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esa

Bridging the gap between surface and subsurface optical estimates of particulate organic carbon concentration

Evaluating multivariable algorithms for global satellite ocean color and BGC-Argo applications

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Algorithms for Ocean Color Science

Three main approaches for deriving in-water particle properties from satellite data:

1. **Empirical algorithms** rely on purely statistical relationships between observed signals and in-water properties, such as using top-of-atmosphere radiance to estimate Chla concentration with machine learning approaches (e.g., neural networks).

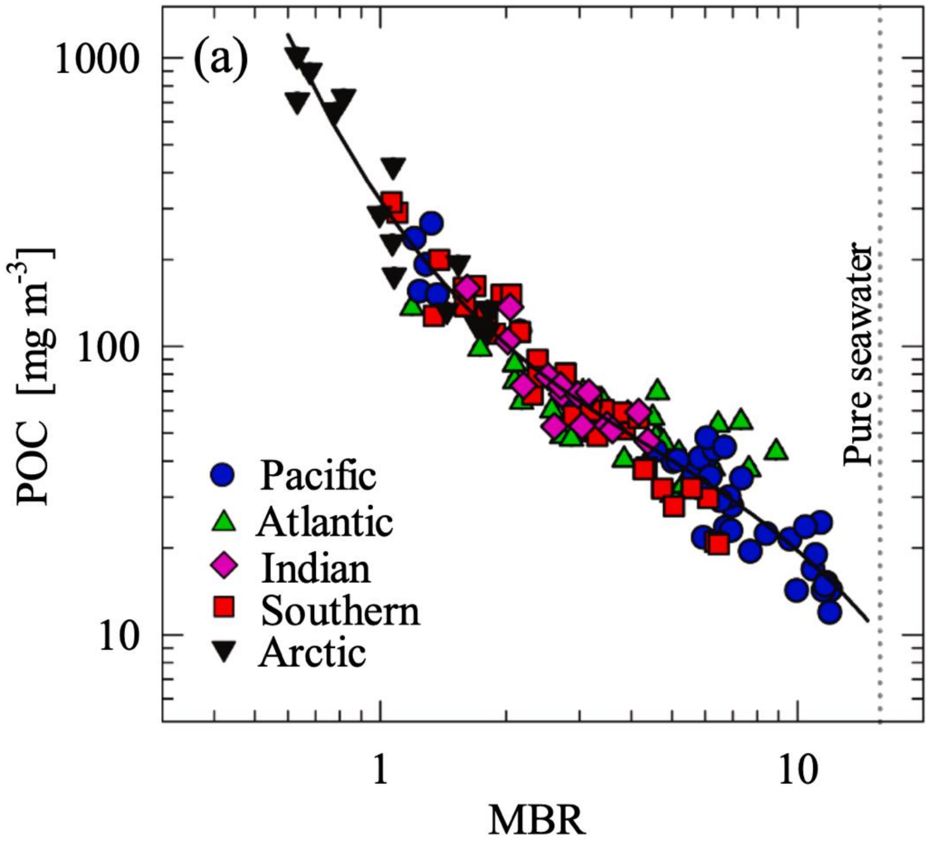
2. **Semi-empirical algorithms** combine empirical relationships with some physical understanding, e.g., using the ratio of R_{rs} in blue and green bands to infer Chla concentration due to relationships between increasing phytoplankton absorption and Chla.

3. **Mechanistic or physics-based algorithms** provide a more process-oriented approach, e.g., radiative transfer models or retrieval of inherent optical properties from R_{rs} to then derive in water particle characteristics.

Optical methods for POC estimation

Particulate Organic Carbon concentration (POC) – mass concentration of carbon containted all organic particles

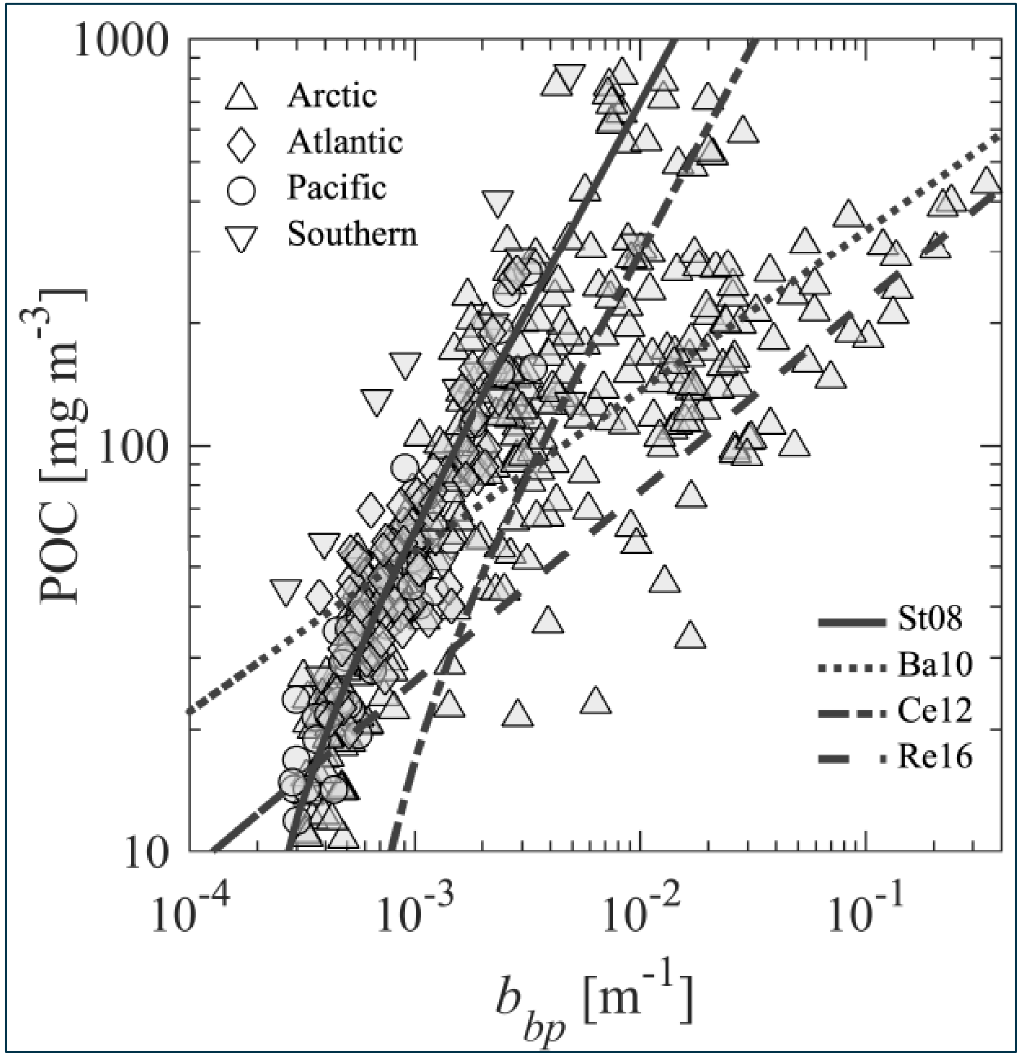
- Predominantly rely on semi-empirical algorithms using R_{rs} ratios
  - Blue:Green (B:G) ratio decreases → associated with ↑ Chla
  - Polynomial functions of maximum band ratios often outperform simpler models
- Other constituents (e.g., absorption by non-algal particles) also influence B:G
  - Provides basis for R_{rs} → POC algorithms, potentially more robust than Chla approaches since POC includes both algal and non-algal particles



Stramski et al. (2022)

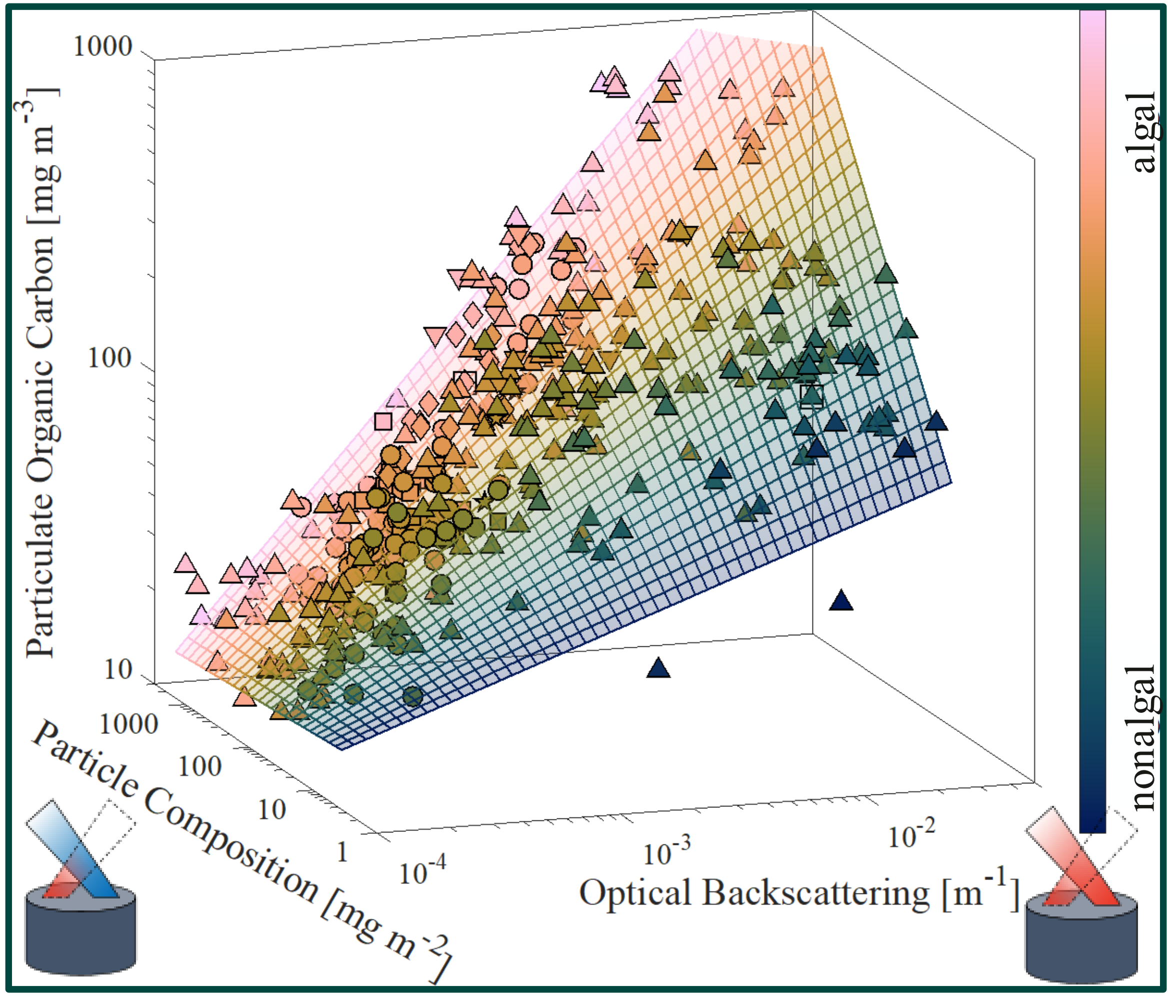
The two-step approach

- Step 1: Invert R_{rs} to derive particulate backscattering coefficient (b_{bp})
- Step 2: Derive POC from b_{bp}
- More theory-driven: links inherent optical properties (IOPs) to particle characteristics
- Limitations:
  - Large variability in b_{bp}–POC relationships
  - Uncertainty in $R_{rs} \rightarrow b_{bp}$ inversion
- Consequently, best-performing POC algorithms still use direct R_{rs} input in semi-empirical models (Stramski et al. 2022)



Recent advances

- Incorporate optical proxies for particle composition:
    - Chla:b_{bp} → indicator of algal vs. non-algal dominance
- Potential applications:
    - Global BGC-Argo float array for in-water POC estimation
    - Satellite-based POC retrieval
    - Integration of surface (satellite) and subsurface (BGC-Argo) POC estimates
- Key challenge: identify external variables to strengthen extrapolation for merging datasets



Koestner et al. (2024)

Objectives

The purpose of this work is focused primarily on examining the performance of the improved relationships for POC utilizing satellite and *in situ* data. The main objects are:

1. Compare/validate POC estimations from a R_{rs}–POC algorithm (Stramski et al. 2022) and a two-step approach (Koestner et al. 2024) with concurrent *in situ* measures of POC and R_{rs}.
2. Compare/validate POC estimations from each method using match-ups of *satellite* R_{rs} and *in situ* measured POC
3. Compare POC estimations from *satellite* R_{rs} and *in situ* estimated POC from BGC-Argo floats over the MODIS timeseries
4. Identify factors to exploit for merging of satellite and BGC-Argo data (POC and corrections for Chla F)
    1. Allow satellites to guide the interpolation at the surface and the entire BGC-Argo array to guide interpolation at depth
    2. Develop predictive relationships between satellite POC and water-column integrated POC based on the current dataset.

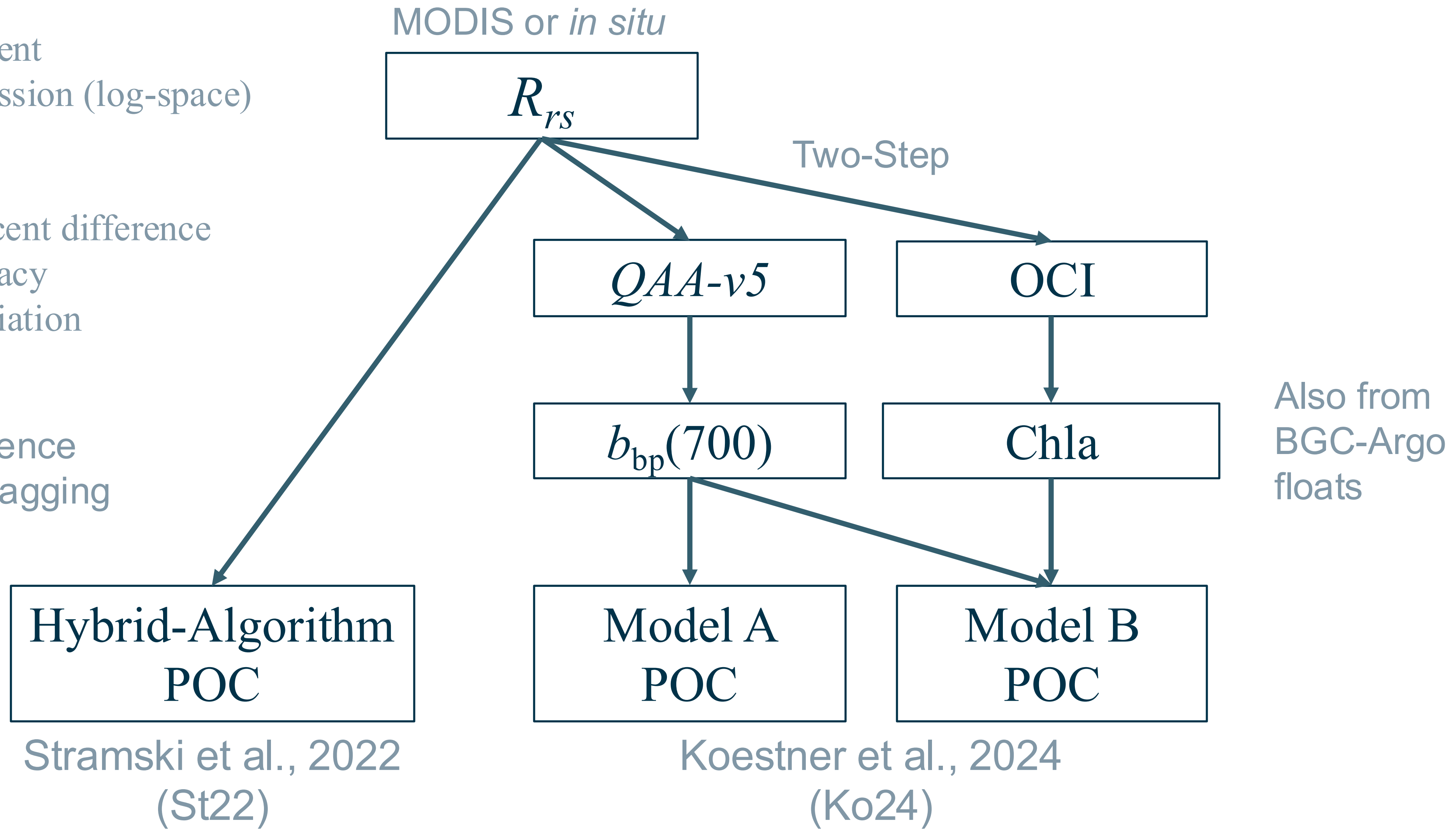
Methods

Statistical metrics:

R: Pearson correlation coefficient
S: Slope of type-II linear regression (log-space)
MdR: Median ratio
MnB: Mean bias
MdAPD: Median absolute percent difference
MnSA: Mean symmetric accuracy
RMSD: Root mean square deviation

Matchup-criteria:

3-hour maximum time difference
3x3 pixels; at least 3 pass flagging and hampel filter



Objective 1: *in situ* measures of POC and R_{rs}

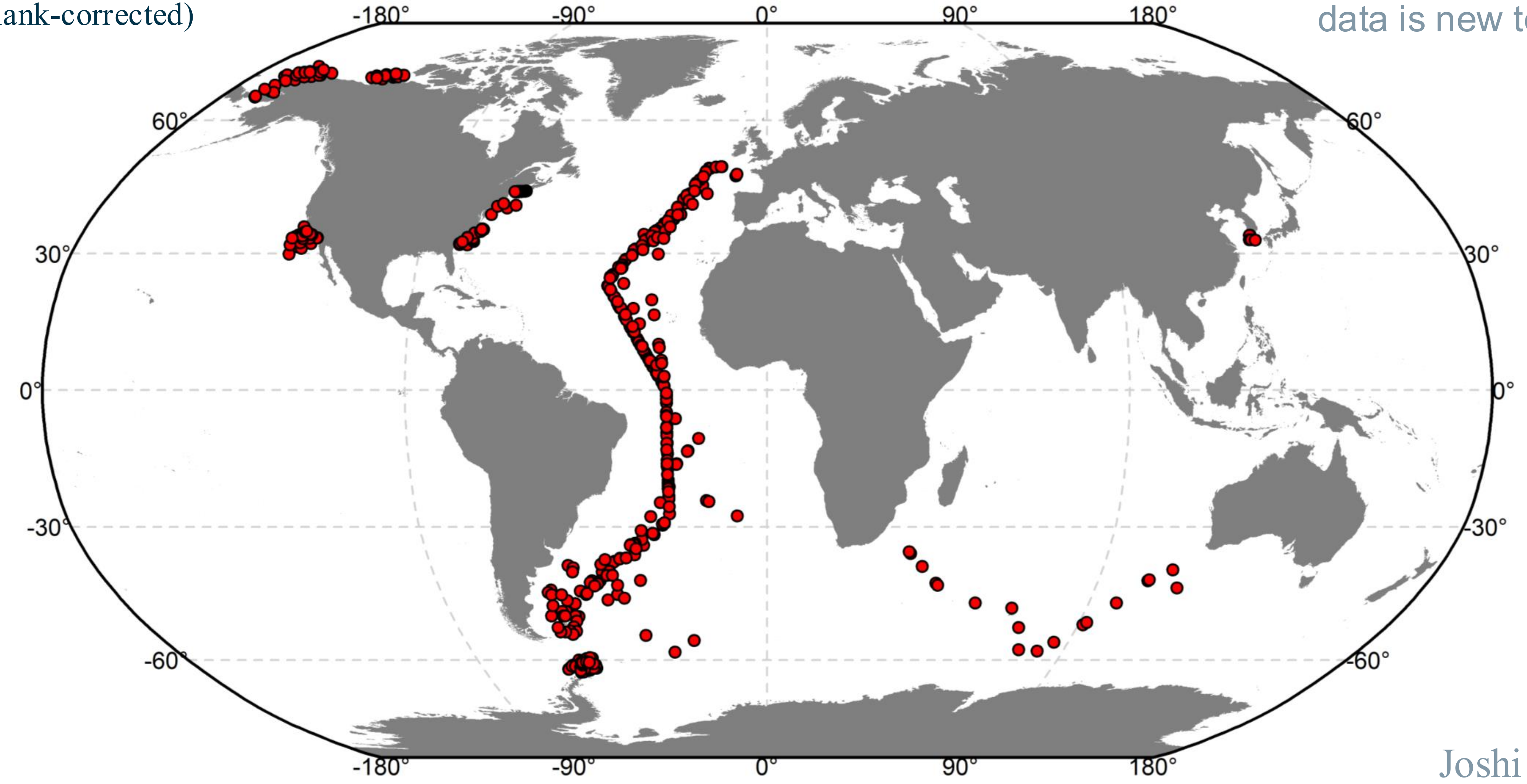
<u>Available variables:</u>

In situ $R_{rs}(\lambda)$ (In-water and above-water radiometry)

In situ POC (Blank-corrected)

In-situ Dataset ($N = 509$)

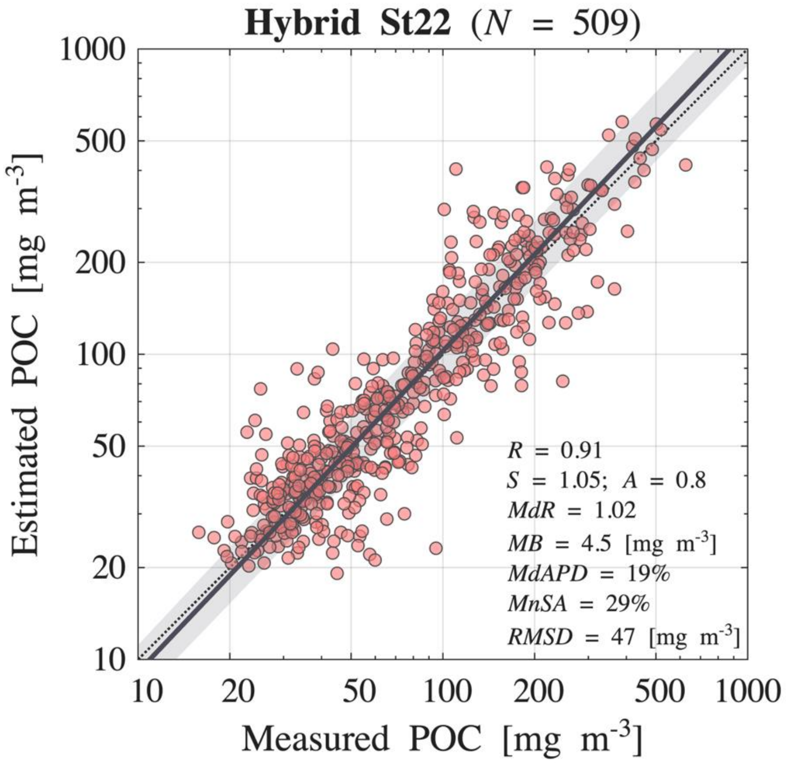
Nearly all comparison data is new to models

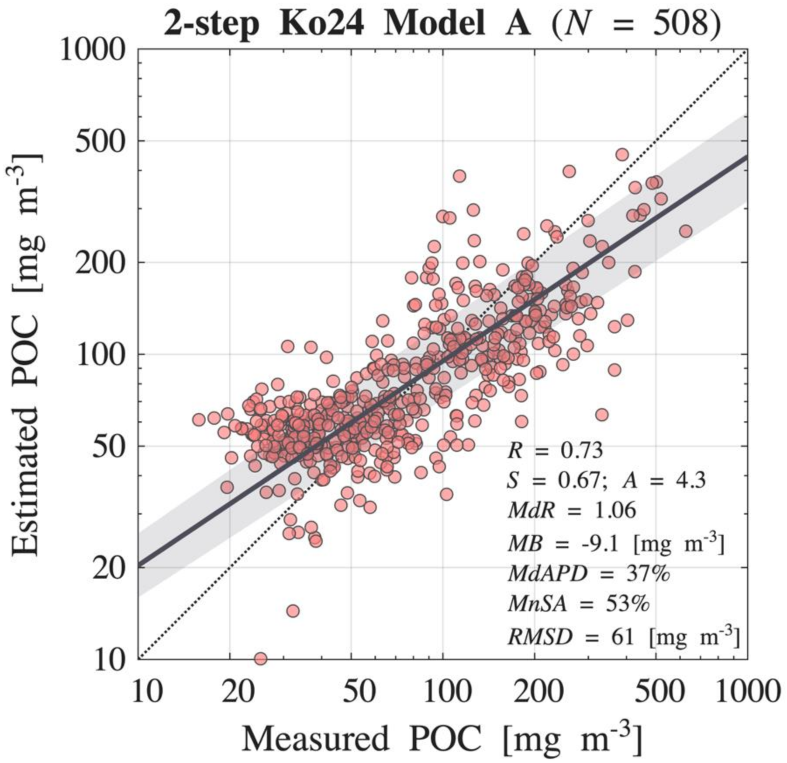


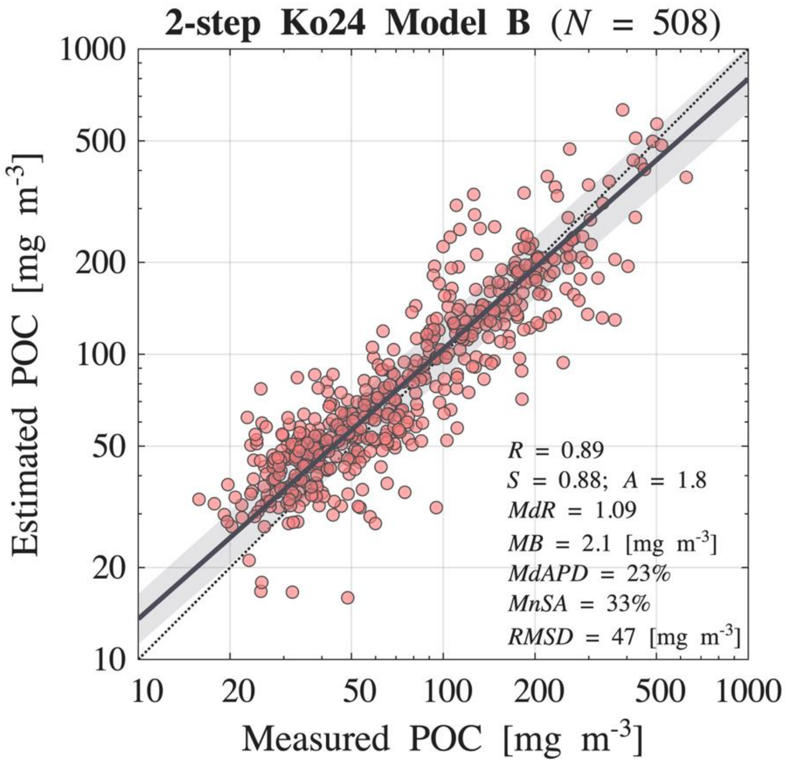
Joshi et al. (2023)

Objective 1: *in situ* measures of POC and R_{rs}

Performance is noticeably improved with multivariable Model B compared to univariate Model A





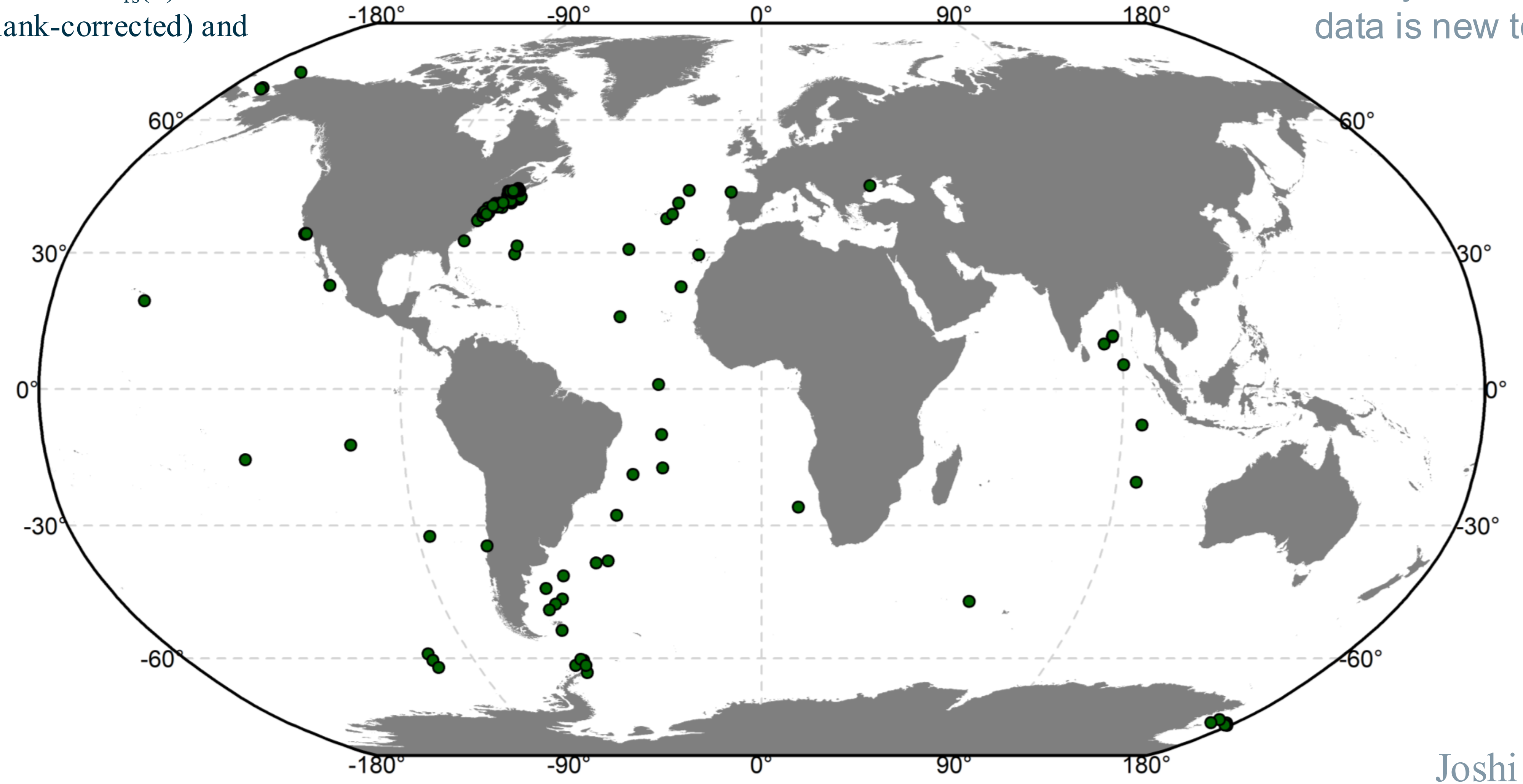


Model B performance is comparable to Hybrid, with only some minimal increase in bias at lower POC (< 50 mg m^{-3})

Objective 2: *satellite* R_{rs} and *in situ* measured POC

<u>Available variables:</u>
MODIS-Aqua-derived $R_{rs}(\lambda)$
in situ POC (Blank-corrected) and
HPLC Chl-a

Satellite–In-situ Matchup Dataset (N = 223)

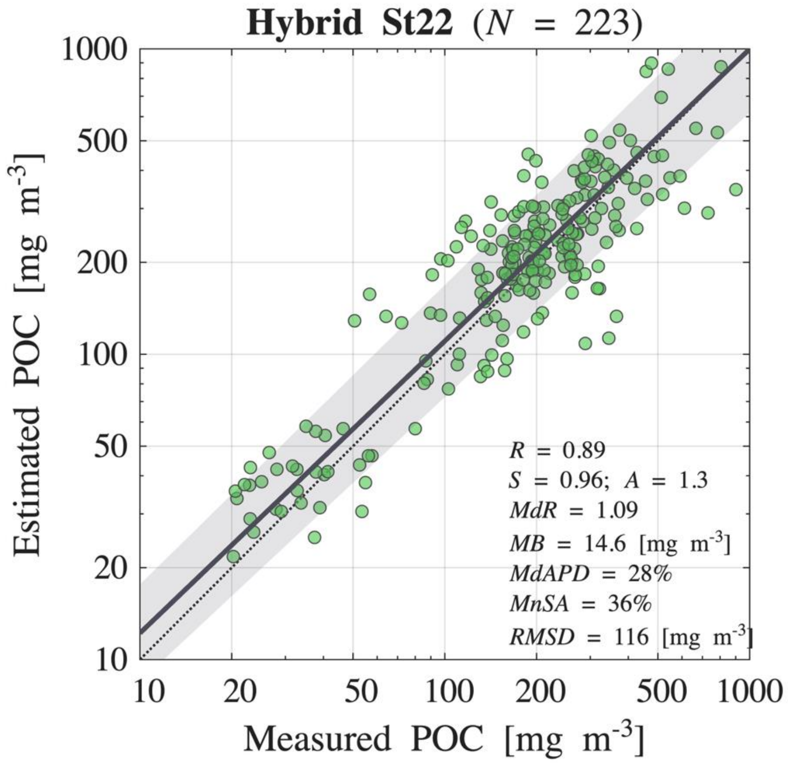


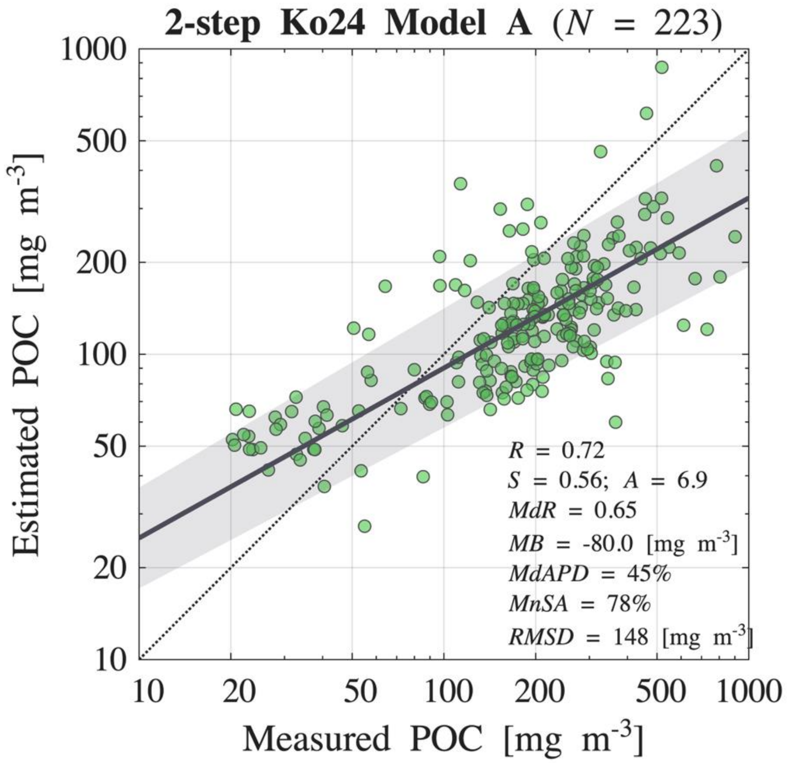
Nearly all comparison data is new to models

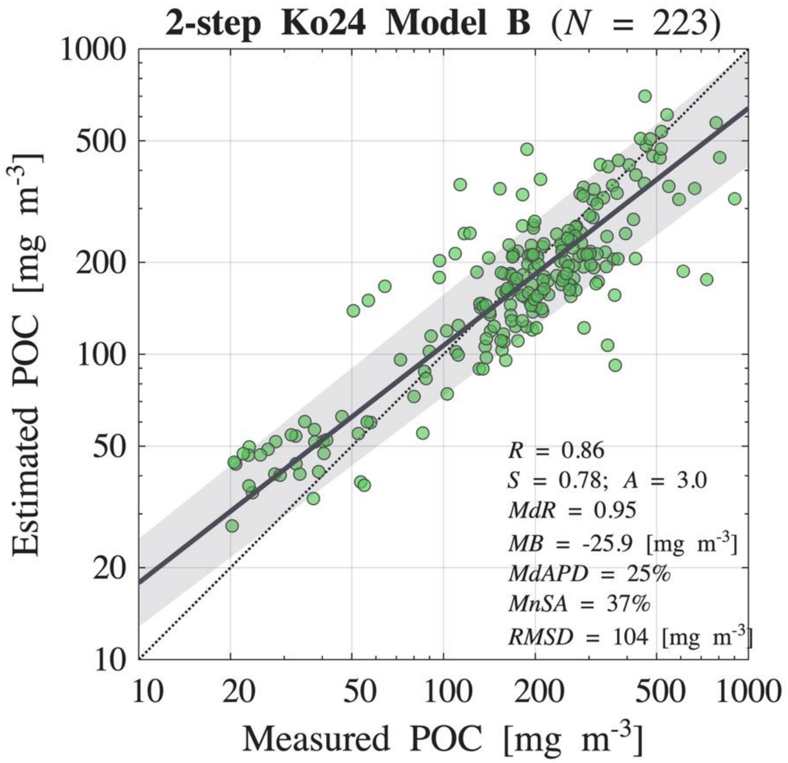
Joshi et al. (2023)

Objective 2: *satellite* R_{rs} and *in situ* measured POC

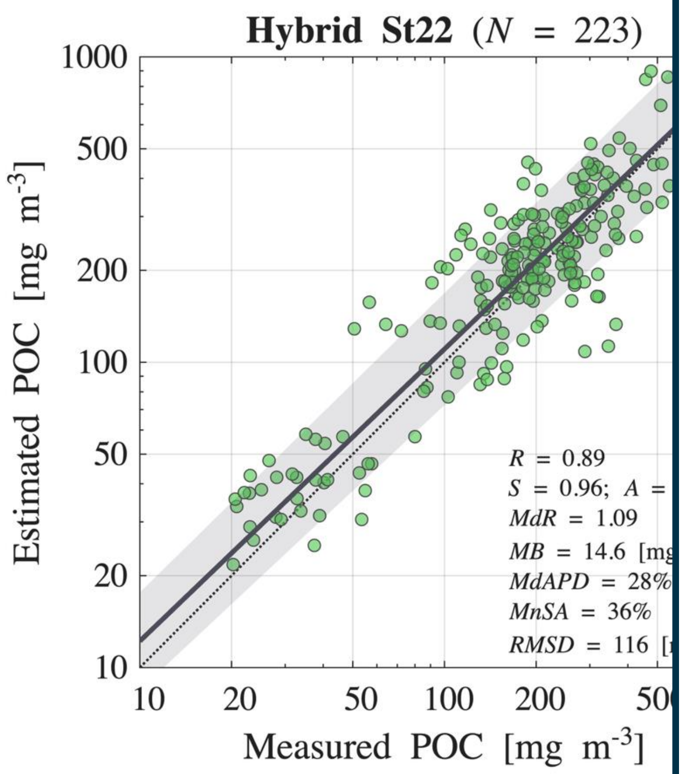
Again, comparable results between St22 and 2-step Ko24

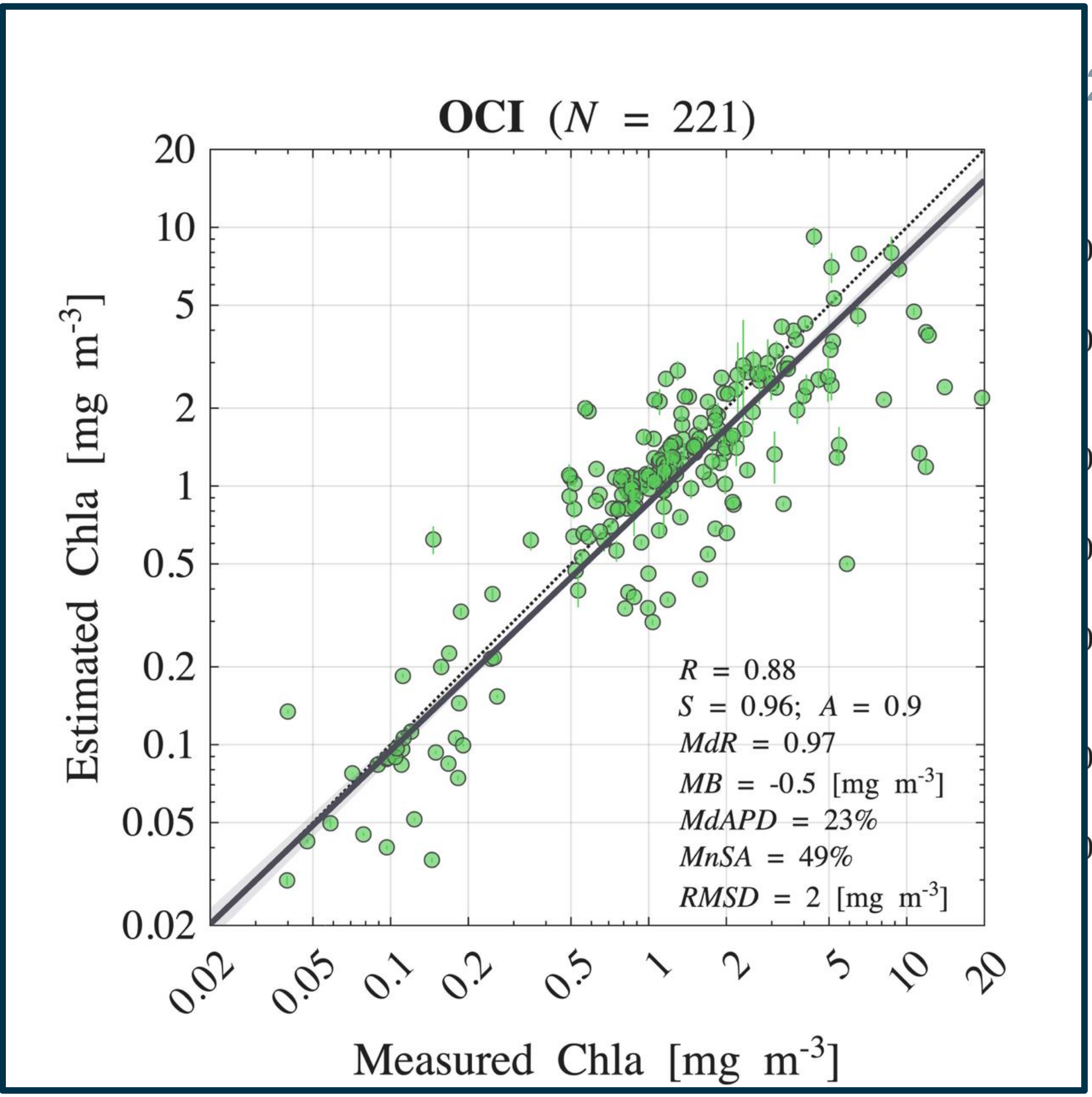


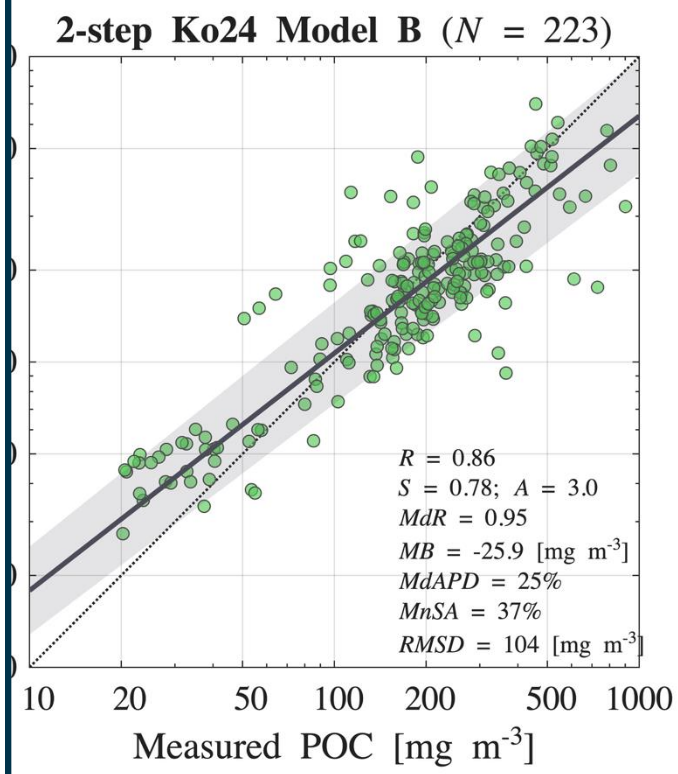




Objective 2: *satellite* R_{rs} and *in situ* measured POC



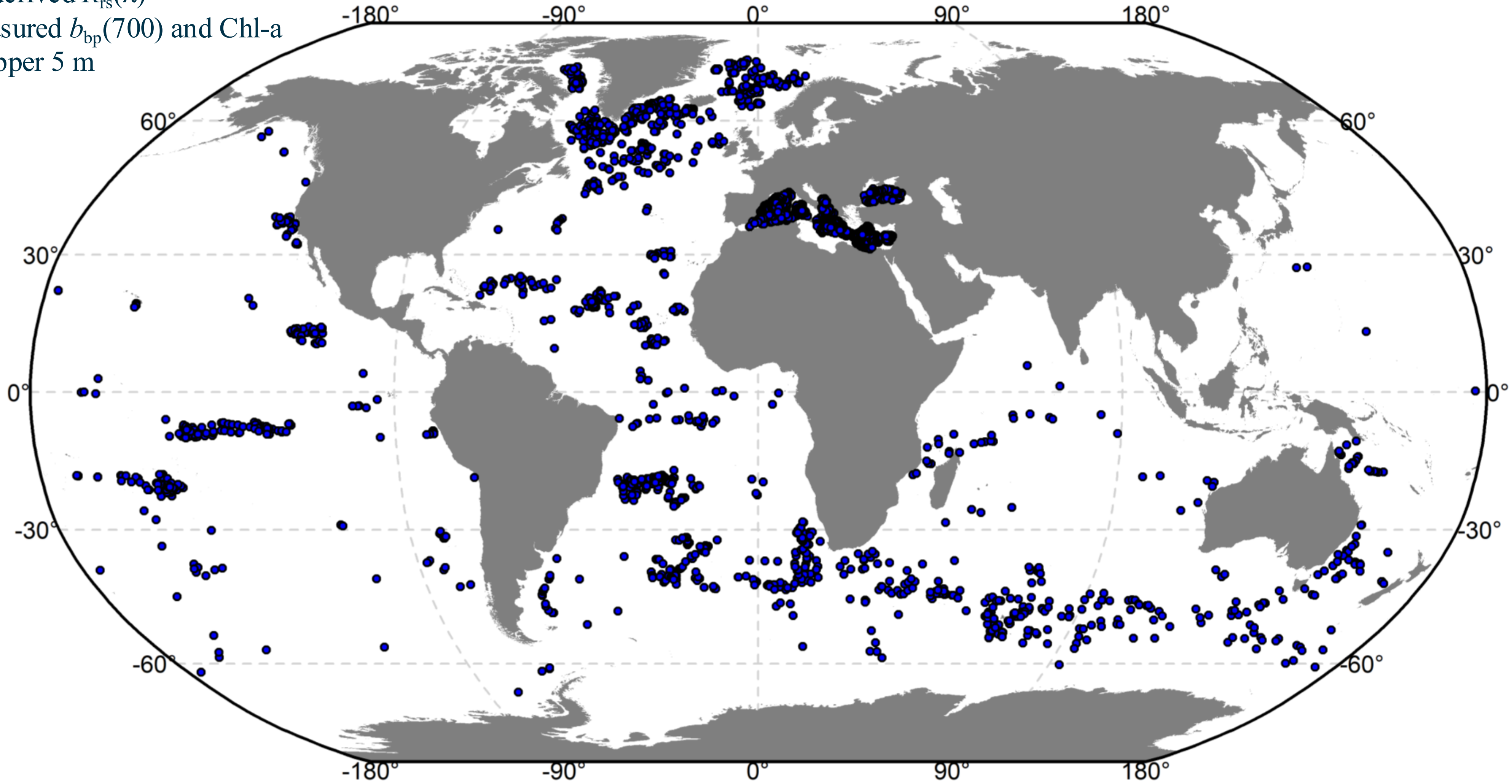




Objective 3: *satellite* R_{rs} and *in situ* estimated POC

<u>Available variables:</u>
MODIS-Aqua-derived $R_{rs}(\lambda)$
BGC-Argo-measured $b_{bp}(700)$ and Chl-a averaged into upper 5 m

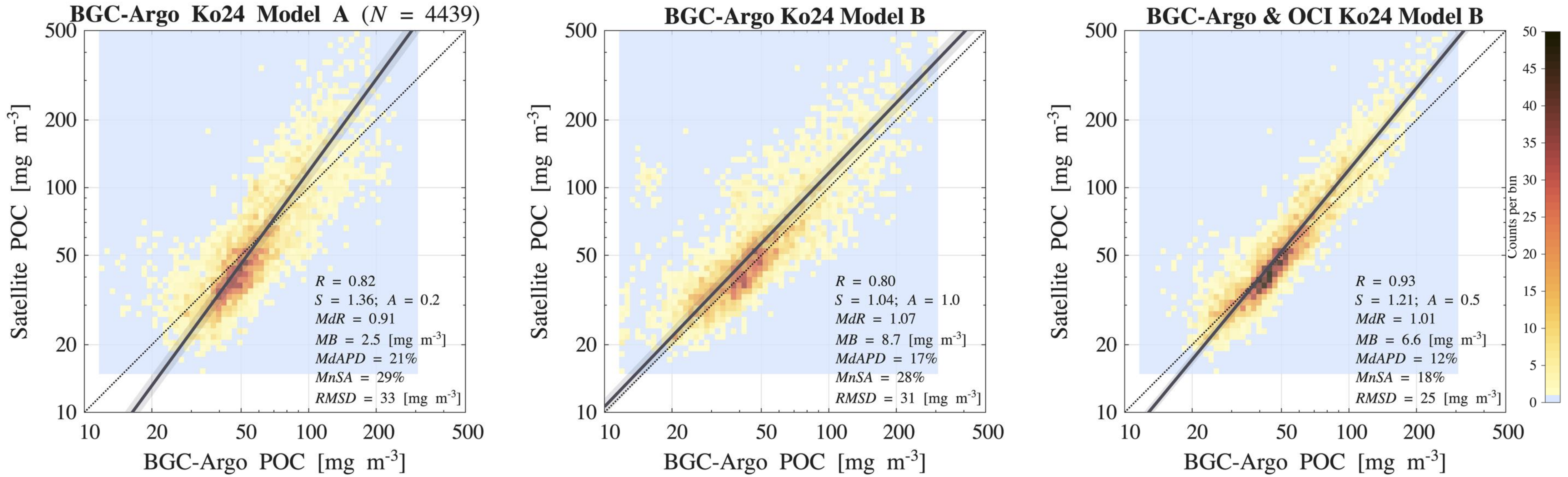
Satellite–BGC-Argo Matchup Dataset (N = 4448) [2012 – 2024]



Objective 3: *satellite* R_{rs} and *in situ* estimated POC

Reasonably good agreement between Satellite and BGC-Argo (Model B) POC

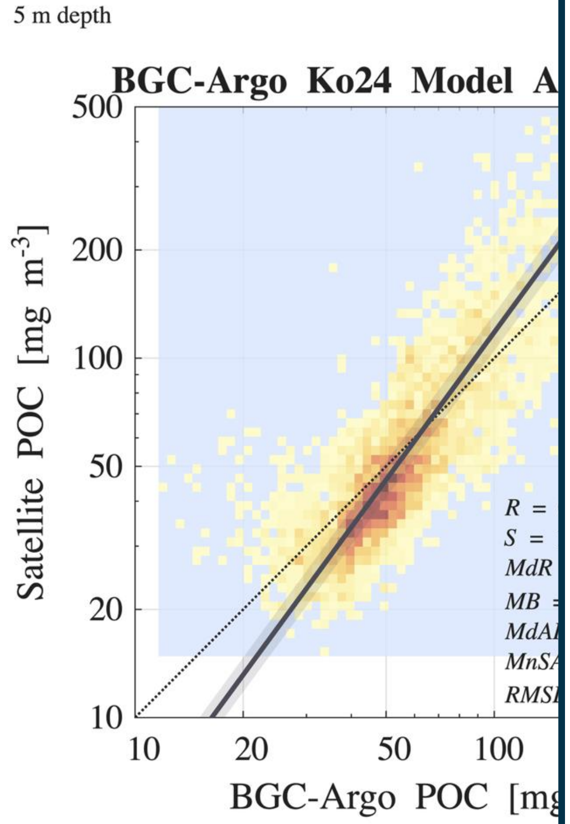
5 m depth



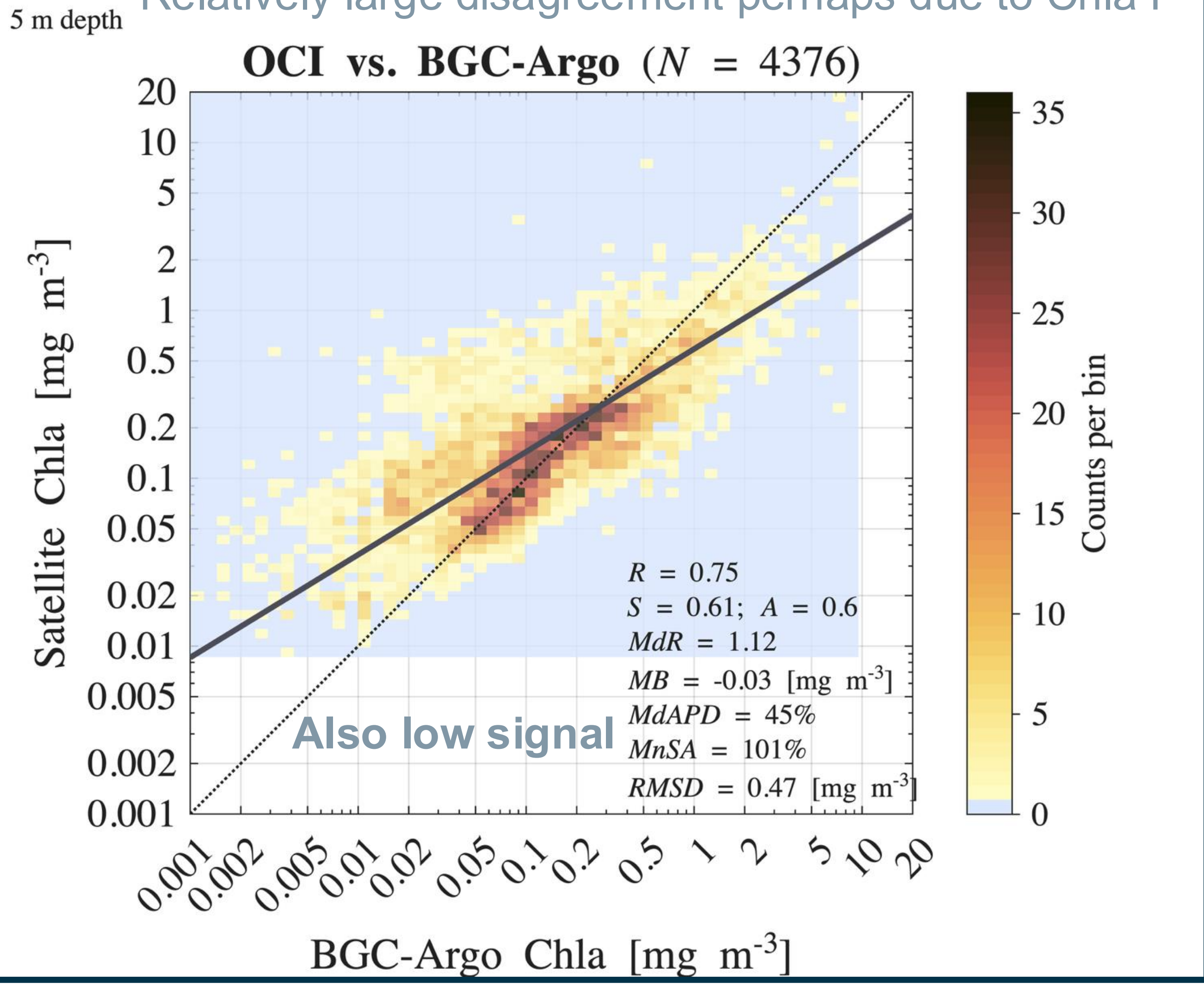
Even better agreement if input Chla is from Satellite (OCI)

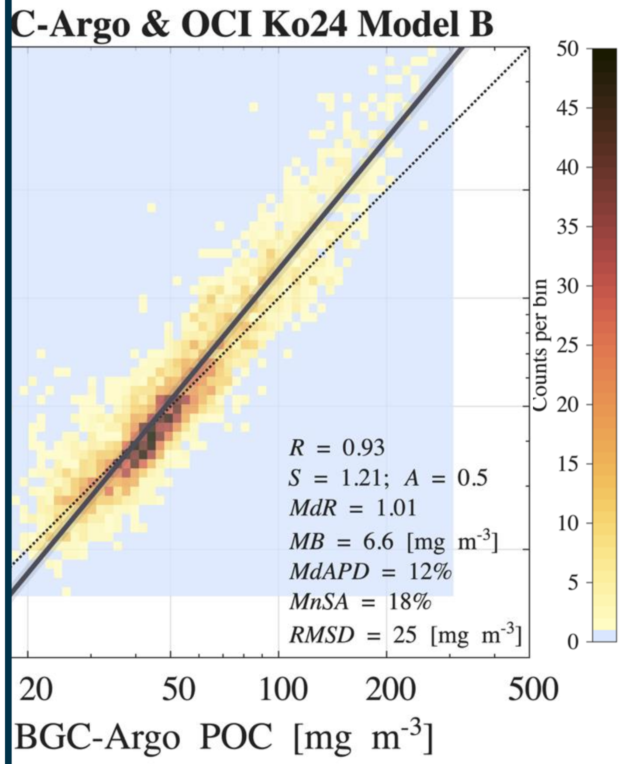
Objective 3: *satellite* R_{rs} and *in situ* estimated POC

Reasona ... B) POC



Relatively large disagreement perhaps due to Chla F





Chla is from Satellite (OCI)

Objective 4: Identify factors to exploit for merging of satellite and BGC-Argo data

Interest in developing:
1. Chla F correction factors
2. Estimations of integrated POC

No strong correlations on global scale.

Naturally, satellite POC correlates strongest with iPOC in the mixed layer compared with 1000 m water column, but still promising relationships with 200 m integration if we can leverage other information

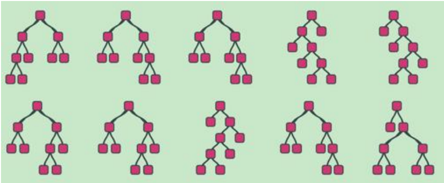
Best options currently include information about location and time of year.

Correlation Matrix: All Variables

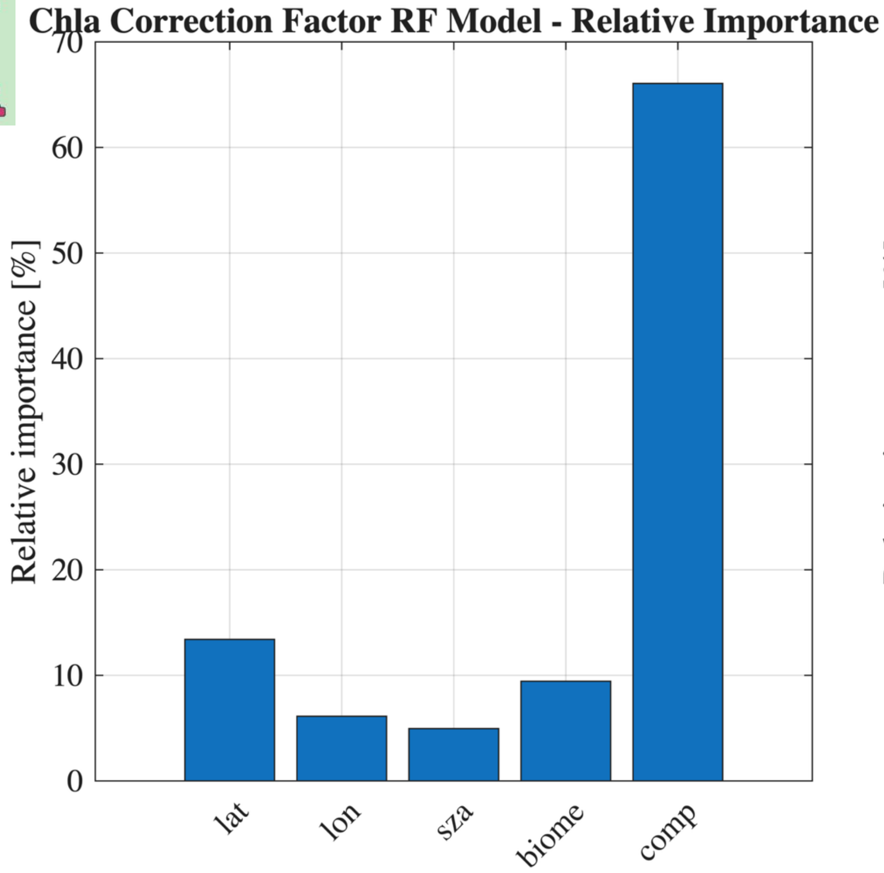
	satPOC	satChla	Chla	comp	Chla CF	iPOC	$iPOC_{200}$	$iPOC_{mld}$	lat	lon	sza	MonthsSinceWinter	parProxy
satPOC	1	0.98	0.72	0.52	0	0.39	0.54	0.65	0.25	-0.06	0.28	-0.1	-0.08
satChla	0.98	1	0.68	0.46	0.01	0.27	0.42	0.45	0.18	-0.04	0.17	-0.07	-0.04
Chla	0.72	0.68	1	0.81	-0.12	0.45	0.65	0.67	0.05	-0.04	0.12	-0.09	0.03
comp	0.52	0.46	0.81	1	-0.23	0.36	0.52	0.58	0.01	-0.05	0.22	-0.14	-0.13
Chla CF	0	0.01	-0.12	-0.23	1	-0.09	-0.12	-0.14	0.07	-0.05	-0.03	0.03	0.06
iPOC	0.39	0.27	0.45	0.36	-0.09	1	0.77	0.5	-0.19	0.03	-0.05	-0.16	0.2
$iPOC_{200}$	0.54	0.42	0.65	0.52	-0.12	0.77	1	0.65	-0.1	0.09	0.05	-0.2	0.17
$iPOC_{mld}$	0.65	0.45	0.67	0.58	-0.14	0.5	0.65	1	0.01	0.01	0.21	-0.1	-0.04
lat	0.25	0.18	0.05	0.01	0.07	-0.19	-0.1	0.01	1	-0.06	0.19	0	-0.08
lon	-0.06	-0.04	-0.04	-0.05	-0.05	0.03	0.09	0.01	-0.06	1	0.01	-0.04	-0.03
sza	0.28	0.17	0.12	0.22	-0.03	-0.05	0.05	0.21	0.19	0.01	1	0.08	-0.83
MonthsSinceWinter	-0.1	-0.07	-0.09	-0.14	0.03	-0.16	-0.2	-0.1	0	-0.04	0.08	1	-0.1
parProxy	-0.08	-0.04	0.03	-0.13	0.06	0.2	0.17	-0.04	-0.08	-0.03	-0.83	-0.1	1

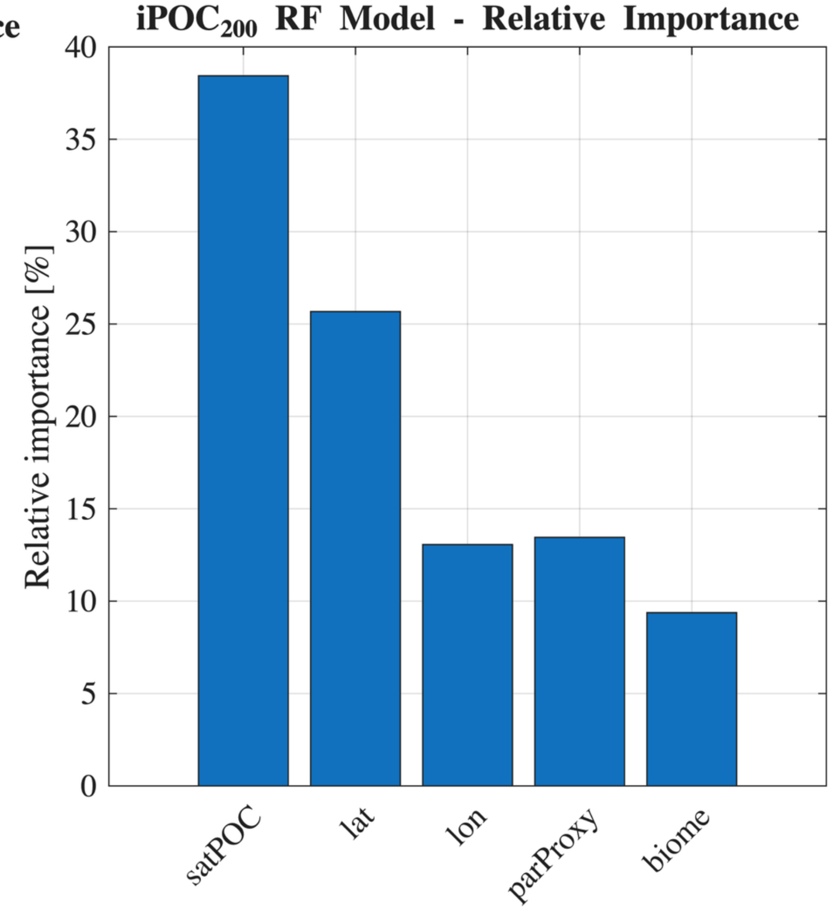
Objective 4: Identify factors to exploit for merging of satellite and BGC-Argo data

Random Forest ensemble model (100 trees) was developed explore relative importance of variables in predicting Chla Correction Factor (CF) for BGC-Argo float data and POC integrated from surface to 200 m ($iPOC_{200}$)



For Chla CF, we find particle composition (Chla:b_{bp}) to be a strong determinant, then latitude, (aggregate) biome, solar zenith angle (sza) of measurement, and longitude

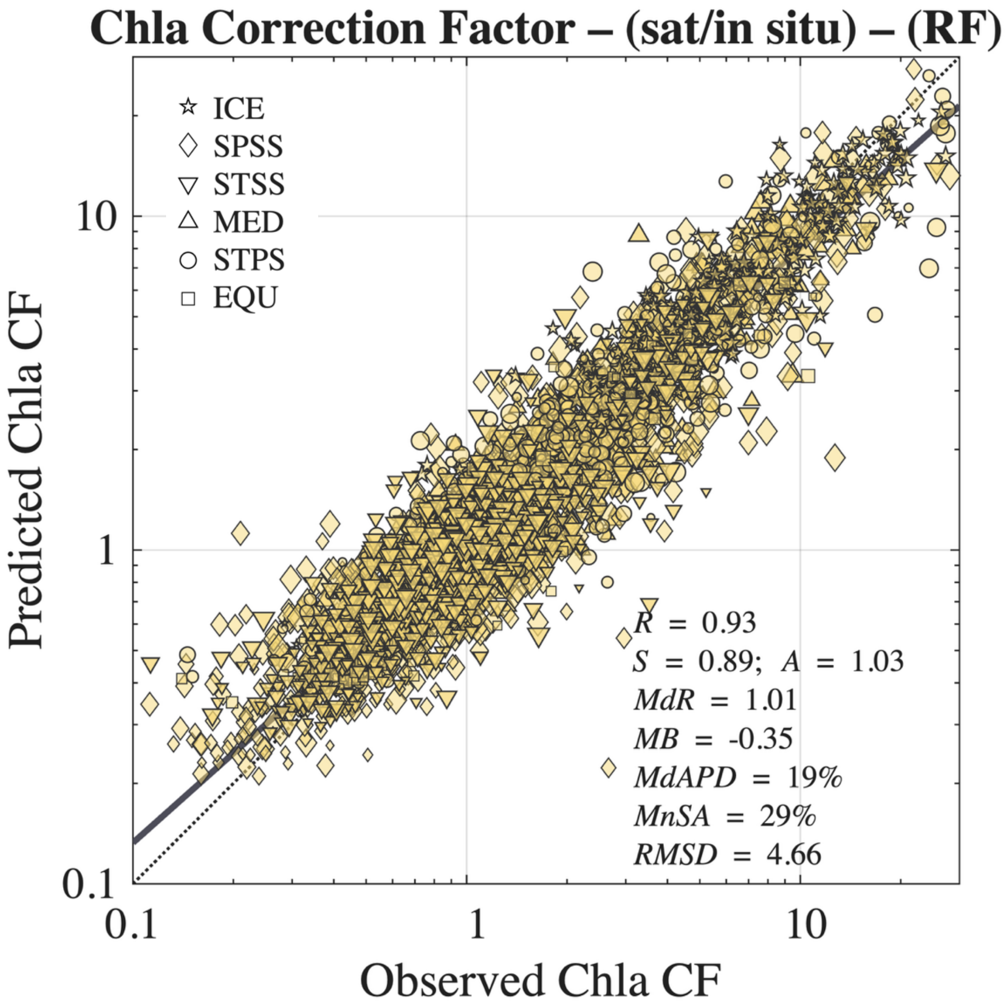


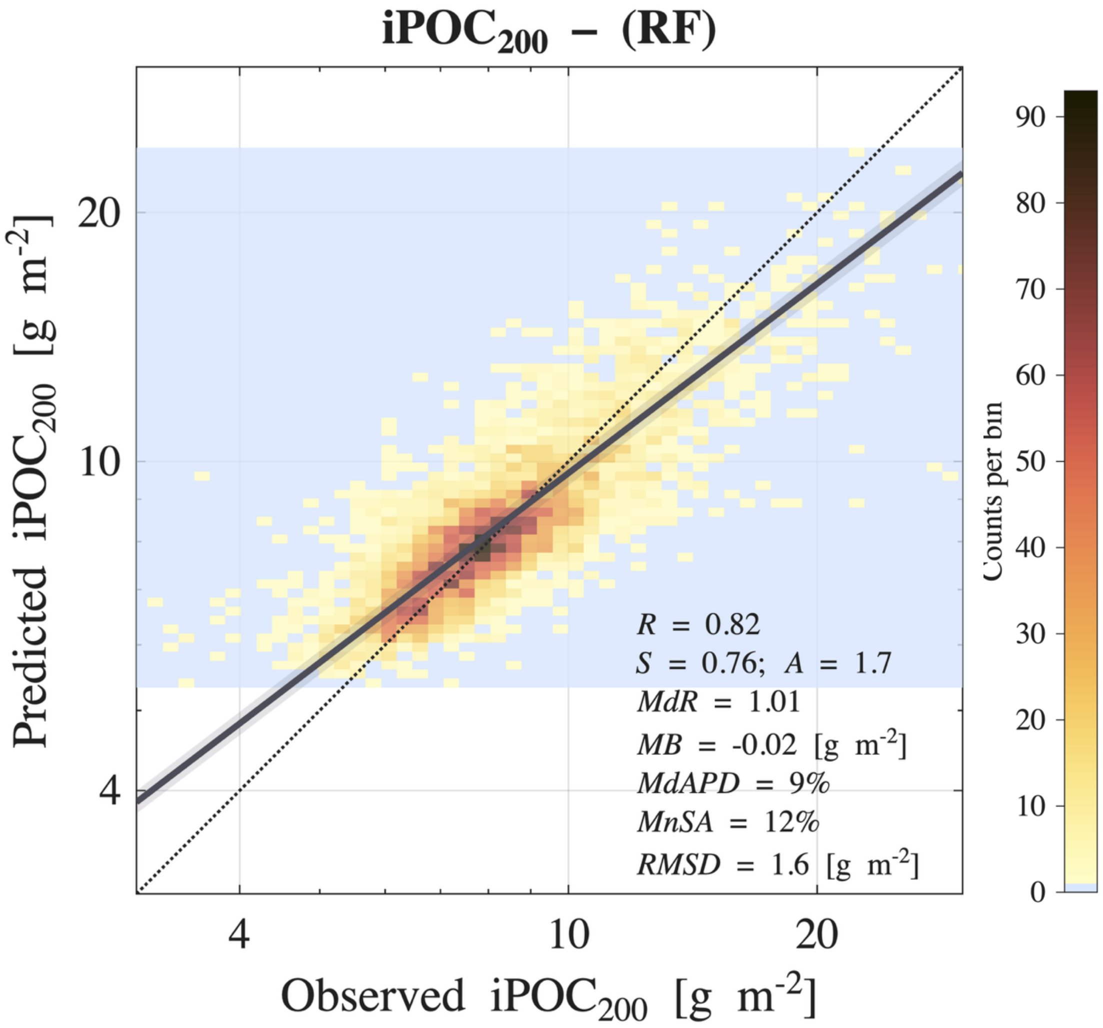


For $iPOC_{200}$, Satellite POC and latitude are strongest predictors, but a proxy for daily PAR potential based on day-of-year and latitude is also useful

Mean biomes from Fay et al. (2014)

Objective 4: Identify factors to exploit for merging of satellite and BGC-Argo data

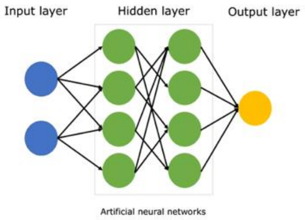


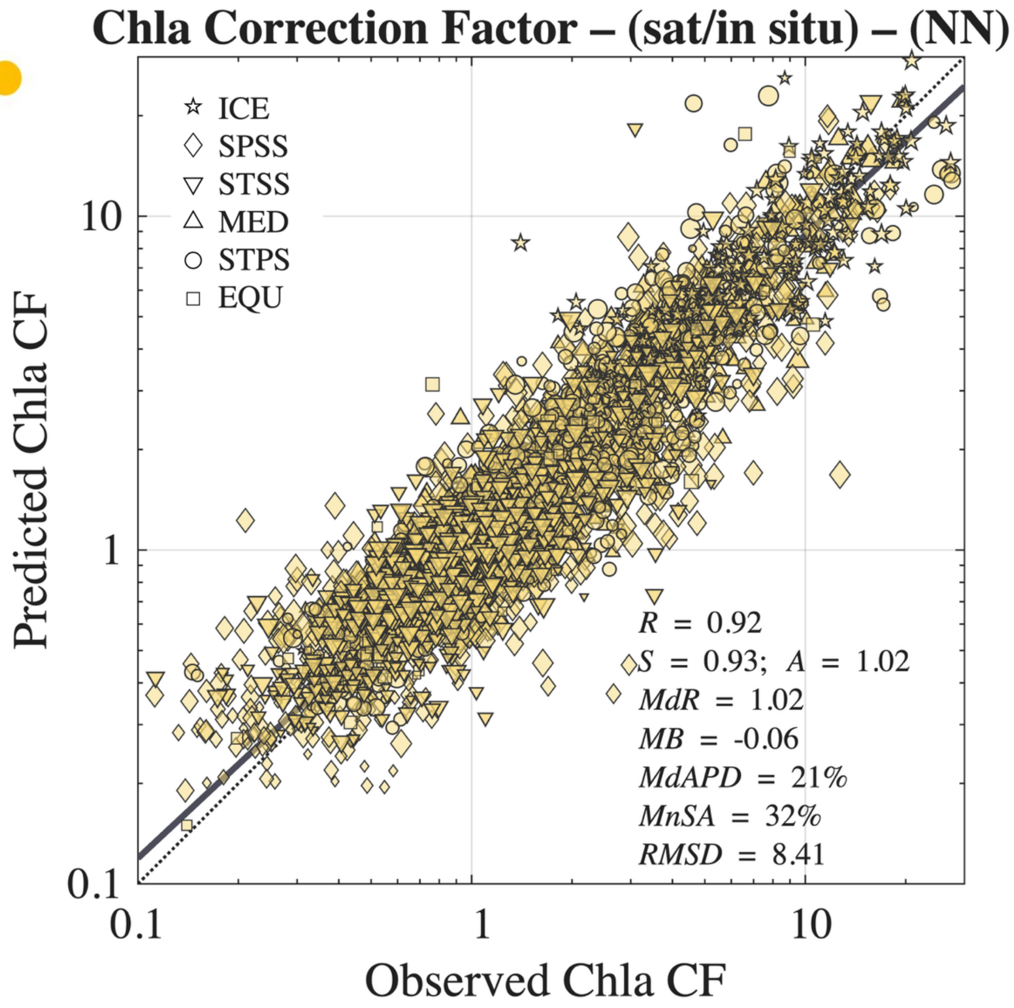


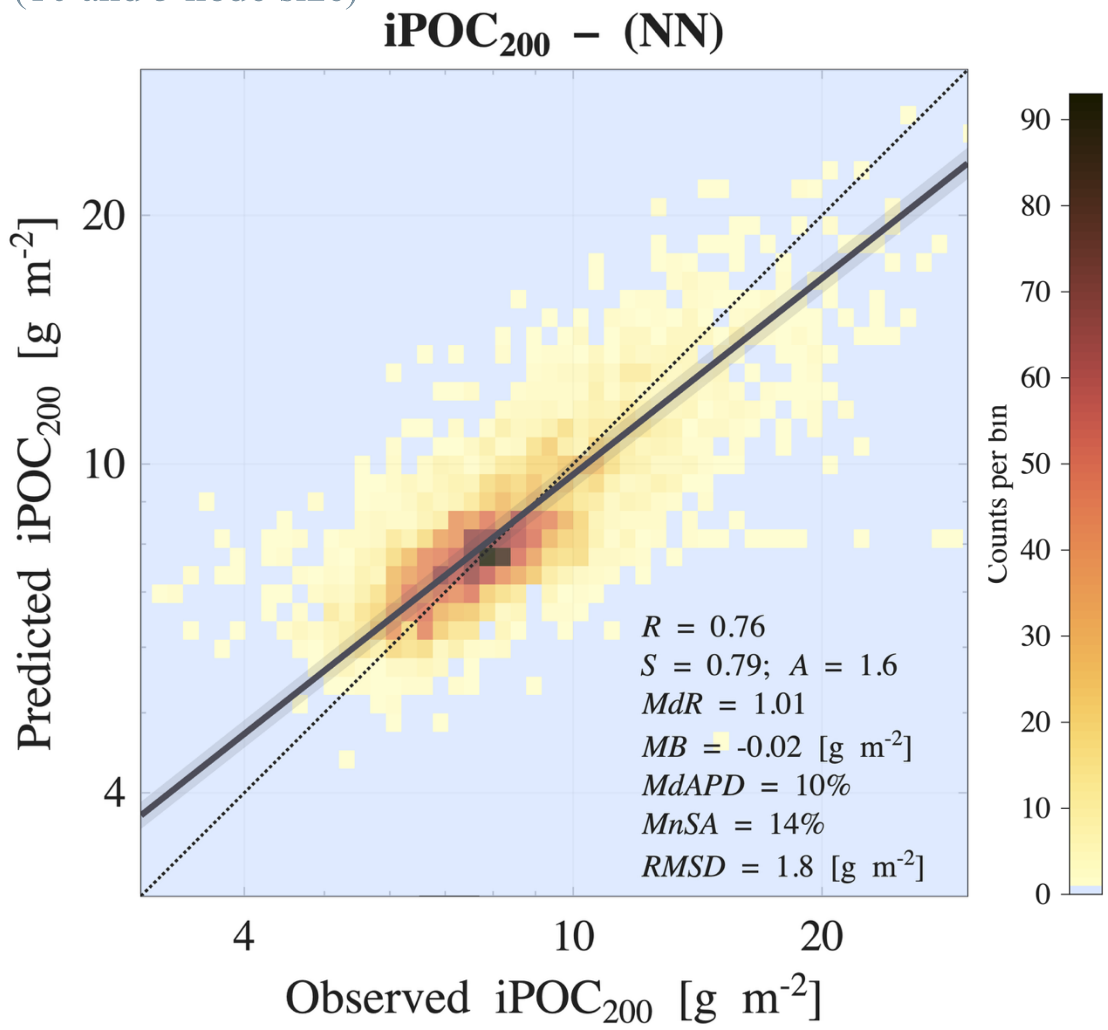
Out-of-bag validation from 5 k-folds

Objective 4: Identify factors to exploit for merging of satellite and BGC-Argo data

Two layer NN (10 and 5 node size)

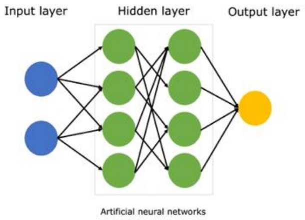


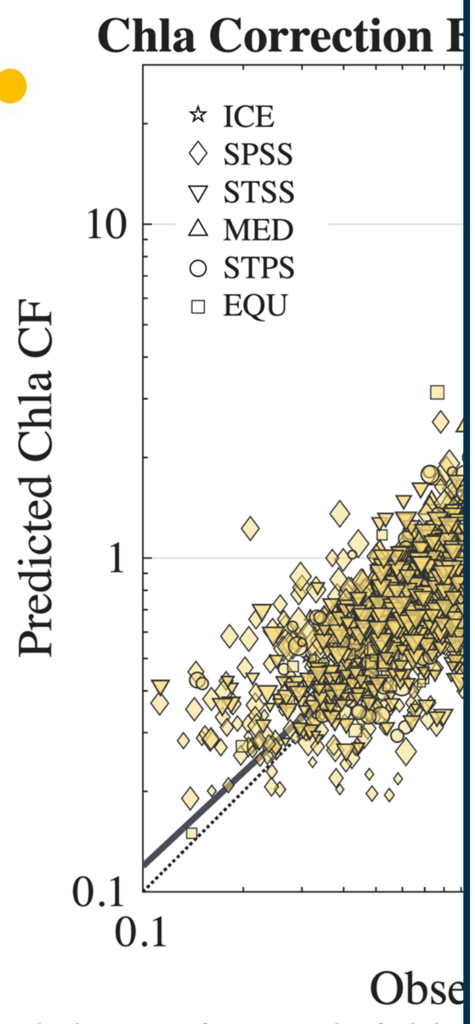


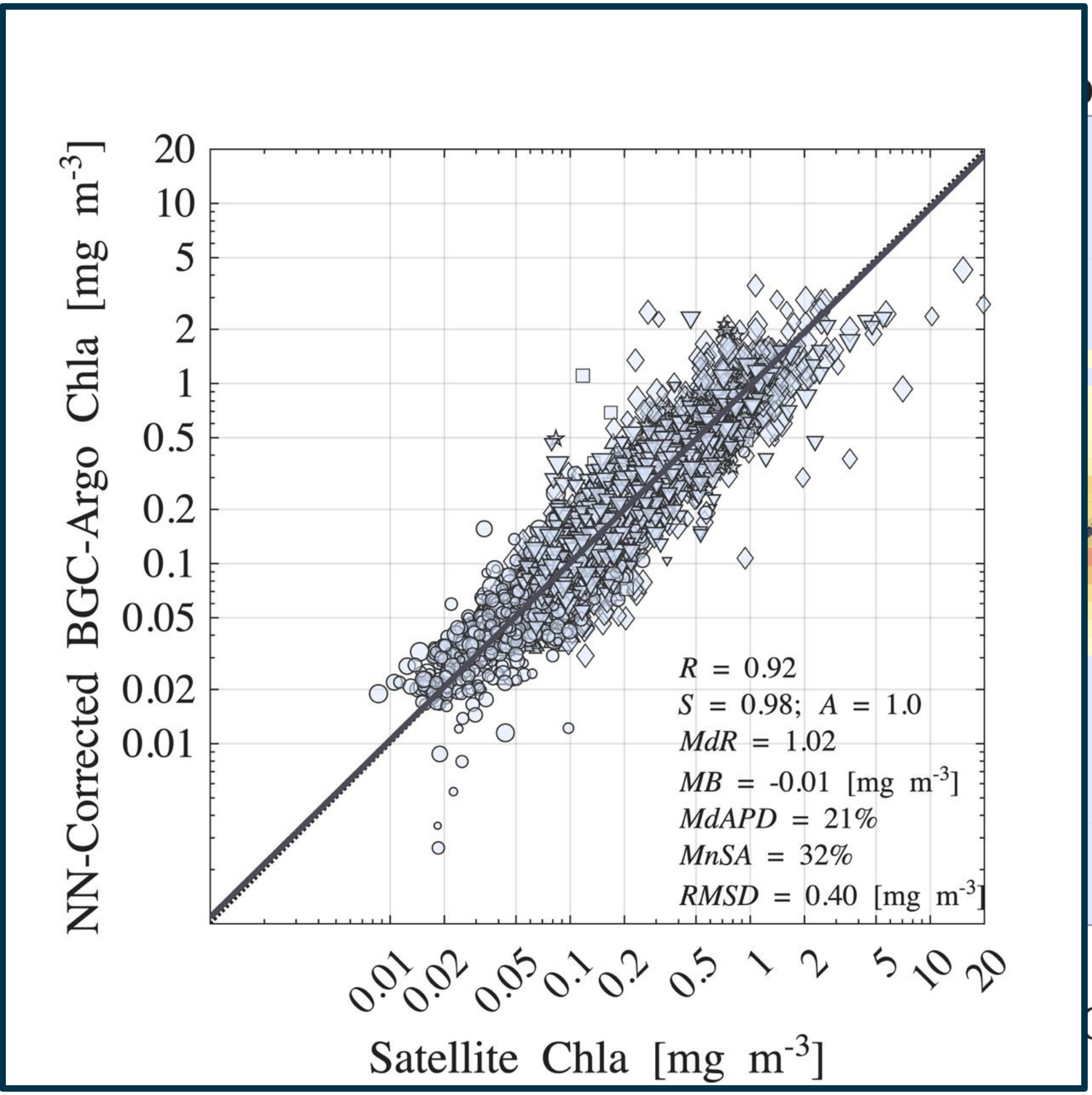


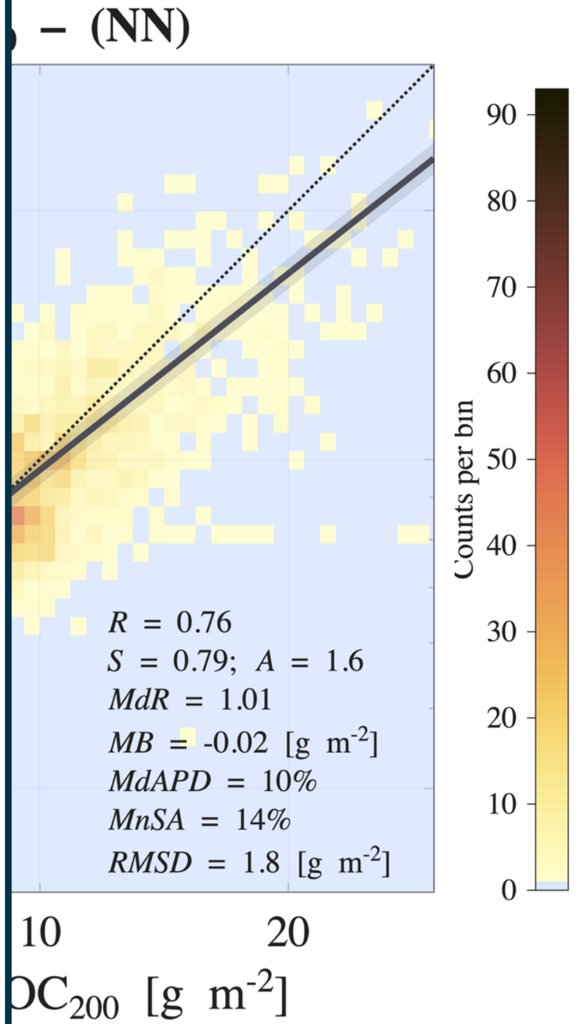
Out-of-bag validation from 5 k-folds

Objective 4: Identify factors to exploit for merging of satellite and BGC-Argo data









Out-of-bag validation from 5 k-folds

Conclusions

- Revisiting the two-step approach to estimating POC from R_{rs} by first retrieving b_{bp} and leveraging a particle composition proxy suggests comparable results with a semi-empirical band-ratio based approach
- A global comparison of *in situ* estimated surface POC from BGC-Argo floats reveals overall good agreement with satellite estimates, with some potential for large errors for low POC values
    - Likely linked to relatively large disagreements between Chla estimated from *in situ* fluorometers and satellite estimates (typically developed with extracted pigment measurements)
- Corrections have been developed for improving Chla estimations from *in situ* fluorometers on BGC-Argo floats by leveraging ancillary information
    - Average disagreement between BGC-Argo and satellite Chla is reduced from ~100% to 30%
- Using the relatively large dataset of MODIS and BGC-Argo matchups, satellite POC can be combined with limited ancillary information to produce predictive models for reasonable estimates of POC integrated within the upper 200 m
    - *Can we really go any deeper without more information?*
- Development of these ideas, identification of additional predictor variables, refinement of models, and expansion of BGC-Argo float array is expected to support future 3-D products of POC in the ~near future

In situ data

Satellite L2 product

Select L2 scene acquired within ±3 hours of field measurement

A 3 x 3 pixel box (9 pixels) centered at in situ station is extracted.

$R_{rs}(\lambda)$ (9 pixels)

Pixel is rejected if flagged by at least one of 15 L2 quality flags. [ATMFAIL, LAND, HIGLINT, HISATZEN, STRAYLIGHT, CLDICE, COCOLITH, HISOLZEN, LOWLW, CHLFAIL, NAVWARN, MAXITER, CHLWARN, ATMWARN, NAVFAIL]

If number of remaining pixels is greater than 3 for all bands then process continued.

If number of remaining pixels is less than 3 in any band then the entire 3 x 3 pixel box is rejected and search begun for the next station.

QAA-v5

$b_{bp}(700)$

Chla from OCI

Hybrid POC algorithm

Model A or B POC algorithms

Hempel filter was applied to remaining pixels to identify and remove outliers if any.

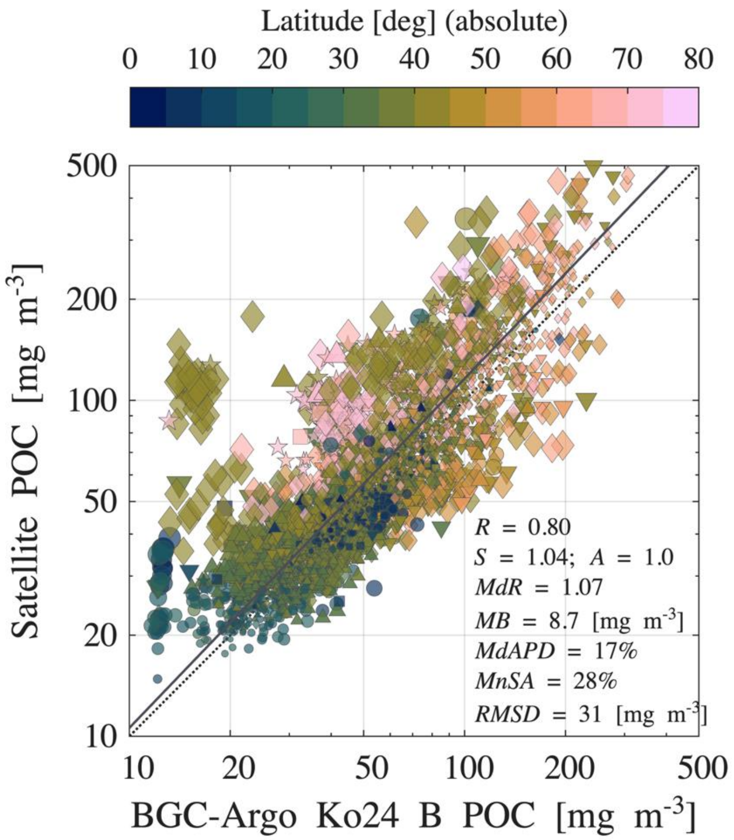
If number of remaining pixels is less than 3 then matchup is rejected

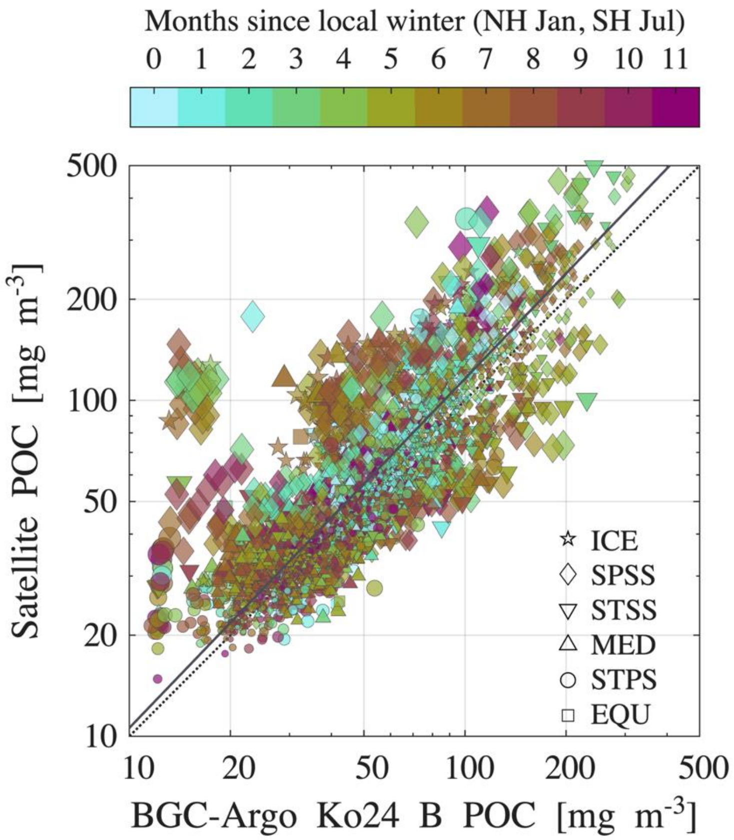
If number of remaining pixels is greater than 3 then process continued.

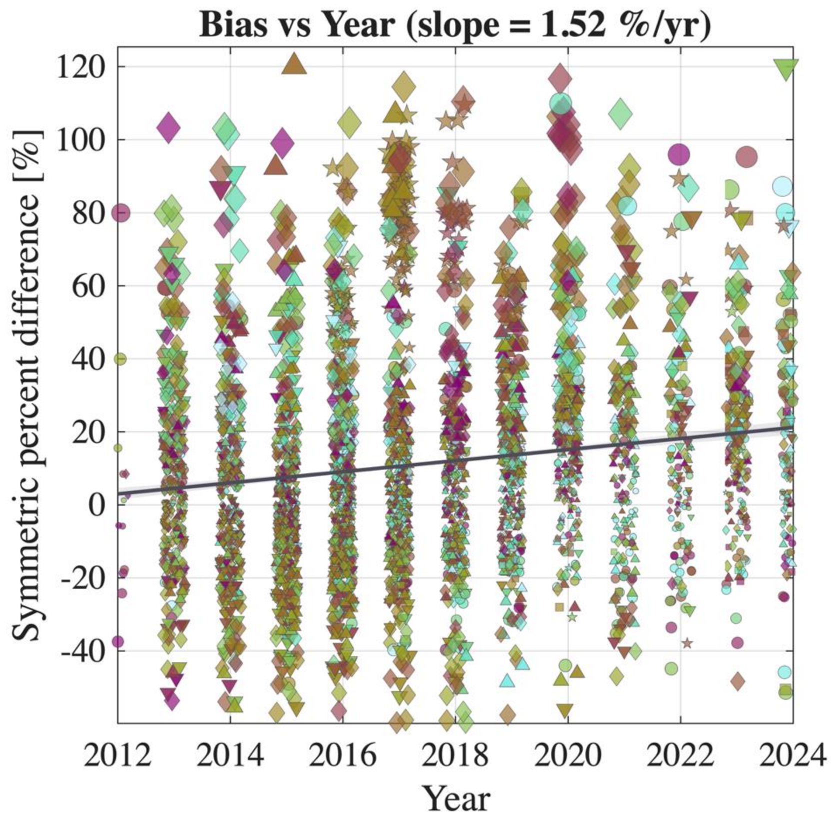
Mean and standard deviation are computed and considered as valid satellite matchup.

Objective 3: *satellite* R_{rs} and *in situ* estimated POC

Other factors potentially influencing disagreement?
Higher latitude SPSS and ICE biomes appear to have larger disagreement







Objective 3: *satellite* R_{rs} and *in situ* estimated Chla