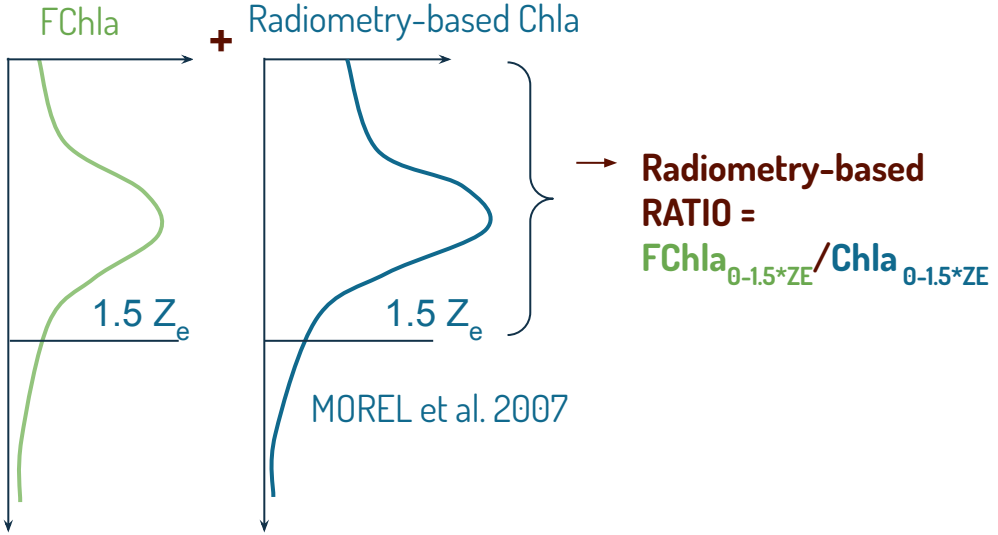


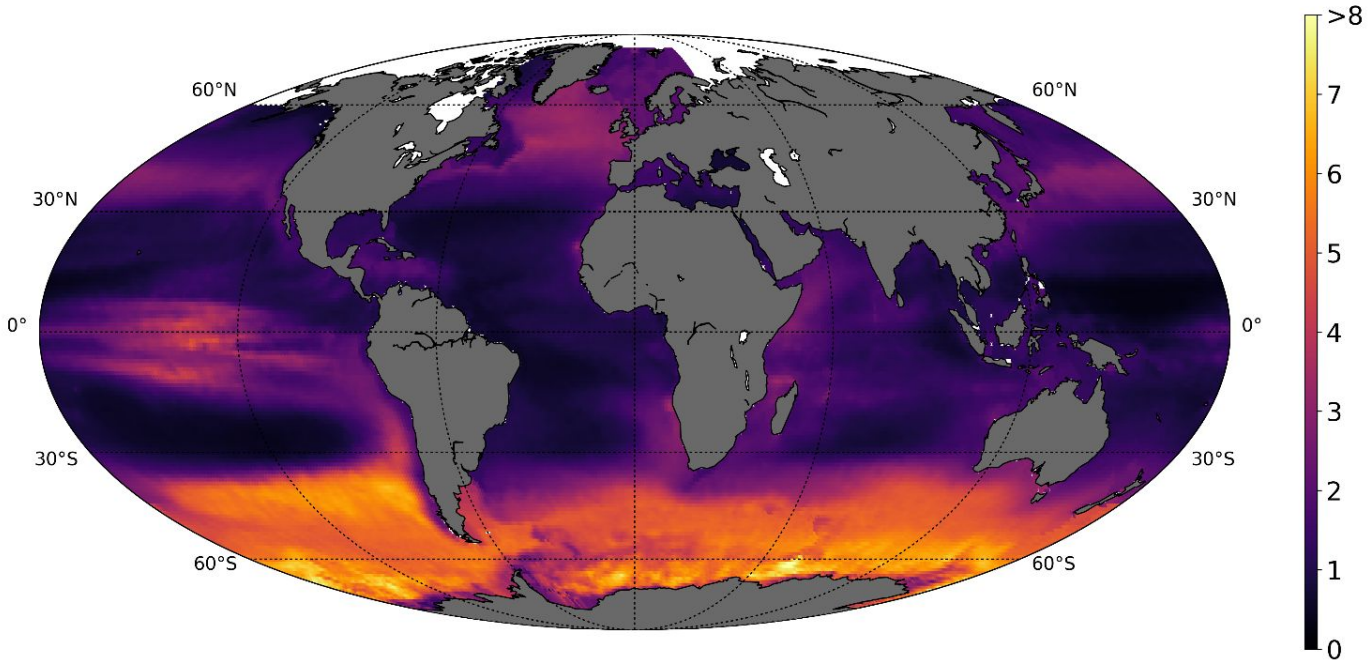
FChla

dark and NPQ corrected (Xing et al., 2012)

Light (Ed490)



Radiometry-based physiological ratios between FChla and Chla



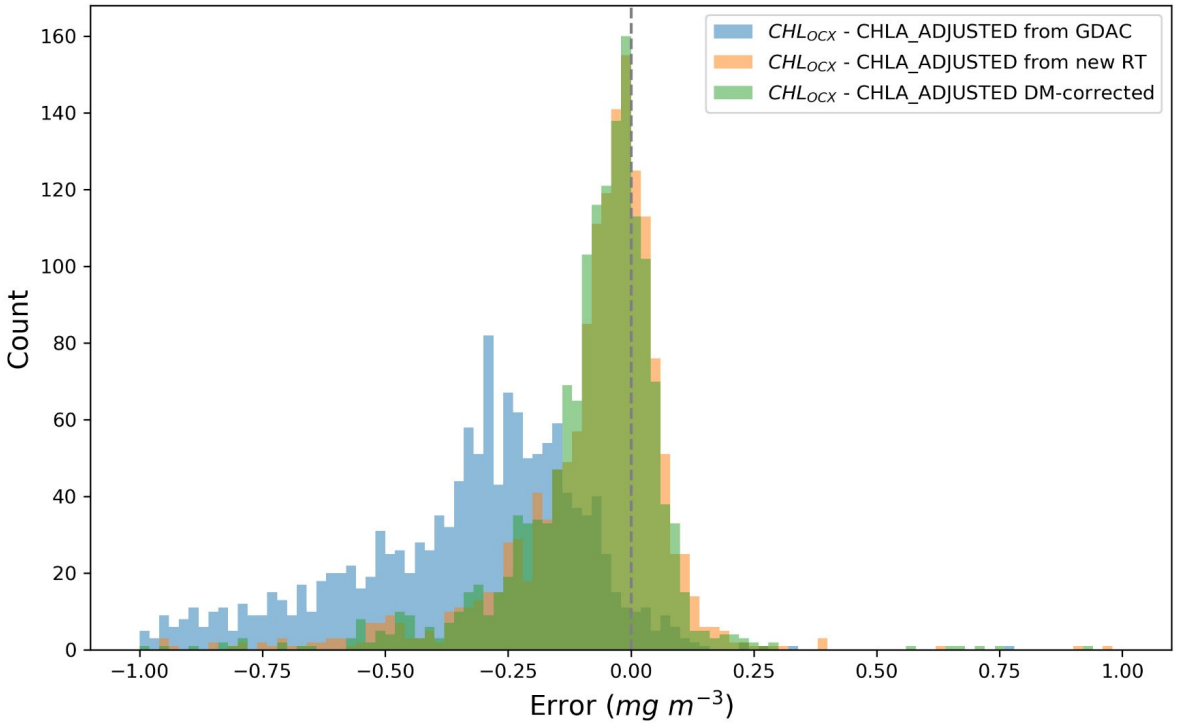
These ratios are expected to be operationally implemented in the Argo datastream by next year.

DM and AM correction – comparison with satellite ocean color Chla

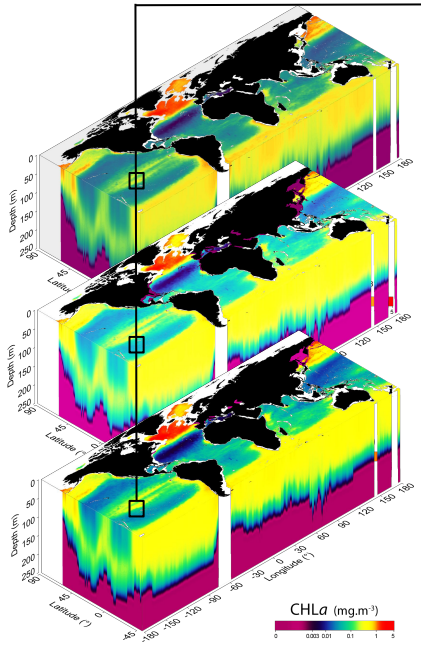
Southern Ocean (>45°S)

The new RT correction of the physiological ratio between FChla and Chla exhibits the same debiased errors as the DM correction and helps correct the overestimation of BGC-Argo Chla in the Southern Ocean.

However, satellites have their own bias and limitations...



New machine learning (SOCA)-based workflow



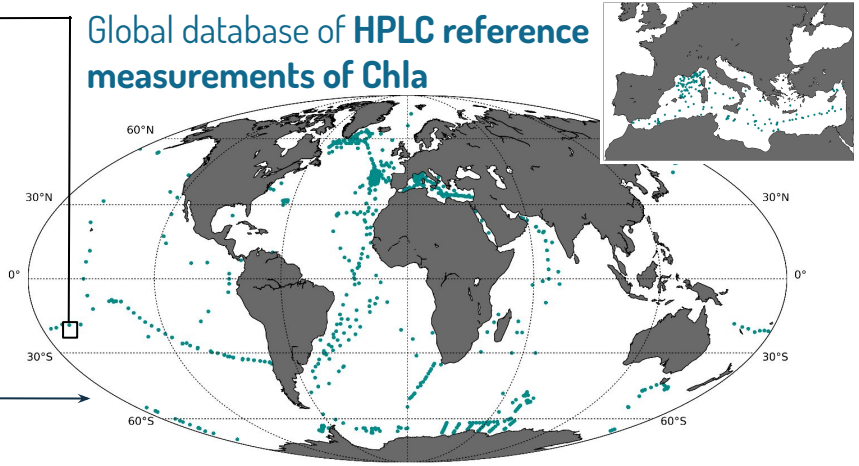
MODEL A

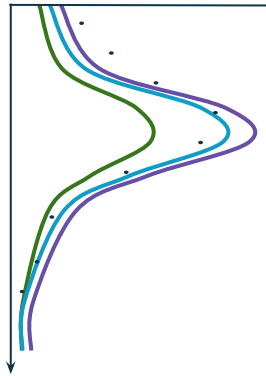
MODEL B

...

MODEL X

Global database of **HPLC reference measurements of Chla**

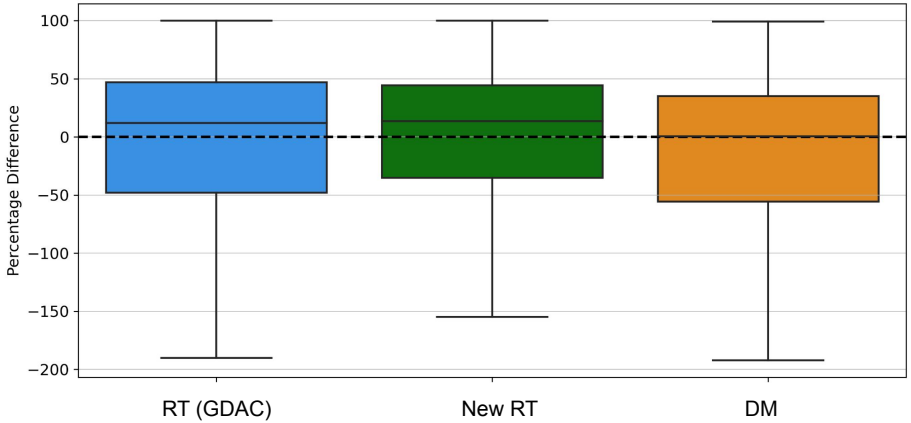




Global (or regional) **statistics**:
R^2, bias, MAPD, RMSD...
→ **Best statistics** = Chla from BGC-Argo with the correction the more **representative of HPLC** reference measurements
= Best correction

$$\text{Percentage Difference} = (Chla_{HPLC} - Chla_{BGC\text{-}Argo})/Chla_{HPLC}$$

Global Ocean



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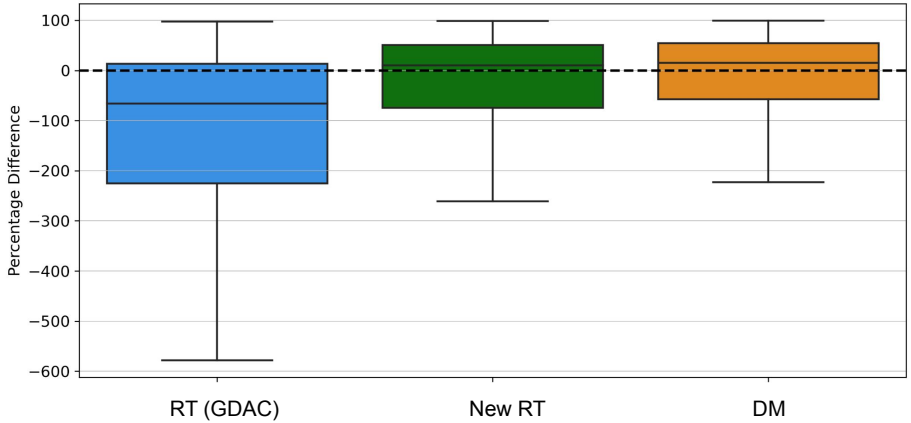

The new real-time correction still results in a **slight underestimation of Chla at the global scale**, likely due to the current limitations in improving the NPQ correction within the real-time correction. However, this correction **successfully addresses the overestimation of Chla in the Southern Ocean.**

- A **delayed-mode Chla dataset is available on SEANOE,** but integration into the Argo stream is challenging due to large differences with real-time corrections, especially in the Southern Ocean.

- **Machine learning (SOCA)** has greatly enhanced the **delayed-mode** procedure, making it applicable across the entire fleet—not just floats with radiometers—and offering a new path to improved **real-time** corrections.

- A new **SOCA-based workflow** was developed to assess the accuracy of the BGC-Argo Chla dataset, enabling comparison and evaluation of various corrections methods.

- This validation workflow, which compares synthetic BGC-Argo data with **reference in situ measurements**, shows that corrections based on radiometry-based physiological factors (in both RT and DM) provide **more accurate Chla estimates** than current corrections, offering better alignment with ocean color data.

- As part of the **BGC-OptiQ** Copernicus Service Evolution project, we aim to expand this workflow to evaluate corrections globally, regionally, seasonally, and in specific layers (e.g., surface layer for NPQ correction), to **further improve BGC-Argo Chla dataset accuracy**, especially within the Copernicus Marine Service.

- This more accurate BGC-Argo Chla dataset supports **biogeochemical modeling**, particularly in data assimilation, by reducing biases with satellite-derived data and increasing overall data accuracy.

Thank you
Questions?

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