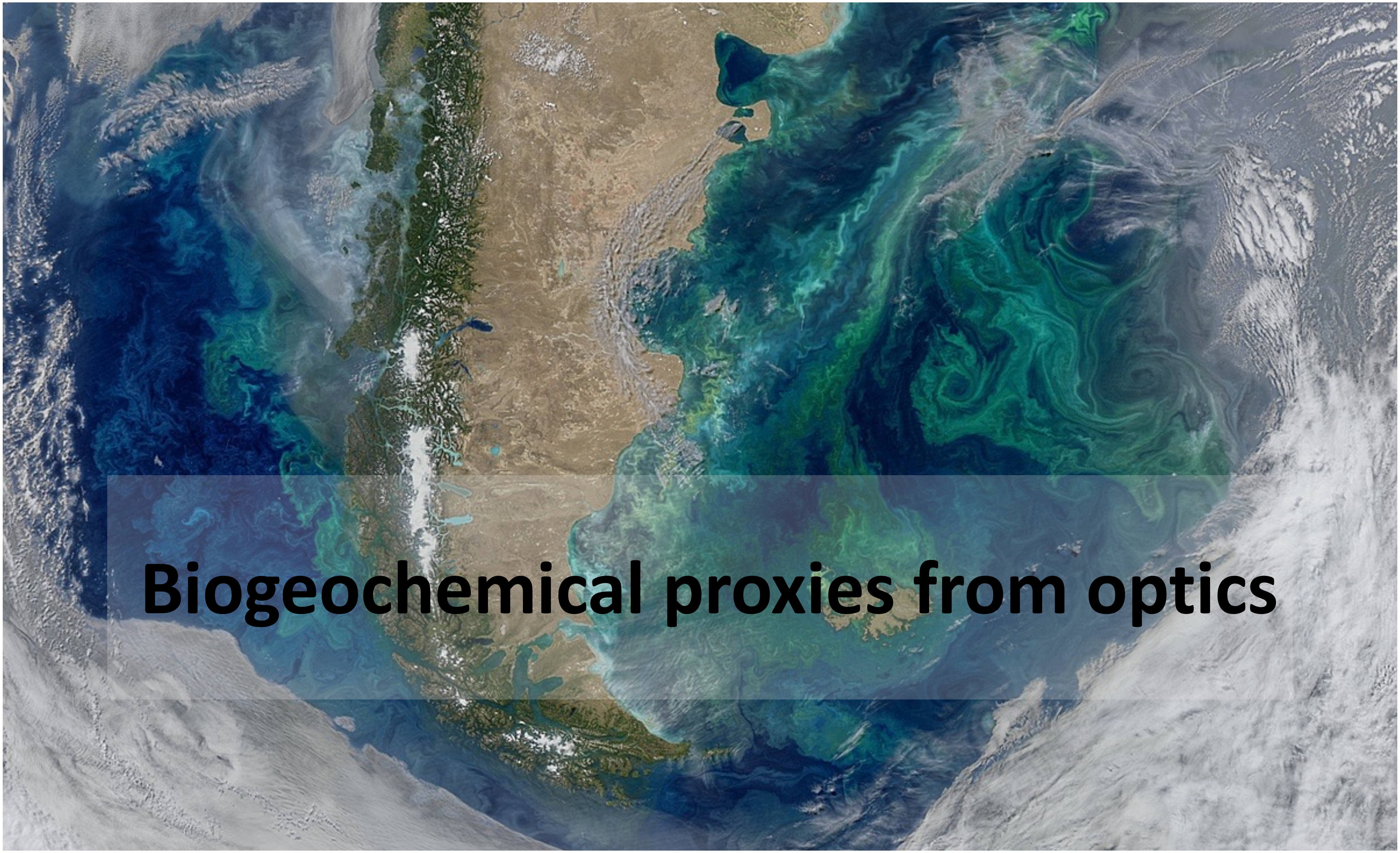
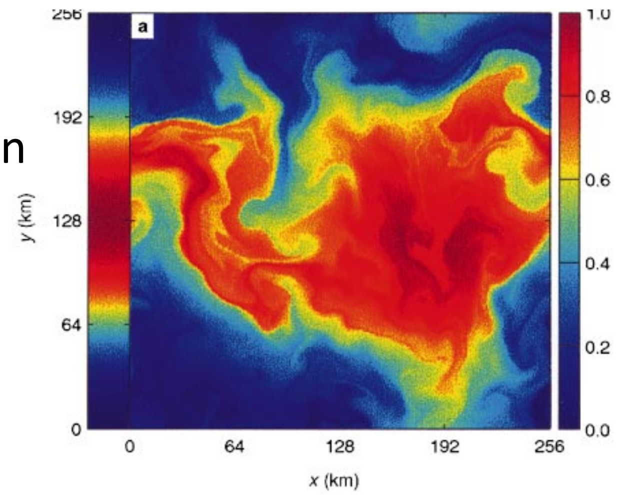


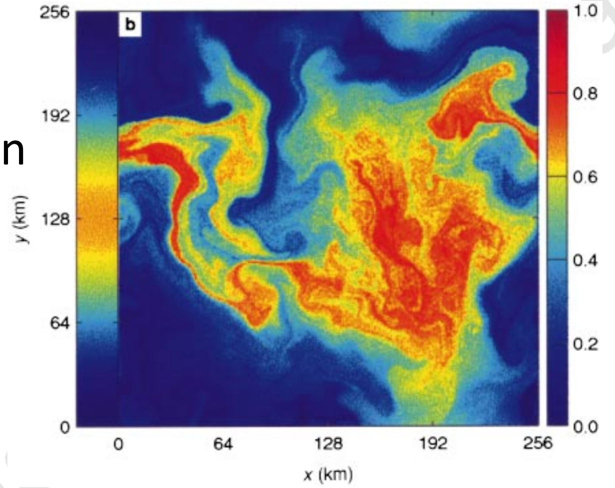
Biogeochemical proxies from optics

Meg Estapa, UMaine
Slides borrowed heavily from Ivona Cetinić, NASA GSFC

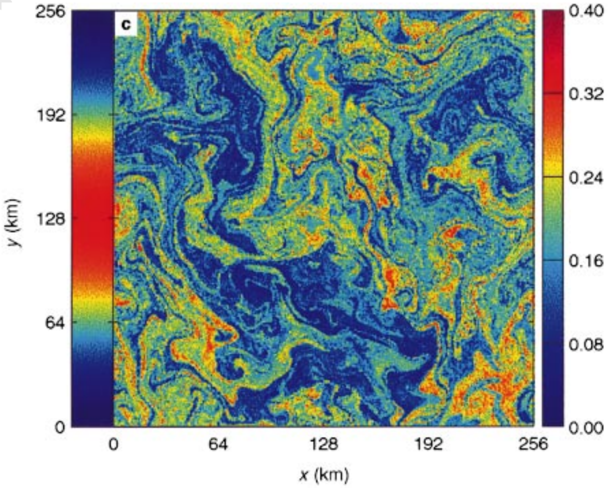
Phytoplankton
“carrying
capacity”



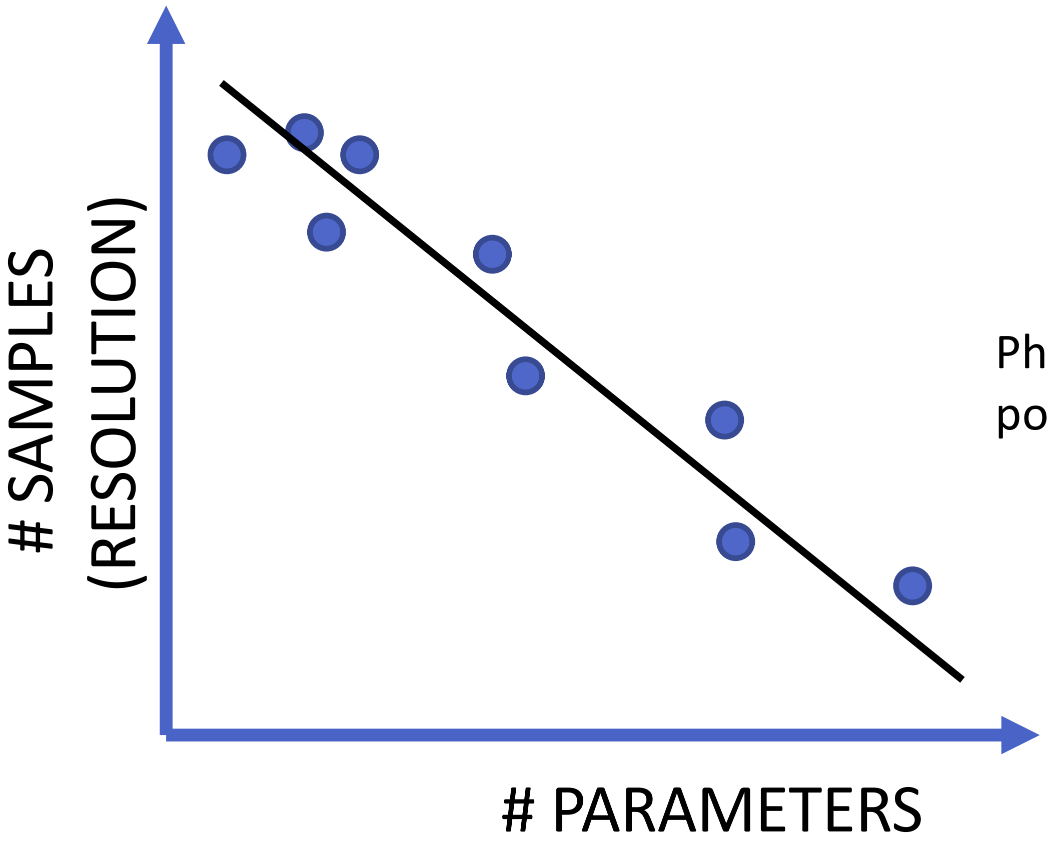
Phytoplankton
population

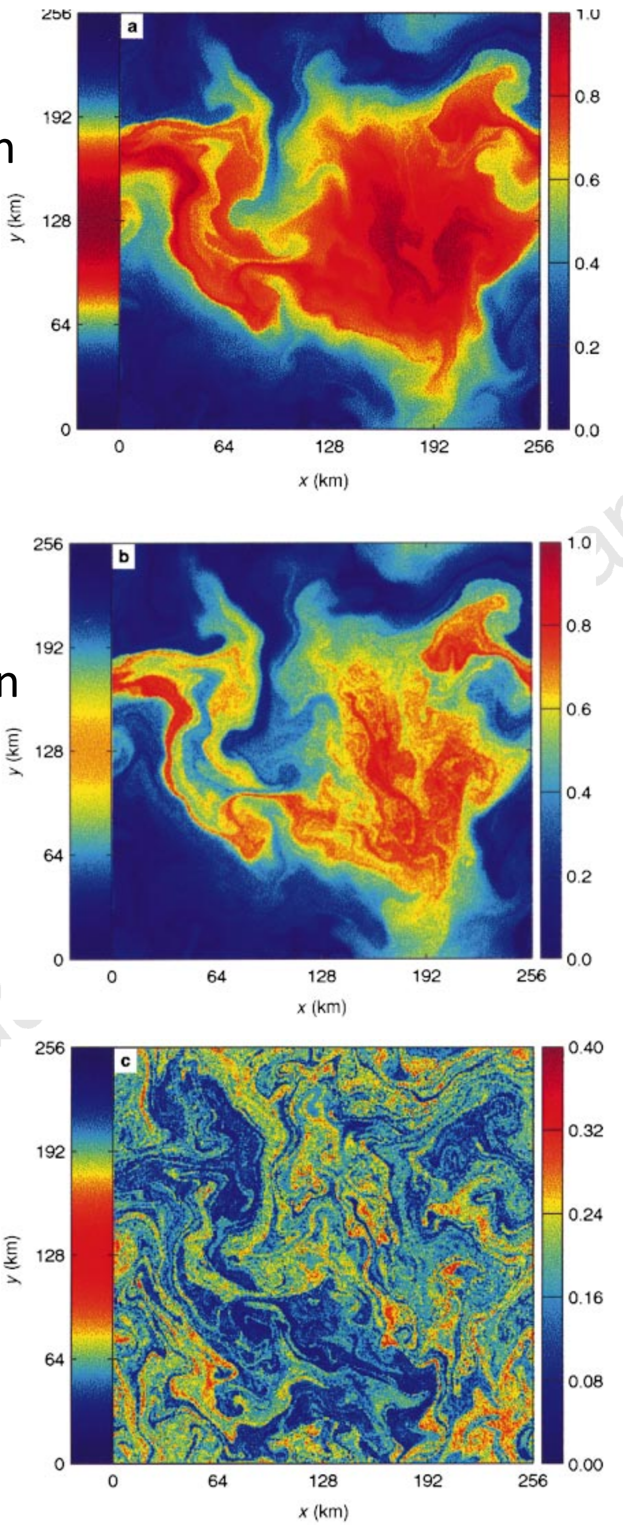


Zooplankton
population



Abraham, 1998



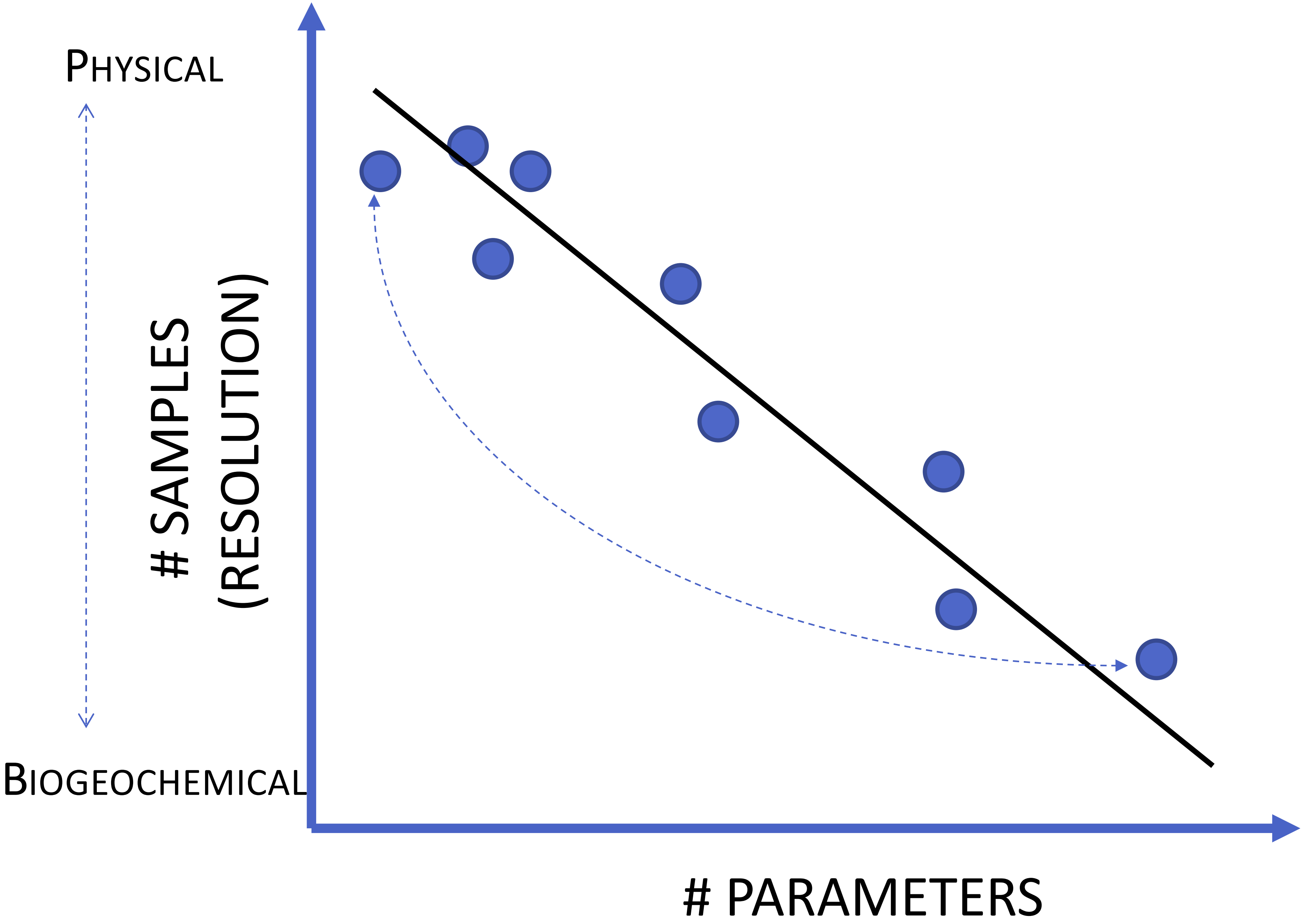


Phytoplankton “carrying capacity”

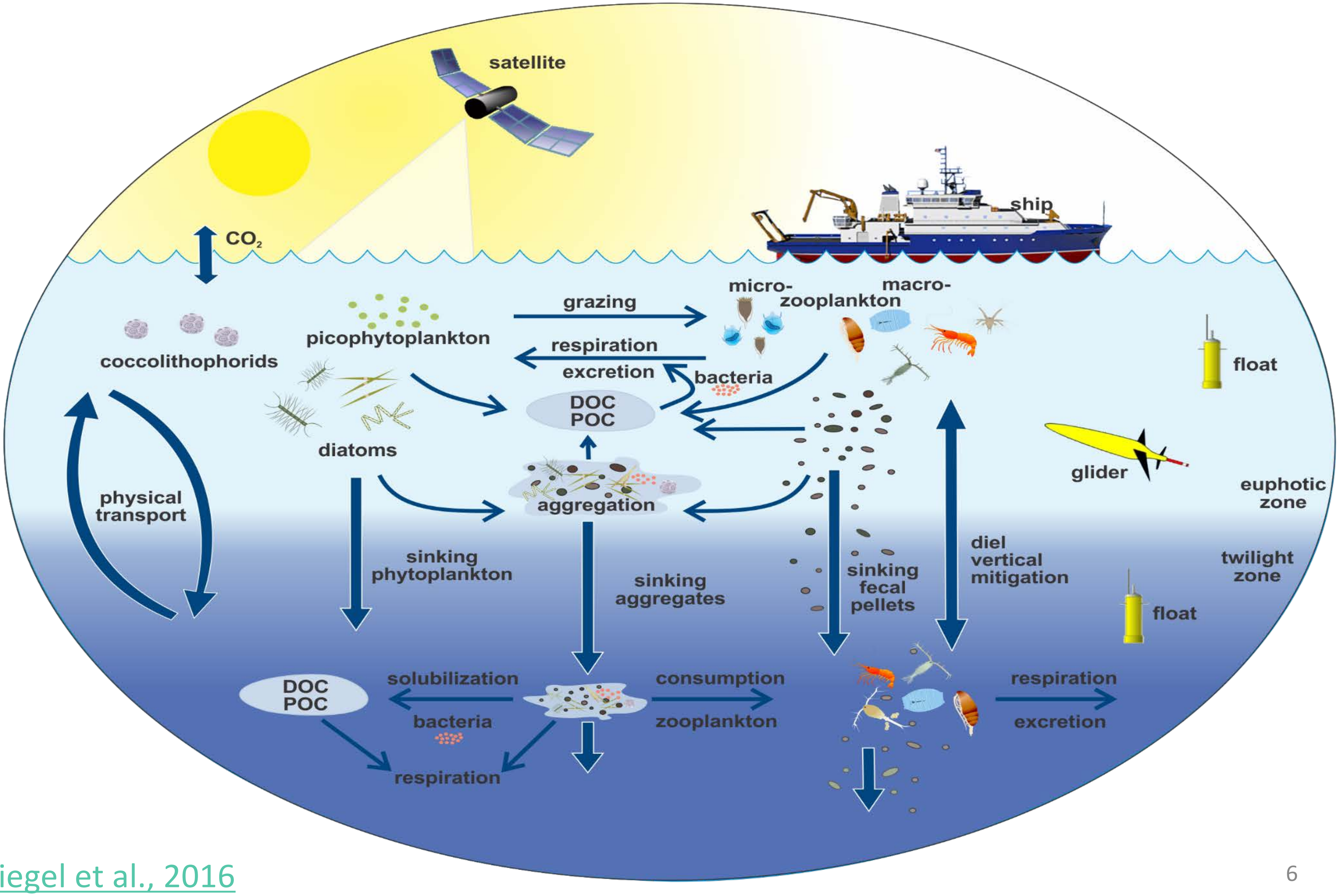
Phytoplankton population

Zooplankton population

Abraham, 1998


Physical
Biogeochemical
SAMPLES
(RESOLUTION)
PARAMETERS

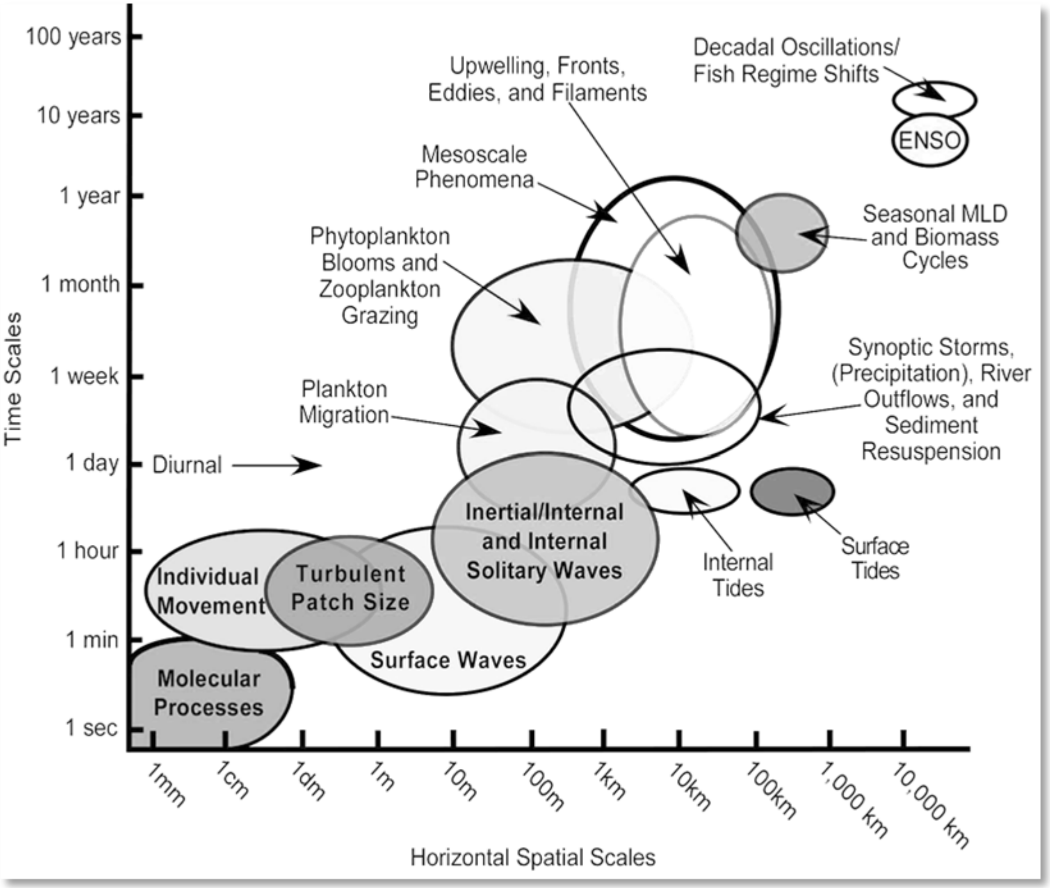
Proxies are at the heart of major sampling programs



Siegel et al., 2016

Why?

- Optics – in situ or remote sensed gives us higher resolution dataset
- Traditional methods (discrete) often expensive and time consuming
- Sampling the parameters on the scales of importance
- Validation for remote sensing and hi-res biogeochemical models (e.g. Haëntjens et al, 2017)



Chang, G. and T. Dickey (2008).

Why?

- Optics – in situ or remote sensed gives us higher resolution dataset
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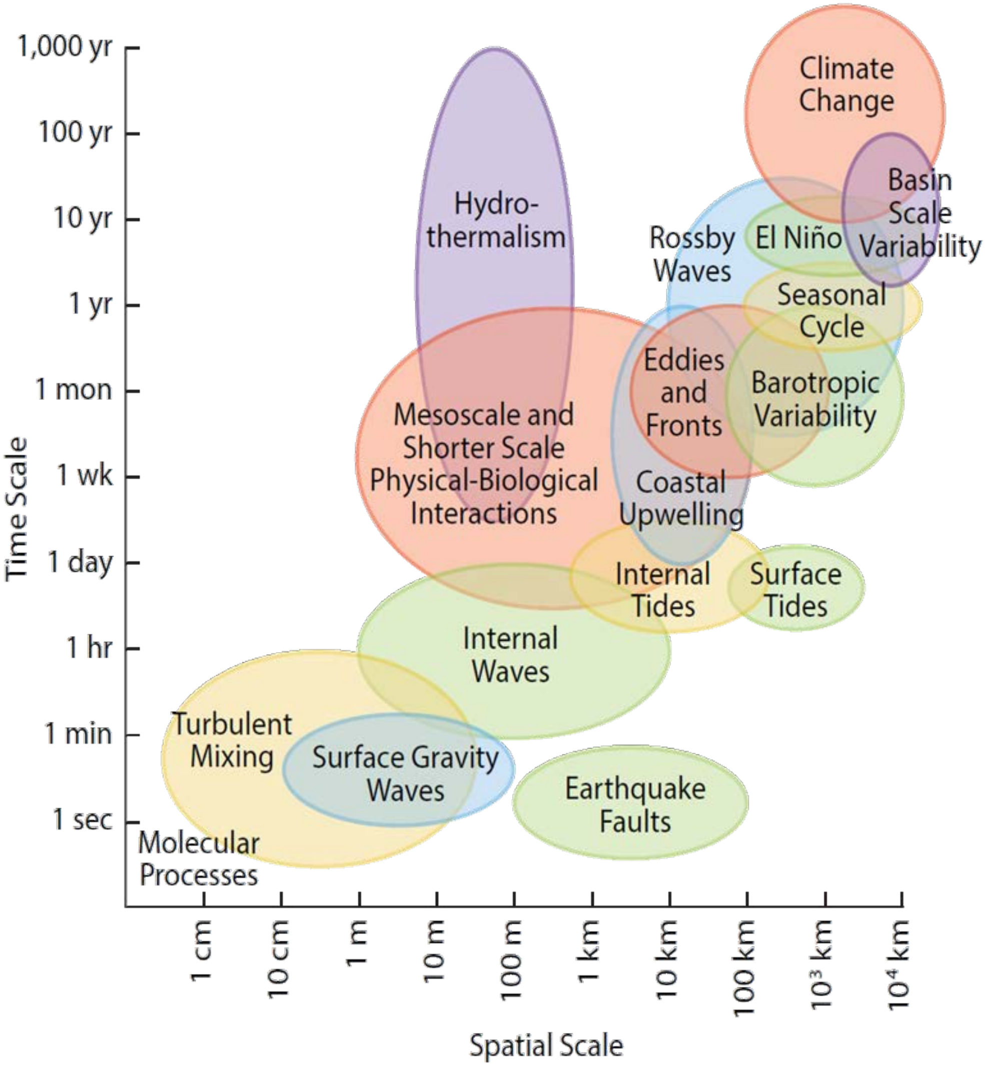


Zykov and Miller (2019).

Why?

- Optical instruments are getting smaller, more robust and diverse
- They can be deployed over extended periods of time and in hard to reach areas

What are some *in situ* optical proxies (and associated biogeochemical quality/quantity)?

Check out - Boss et al (2014) and Babin, Roesler and Cullen (2008)

Overview

- ✓ Where proxies fit, why to construct them
- Concentration proxies
  - “To first order, concentration controls IOPs”
    Emmanuel Boss, yesterday
- Composition and rate proxies
- Caveats

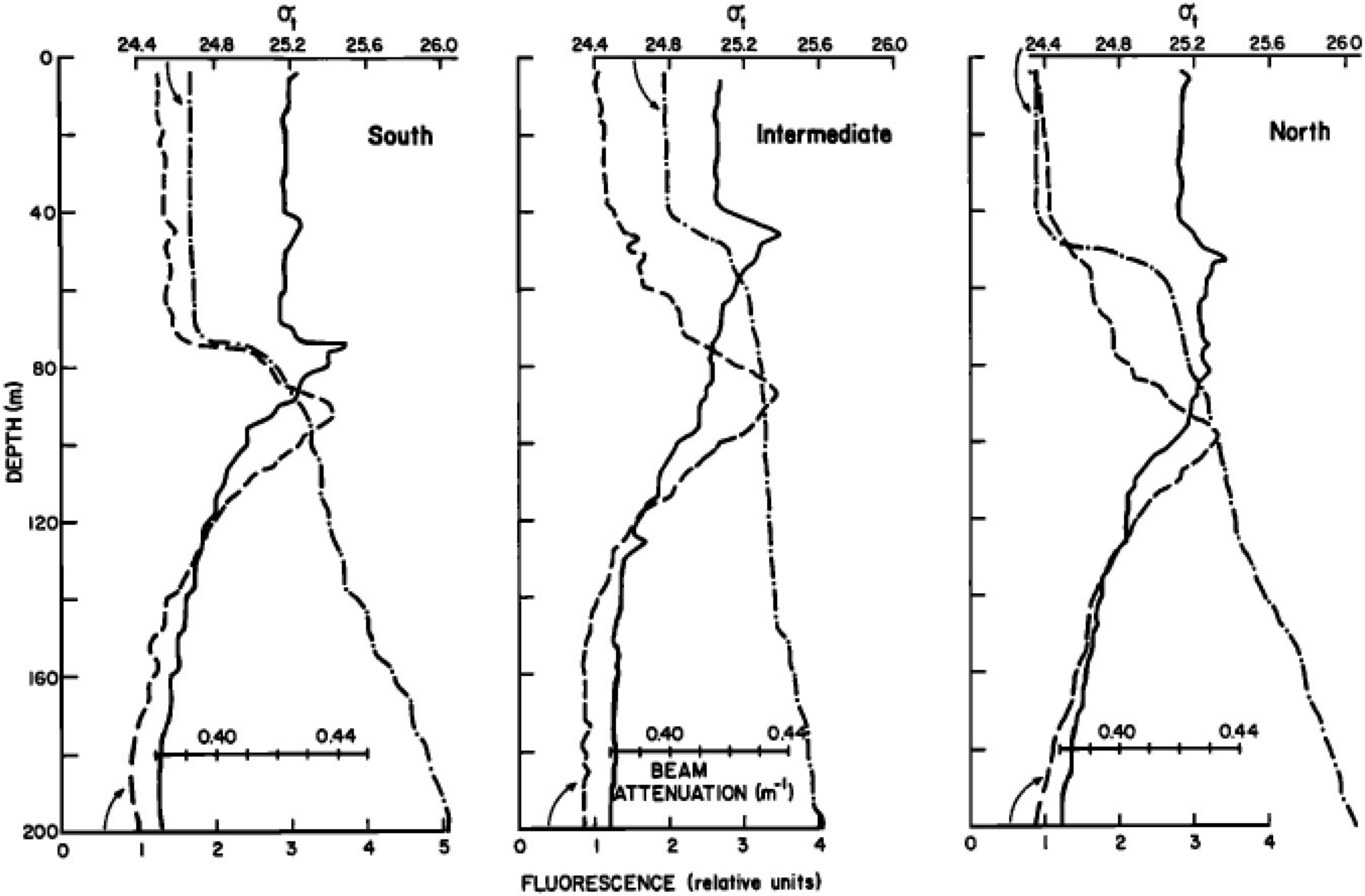
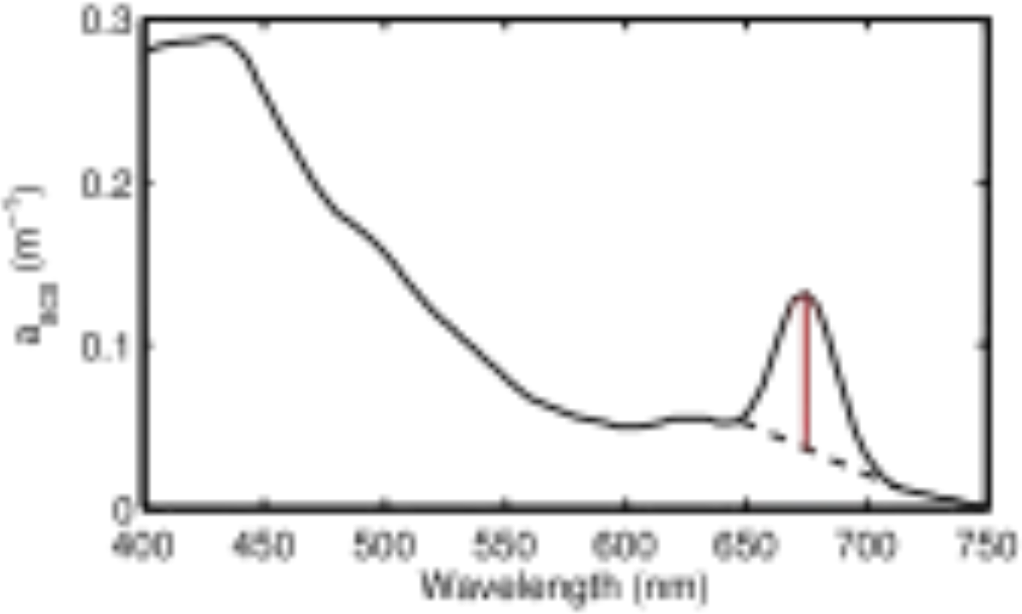
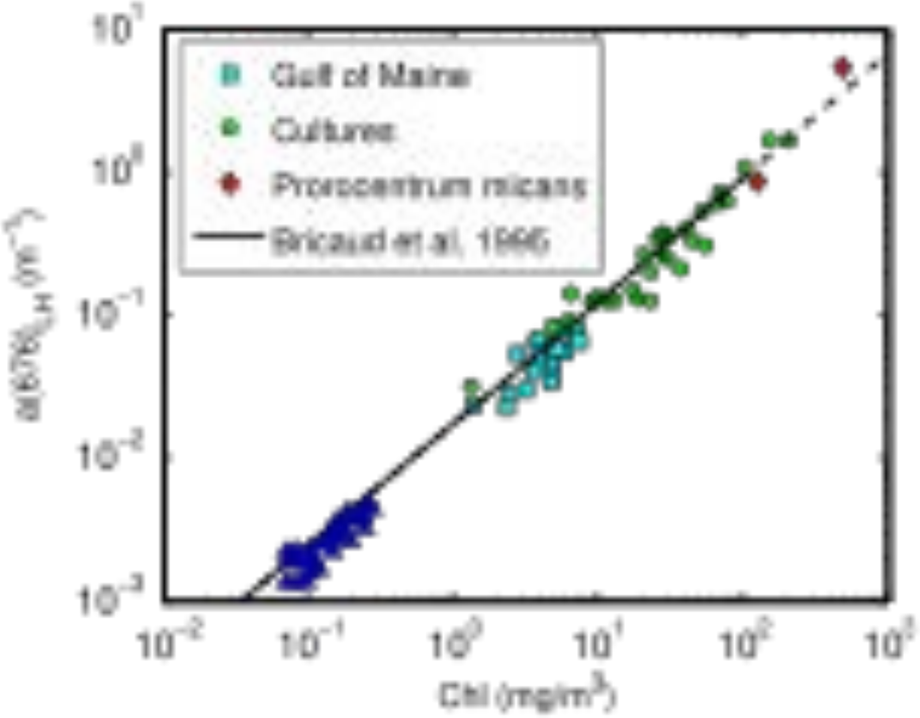


Fig. 1. Profiles of fluorescence, beam attenuation (665 nm) and σ_t for Pacific Central Gyre stations typical of waters north, south and in the Subtropical Front, Oct.-Nov., 1982.

Kitchen and Zaneveld, 1990

Absorption Line Height → Chlorophyll proxy





Roesler and Barnard, 2013

Chlorophyll from absorption band effects on beam attenuation (Housekeeper et al., 2020)

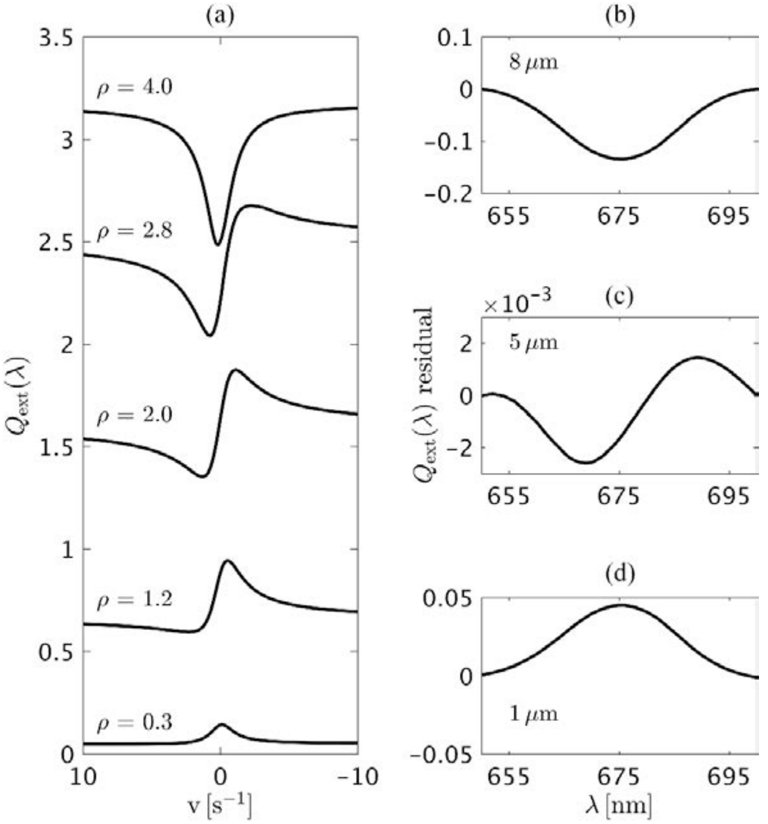
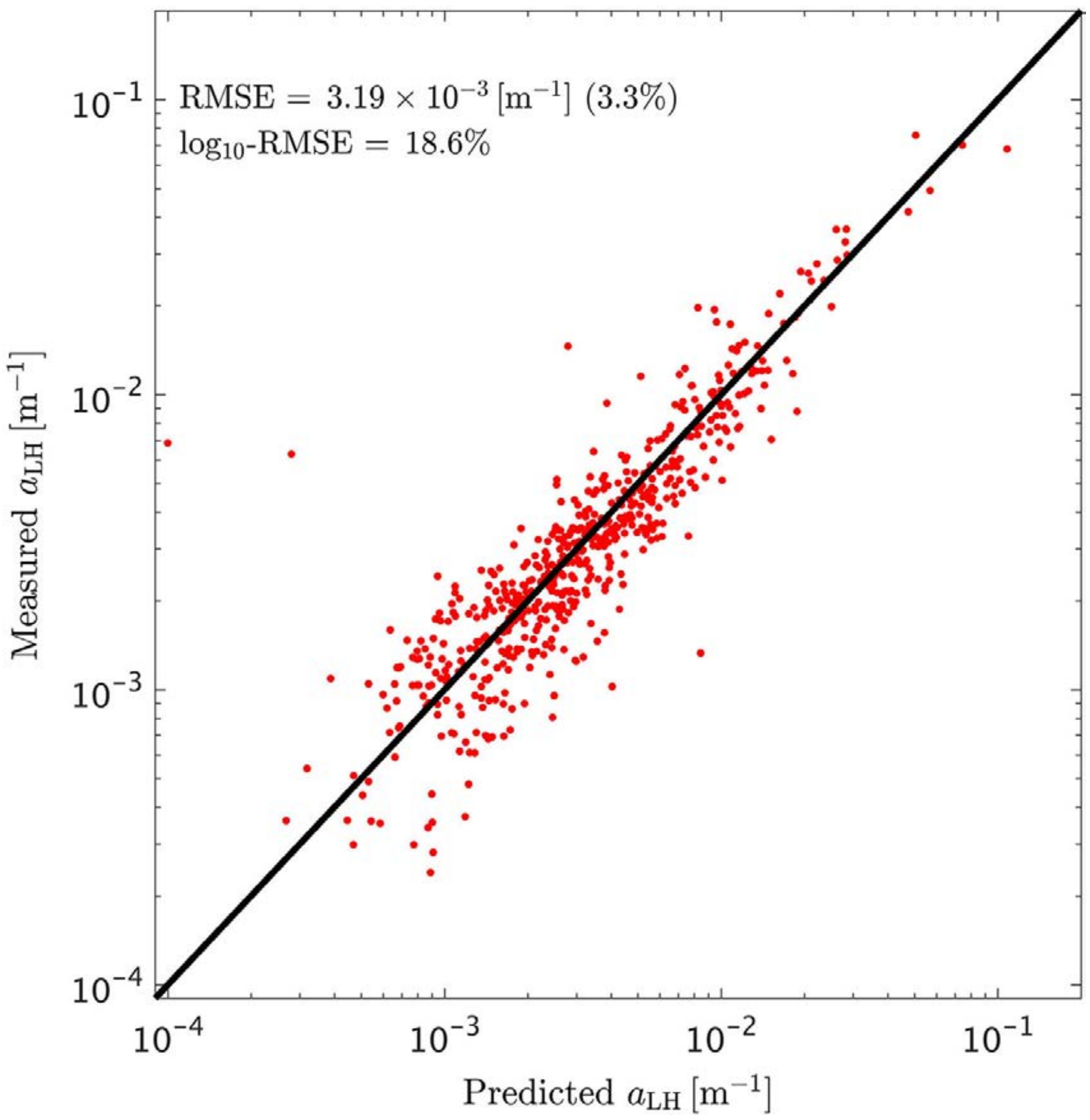
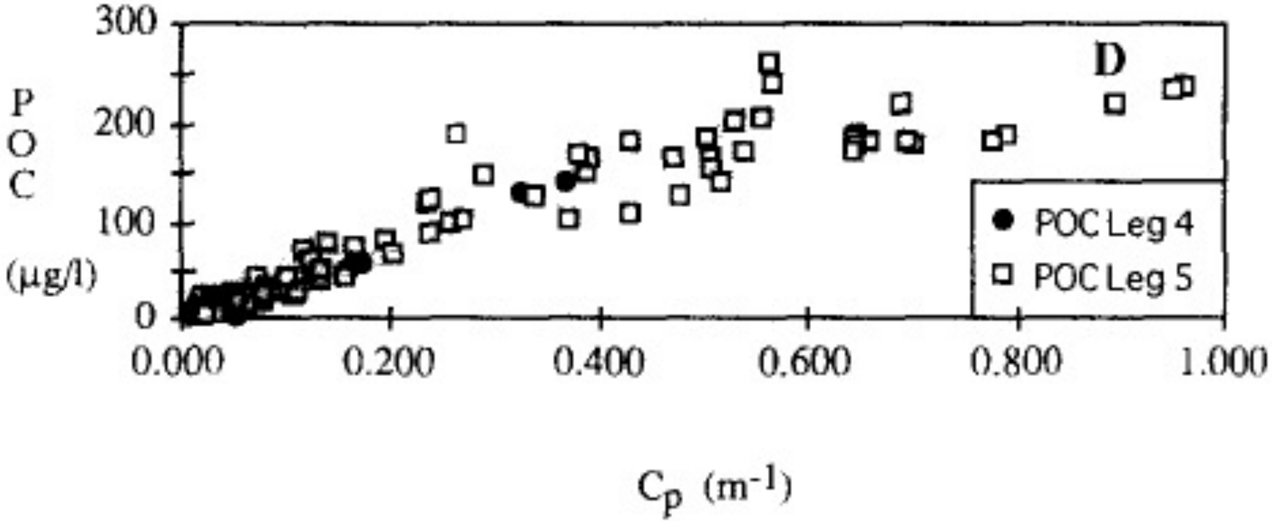


Fig. 1. (a) Anomalous diffraction approximation for $Q_{\mathrm{ext}}(\lambda)$ at a narrow absorption band as a function of light frequency for various ρ values, recreated from van de Hulst [8] using a lookup table; and (b)–(d) illustrative examples of $Q_{\mathrm{ext}}(\lambda)$ residuals for various small-sized phytoplankton (diameters 8, 5, and 1 µm, respectively), with a fixed n of 1.0344 and spectral n' with a maximum value of 0.0024 at the Chl *a* red absorption peak. The sizes presented in (b)–(d) are sensitive to the selection of real and imaginary refractive index; for example, as [14] illustrates, an anomalous dispersion curve for $Q_b(\lambda)$ using a 1 µm absorbing sphere and spectral dependencies in both n and n'.



Particulate Organic Carbon & Suspended Particulate Material proxy

- Backscattering and attenuation are associated with particle concentration / size.
- Backscattering is also highly dependent on morphology and type of the particle
- Carbon density in all oceanic particles / phytoplankton are not the same.



Gardner et al 1993

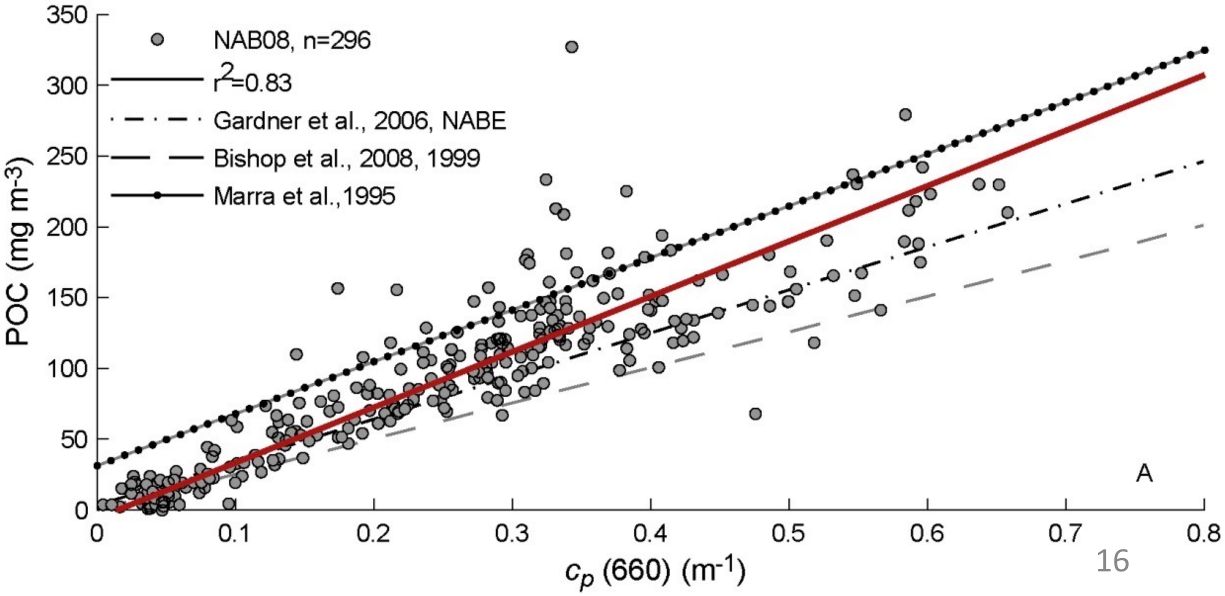
Also see:

Kitchen and Zaneveld, 1990

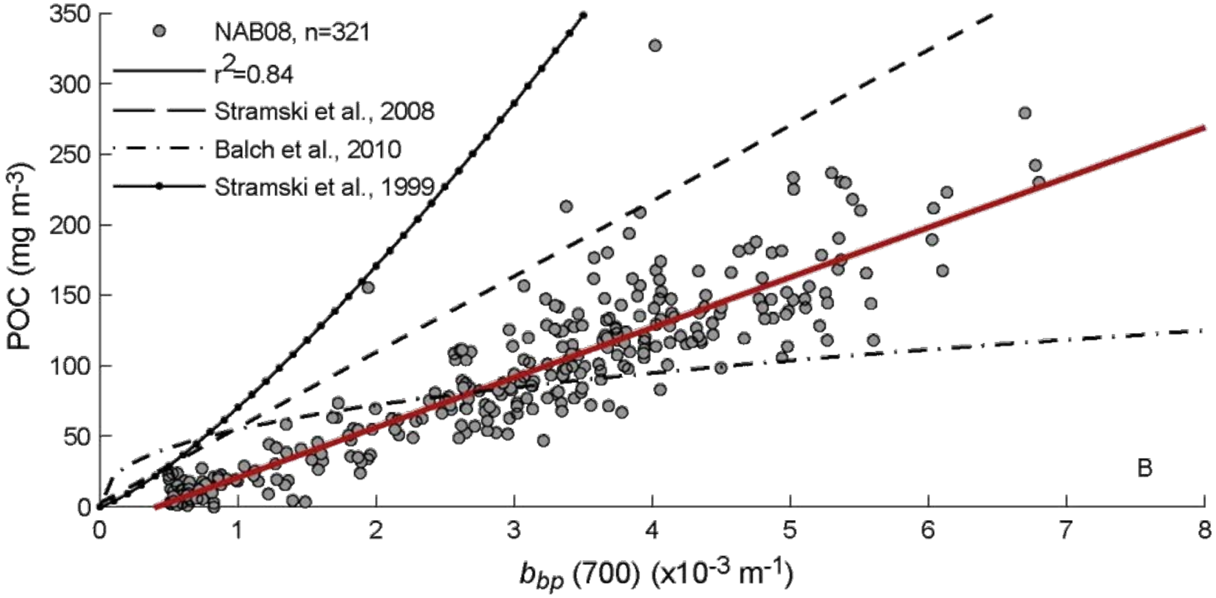
Particulate Organic Carbon

Beam attenuation (c_p)

Cetinić et al., 2012, JGR

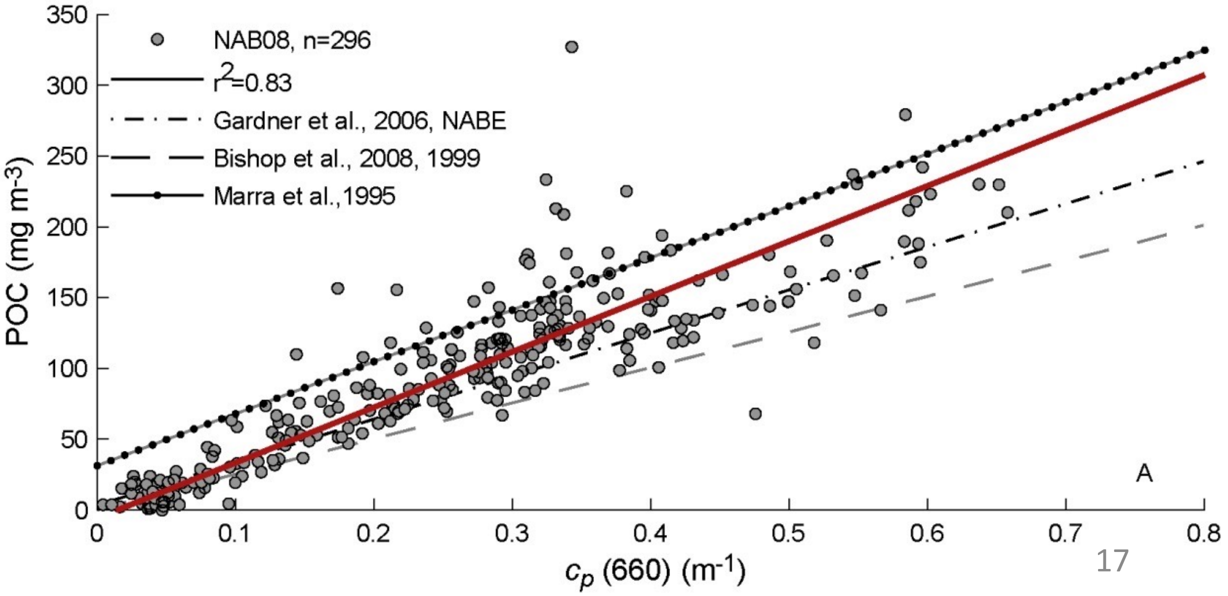


Particulate Organic Carbon



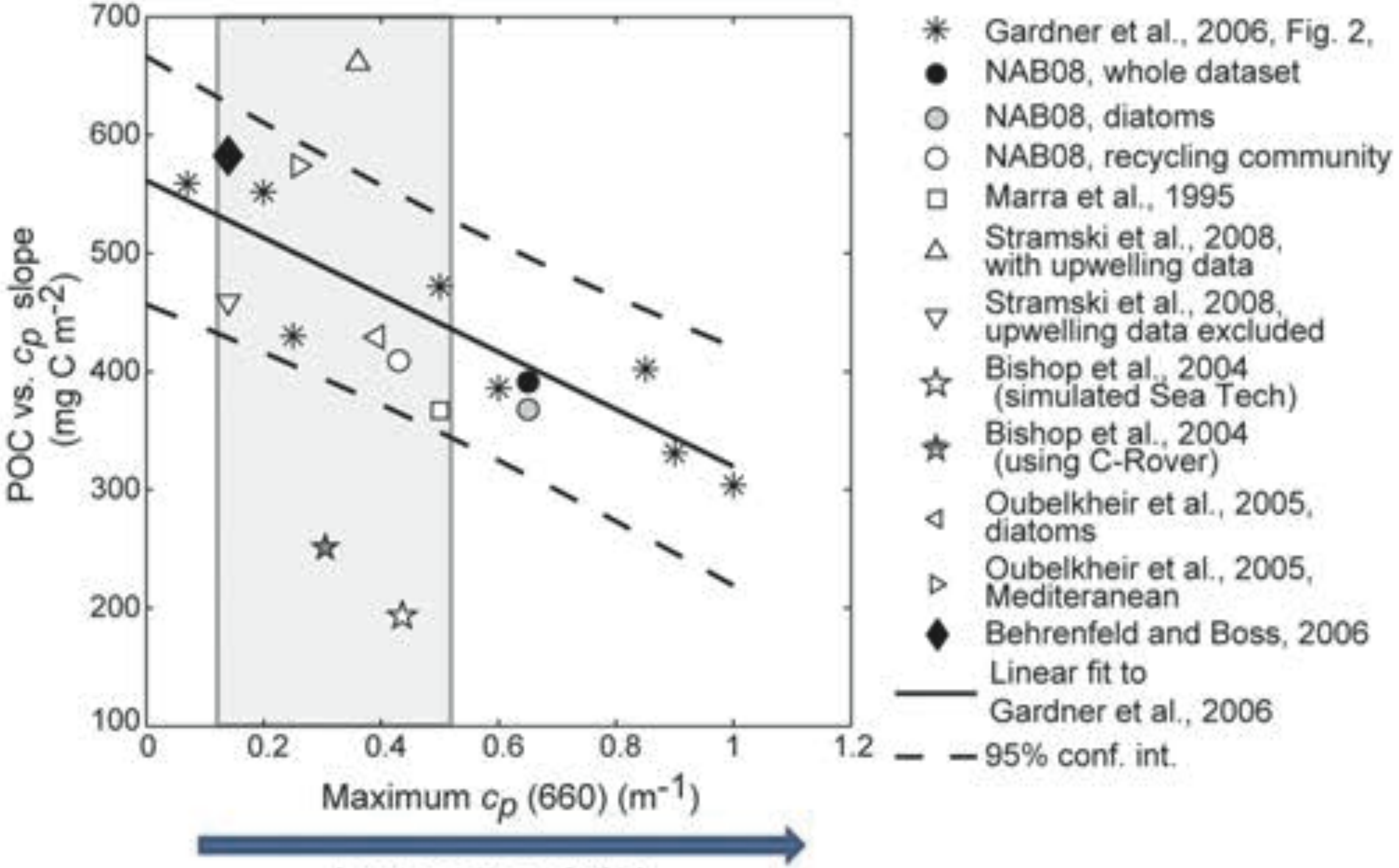
Particulate backscattering (b_{bp})

Beam attenuation (c_p)



Cetinić et al., 2012, JGR

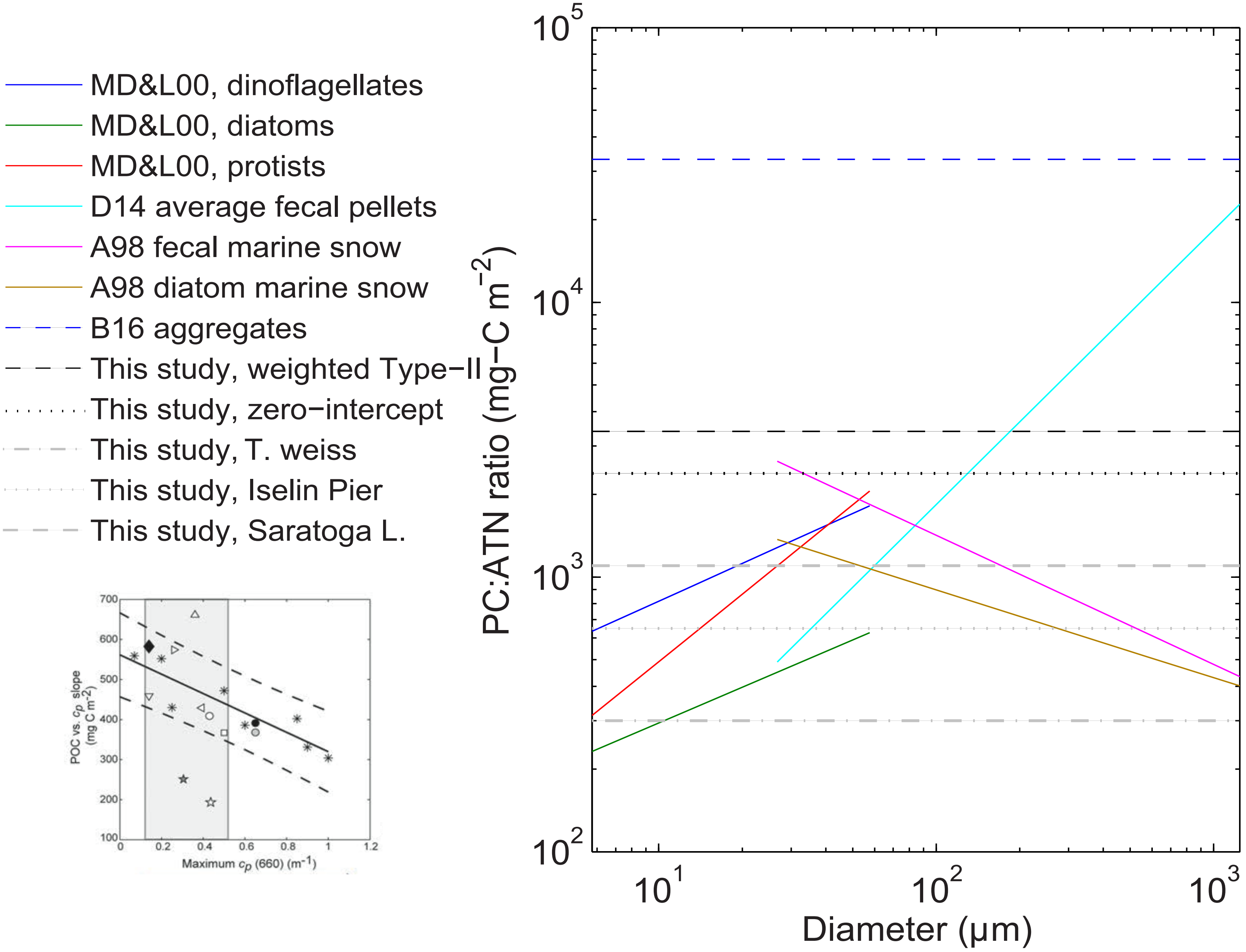
POC/c_p slope comparison (mg C m^{-2})



Increase in c_p & Chl
Smaller to larger cells
Oligotrophic to Eutrophic system
Pico/nano plankton to micro plankton

Cetinić et al., 2012, JGR

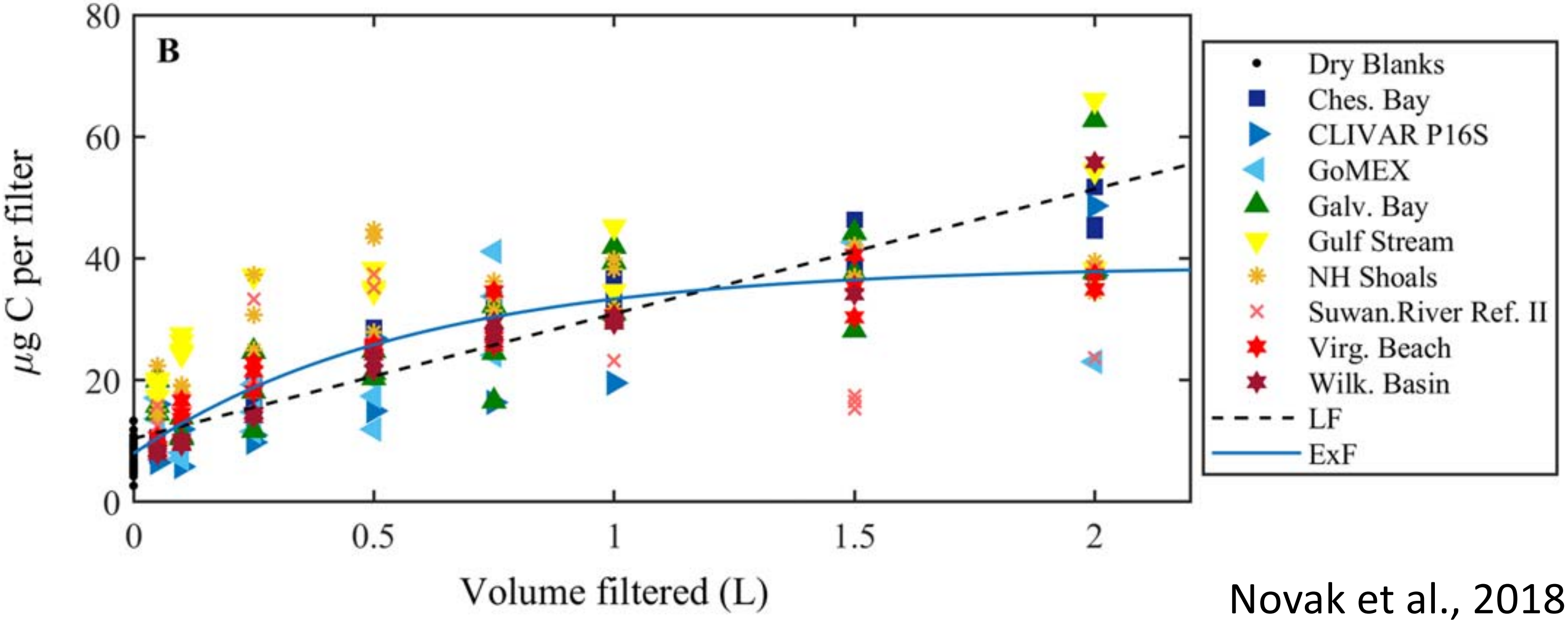
Extend POC:cp relationship to sinking particles



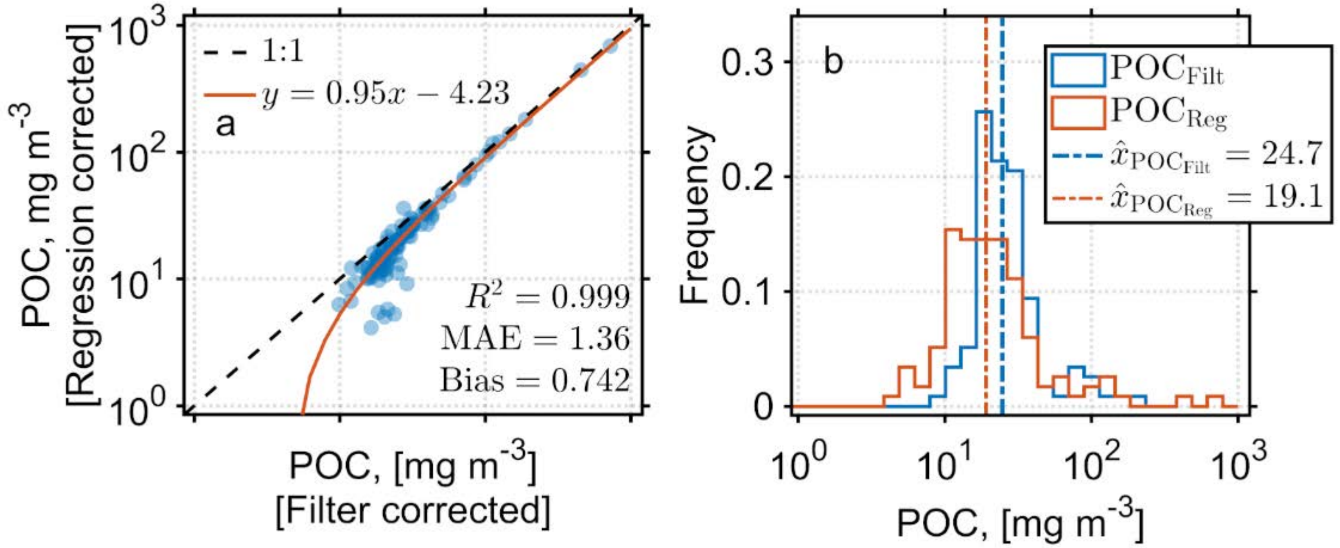
Estapa et al., 2017

Good POC proxies require accurate in-water measurements:

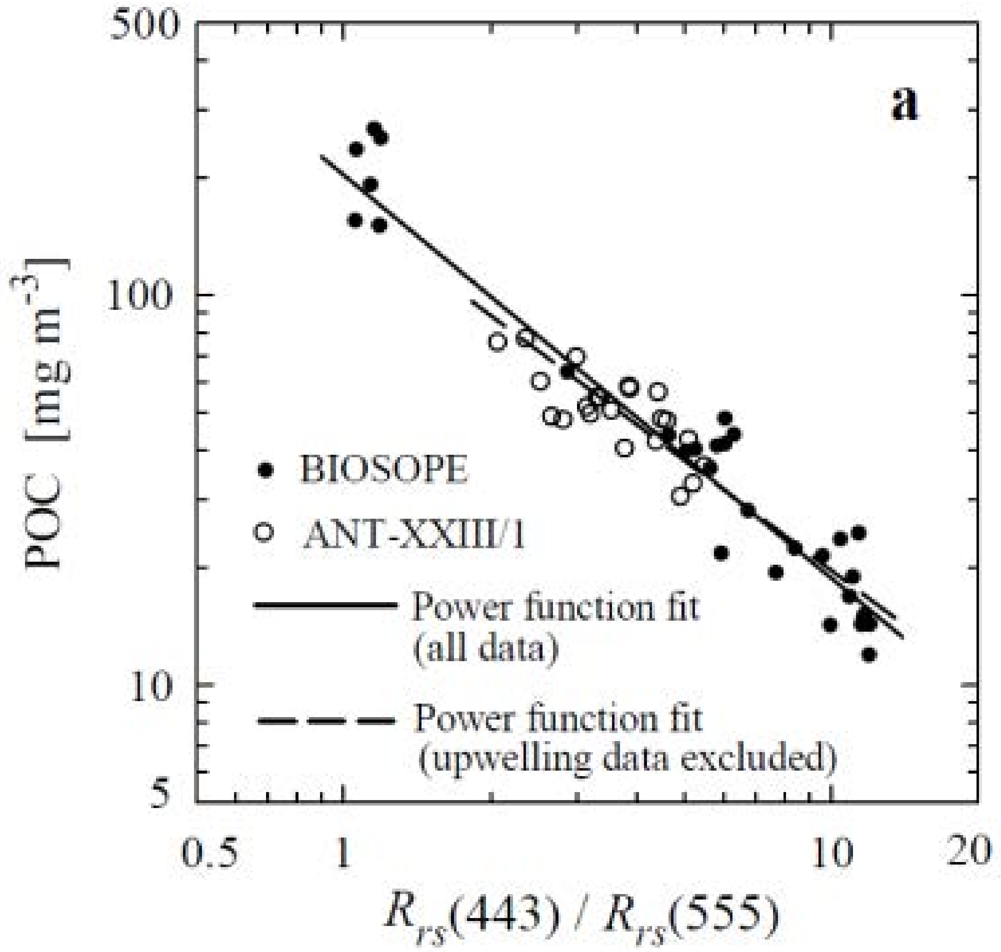
Bias in discrete POC measurements from DOC adsorption to filters



Novak et al., 2018



Chaves et al., 2021



Current POC algorithm

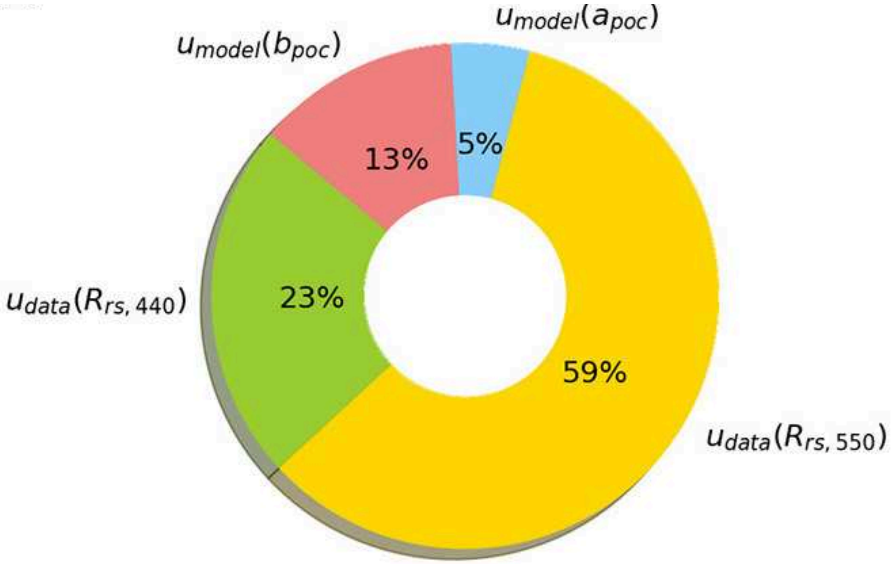
Stramski et al., 2008

No DOC adsorption blanks

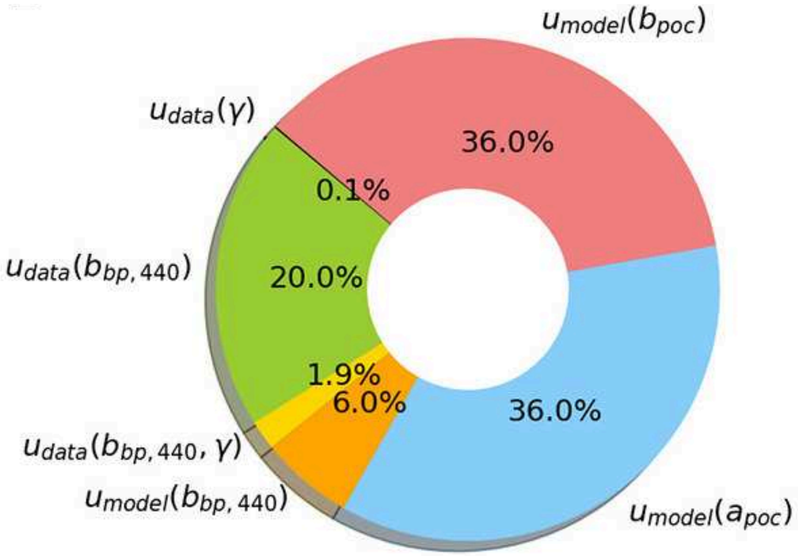
- DOC adsorption can be up to 30.86±0.62 µg C per filter (Novak et al. 2018)
- We need original data
- We need filtered volumes to apply the correction

Contributions of different uncertainty sources to RS algorithms – example for two different POC algorithms

Stramski et al. 2008 band-ratio



Rasse et al. 2017 IOP-based

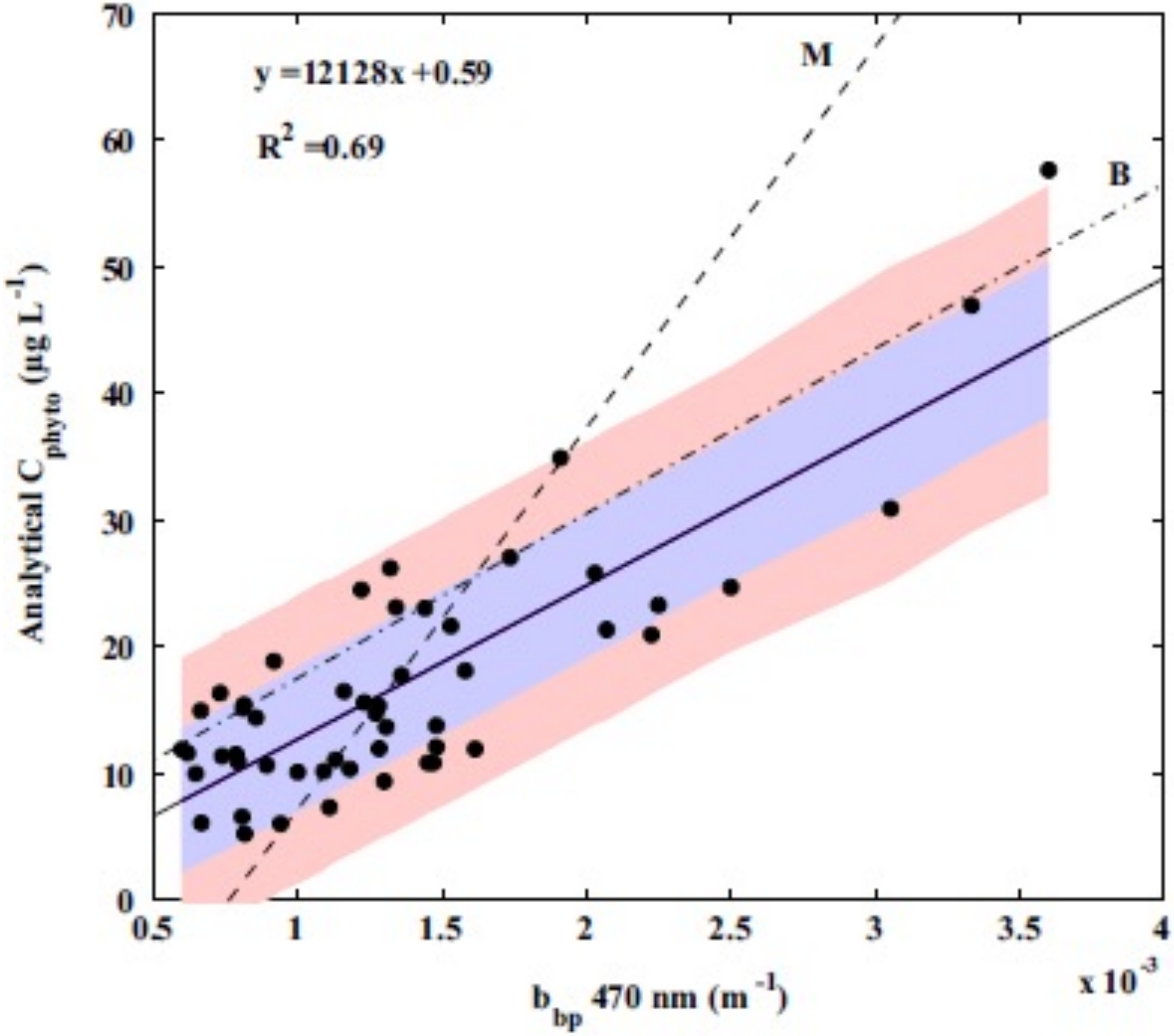


- u_{model} terms include uncertainty in the POC measurements used to construct the algorithms (here, uncorrected DOC adsorption)
- u_{data} terms include uncertainty in radiometric measurements

McKenna et al., 2019

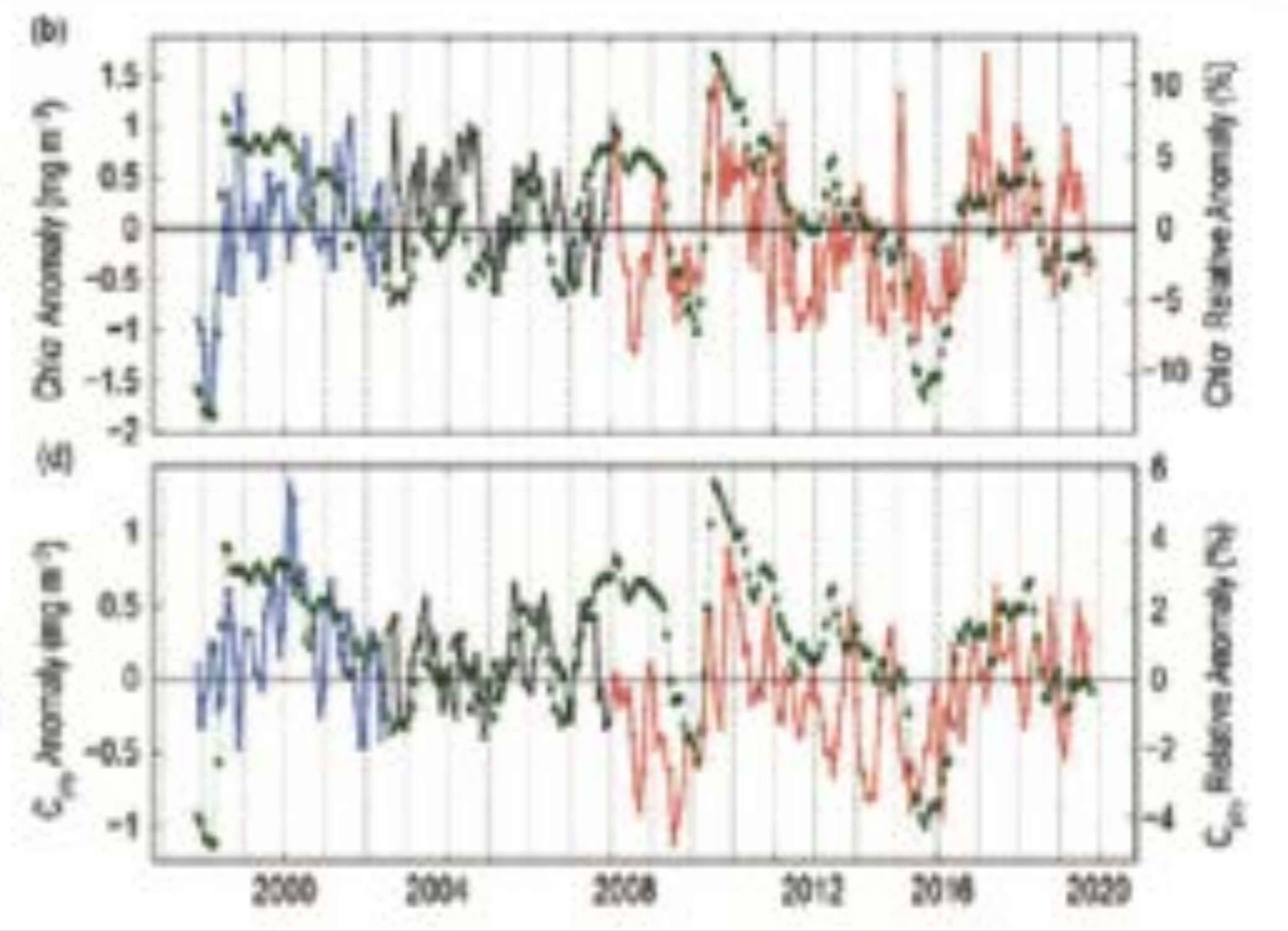
Phytoplankton carbon

- Cell sorting technique in combination with optics
- Traditionally – calculation from of imaging/flow cytometry based biovolumes and cell/C values



Graff et al., 2015

GIOP backscattering --> Phytoplankton carbon



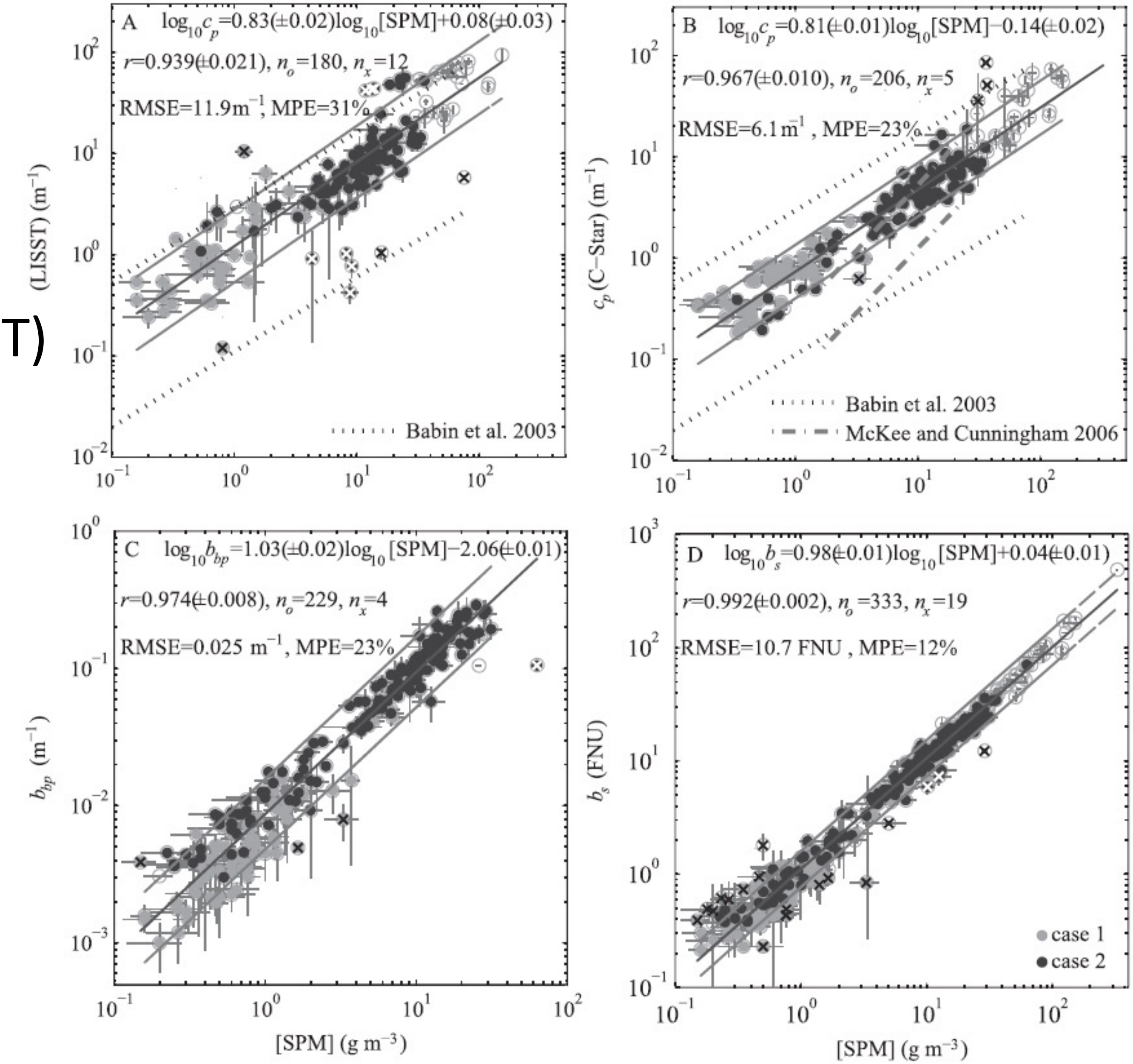
Green dots = Multivariate ENSO Index, inverted

Franz et al. 2020, ”Global Ocean Phytoplankton”, in Baringer et al. [eds], *State of the Climate in 2019*

Suspended Particulate Matter

Gray dots: Case I
Black dots: Case II

c_p(LISST)



c_p(C-Star)

b_{bp}

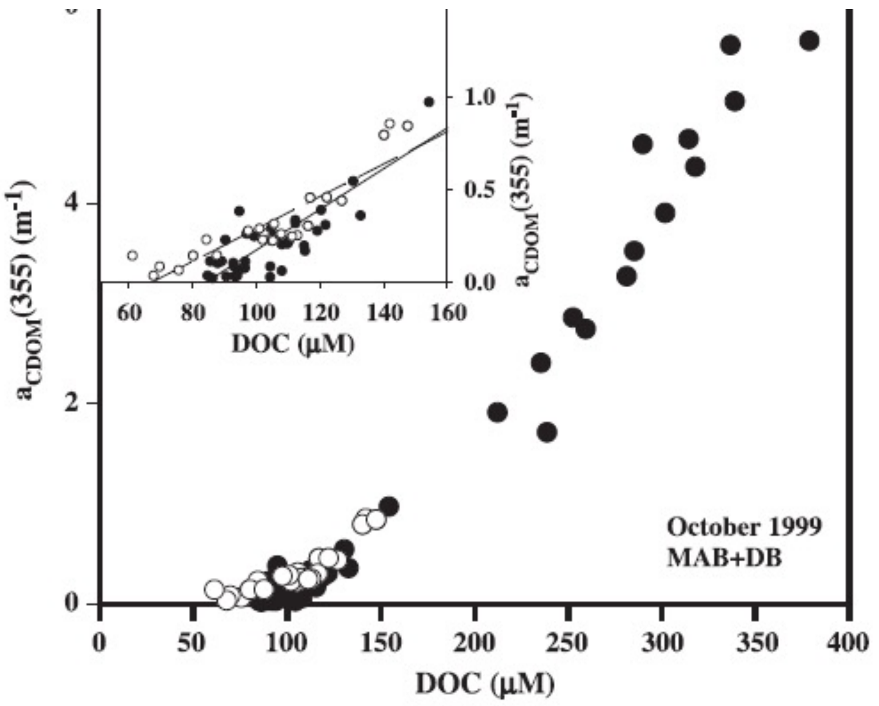
b_s (discrete samples in turbidity sensor)

Neukermans et al. 2012

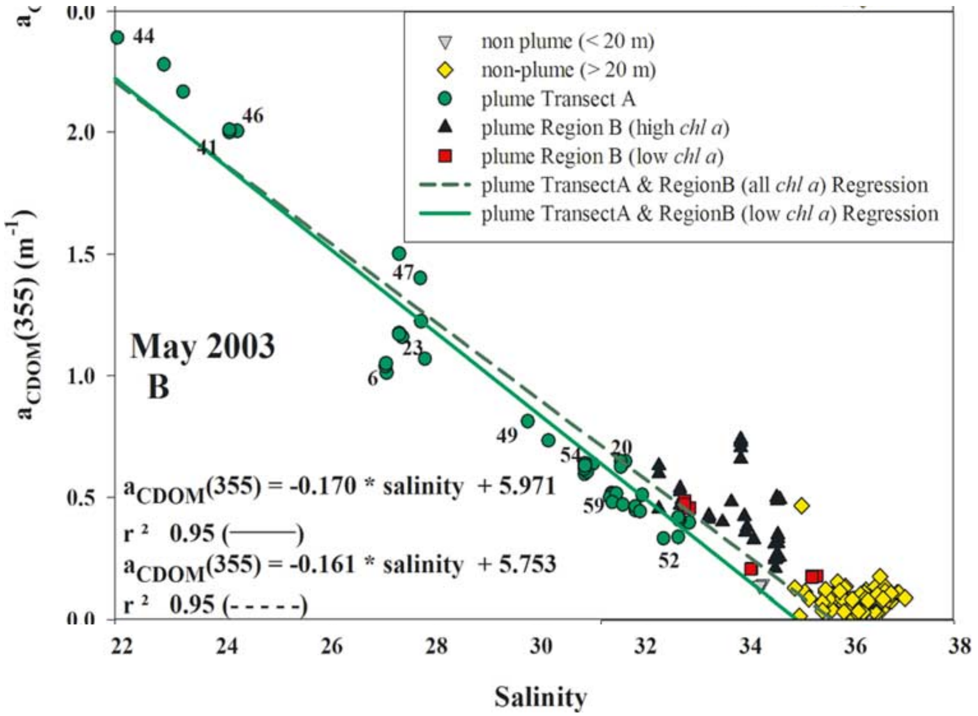
SPM (g m^{-3})

Dissolved Organic Carbon

CDOM can approximate DOC in the coastal ocean



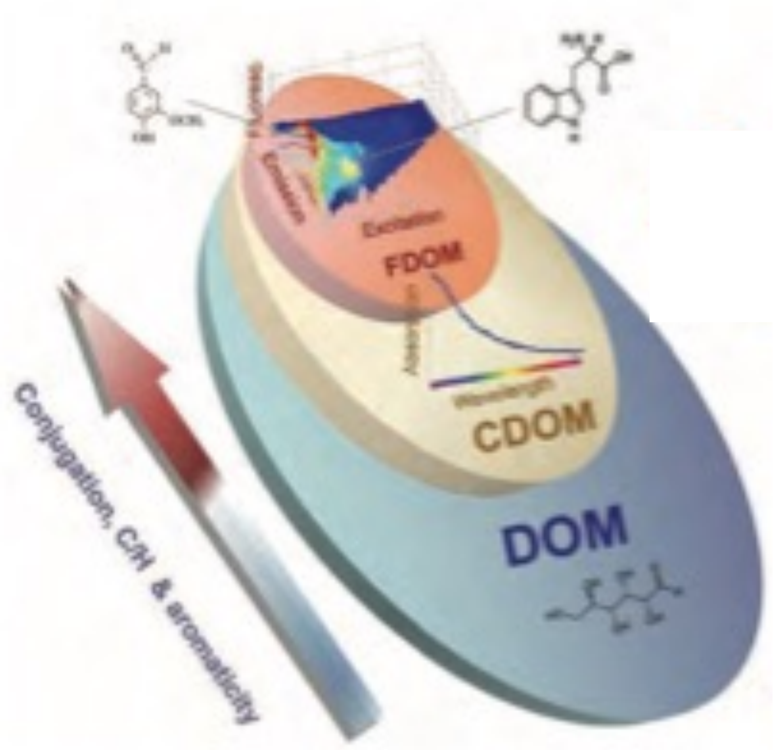
Del Vecchio and Blough, 2004



Del Vecchio and Subramaniam, 2004

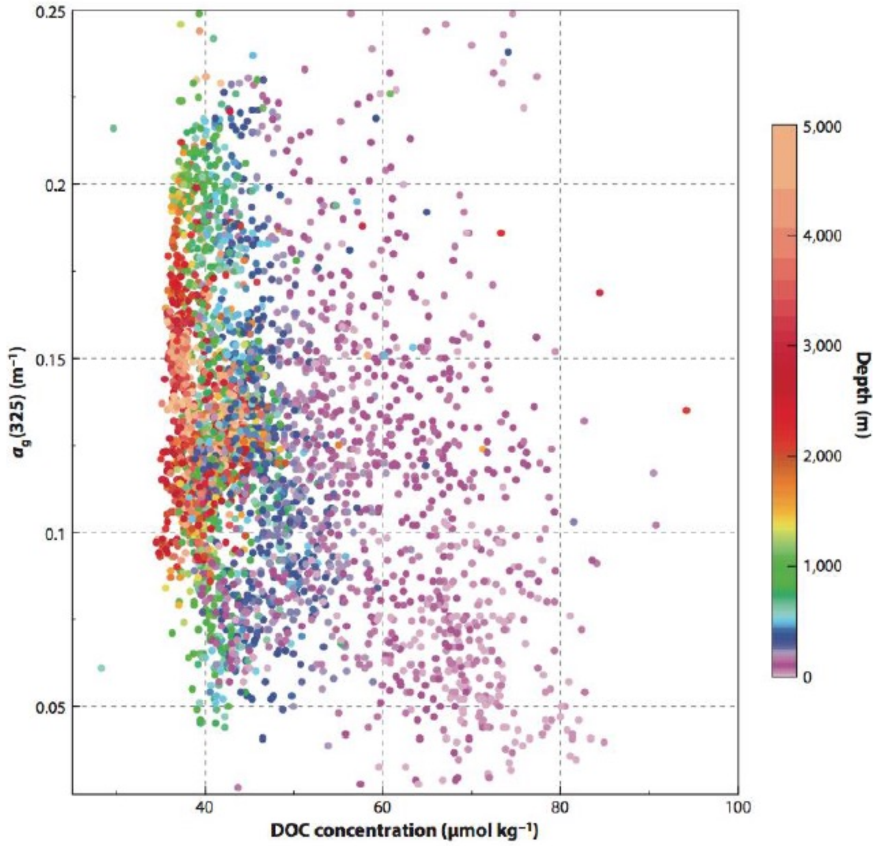
- Every coastal region will probably be different
- Better relationships when there is one strong source (e.g. river plume) and one major loss process (e.g. dilution into ocean)

Dissolved Organic Carbon...



Stedmon and Alvarez-Salgado, 2011

CDOM ≠ DOC in the open ocean



Nelson and Siegel 2013

DOC from space – Aurin et al., 2018.
Empirical regression against 4 wavebands (440-555 nm) + salinity required, RMSE still 27-29 μmol L^{-1}

Overview

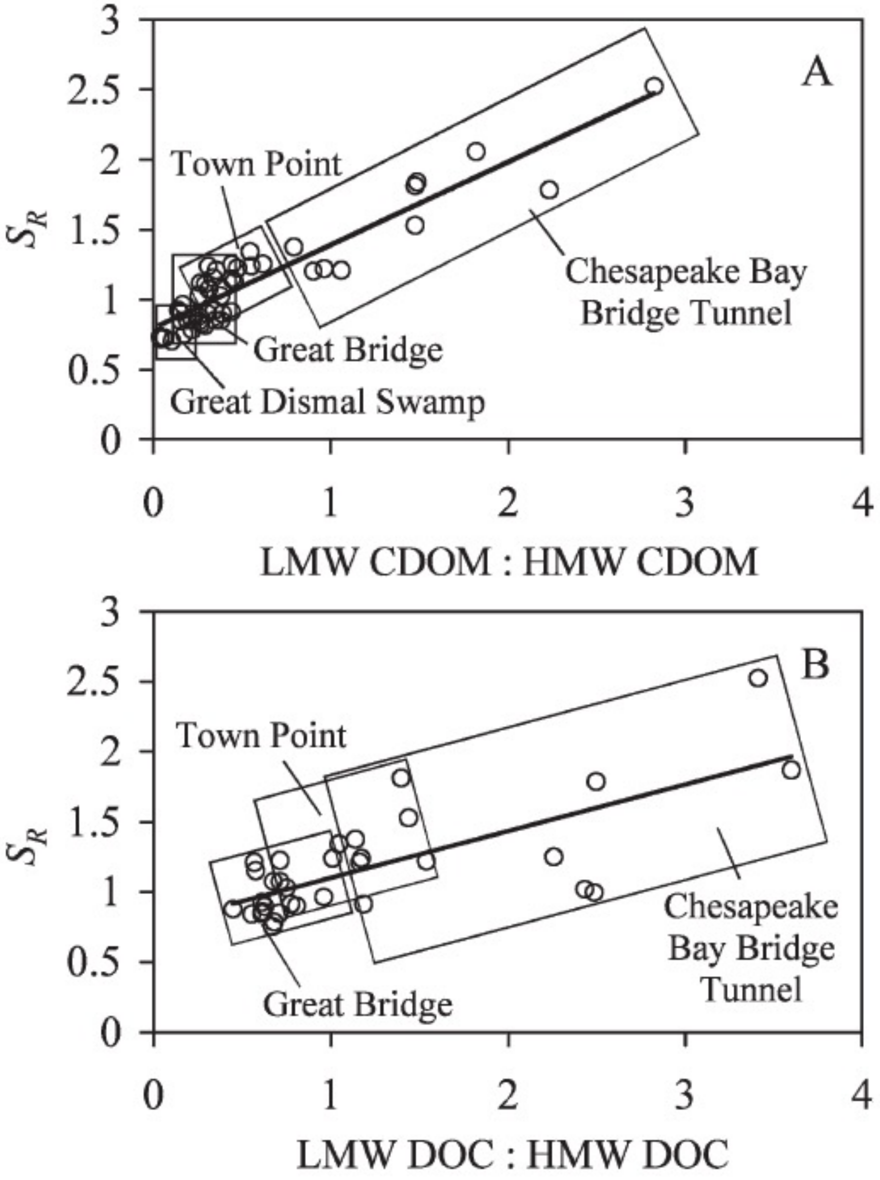
- ✓ Where proxies fit, why to construct them
- ✓ Concentration proxies
- Composition and rate proxies
  - "ANYTHING THAT CAUSES VARIABILITY IN THE SAMPLE IS AN OPPORTUNITY TO EXTRACT ADDITIONAL INFORMATION FROM THAT SAMPLE" - COLLIN ROESLER
- Caveats

As Rufus well knows, there's opportunity in chaos.

OPPORTUNITY IN CHAOS
QUALITY (COMPOSITION, SIZE)

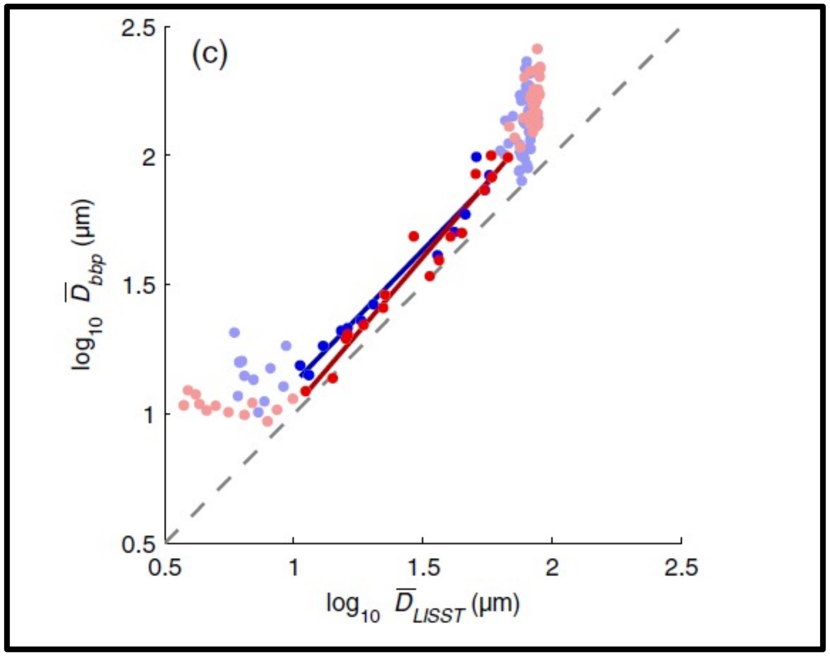
CDOM slope ~ DOC molecular mass

CDOM slope ratio



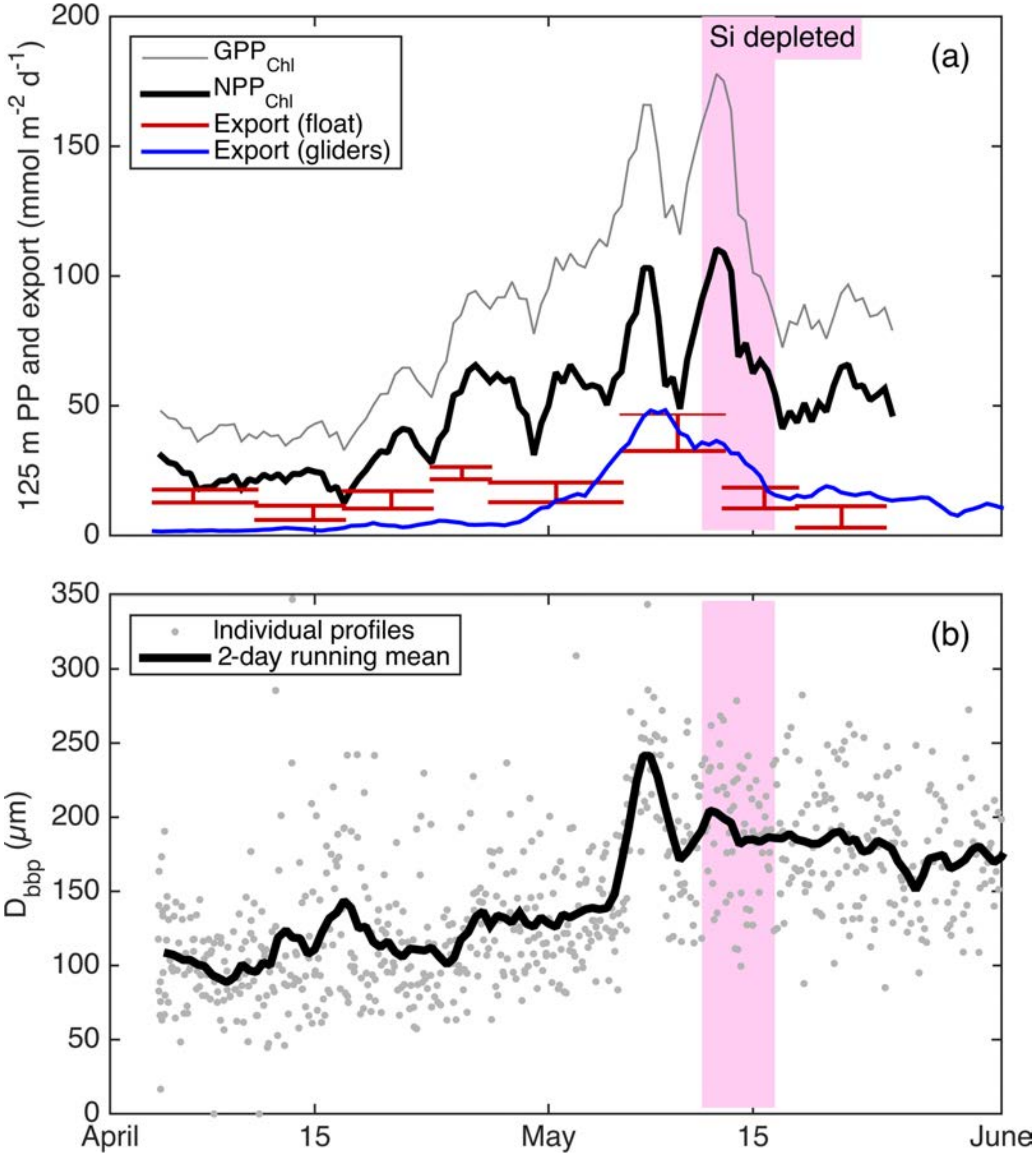
Helms et al., 2008

Particle size – fluctuation based

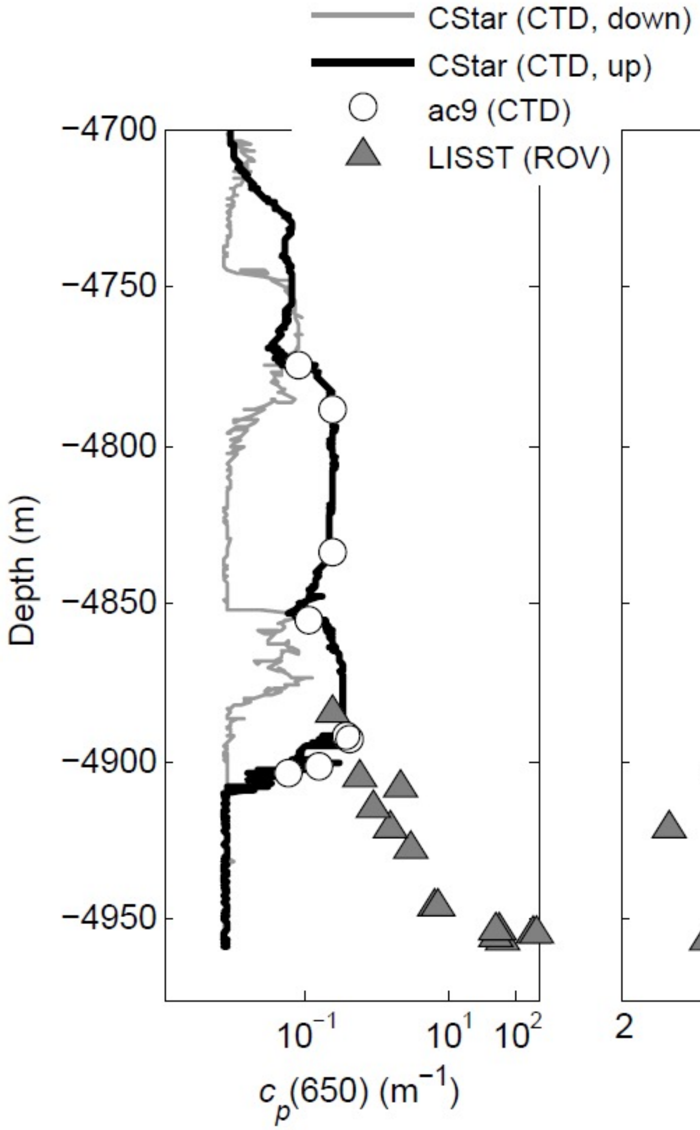


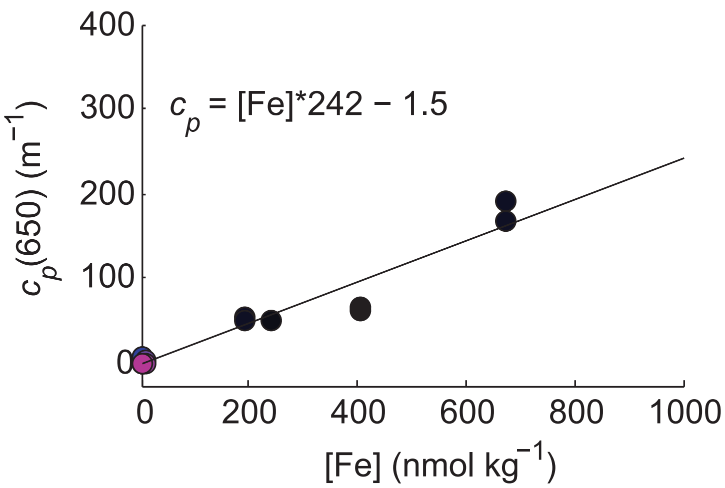
Briggs et al, 2013

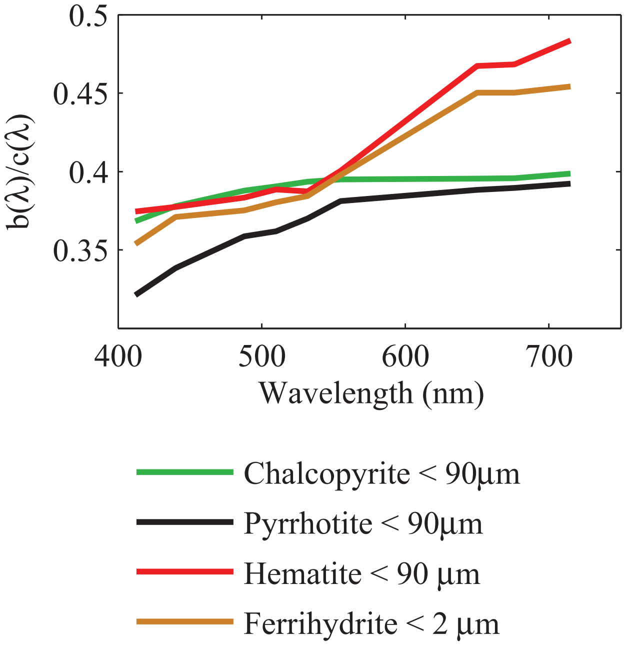
Application – Briggs et al., 2018



Particle composition in a hydrothermal plume

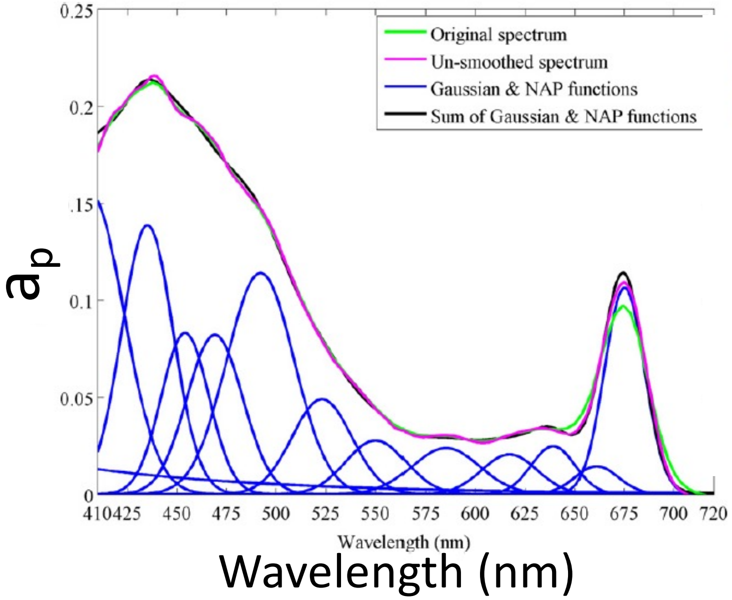






Estapa et al, 2015

Phytoplankton community composition



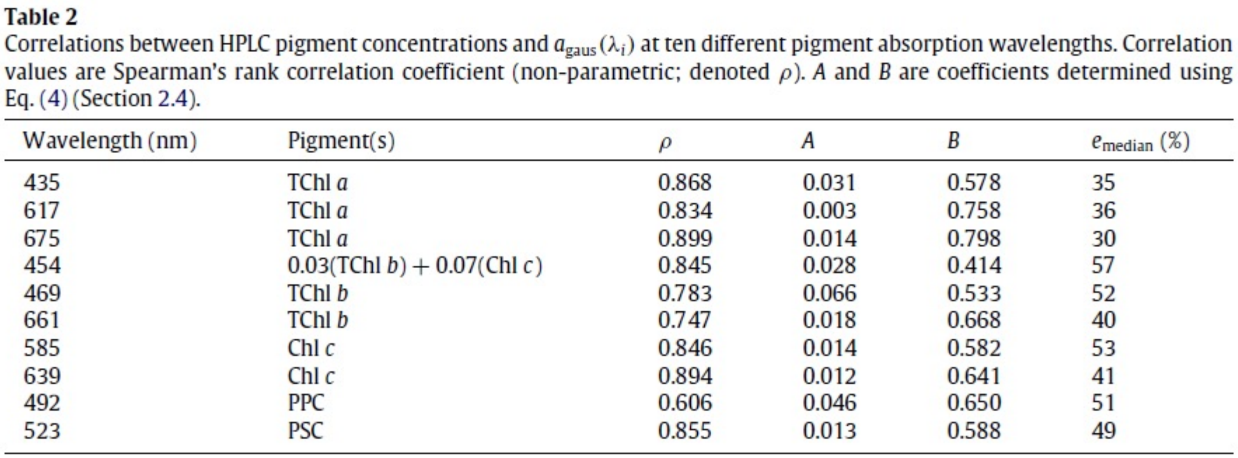
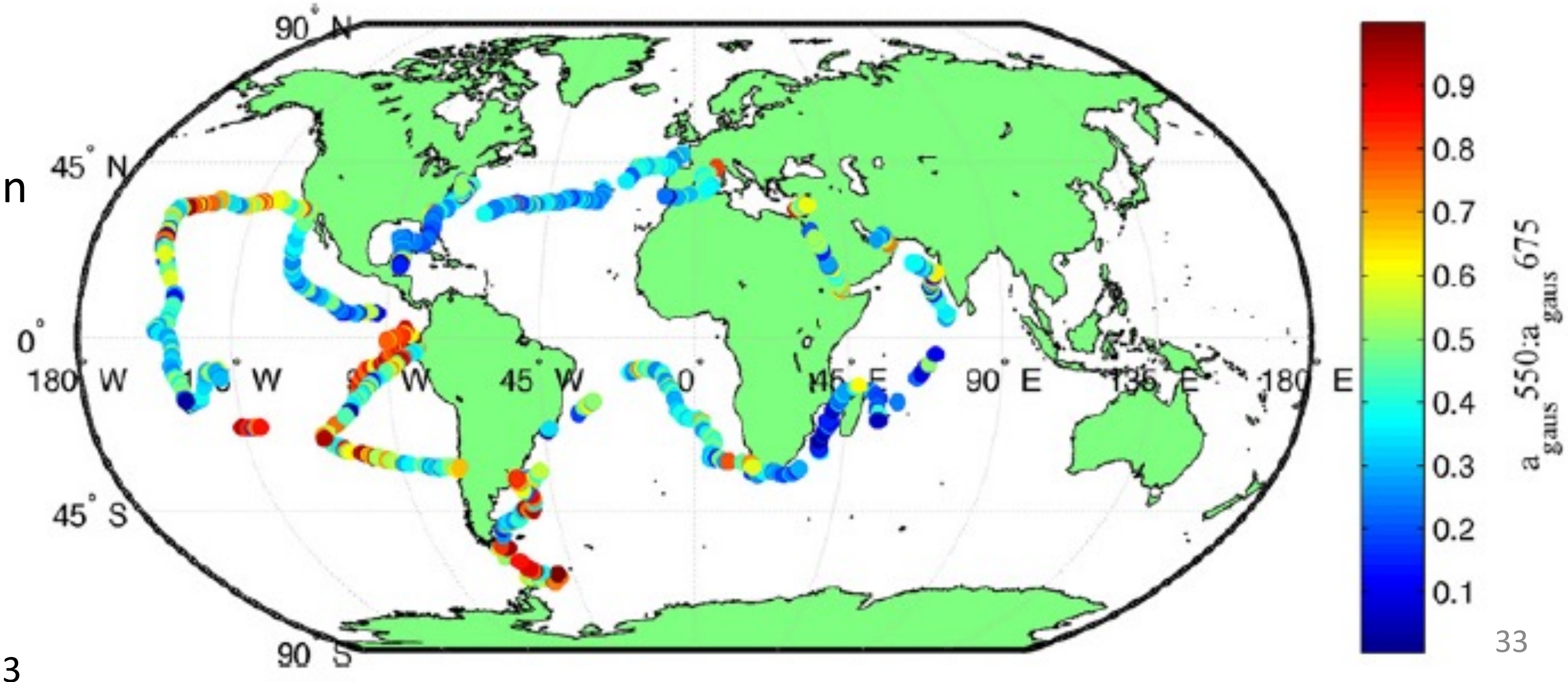


Table 2

Correlations between HPLC pigment concentrations and $a_{gaus}(\lambda_i)$ at ten different pigment absorption wavelengths. Correlation values are Spearman's rank correlation coefficient (non-parametric; denoted ρ). A and B are coefficients determined using Eq. (4) (Section 2.4).

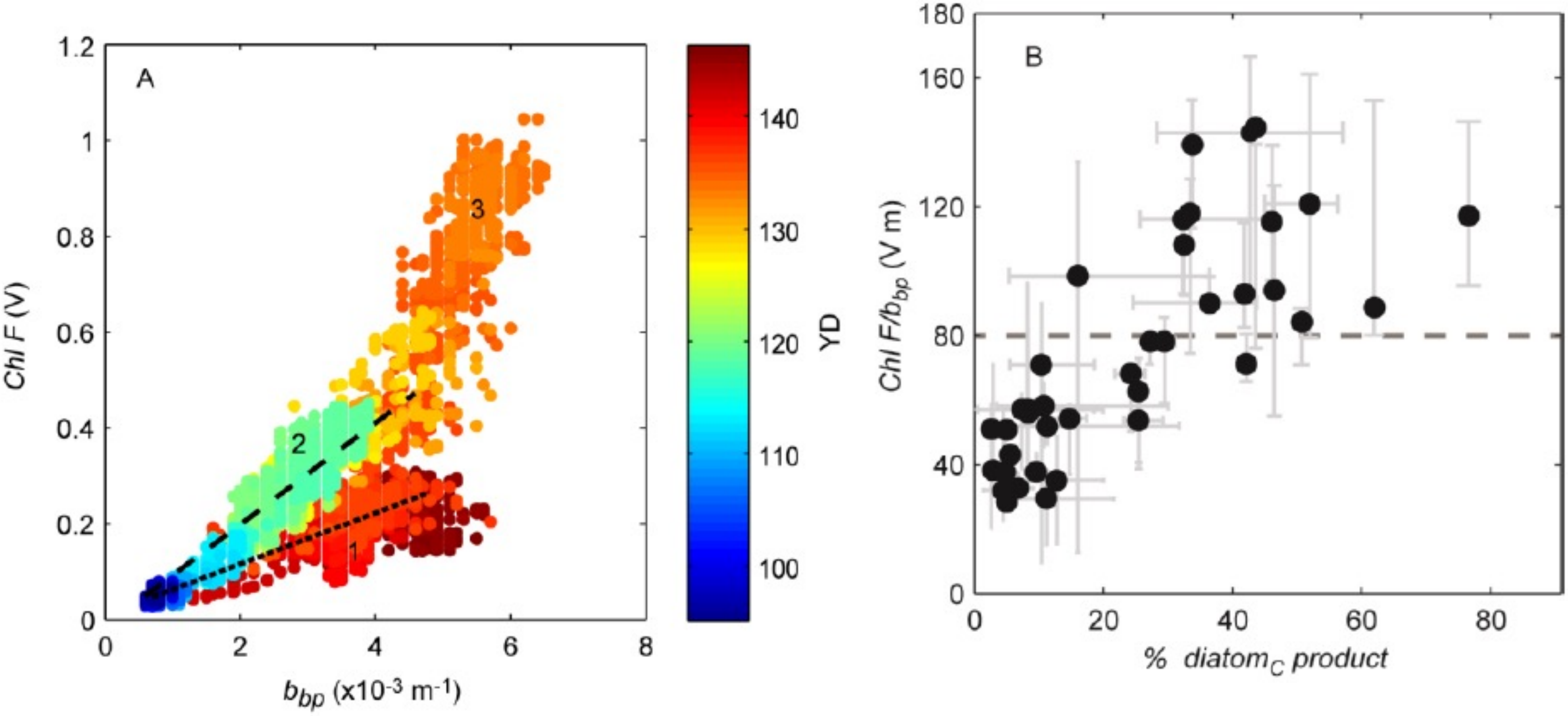
Wavelength (nm)	Pigment(s)	ρ	A	B	e_{median} (%)
435	TChl *a*	0.868	0.031	0.578	35
617	TChl *a*	0.834	0.003	0.758	36
675	TChl *a*	0.899	0.014	0.798	30
454	0.03(TChl *b*) + 0.07(Chl *c*)	0.845	0.028	0.414	57
469	TChl *b*	0.783	0.066	0.533	52
661	TChl *b*	0.747	0.018	0.668	40
585	Chl *c*	0.846	0.014	0.582	53
639	Chl *c*	0.894	0.012	0.641	41
492	PPC	0.606	0.046	0.650	51
523	PSC	0.855	0.013	0.588	49

Phycoerythrin proxy distribution

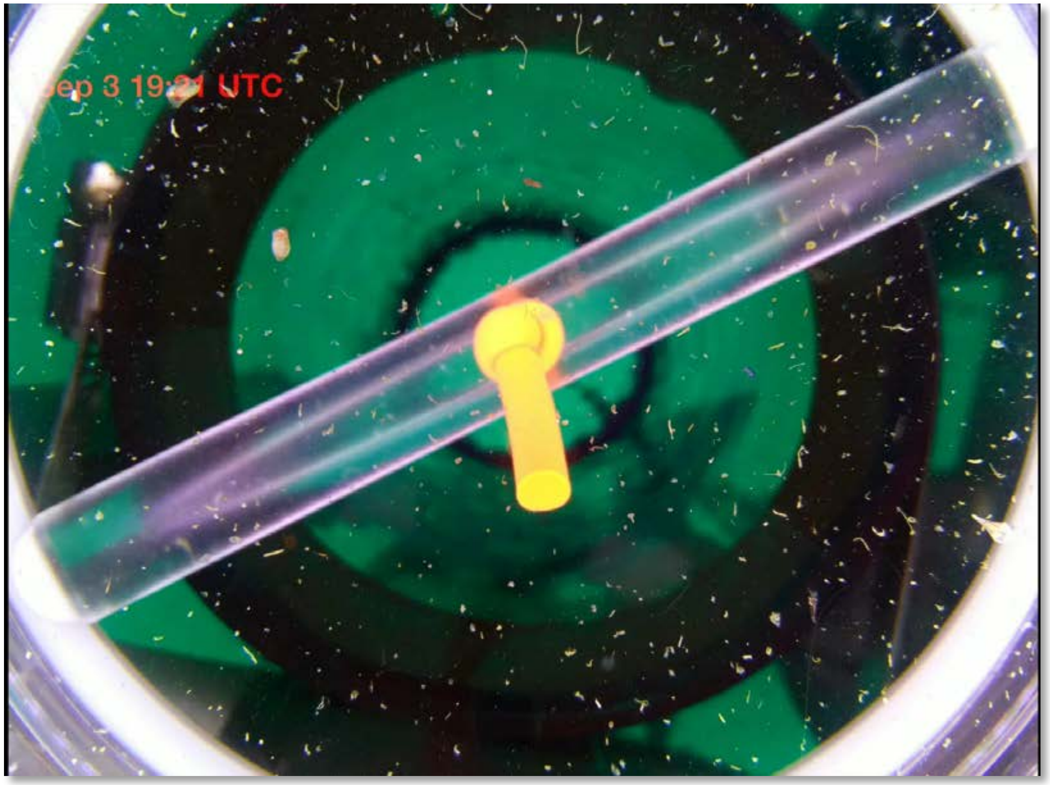


Chase et al, 2013

Phytoplankton Community composition



Cetinic et al, 2015



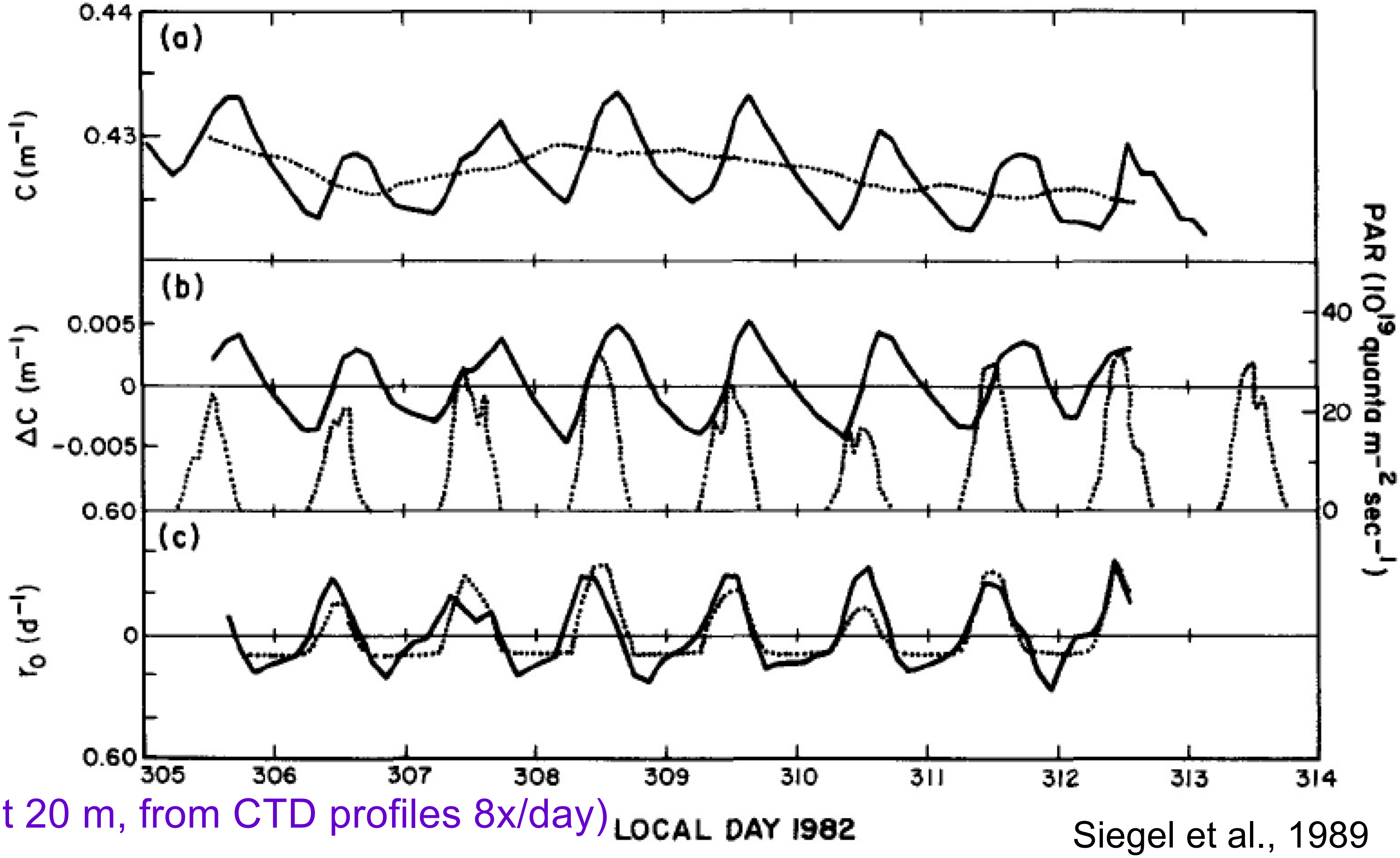
Omand et al, unpublished

OPPORTUNITY IN CHAOS
RATES AND FLUXES

Change in *in situ* optical proxies will tell us something about **rates and fluxes**

- Space - e.g. carbon export from mixed layer to deeper ocean
- Time – productivity - e.g. primary production
- Type – e.g. phytoplankton to detritus, POC to DOC
- Typical units could be:
  - mol m^{-2} y^{-1}
  - μmol L^{-1} h^{-1}
  - d^{-1}

PRODUCTIVITY/GROWTH

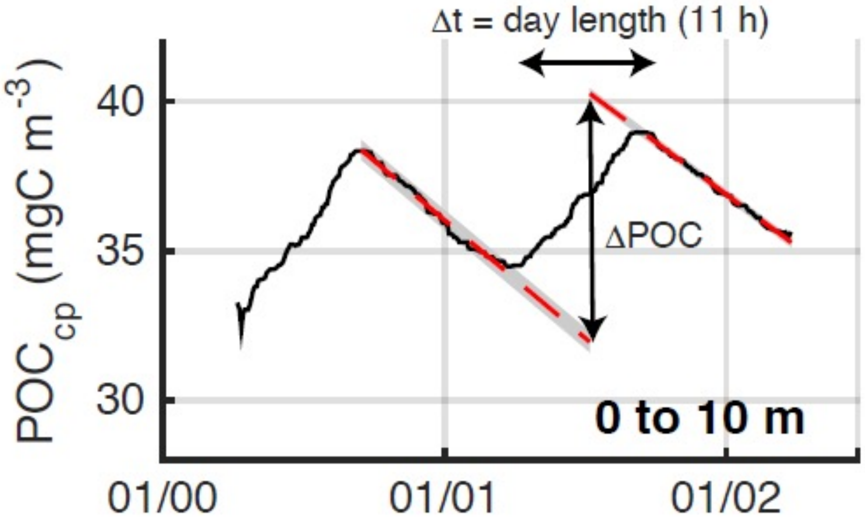


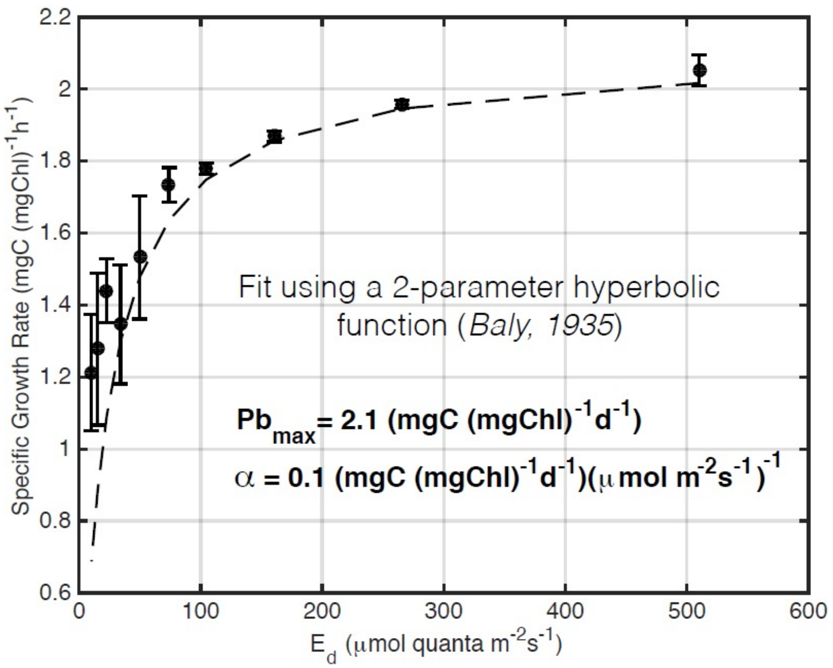
(at 20 m, from CTD profiles 8x/day)

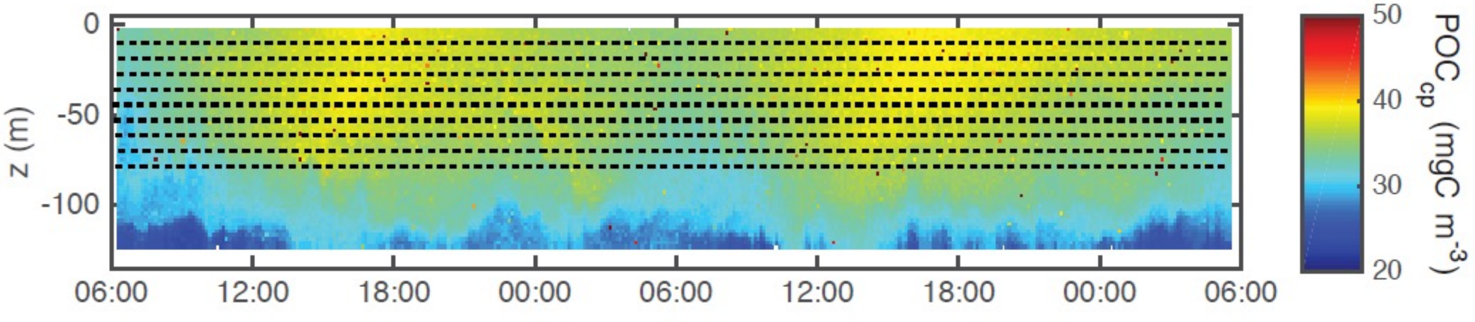
Siegel et al., 1989

+relevant work by many others

PRODUCTIVITY/GROWTH



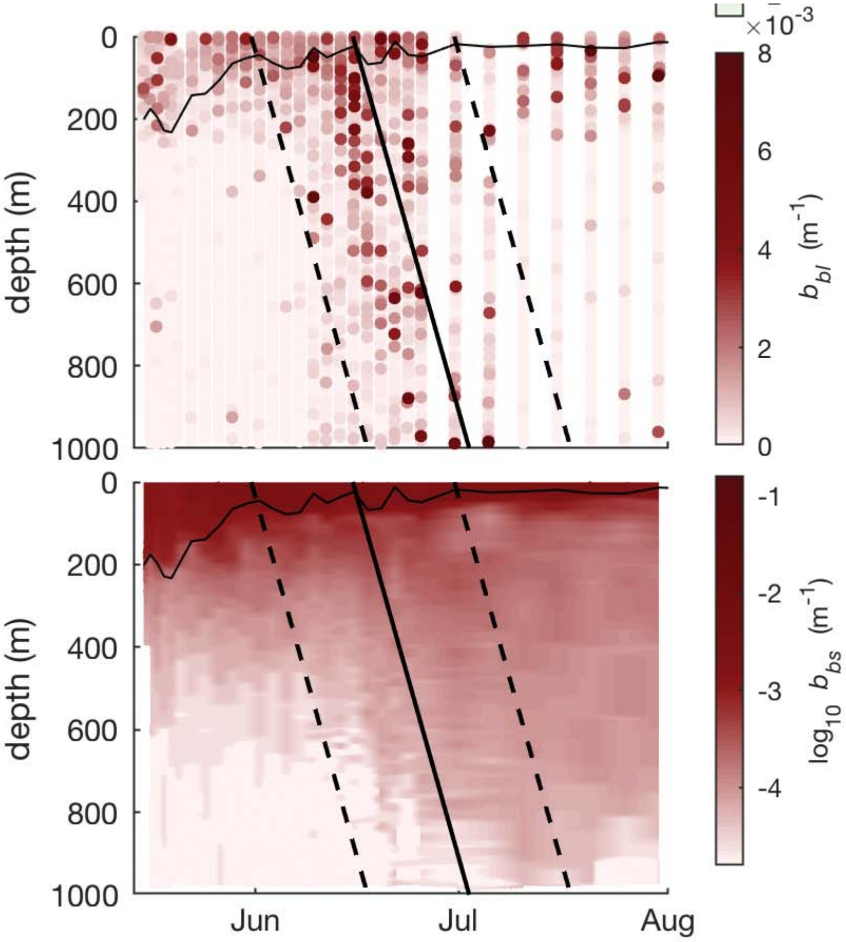




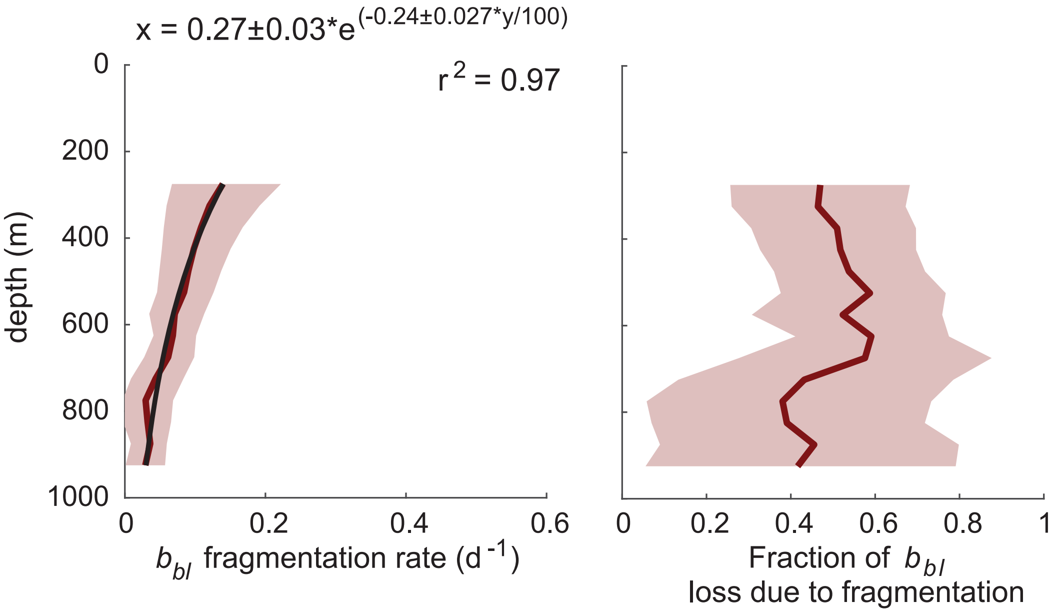
Omand et al, *unpublished*

DISSAGGREGATION

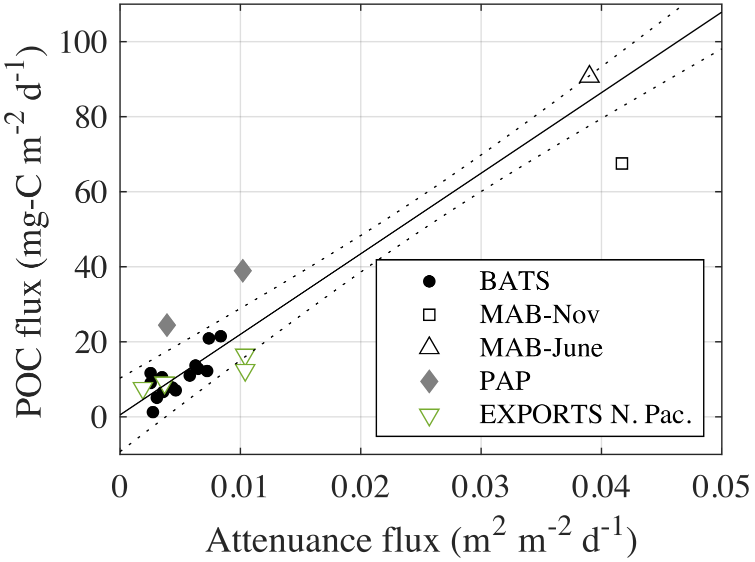
Briggs et al, 2020

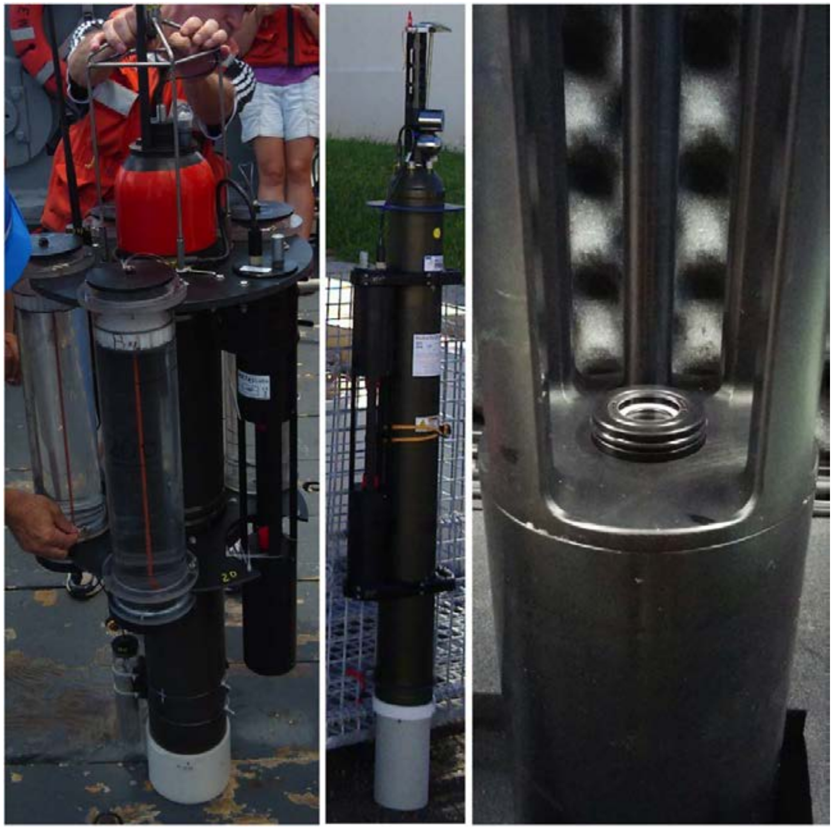


- Use “spikes” to quantify large- and small-particle backscattering
- Find well-defined export events in BGC-Argo data
- → Disaggregation during such events accounts for ~ half of C flux attenuation

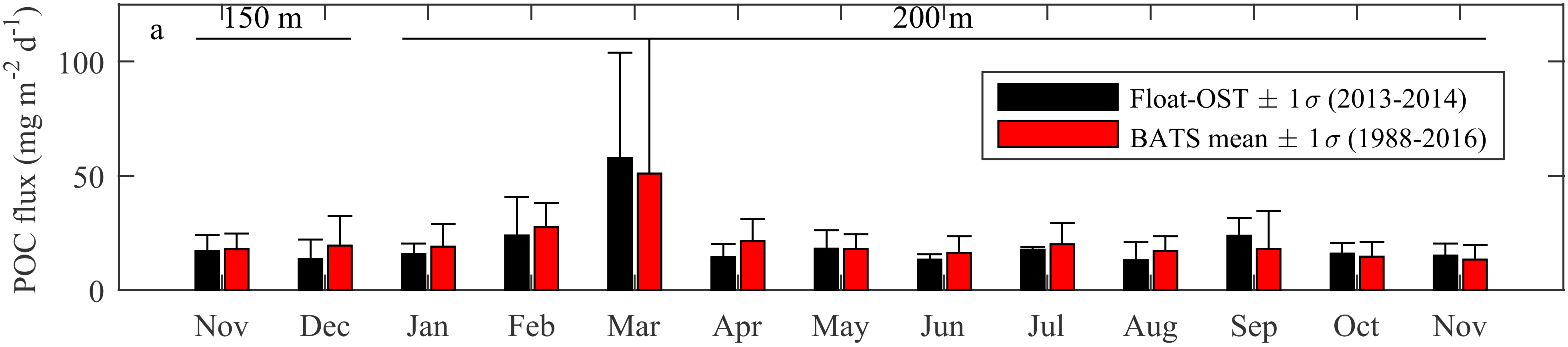


“Optical sediment trap”



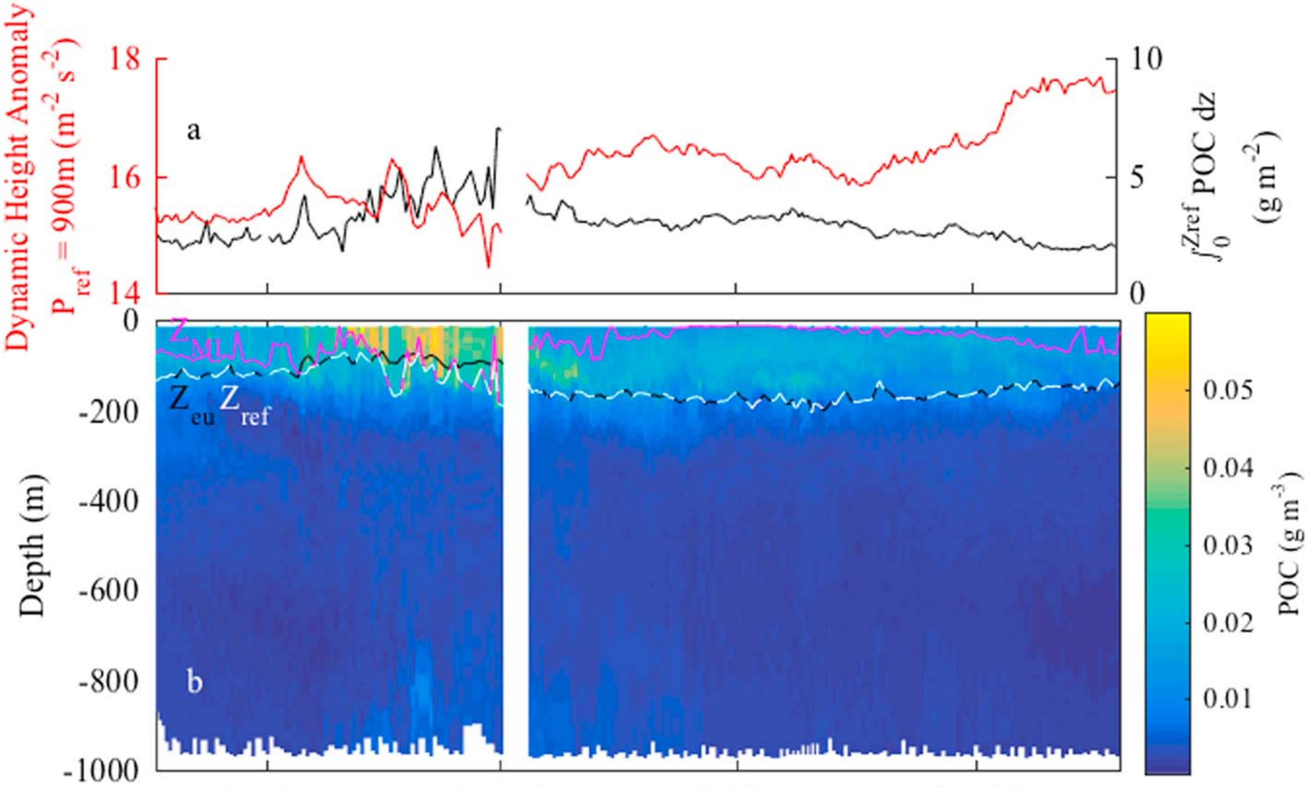


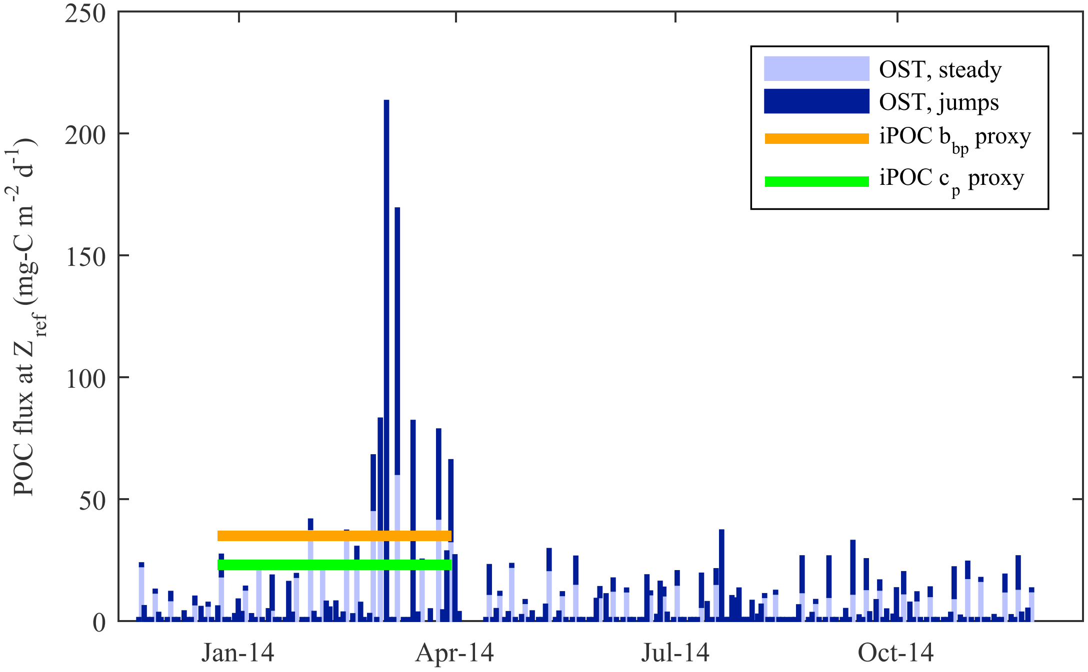
Estapa et al., 2017



Estapa et al. 2019, plus unpublished EXPORTS data

“Optical sediment trap”





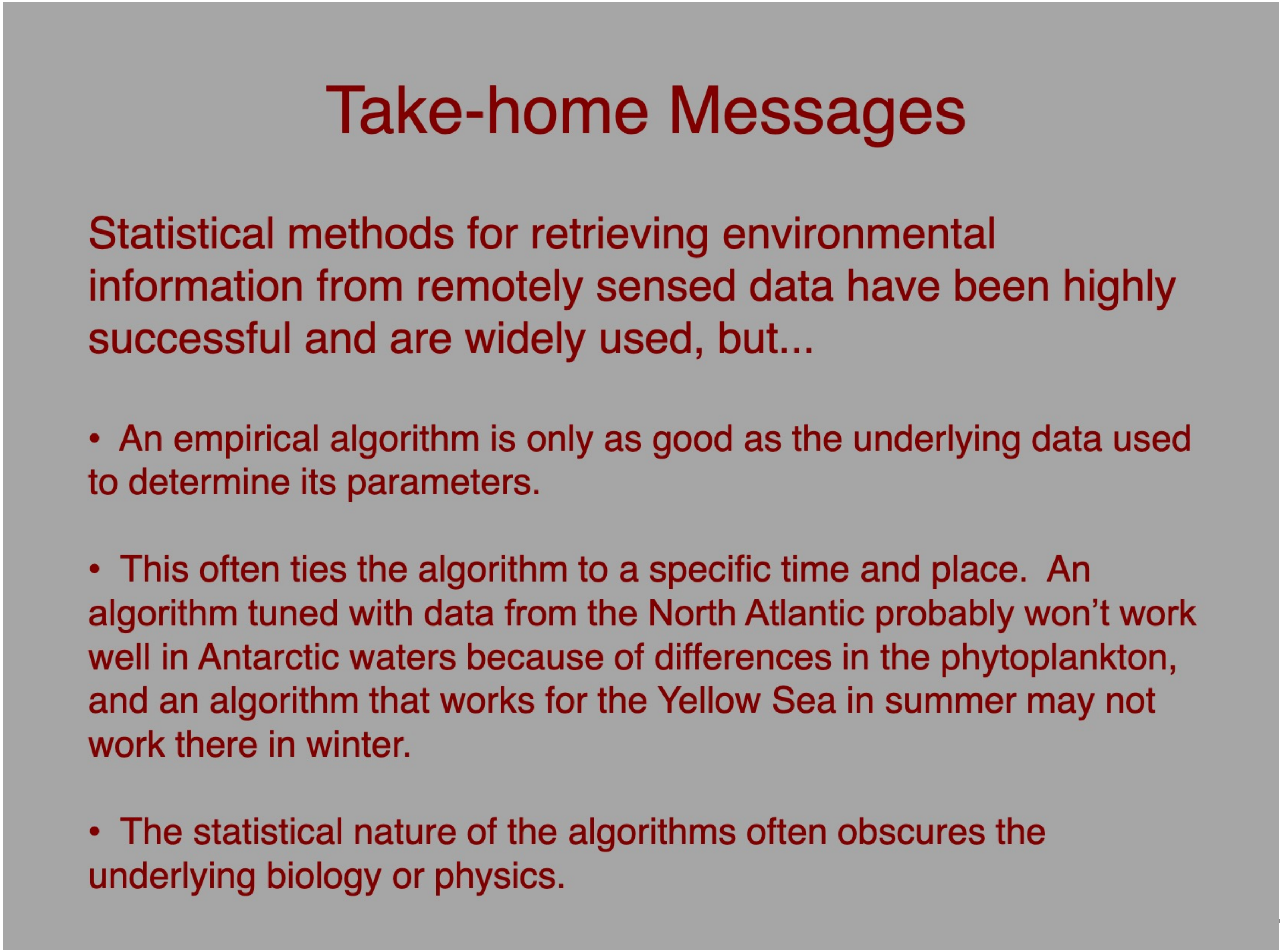
Intercomparison of three optical proxies for POC flux

Estapa et al., 2019

Overview

- ✓ Where proxies fit, why to construct them
- ✓ Concentration proxies
- ✓ Composition and rate proxies
- Caveats

Curt’s slide from Monday morning...



Take-home Messages

Statistical methods for retrieving environmental information from remotely sensed data have been highly successful and are widely used, but...

- An empirical algorithm is only as good as the underlying data used to determine its parameters.

- This often ties the algorithm to a specific time and place. An algorithm tuned with data from the North Atlantic probably won’t work well in Antarctic waters because of differences in the phytoplankton, and an algorithm that works for the Yellow Sea in summer may not work there in winter.

- The statistical nature of the algorithms often obscures the underlying biology or physics.

Caveats

1. Validate – make sure your proxies are based on strong and meaningful relationship with biogeochemical parameters
2. Interpolate rather than extrapolate – know the limits of your method, spatial, temporal and logical
3. Same as Rufus the dog, seize the variability and chaos (but remember 1 and 2)

As Rufus well knows, there's opportunity in chaos.

“PROXIES WORK UNTIL THEY DON’T” – Mary Jane Perry