A Multivariable Model for Estimating Particulate Organic Carbon Concentration in Marine Environments using Optical Backscattering and Chlorophyll-a Measurements

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Background/Motivation

- In situ optical measurements can be useful for calibrating satellite observations, high temporal resolution monitoring of point-source locations, and understanding vertical structure.
- In situ estimates of POC have typically relied on simple models relating particulate backscattering coefficient (b_{bp}) or chlorophyll-a concentration (Chla) to POC and can be subject to high uncertainties under various oceanic conditions.
- Chla-based estimates of POC can be accurate for oceanic surface waters; however, often fail to estimate POC when POC is non-phytoplankton dominated such as in mesopelagic or coastal waters, or for varying phytoplankton type/health.
- b_{bp}-based estimates of POC can also be accurate, but POC-specific b_{bp} values vary throughout the ocean, also driven by changes to particle assemblage (e.g., composition, size distribution).

$G = \frac{\pi}{4} D^2$ (sphere)
$m = n - i\,n'$
$n' = a_s \lambda / 4\pi$
$\rho = 2\alpha(n-1)$
$\alpha = \pi D/\lambda$

Theory

$$b_b = Q_{bb} \frac{N}{V} G$$

$b_b \propto \frac{N}{V}$ (single particle type)

$$POC = \frac{N}{V} poc_i v$$

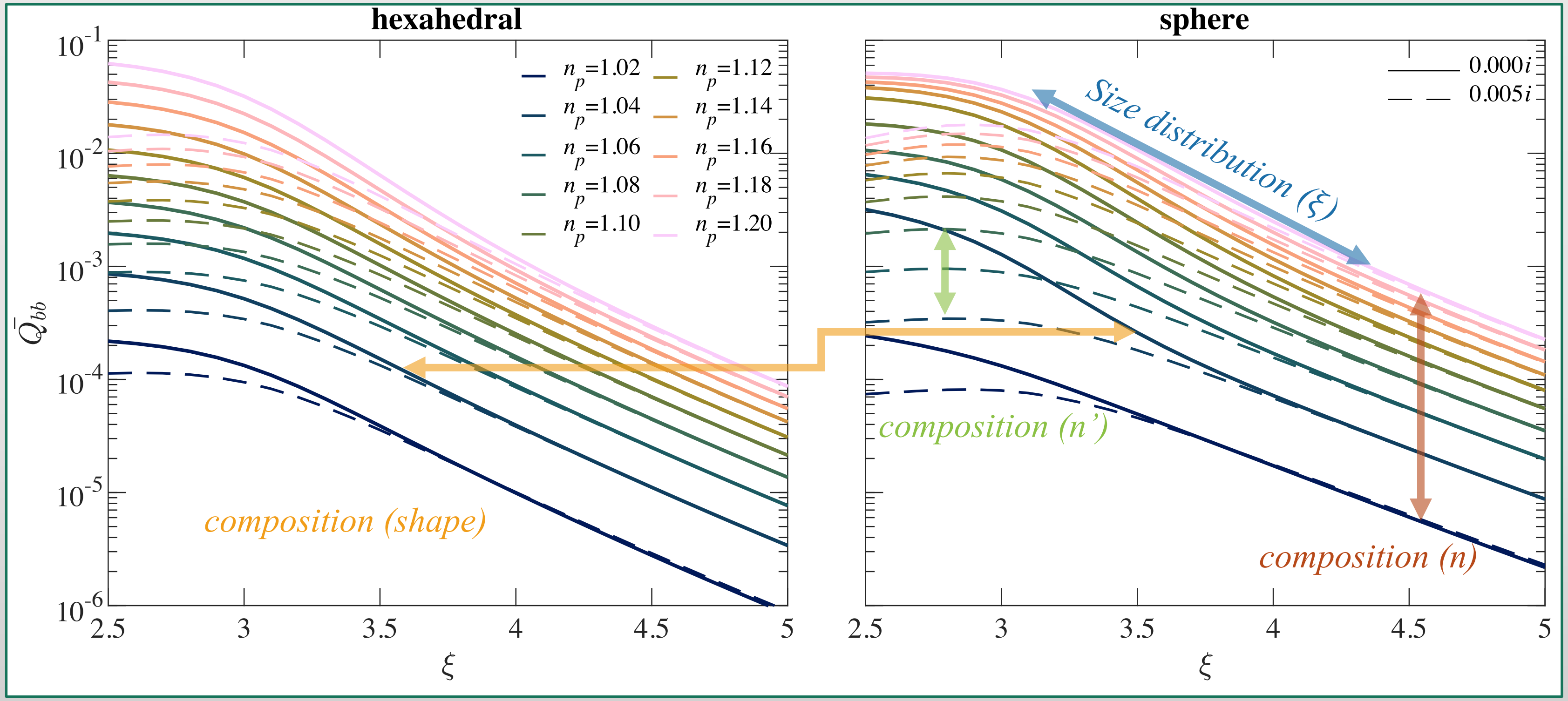
$$b_b^* = \frac{b_b}{POC}$$

$b_b^* = \frac{3Q_{bb}}{2Dpoc_i}$ (sphere)

Particle properties influencing b_b^*?

$Q_{bb}(n,D,n')$ – sensitive to comp and size

poc_i also has variability related to particle type



PSDs assume Junge shape with 200 log-spaced bins 10 nm to 100 µm (at 532 nm) with varying slope ξ

Intraparticle poc and Q_{bb} have sensitivity to composition and size distribution.

Without accounting for these effects, estimates of POC using backscattering will be limited to systems exhibiting minimal variability in composition and size distribution.

Research question

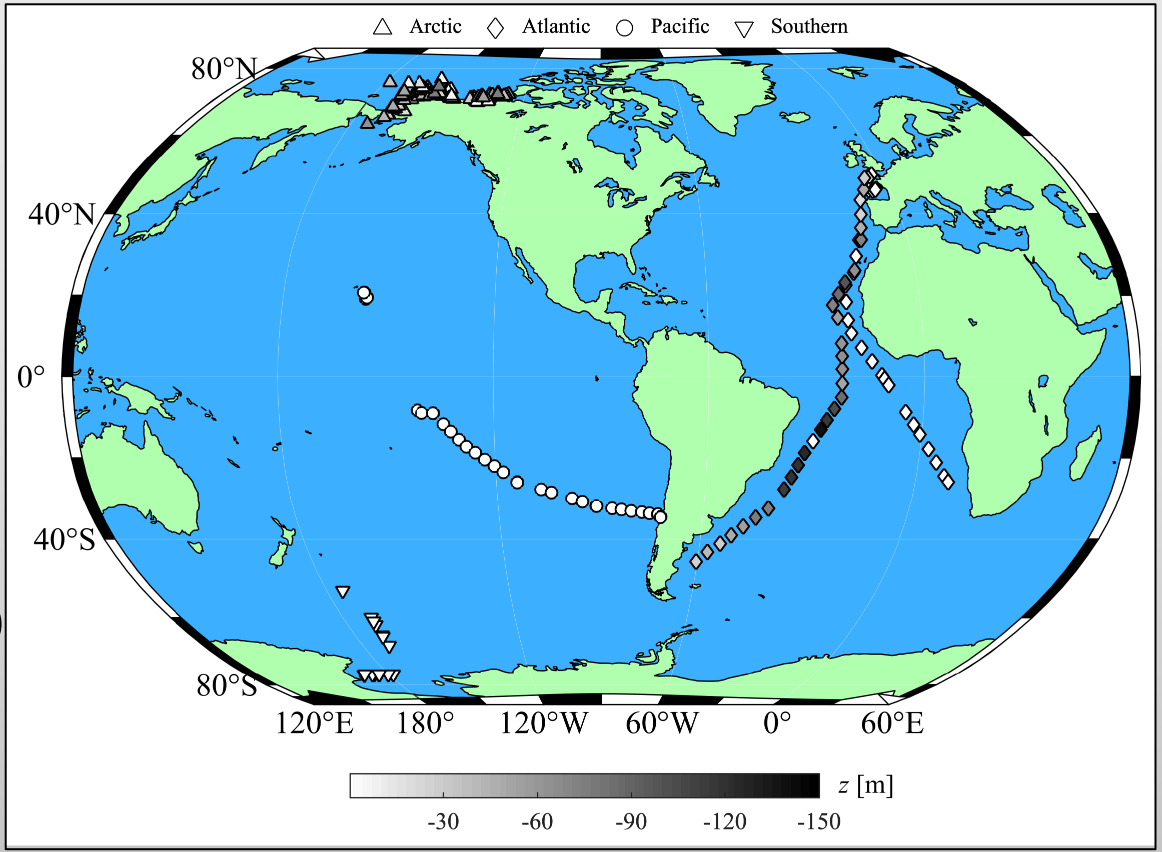
- Can the inclusion of a composition term in optically-based models improve POC estimations for various conditions encountered in the ocean (e.g., organic/inorganic, algal/nonalgal, coastal/open, epipelagic/mesopelagic)?
    - POC = $\boldsymbol{f(b_{bp})}$ vs. POC = $\boldsymbol{f(b_{bp}, composition)}$

Objectives

1. Develop a more sophisticated model for the in situ determination of POC using a global database of surface and subsurface measurements
2. Apply new model to BGC-Argo data

Dataset

- Global dataset of over 400 surface and subsurface samples from Arctic, Atlantic, Pacific, and Southern Oceans
- Spectral b_{bp} measured in situ with HydroScat instruments, generally 6–11 wavelengths ~400–800 nm
- POC determined with 25 mm diameter GF/Fs
- TChla from HPLC analysis (also 25 mm GF/Fs)

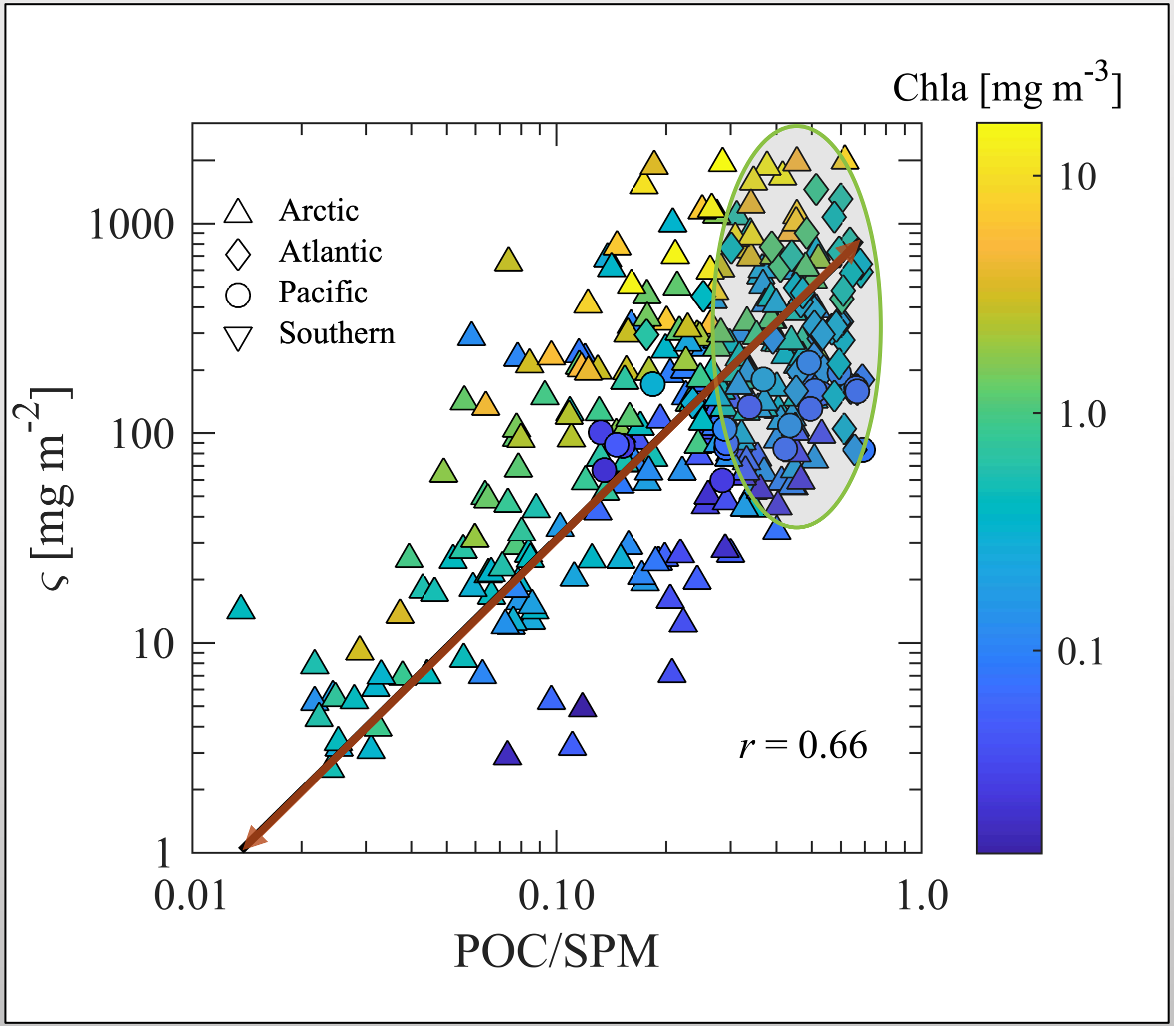


Dataset

Ocean	Sub-Location	Cruise(s)	Year(s)	Depth [–m] range	$b_{bp}(550)$ [m^{-1}] range; median(iqr)	POC [mg m^{-3}] range; median(iqr)	Chla [mg m^{-3}] range; median(iqr)	ς [mg m^{-2}] range; median(iqr)	POC/SPM [g g^{-1}] range; median(iqr)	N
Arctic	Chuckchi/Beafort	HLY1001 HLY1101	2010 2011	1–150	0.0004–0.038; 0.004(0.010)	16–816; 138(139)	0.01–17; 0.56(2.6)	5–1988; 146(245)	0.01–0.6; 0.28(0.25)	128
	SE Beaufort	MALINA	2009	1–80	0.0003–0.34; 0.0006(0.027)	11–493; 32(57)	0.02–3.3; 0.09(0.22)	3–1101; 103(160)	0.03–0.4; 0.22(0.13)	81
	Chuckchi/Beafort	MR17-05C	2017	1–300	0.0005–0.20; 0.0030(0.014)	23–789; 129(110)	0.02–11; 0.42(0.82)	3–869; 221(319)	0.02–0.5; 0.32(0.32)	46
	S Beaufort	PB18 PB19	2018 2019	1–17	0.0018–0.22; 0.047(0.067)	70–388; 181(93)	0.1–1.9; 0.45(0.44)	3–76; 13(15)	0.02–0.3; 0.04(0.04)	23
	All Arctic	All Arctic	2009–2019	1–300	0.0003–0.34; 0.0034(0.012)	11–816; 117(152)	0.01–16; 0.39(1.0)	3–1988; 120(228)	0.01–0.6; 0.25(0.23)	278
Atlantic	Meridional	ANTXXIII1/1 ANTXXVI/4	2005 2010	1–140	0.0004–0.0028; 0.0008(0.0005)	20–265; 49(26)	0.09–1.5; 0.28(0.27)	77–1702; 318(341)	0.18–0.7; 0.54(0.15)	90
Pacific	SE Pacific Central Pacific	BIOSOPE KM12-10	2004 2012	1	0.0003–0.0034; 0.0008(0.0005)	12–267; 38(28)	0.02–1.5; 0.08(0.12)	58–523; 121(108)	0.13–0.7; 0.37(0.26)	42
Southern	Southern Ocean	NBP97-8 REV98 01/02	1997 1998	1	0.0003–0.0096; 0.0017(0.0017)	27–822; 131(164)	0.12–9.6; 0.81(1.1)	93–1970; 530(1279)	-	17
ALL	**ALL**	**ALL**	**1997–2019**	**1–300**	**0.0003–0.34; 0.0018(0.0058)**	**11–822; 81(120)**	**0.01–17; 0.31(0.70)**	**3–1988; 165(264)**	**0.01–0.7; 0.28(0.27)**	**427**

Composition parameter ς

- $\varsigma = \frac{1}{b_{bp}^{*C}} = \frac{Chla}{b_{bp}}$
- Inverse of chlorophyll-a specific particulate backscattering coefficient
- Can be easily measured in situ
- Represents bulk changes in organic vs. inorganic – *n*
- Can represent changes in phytoplankton composition (e.g., pico vs. micro, phytoplankton vs. detritus) – *n*, *n'*, *ξ*, shape

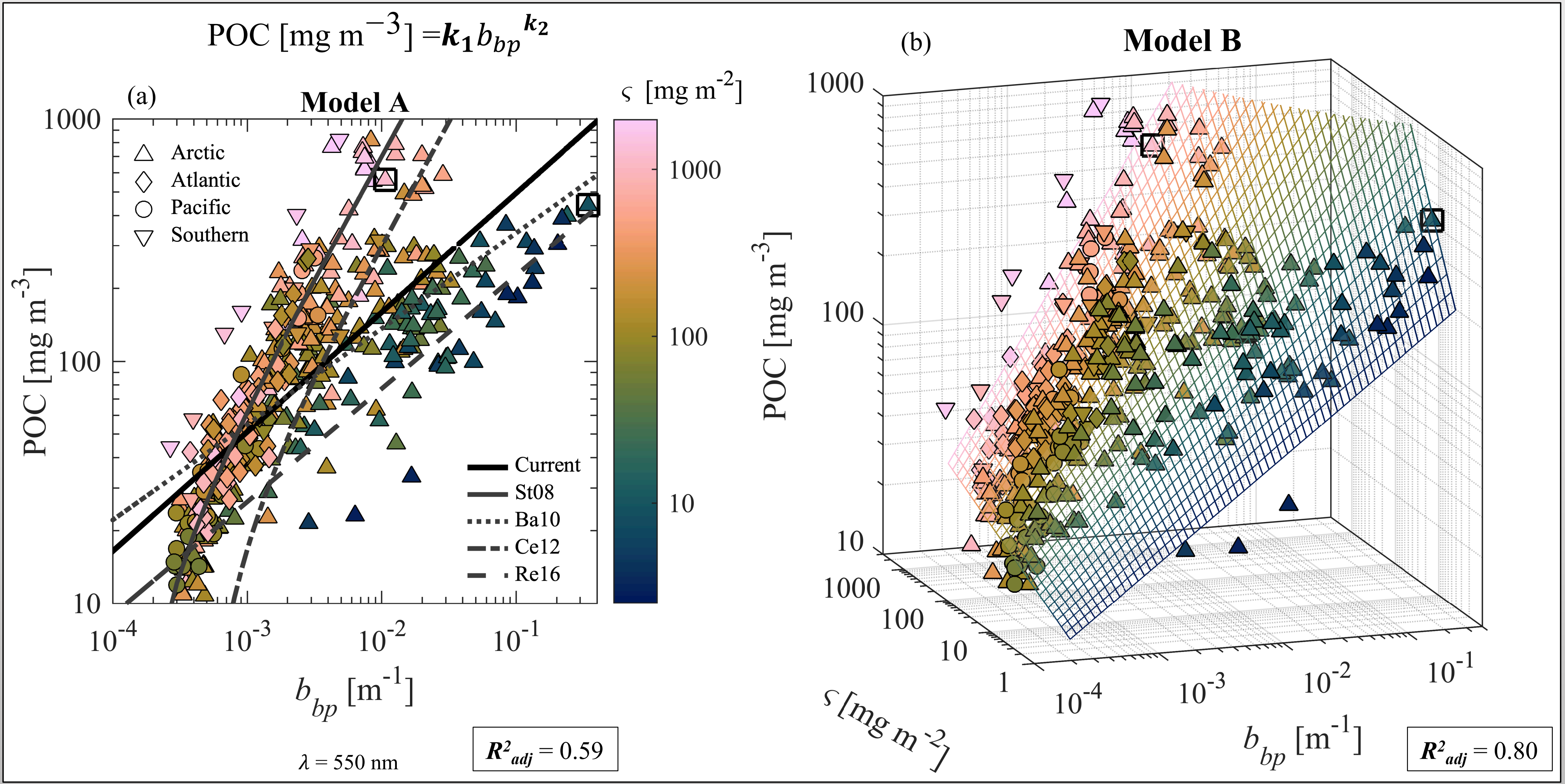


Model development

$$\mathrm{POC} = b_{bp} + \varsigma$$

$$\mathrm{POC} = b_{bp} + \varsigma \times b_{bp}$$

$$\mathrm{POC}\ [\mathrm{mg\ m^{-3}}] = \boldsymbol{k_1} b_{bp}^{\boldsymbol{k_2}} \varsigma^{\boldsymbol{k_3}} \varsigma^{\boldsymbol{k_4} \log b_{bp}}$$



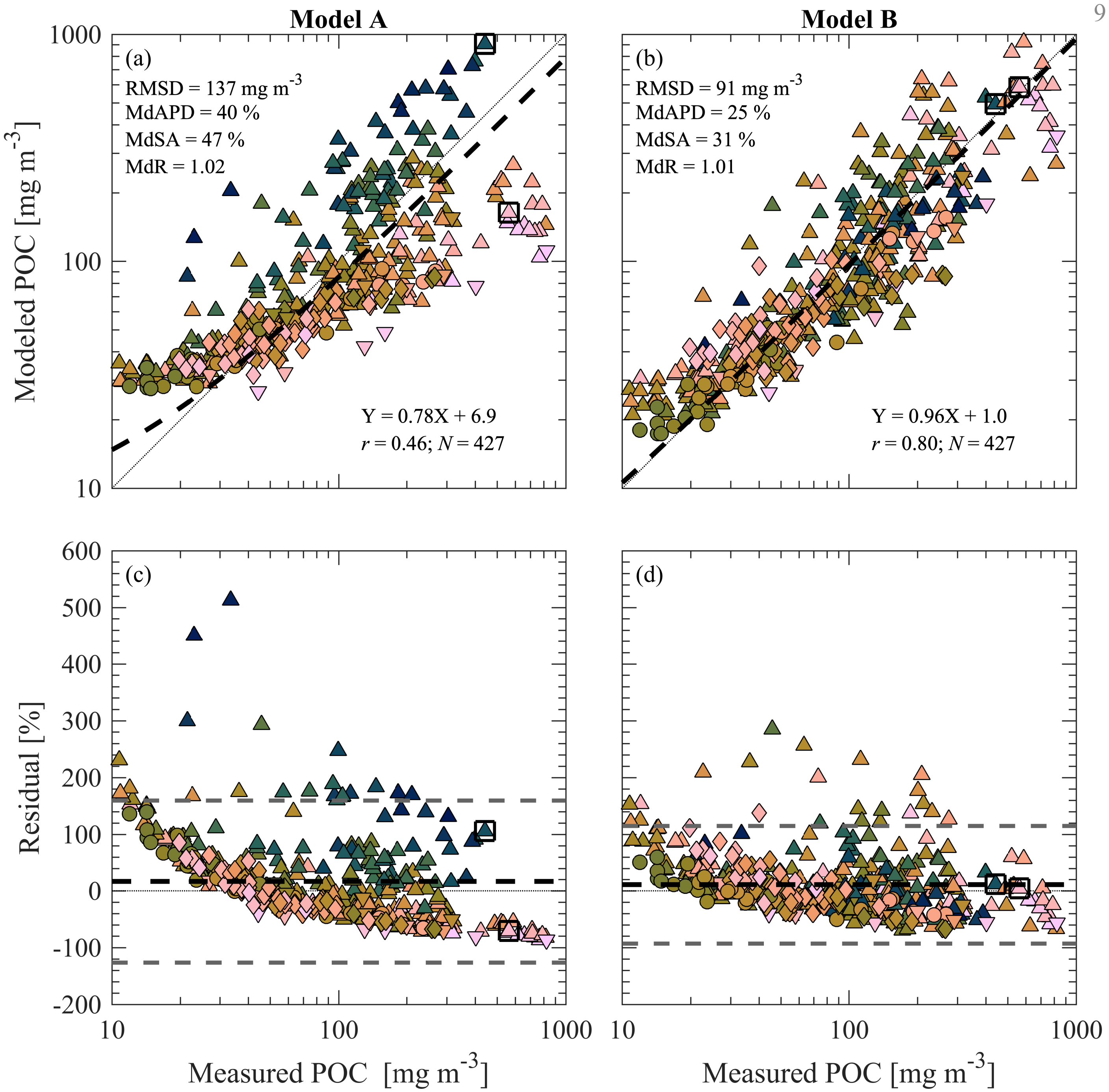
Validation

Model A: POC [mg m^{-3}] $= \boldsymbol{k_1} b_{bp}^{\boldsymbol{k_2}}$

Model B: POC [mg m^{-3}] $= \boldsymbol{k_1} b_{bp}^{\boldsymbol{k_2}} \varsigma^{\boldsymbol{k_3}} \varsigma^{\boldsymbol{k_4} \log b_{bp}}$

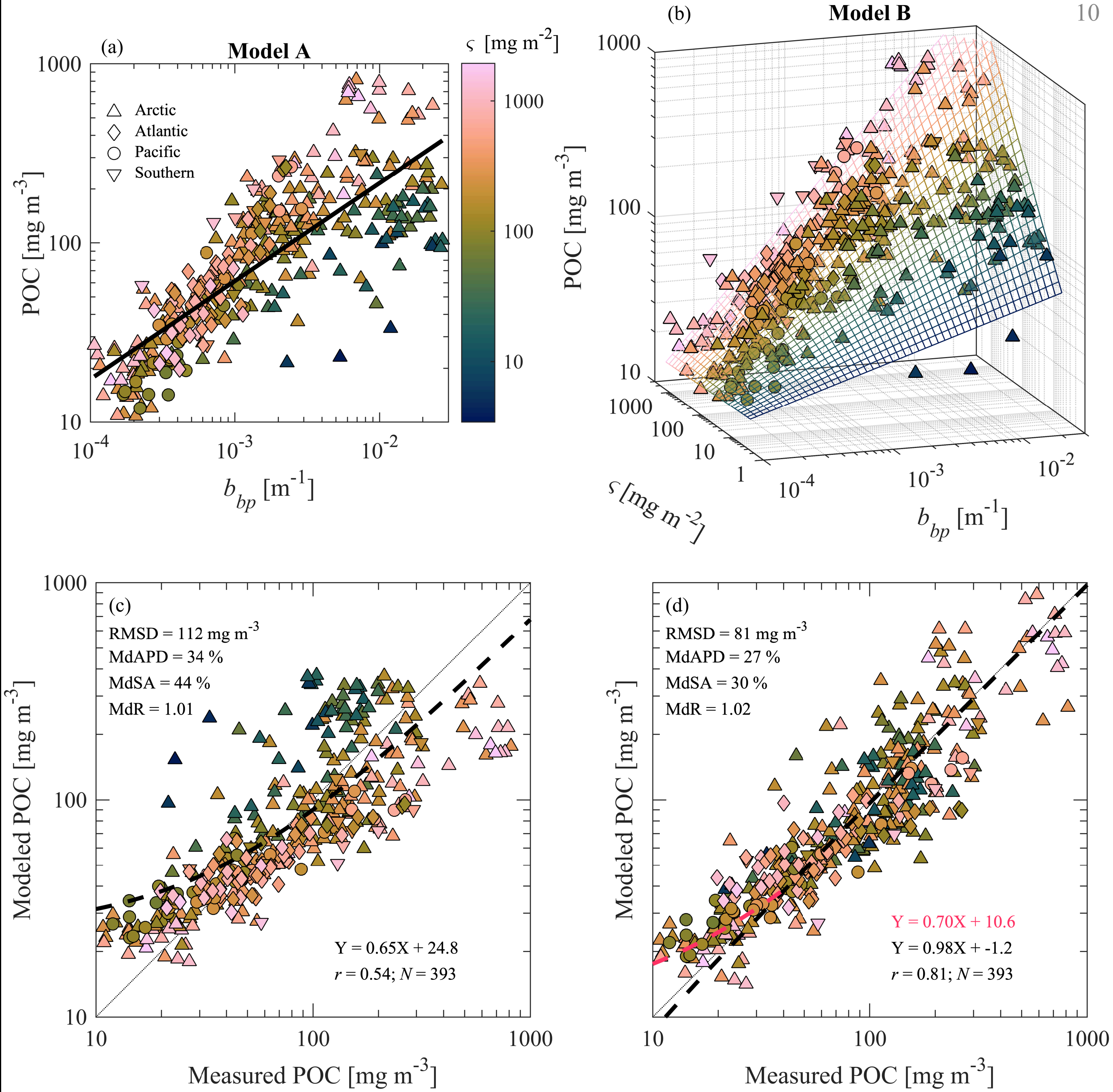
Model-assessment variables	
N	Number of samples
x_i or y_i	Measured value for sample i of N
x or y	Mean value; $x = \frac{1}{N}\sum_{i=1}^{N} x_i$, and likewise for y
O_i or P_i	Observed or model-predicted value for sample i of N
r	Pearson correlation coefficient; $\frac{\sum_{i=1}^{N}(x_i - x)(y_i - y)}{\sqrt{\sum_{i=1}^{N}(x_i - x)^2}\sqrt{\sum_{i=1}^{N}(y_i - y)^2}}$
Md	Median operator
RMSD	Root mean square deviation; $\sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2}$
MdAPD	Median absolute percent difference; $Md\left\|\frac{P_i - O_i}{O_i}\right\| \times 100\%$
MdSA	Median symmetric accuracy; $\left(10^{Md\left\|\log_{10}\frac{P_i}{O_i}\right\|} - 1\right) \times 100\%$
MdR	Median ratio; $Md(\frac{P_i}{O_i})$

Model B has improvements in all statistical metrics evaluated!



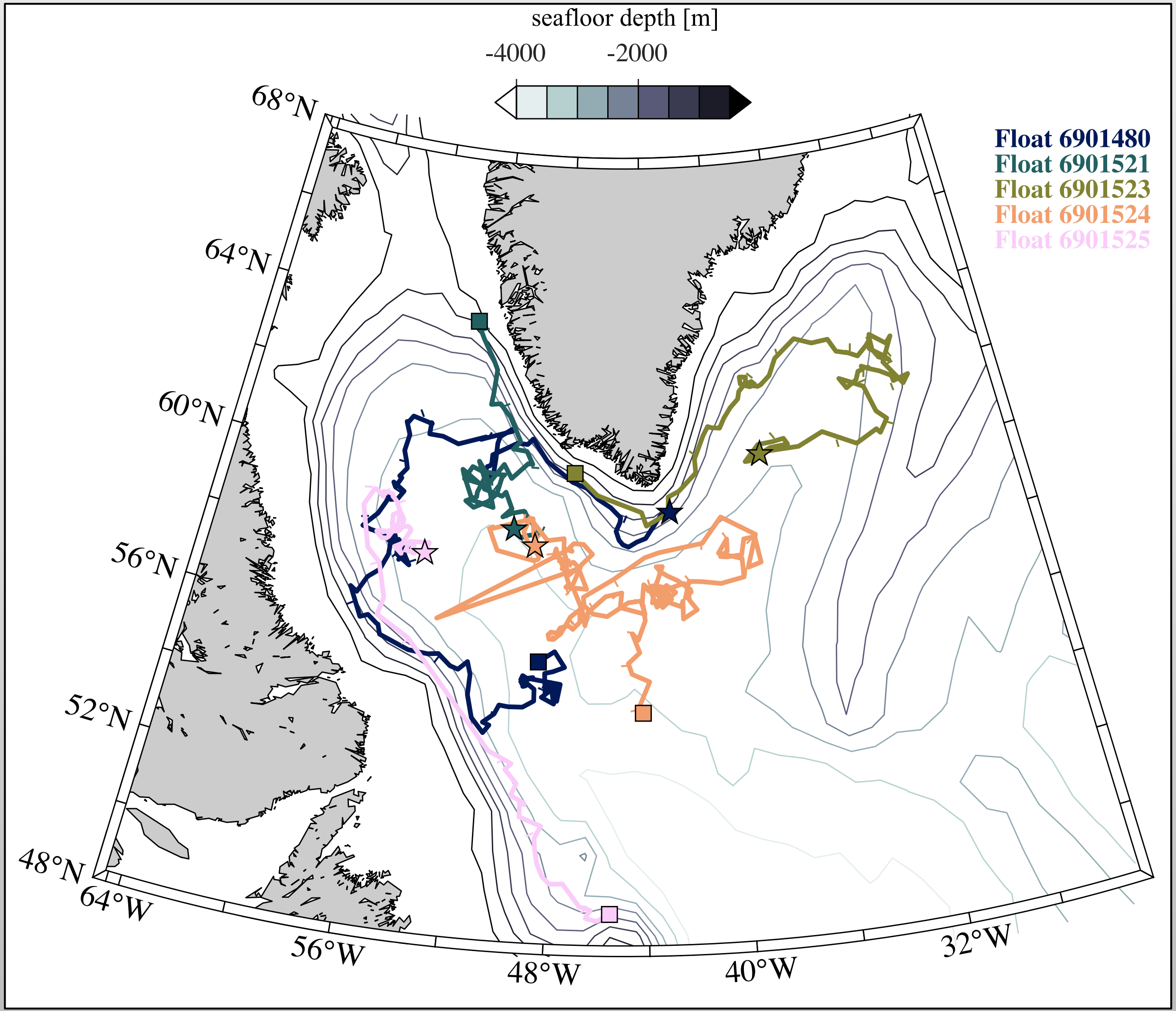
Reformulation for application to BGC-Argo

- λ = 700 nm
- Reduced range of b_{bp}
- Bias term for low modeled POC
    - Consequential for mesopelagic POC



Application to BGC-Argo floats deployed in Labrador Sea (LAS)

- Excellent QC'ed dataset provided by Barbieux, Organelli, Claustre and others
- Over 500 vertical profiles of b_{bp}, Chla F, PAR, and temp/sal from about May 2013 to December 2015.
- Applied our global models to derive vertical profiles of POC
  - Focus analysis on multivariable Model B

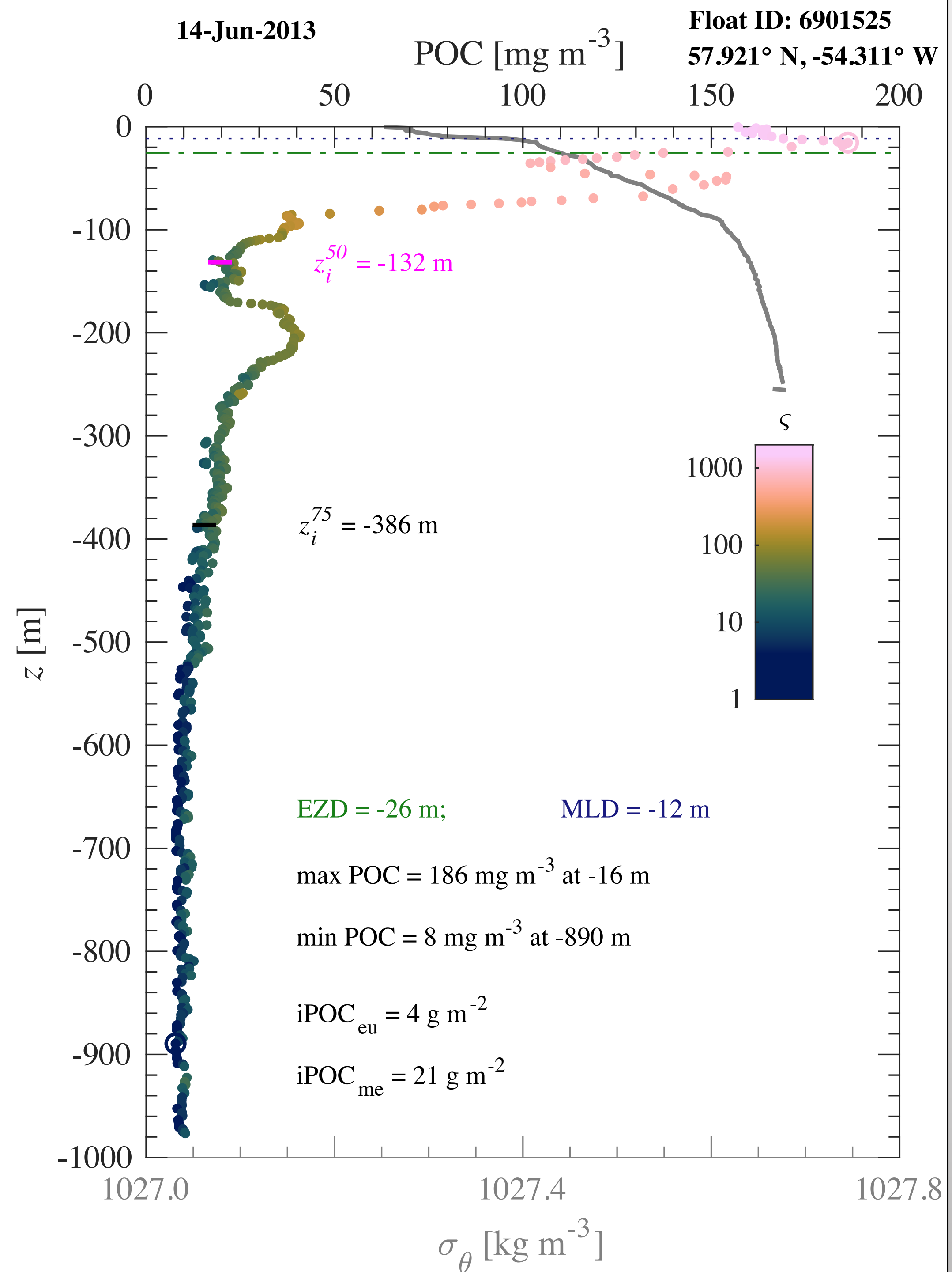


Barbieux, M., Organelli, E., Claustre, H., Schmechtig, C., Poteau, A., Boss, E., Bricaud, A., Briggs, N., Dall'Olmo, G., D'Ortenzio, F., Prieur, L., Roesler, C., Uitz, J., Xing, X. (2017). A global database of vertical profiles derived from Biogeochemical Argo float measurements for biogeochemical and bio-optical applications. SEANOE. https://doi.org/10.17882/49388

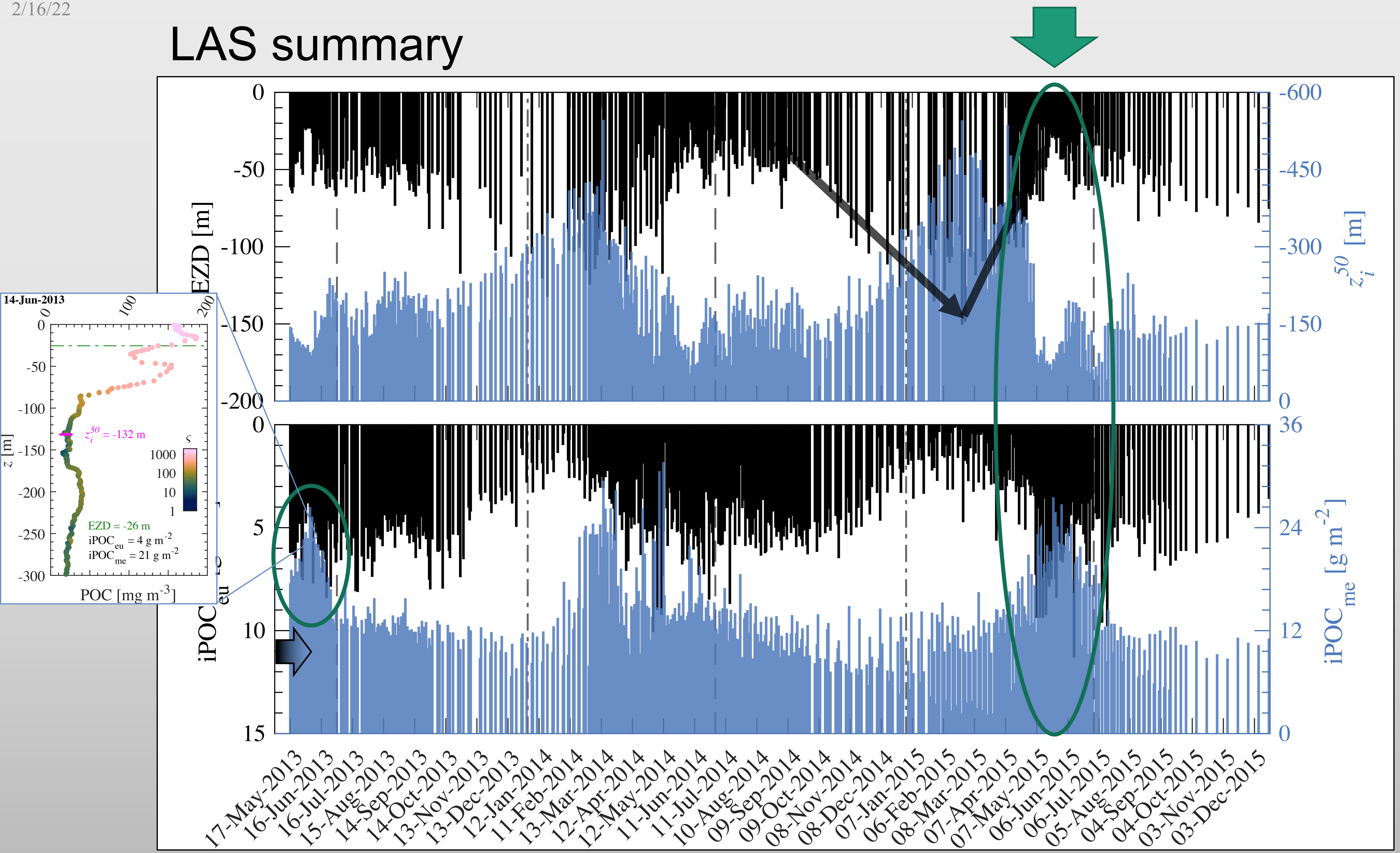
Organelli, E., Barbieux, M., Claustre, H., Schmechtig, C., Poteau, A., Bricaud, A., Boss, E., Briggs, N., Dall'Olmo, G., D'Ortenzio, F., Leymarie, E., Mangin, A., Obolensky, G., Penkerc'h, C., Prieur, L., Roesler, C., Serra, R., Uitz, J., and Xing, X. (2017) Two databases derived from BGC-Argo float measurements for marine biogeochemical and bio-optical applications, Earth Syst. Sci. Data, 9, 861–880, https://doi.org/10.5194/essd-9-861-2017

Example profile and parameters

- $\mathrm{PAR}(\mathbf{EZD}) = \frac{\mathrm{PAR}(0^{-})}{100}$
- $\mathrm{iPOC_{eu}} = \int_{z=1}^{z=\mathbf{EZD}} \mathrm{POC}\, dz$
- $\mathrm{iPOC_{me}} = \int_{z=\mathbf{EZD}}^{z=1000} \mathrm{POC}\, dz$
- $\frac{X}{100} = \frac{\int_{z=1}^{z=z_i^X} \mathrm{POC}\, dz}{\int_{z=1}^{z=1000} \mathrm{POC}\, dz}$



LAS summary



14-Jun-2013
POC [mg m-3]
z [m]
z_i^{50} = -132 m
EZD = -26 m
iPOC$_{eu}$ = 4 g m^{-2}
iPOC$_{me}$ = 21 g m^{-2}
1000
100
10
1
EZD [m]
z_i^{50} [m]
iPOC$_{eu}$
iPOC$_{me}$ [g m^{-2}]
17-May-2013
16-Jun-2013
16-Jul-2013
15-Aug-2013
14-Sep-2013
14-Oct-2013
13-Nov-2013
13-Dec-2013
12-Jan-2014
11-Feb-2014
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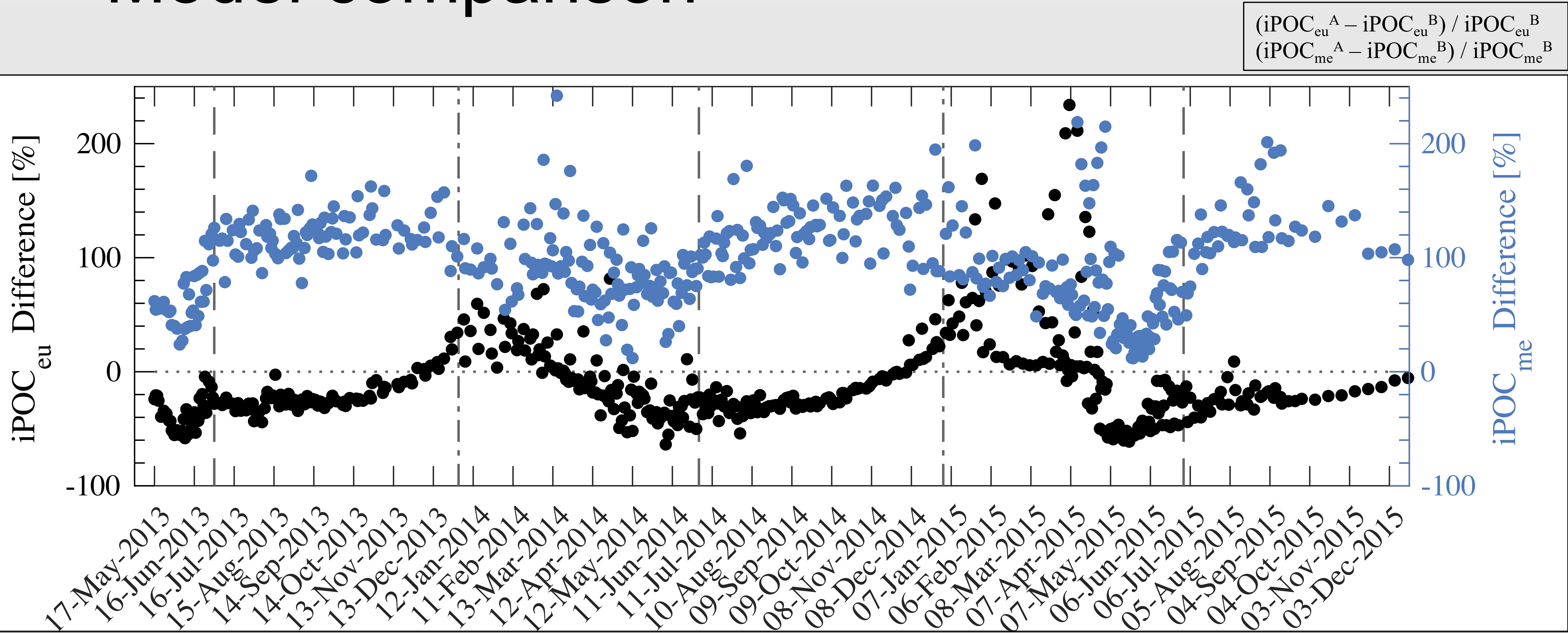
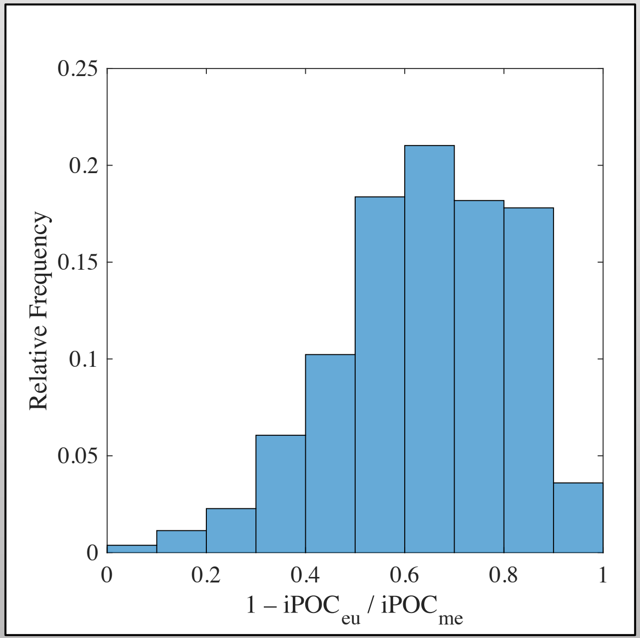
04-Oct-2015
03-Nov-2015
03-Dec-2015

Model comparison



Summary

- A multivariable model to estimate POC from optics is more effective than a univariate model for a global dataset of contrasting surface and subsurface water samples
  - Errors less than 30% and minimal bias
  - Model has been specially formulated for use with BGC-Argo
- We observe notable increase in $iPOC_{me}$ during late spring in LAS, sometimes time-delayed from increases in $iPOC_{eu}$ (evidence of vertical transport)
- Mesopelagic POC is a significant part (typically 50–90%) of POC within the upper 1000 m of the water column
  - $iPOC_{me}$ values generally range 5–15 g m^2 in winter months and 10–25 g m^2 in late spring/early summer



Knowledge gaps and priorities

- 1–5 year – Validation of POC estimates with independent data, especially in deep mesopelagic waters
- 1–5 year – What more can we learn from high resolution vertical profiles of POC?
  - Ways to parameterize profiles for analysis and how to understand horizontal advection
- 1–5+ year – Centralized pipeline of BGC-Argo optical data, analogous to some satellites, with QC'd data and standard processing protocols
  - Routine implementation of POC data product?
- 5–10+ year – Global network of floats, gliders, wirewalkers, and moorings with optics
- 5–10 year – Implementation/development of new "low-cost" sensors to target composition/size more explicitly on autonomous platforms
  - see Koestner et al. 2020 and 2021 in Applied Optics

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- Ocean Optics Research Lab at SIO
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  - Steve Ackleson
  - Ahmed El-Habashi
- NRC Research Associateship Program
- Cruise operators/crew/scientists
- Barbieux, Organelli, Claustre and many others working on deploying and processing data from BGC-Argos
- Workshop organizers and participants!
- Wife and cats!

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Questions?
Feedback?

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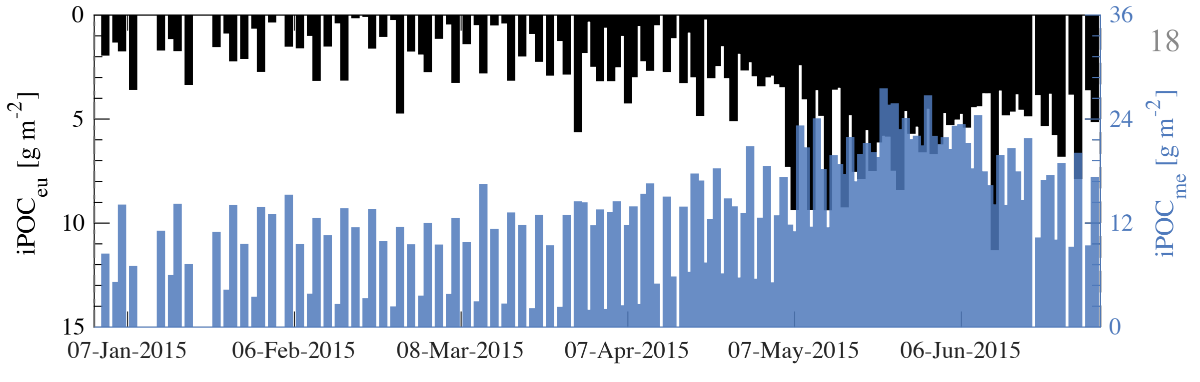
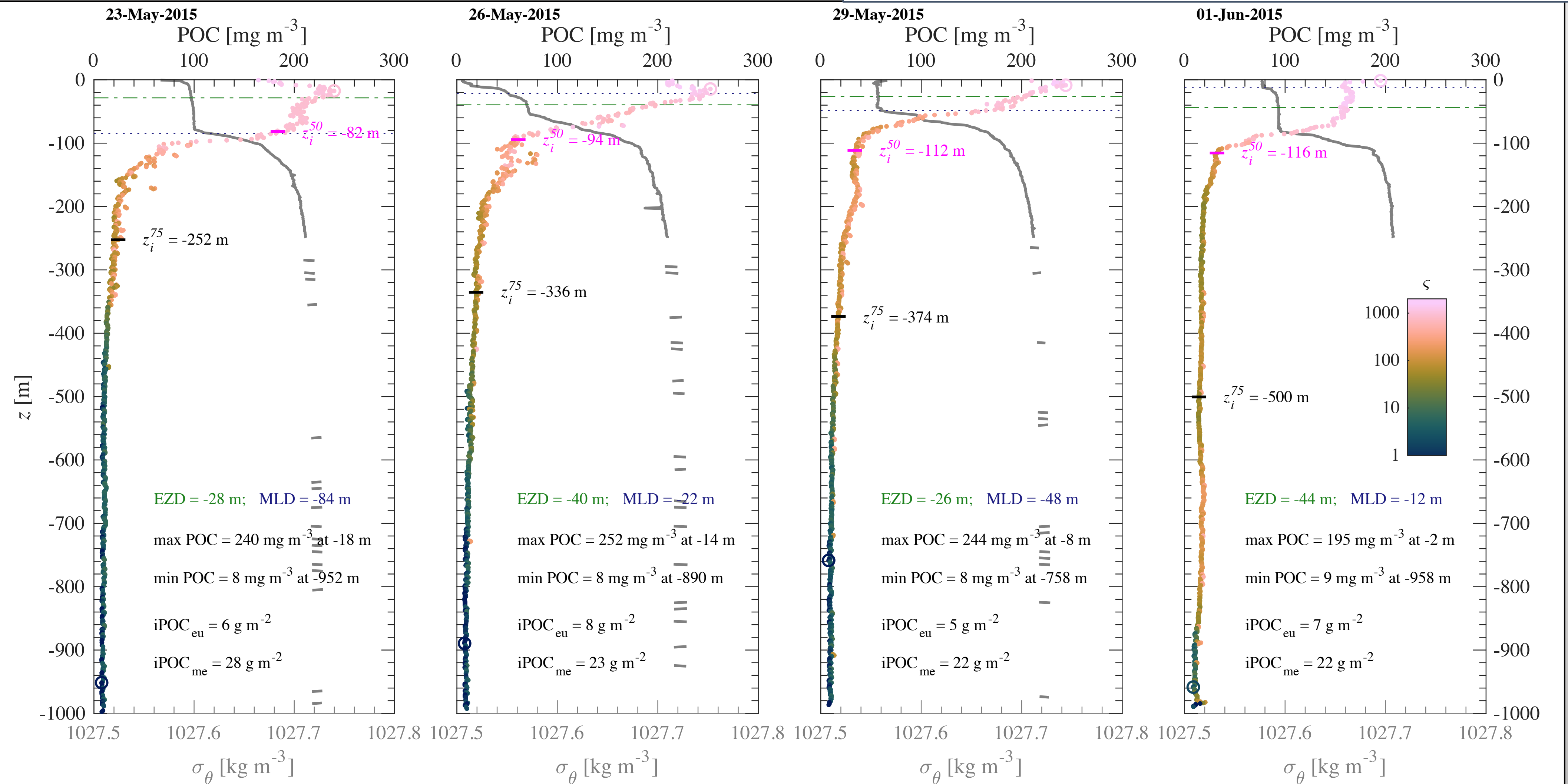
Supplemental: Example profiles May 2015





Supplemental: Uncertainty Estimates

Three sets of nonparametric box plots are presented based on data from each month, left represents lower estimates of POC based on lower 95% confidence interval of estimations, right represents upper estimates of POC based on upper 95% confidence interval of estimations, and middle represents derivations from best fit Model B coefficients.

Seasonal pattern clearly detected, May is a dynamic month for LAS!
Larger range of uncertainty for iPOCme because integrating over much larger depth