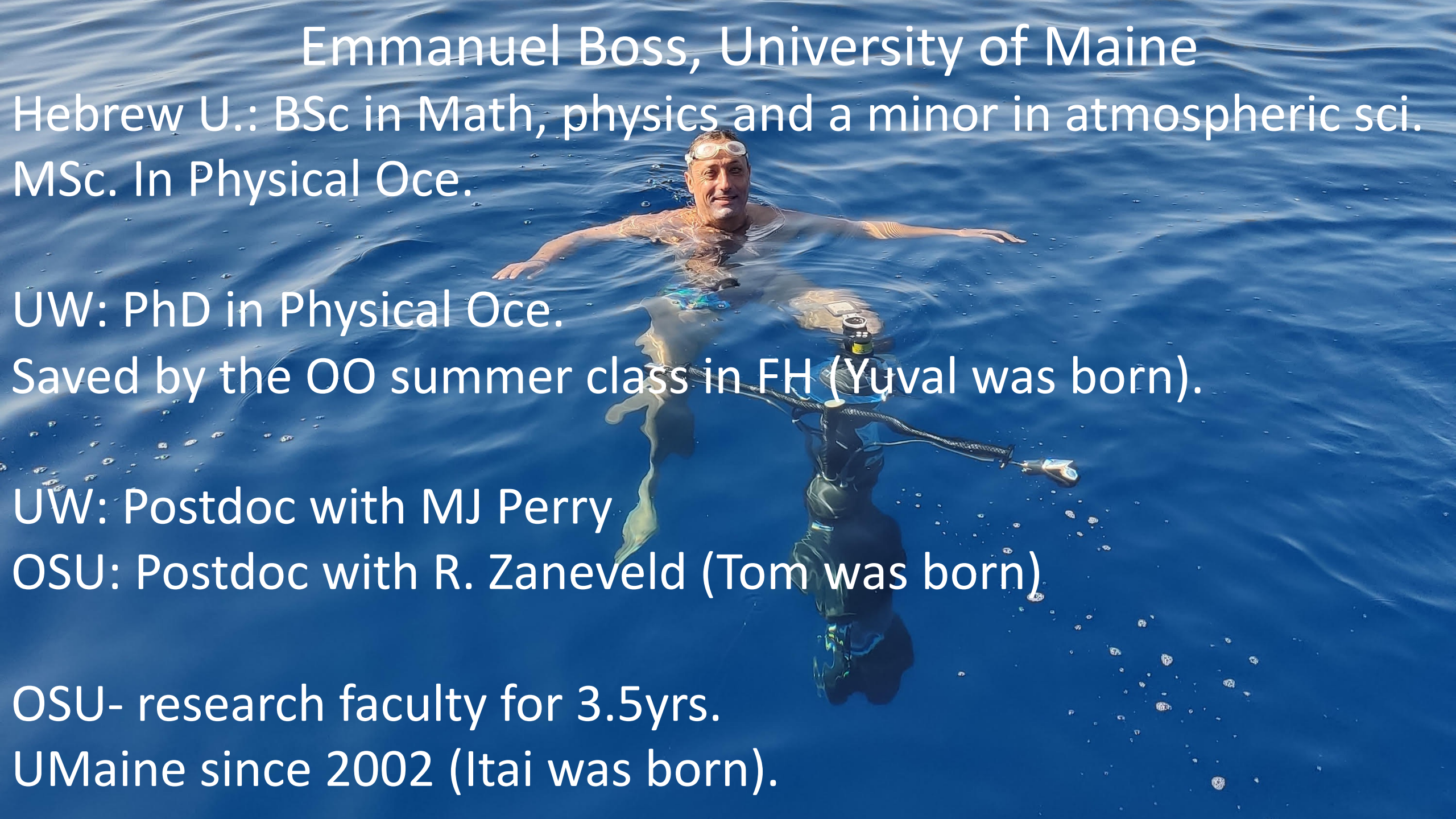
Emmanuel Boss, University of Maine

Hebrew U.: BSc in Math, physics and a minor in atmospheric sci.
MSc. In Physical Oce.

UW: PhD in Physical Oce.
Saved by the OO summer class in FH (Yuval was born).

UW: Postdoc with MJ Perry
OSU: Postdoc with R. Zaneveld (Tom was born)

OSU- research faculty for 3.5yrs.
UMaine since 2002 (Itai was born).



Challenges to obtain IOPs of aquatic environments

Emmanuel Boss, University of Maine

Take home messages:

- What is your reference/blank?
- We almost NEVER measure what we want.
- Do not trust data unless convinced otherwise (closure).
- Know well every instrument you work with data from so ***you*** can recognize when data is reasonable.

What is your reference/blank

Most instruments report a signal even when no real signal comes to the detector. How do we establish what the 'No-signal' level is?

In spectrophotometry, we use a substance of known IOPs (e.g. water). Our measurements are done *relative* to it (we set it to zero with water).

Why does this create problems (think of Mike's talk)?

What is your reference/blank

Problem with using water has a blank:

1. Requires access to an excellent water purifier.

2. How do we know the water is good?

3. Water's IOP are temperature and salinity dependent.

4. Water's IOPs are known, but uncertainties may be large.

And…

Spectroscopy

You are using an AC-S, you calibrate it in the lab or at sea with DIW (H_2O).
From Mike's talk you know that AC=absorption & attenuation.

1. How do you know the calibration was any good (or which calibration to choose in case you are calibrating daily on a cruise)?

2. Assuming you are only interested in properties of particles. What can you use as an alternative reference to water?

Spectroscopy

1. You are at sea/lab and you observe the values of absorption and/or attenuation drifting as function of time for a constant sample. What is likely happening?

2. You are at sea/lab calibrating your AC-S and you are observing the signal to be noisy/spiky. What are possible sources of such spikes? What could you do to deal with it?

3. You have access to a cold and a warm room to perform calibration in. Which is likely to result in better calibrations and why?

Example: Integrating Cavity Absorption Meter (ICAM)

The promise

- Measures absorption in absence of scattering loss
- Huge improvement over the ac meters
- A UV channel

Applied Optics Vol. 45, Issue 35, pp. 8990-8998 (2006) • https://doi.org/10.1364/AO.45.008990

Design and analysis of a flow-through integrating cavity absorption meter

Deric J. Gray, George W. Kattawar, and Edward S. Fry

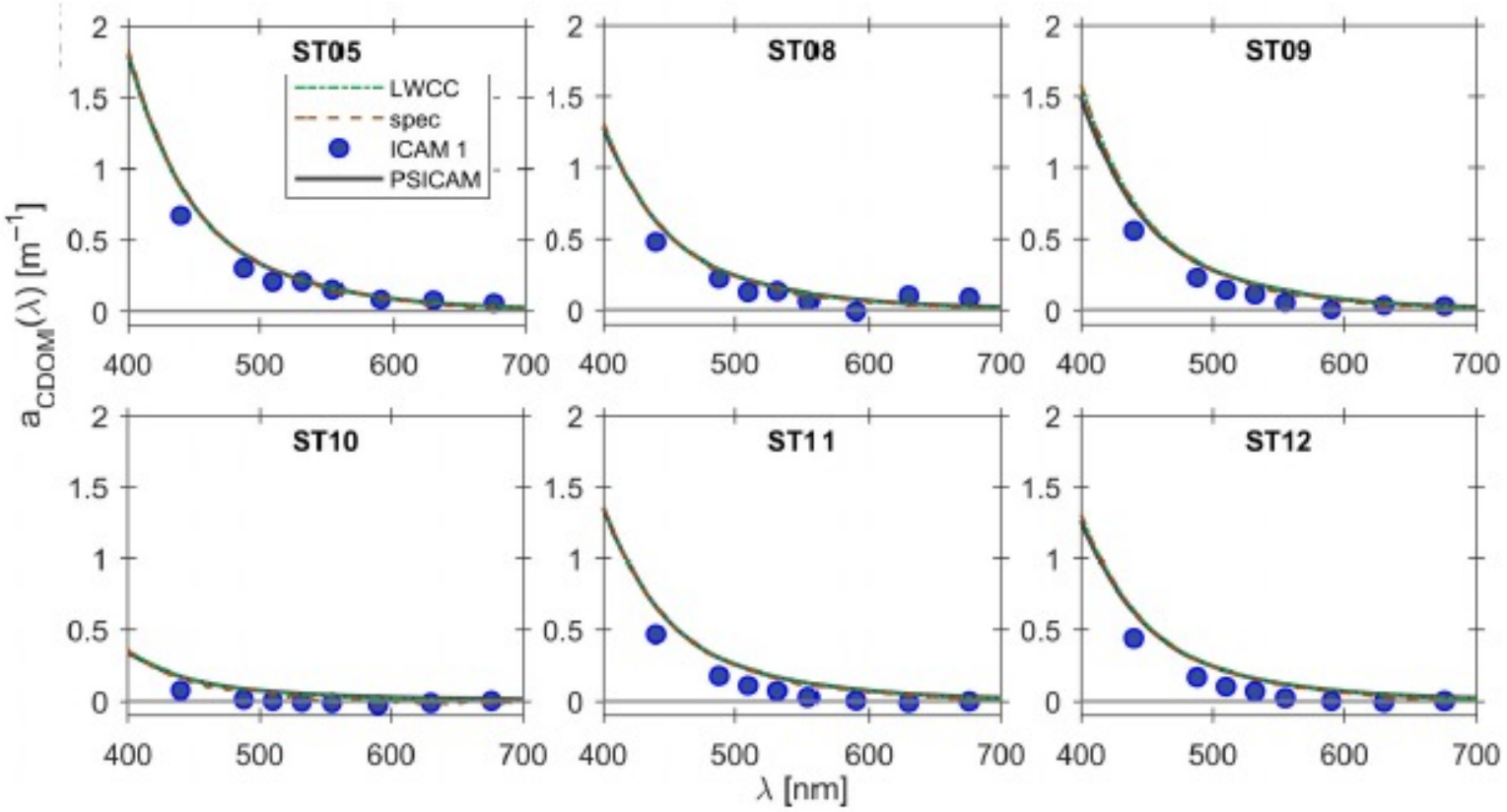
Applied Optics Vol. 48, Issue 19, pp. 3596-3602 (2009) • https://doi.org/10.1364/AO.48.003596

Flow-through integrating cavity absorption meter: experimental results

Joseph A. Musser, Edward S. Fry, and Deric J. Gray

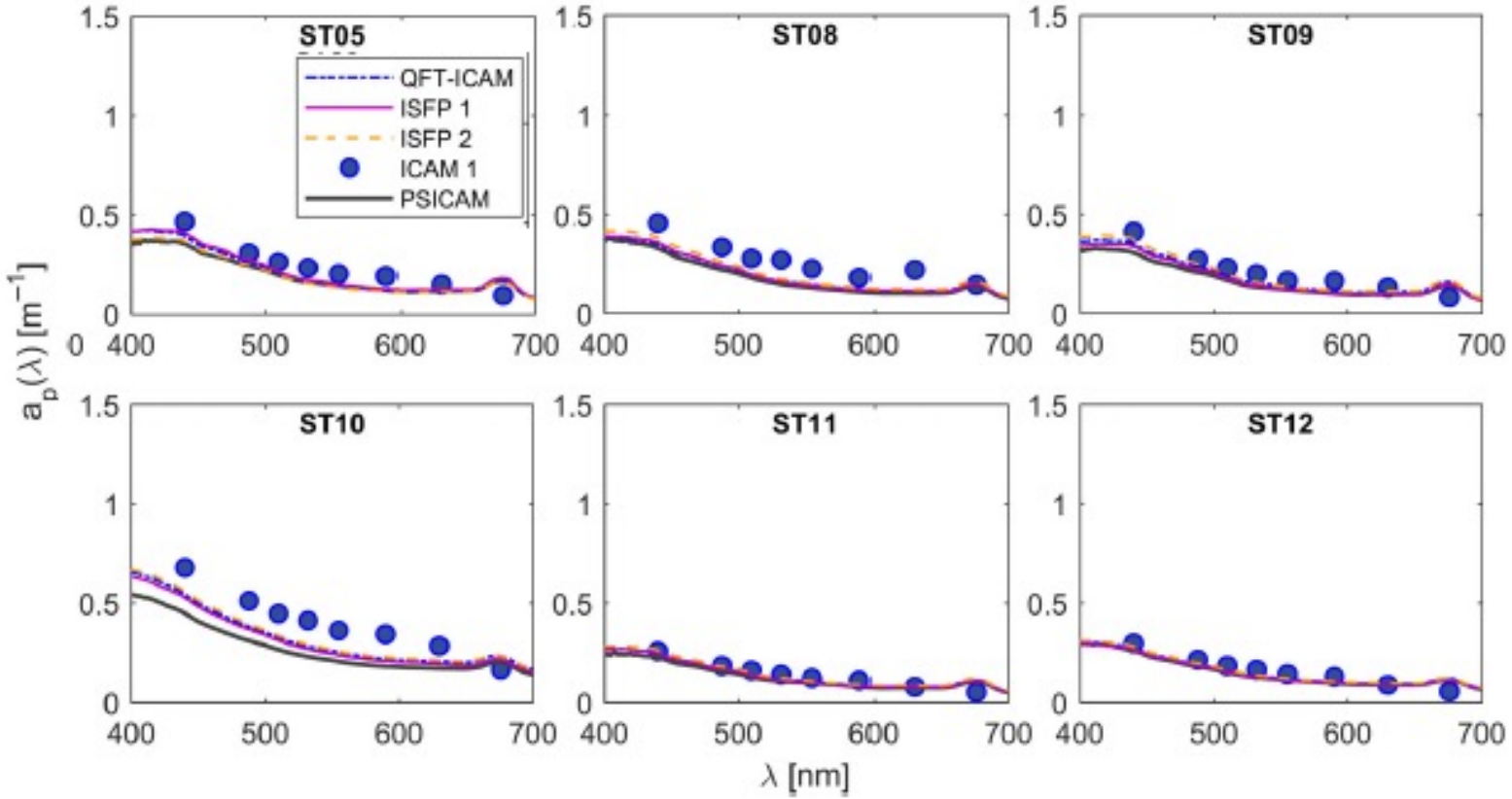
Commercialized by Turner Designs

- Step 1. closure between diverse approaches to compute absorption coefficient.
  - aCDOM (filtered water absorption)
  - Liquid Wave Guide, spectrophotometer, PSICam



Commercialized by Turner Designs

- Step 1. closure between diverse approaches to compute absorption coefficient.
  - ap Filter pad (PsiCAM, Integrating sphere)
  - ap by difference (PsiCam)



Step 2 measure absorption of phytoplankton culture

- last wavelength 676 nm, no resolution of red signal (outside abs band) for scattering correction
- Significant underestimation of absorption at 676 nm due to fluorescence stimulation by white light source

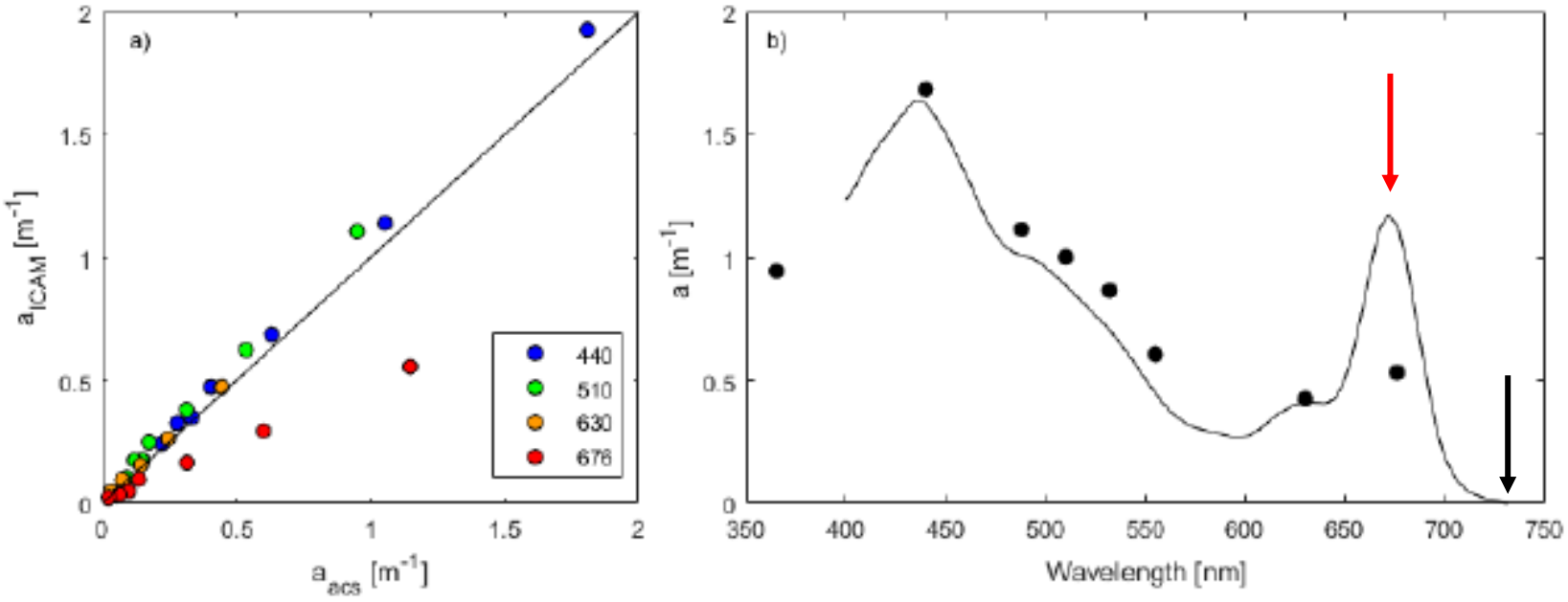


Figure S1. Results of determining the response of the ICAM to seven sequential dilutions of a cultured diatom, Thalassiosira pseudonana, with filtered seawater: a) absorption coefficients at 4 overlapping wavelengths measured with the ICAM and the AC-s; b) absorption spectra determined from the ICAM (black symbols) and the AC-s (black line) for one of the dilutions.

Step 3: sequential bead addition experiments

- add beams to suspension, measure absorption
- Results
  - Top row: ICAM and acs have similar responses (i.e., both show increasing "absorption)
  - Bottom row:
    - scatter corrected acs shows no response to bead additions
    - ICAM shows increased signal in response to bead addition
- ICAM
  - sensitive to scattering interference in absorption measurement but lacks capability for correction
  - Red absorption peak absorption underestimated due to white light stimulation of chlorophyll fluorescence

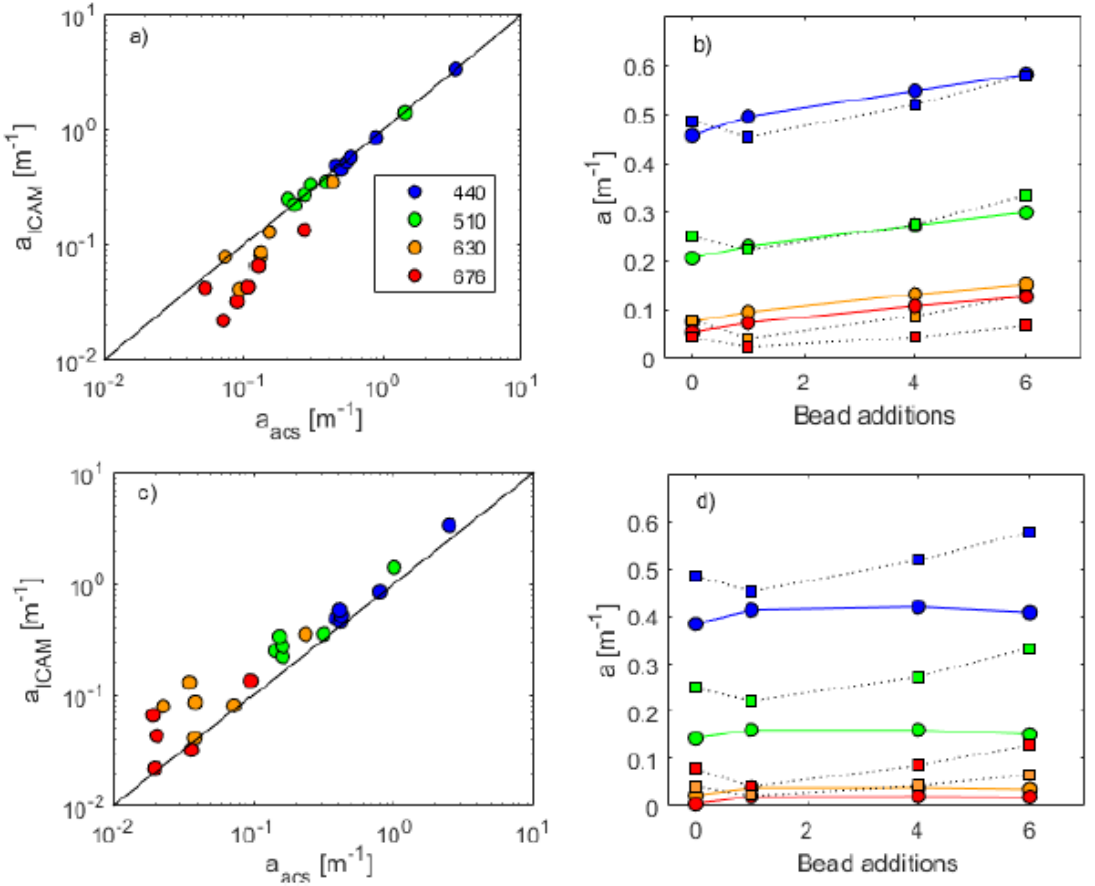


Figure S2. Results of determining absorption coefficients with the AC-s and ICAM in response to sequential additions of non-absorbing polystyrene beads, a) absorption coefficients at 4 comparable wavelengths measured on each sample with the AC-s and ICAM after temperature correction and calibration with MQ© water; b) dependence of apparent absorption coefficients at the four wavelengths as a function sequential bead additions for the AC-s (circle symbols and solid lines) and ICAM (square symbols and dotted lines), symbol colours indicate wavelength as in part a; c) as in part a after scattering corrections applied to the AC-s absorption coefficients; d) as in part b after scattering corrections applied to the AC-s absorption coefficients.

What is your reference/blank

Because the index of refraction of water is salt and temperature dependent, the amount of light crossing the water-window interface varies between blank and sample.

How do we measure the beam attenuation?

$$I(L) = I(0)T^2_{\text{G-}W}e^{-cL}$$

$$T_{\text{G-W}} = \frac{4n_G n_W}{(n_G + n_W)^2}$$

$$I_{DIW}(L) = I(0)T^2_{G\text{-}DIW}e^{-c_{\text{DIW}}L}$$

$$Tr = \frac{I_{sample}(L)}{I_{DIW}(L)} = \frac{T^2_{G\text{-}SW}}{T^2_{G\text{-}DIW}}e^{-\left(c_{sample+SW} - c_{DIW}\right)L}.$$

$$c_{measured} = \frac{log(Tr)}{L} = c_{sample+SW} - c_{DIW} - \frac{2}{L}log\left(\frac{T_{G\text{-}SW}}{T_{G\text{-}DIW}}\right)$$

What is your reference/blank

$$c_{measured} = \frac{log(Tr)}{L} = c_{sample+SW} - c_{DIW} - \frac{2}{L} log\left(\frac{T_{G-SW}}{T_{G-DIW}}\right)$$

Salinity increases the index of refraction of water (makes it more like glass).

→ Transmission term is positive.

Problem is *worst* for short pathlength instruments (e.g. LISST).

Indeed, I measured attenuation = - 0.06m^{-1} for a sample of dead-sea water filtered with a 0.2um filter (Boss et al., 2013, JGR).

Typically, this issue is negligible (*homework*).

Why do we use instruments with different pathlength?

We want to maximize signal/noise.

We want to minimize multiple scattering.

Uncertainty in beam attenuation:

$$c = \frac{\log(Tr)}{L} \rightarrow |\delta c| = \left|\frac{\delta L \log(Tr)}{L^2}\right| + \left|\frac{\delta Tr}{TrL}\right| \rightarrow \frac{|\delta c|}{c} = \left|\frac{\delta L}{L}\right| + \left|\frac{\delta Tr}{Tr\log(Tr)}\right|$$

Largest relative error when $Tr=1$ or $Tr=0$.

Minimal relative uncertainty is when $Tr=1/e$ or when $c=1/L$.

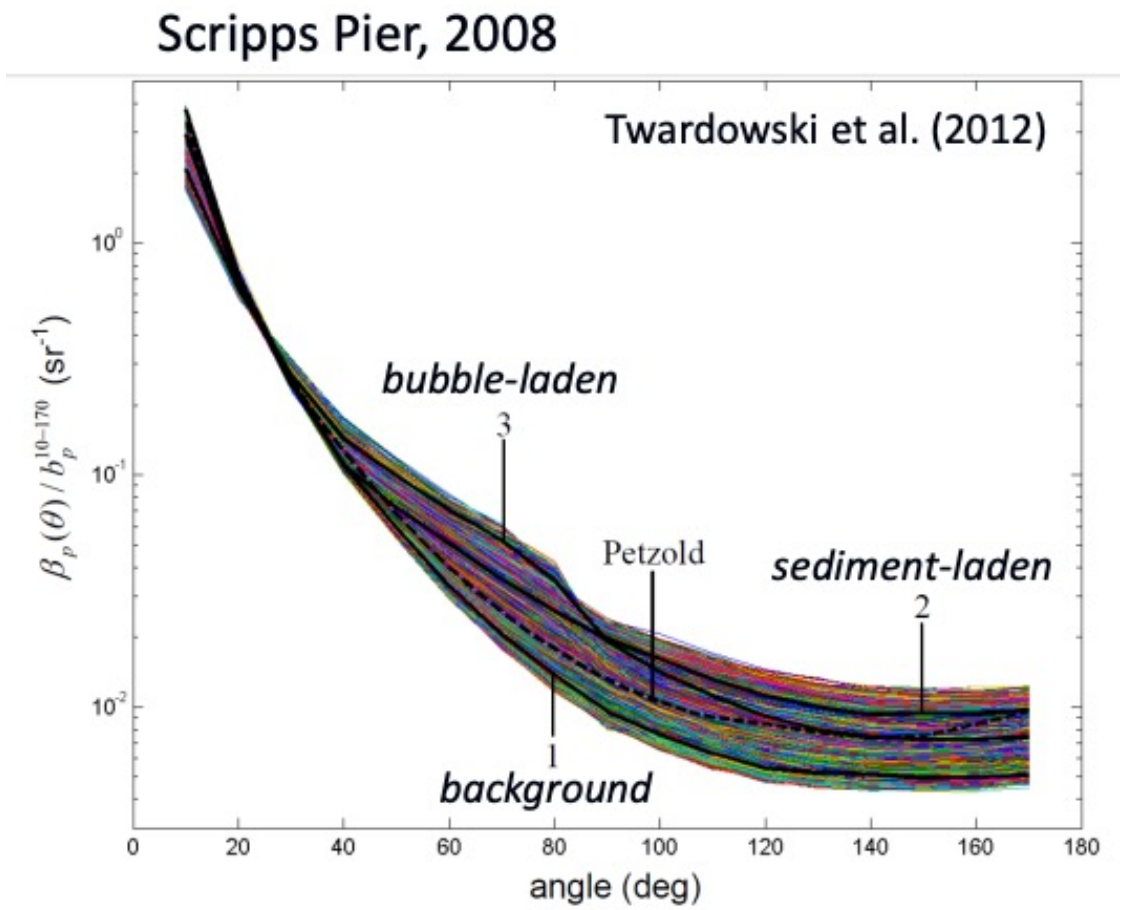
With a 0.25m sensor, $c=$ 4m^{-1}.

We almost NEVER measure what we want

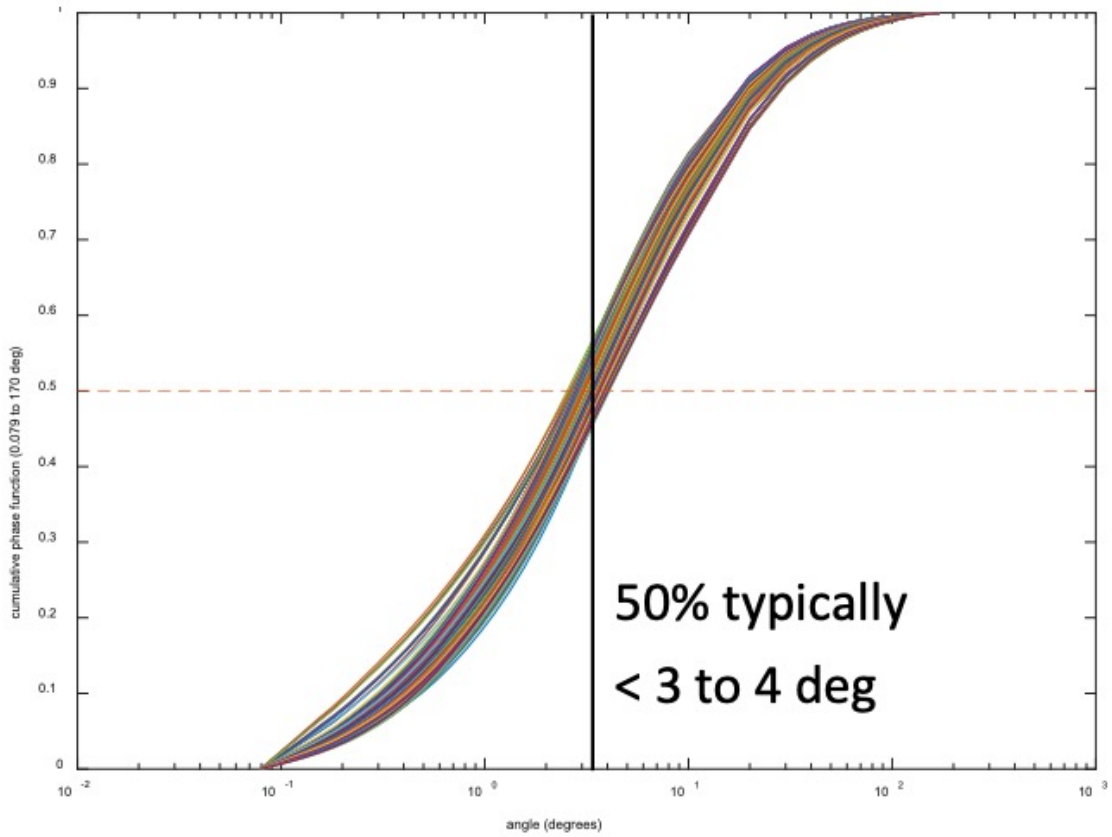
Commercial sensors measuring the beam attenuation comes in many flavors (NB: acceptance angle is in DIW ← why do they vary?):

Instrument	Manufacturer	Acceptance Angle (degrees, in-water)	Pathlength	Wavelength (bandwidth)	Beam Diameter
C-STAR-10	WETLabs	1.2	10cm	650 (20)nm	15mm
C-STAR-25	WETLabs	1.2	25cm	650 (20)nm	15mm
AC-9-10	WETLabs	0.93	10cm	676 (10)nm	8mm
AC-9-25	WETLabs	0.93	25cm	676 (10)nm	8mm
AC-S-25	WETLabs	0.93	25cm	650(15)nm	8mm
LISST-100-B	Sequoia Scientific	0.0269°	5cm	670 (0.1)nm	6mm
LISST-100X-B	Sequoia Scientific	0.0269°	5cm	670 (0.1)nm	6mm
LISST-100X-Floc	Sequoia Scientific	0.006°	5cm	670 (0.1)nm	6mm

How do you expect beam attenuation to change with acceptance angle? From Mike's talk:



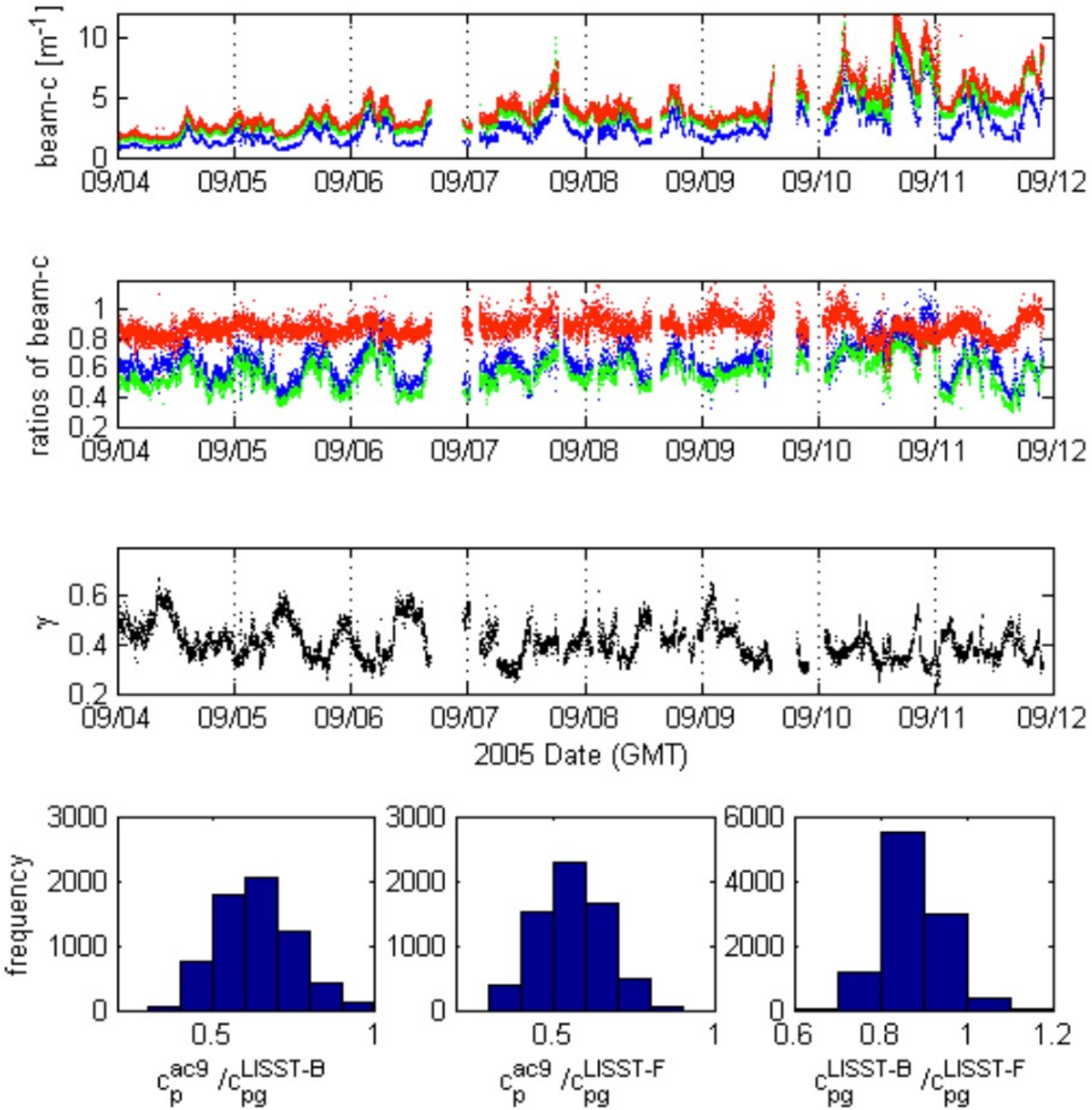
Cumulative scattering contribution:



How does it look in field data:

What do we need to get the theoretical beam-c?

Is it a problem for RT computations associated with Rrs?, For POC?



How much information is there in an IOP?

- How can we assess how much information we can glean from an IOP?
- Should we strive for IOP instruments with 0.1nm resolution?

- When I was a postdoc, everything was described as function of Chl a.
- Indeed, much ***does*** co-vary with Chl a (e.g. species composition and size).
- Provides a benchmark: ***what more is there beyond what Chl a tells us?***

How much information is there in an IOP?

- Information theory (includes the Shannon index, DoF) is designed to answer such questions (given Chl a how surprising is the observed b_b?).

- To what degree (N) can I compress a signal and still be able to describe it to within its noise level. E.g.:

$$a_p(\lambda) = \sum_{n=1}^{N} A_i \dot{a}_{p,i}(\lambda) + \delta(\lambda)$$

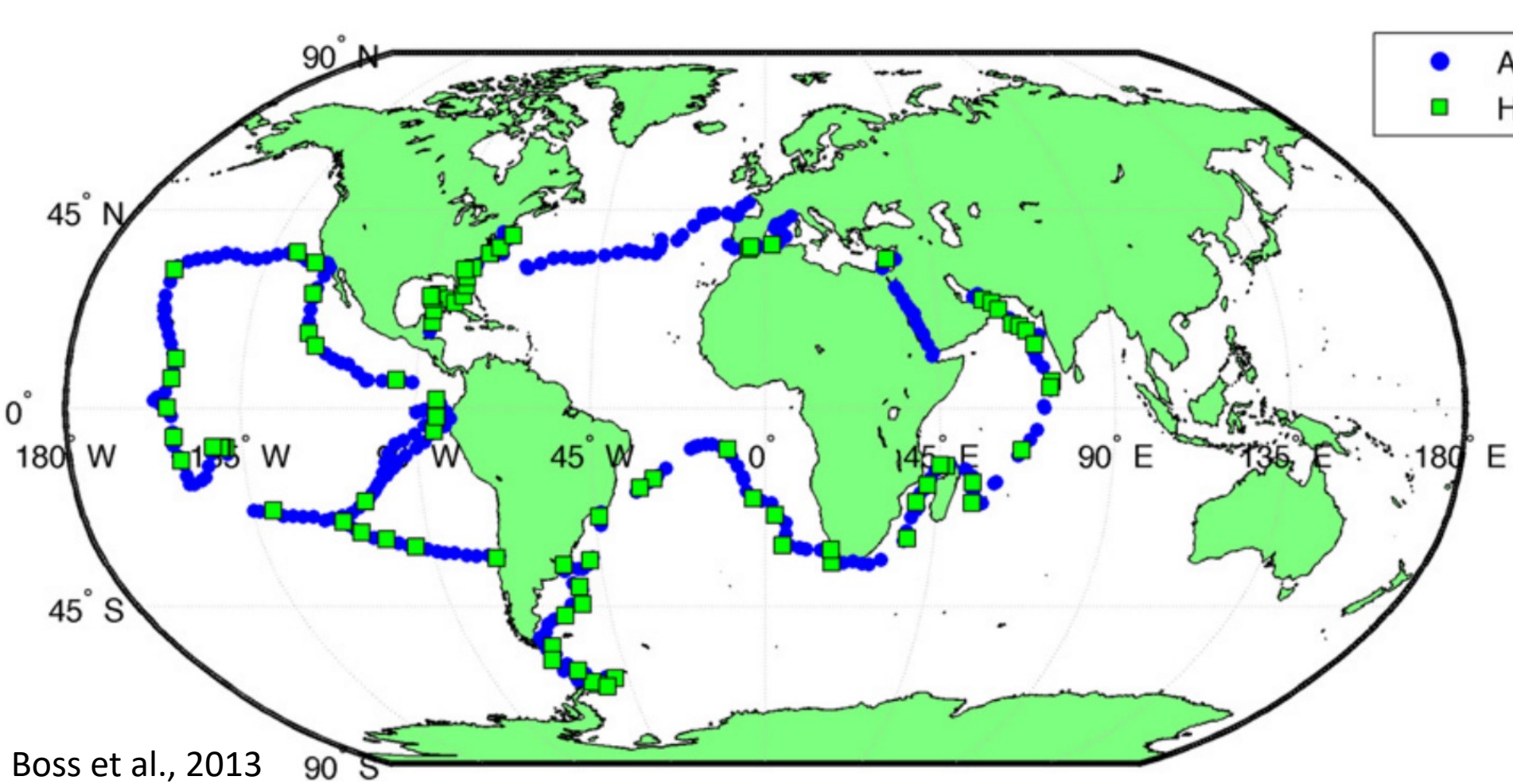
- Linear and non-linear decomposition methods – EOF, PCA – methods to extract variability in signal. Major limitation - what is the meaning of each modes?

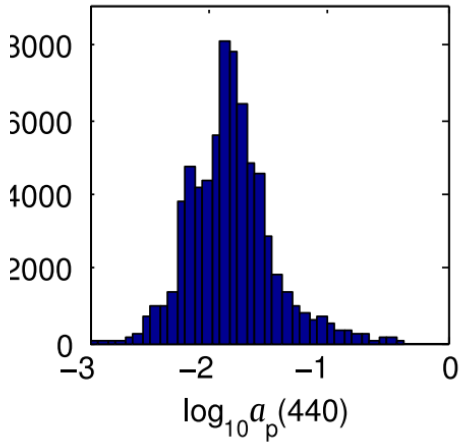
- In atmospheric science, Twomey set a theoretical linear framework.

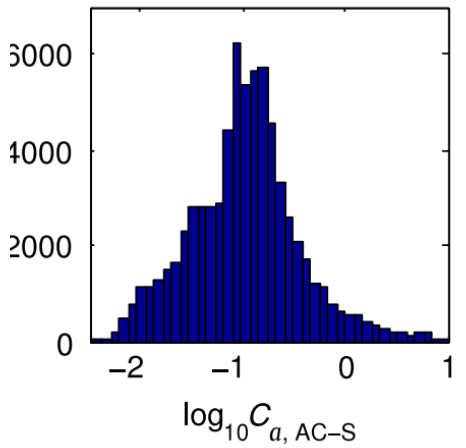
How much information is there in an IOP?

- Need for a large dataset that spans oceans.

- Consistent collection methodology → the Tara dataset.



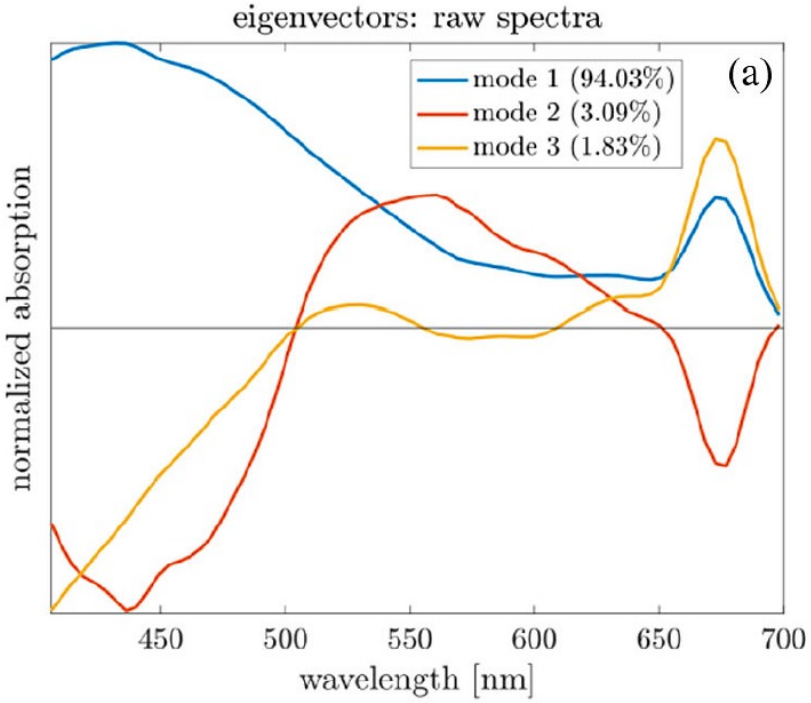


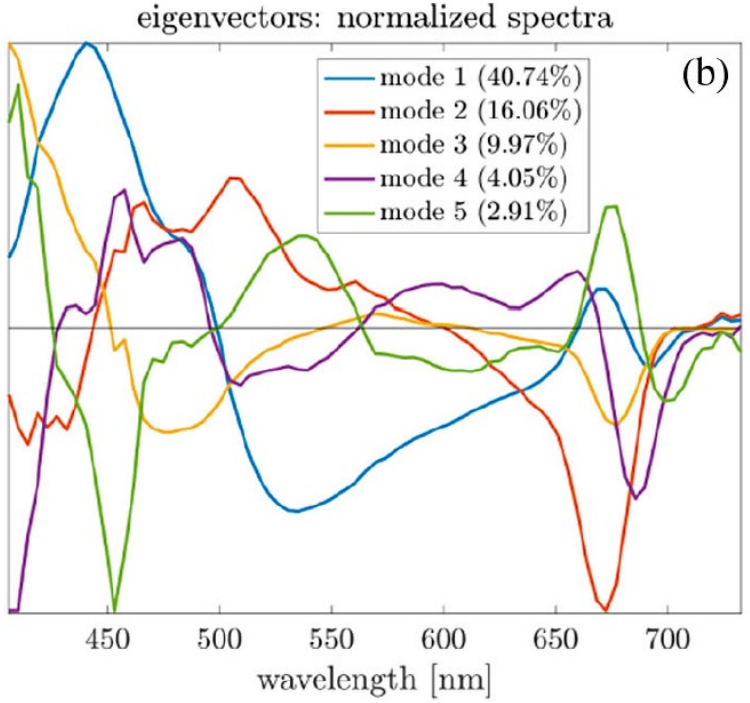


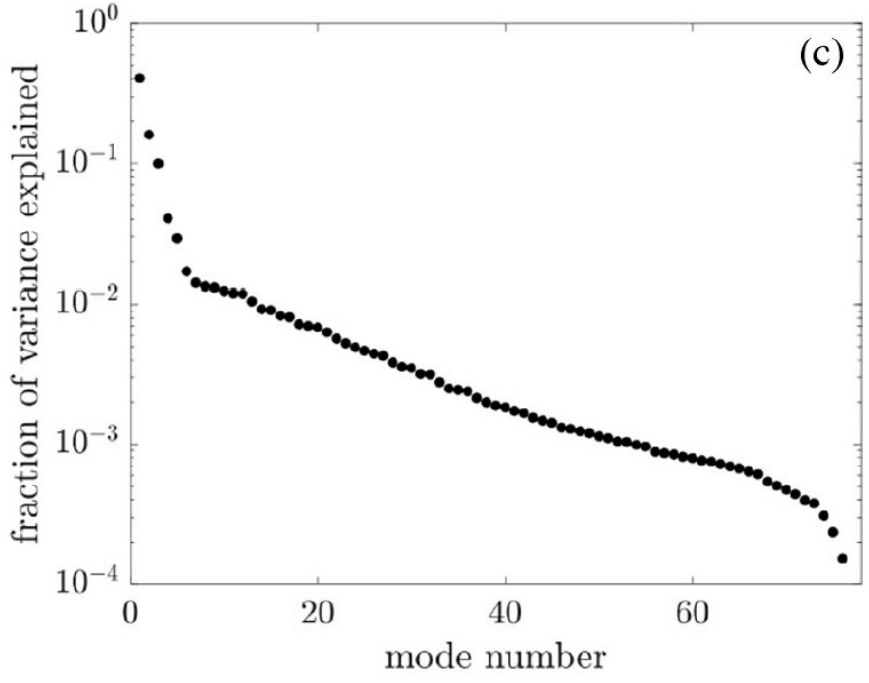
Boss et al., 2013

How much information is there in an IOP?

Example: straight forward PCA analysis:







Cael et al., 2020

How much information is there in an IOP?

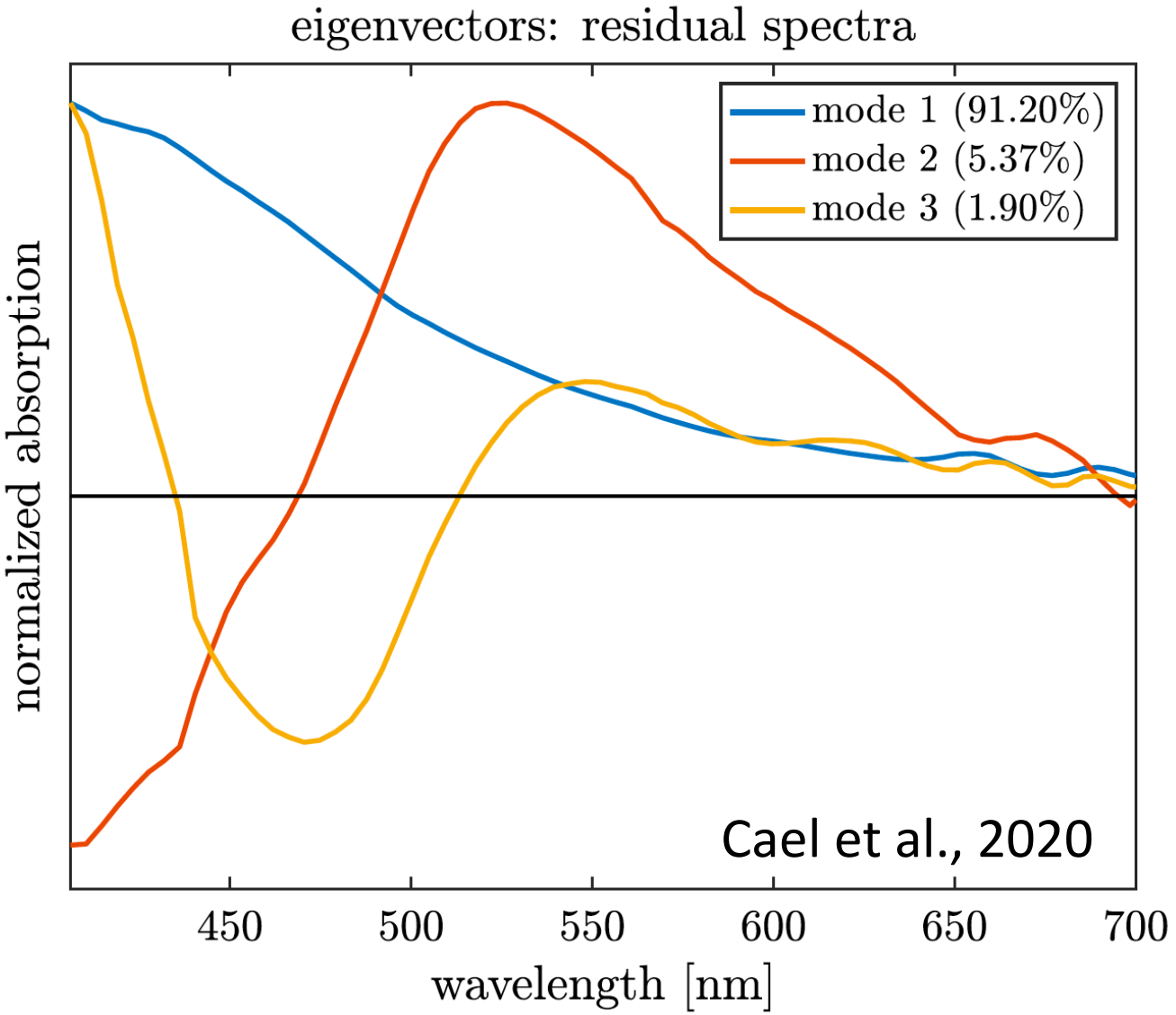
Example: PCA analysis of residuals of a_p (after removing Chl a covarying part)

Covarying part (Bricaud, Chase):

$$a_p(\lambda) = A(\lambda)\mathrm{Chl}_{\mathrm{ALH}}^{B(\lambda)},$$

Lessons:

1. Chl_a domination.
2. 4 DoF.
3. Judicious choices provide more ‘meaningful’ results.
4. 0.1nm resolution will not buy us much.

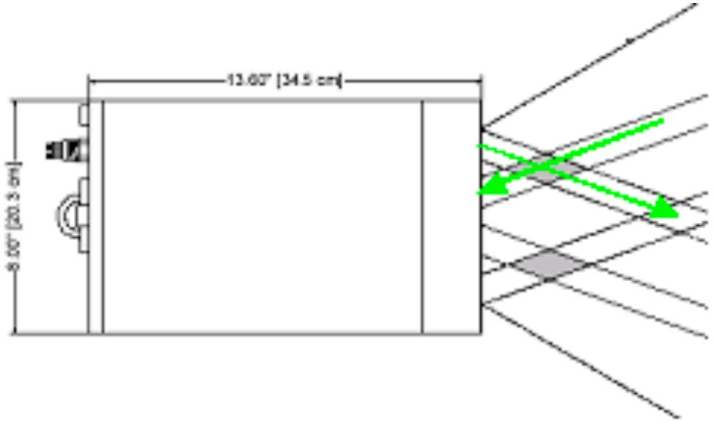


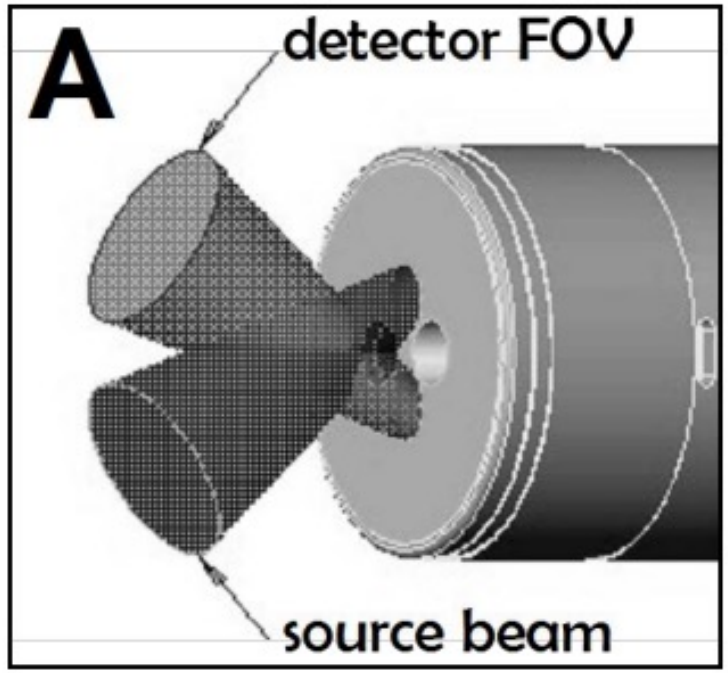
How much information is there? Analysis of anomalies in Rrs.

	412R443,488,547	443R412,488,547	488R412,443,547	531R412,443,547	547 R412,443,488	667R412,443,547	Chl (OC3M)	nflh	Chl (GIOP)	Chl(GSM)	POC	aph(443,GIOP)	aph(443,QAA)	adg(443,GIOP)	adg(443,GSM)	adg(443,QAA)	CDOM index	a(443,QAA)	bbp anomaly	bbp(443,GIOP)	bbp(443,GSM)	PIC	bbp(443,QAA)	Zeu_lee	Zeu_morel	IPAR	PAR	SST4	Rrs(412)	Rrs(443)	Rrs(488)	Rrs(531)	Rrs(547)	Rrs(667)	Rrs(678)	BSI	Kd(490)	Kd(443)_lee	Kd(PAR)_morel	Ångström exp.
443R412,488,547	-59	–																																				
488R412,443,547	-17	0	–																																				
531R412,443,547	1	-5	22	–																																			
547R412,443,488	3	-4	1	45	–																																		
667R412,443,547	-3	8	8	26	20	–																																	
Chl (OC3M)	-4	-2	20	22	12	14	–																																
nflh	-3	-4	14	27	25	15	46	–																															
Chl (GIOP)	6	-14	10	27	29	9	74	43	–																														
Chl(GSM)	3	-9	14	24	21	10	86	44	94	–																													
POC	-4	-3	21	24	13	16	99	41	73	85	–																												
aph(443,GIOP))	6	-14	10	27	29	9	74	43	100	95	70	–																											
aph(443,QAA)	9	-18	11	31	33	9	79	43	93	91	75	93	–																										
adg(443,GIOP)	-16	2	22	12	3	11	84	25	45	59	83	45	44	–																									
adg(443,GSM)	-8	1	19	14	4	12	92	30	57	70	91	57	56	97	–																								
adg(443,QAA)	-18	3	21	12	3	11	88	27	47	63	89	47	48	97	97	–																							
CDOM index	-67	39	14	-4	-14	3	19	2	-5	8	20	-5	-6	47	36	44	–																						
a(443,QAA)	-4	-2	18	20	9	15	98	37	71	84	99	71	74	87	95	92	17	–																					
bbp anomalies	15	-4	-27	-22	-22	-18	-9	-7	3	-5	-12	3	-4	11	11	13	5	12	–																				
bbp(443,GIOP)	-2	-5	31	84	53	26	31	33	36	35	34	36	41	13	18	15	-6	26	-54	–																			
bbp(443,GSM)	-1	-4	30	71	48	20	35	33	33	37	40	33	39	19	24	22	-5	33	-52	95	–																		
PIC	-1	-3	25	69	51	25	43	38	43	46	46	43	48	20	28	24	-3	37	-44	91	93	–																	
bbp(443,QAA)	-1	-3	27	76	55	30	37	37	42	42	39	42	46	15	21	18	-2	30	-55	96	93	91	–																
Zeu_lee	8	2	-22	-28	-20	-22	-93	-48	-69	-80	-93	-69	-73	-73	-81	-78	-12	-89	4	-41	-50	-54	-49	–															
Zeu_morel	4	2	-20	-23	-12	-15	-100	-41	-74	-86	-98	-74	-78	-83	-91	-86	-13	-97	1	-31	-40	-44	-37	95	–														
IPAR	27	-12	-21	-8	-6	-43	-19	-28	-8	-12	-18	-8	-7	-21	-19	-21	-15	-16	17	-17	-16	-17	-19	32	19	–													
PAR	24	-16	-23	-10	-5	-35	-23	-29	-13	-16	-21	-13	-11	-24	-22	-23	-14	-19	12	-14	-13	-15	-17	36	23	86	–												
SST4	28	-11	-27	-9	-5	-25	-24	-27	-12	-16	-24	-12	-11	-28	-25	-27	-17	-21	14	-17	-16	-17	-19	39	25	83	88	–											
Rrs(412)	6	-1	-13	-11	-3	-9	-78	-21	-48	-60	-74	-48	-46	-93	-92	-89	-39	-81	-7	-6	-5	-9	-9	65	77	12	16	11	–										
Rrs(443)	2	0	-9	-9	-2	-7	-75	-20	-52	-63	-70	-52	-49	-85	-87	-81	-28	-78	-11	-4	-3	-7	-7	61	74	7	11	6	96	–									
Rrs(488)	0	0	0	1	1	1	-53	-11	-36	-44	-51	-36	-31	-66	-68	-64	-25	-60	-28	0	2	-1	0	40	53	1	4	2	82	91	–								
Rrs(531)	-1	-4	23	73	55	23	15	20	18	16	18	18	21	9	10	12	-15	14	-71	85	75	70	80	-23	-16	-15	-13	-15	12	9	17	–							
Rrs(547)	-1	-2	27	78	57	29	23	28	29	27	25	29	33	8	11	10	-5	17	-65	93	85	84	94	-34	-24	-19	-15	-16	-3	-2	3	94	–						
Rrs(667)	-1	0	16	48	48	66	36	38	35	37	37	35	40	16	22	19	-1	30	-41	73	72	73	80	-51	-38	-30	-29	-23	-8	-6	-1	58	72	–					
Rrs(678)	-1	-1	18	48	46	49	45	58	47	49	46	47	50	22	30	25	-1	39	-29	70	71	72	77	-61	-47	-33	-30	-25	-13	-11	-4	51	67	91	–				
BSI	-9	2	19	11	8	14	73	41	32	48	72	32	36	61	65	69	15	69	-5	25	36	37	29	-84	-74	-35	-40	-31	-44	-37	-22	8	19	34	44	–			
Kd(490)	-5	-3	18	26	17	19	98	44	77	87	97	77	81	76	86	81	10	95	-1	33	40	46	40	-96	-98	-19	-25	-17	-66	-68	-50	12	26	37	48	61	–		
Kd(443)_lee	-8	-2	23	23	12	18	98	43	68	81	98	68	71	85	92	89	18	96	-2	31	40	43	37	-97	-98	-26	-32	-23	-75	-73	-53	10	24	34	44	72	96	–	
Kd(PAR)_morel	-4	-2	20	22	12	14	100	41	74	87	98	74	78	83	91	87	13	97	-1	30	39	44	36	-94	-100	-18	-24	-17	-73	-73	-53	10	23	32	43	62	99	98	–	
Ångström exp.	3	0	-5	-5	-2	-5	5	-9	-3	-4	5	-3	4	4	5	5	1	5	3	-4	-3	-3	-3	4	-5	16	11	8	-5	-5	-5	-4	-4	-4	-6	-4	4	4	5	–
Aer. opt. thick. 869	0	-1	1	0	-4	-6	1	-1	0	0	1	0	0	2	1	1	2	1	8	-4	-4	-4	-5	1	-1	5	4	2	-2	-3	-4	-5	-5	-9	-4	-1	-1	1	1	-8

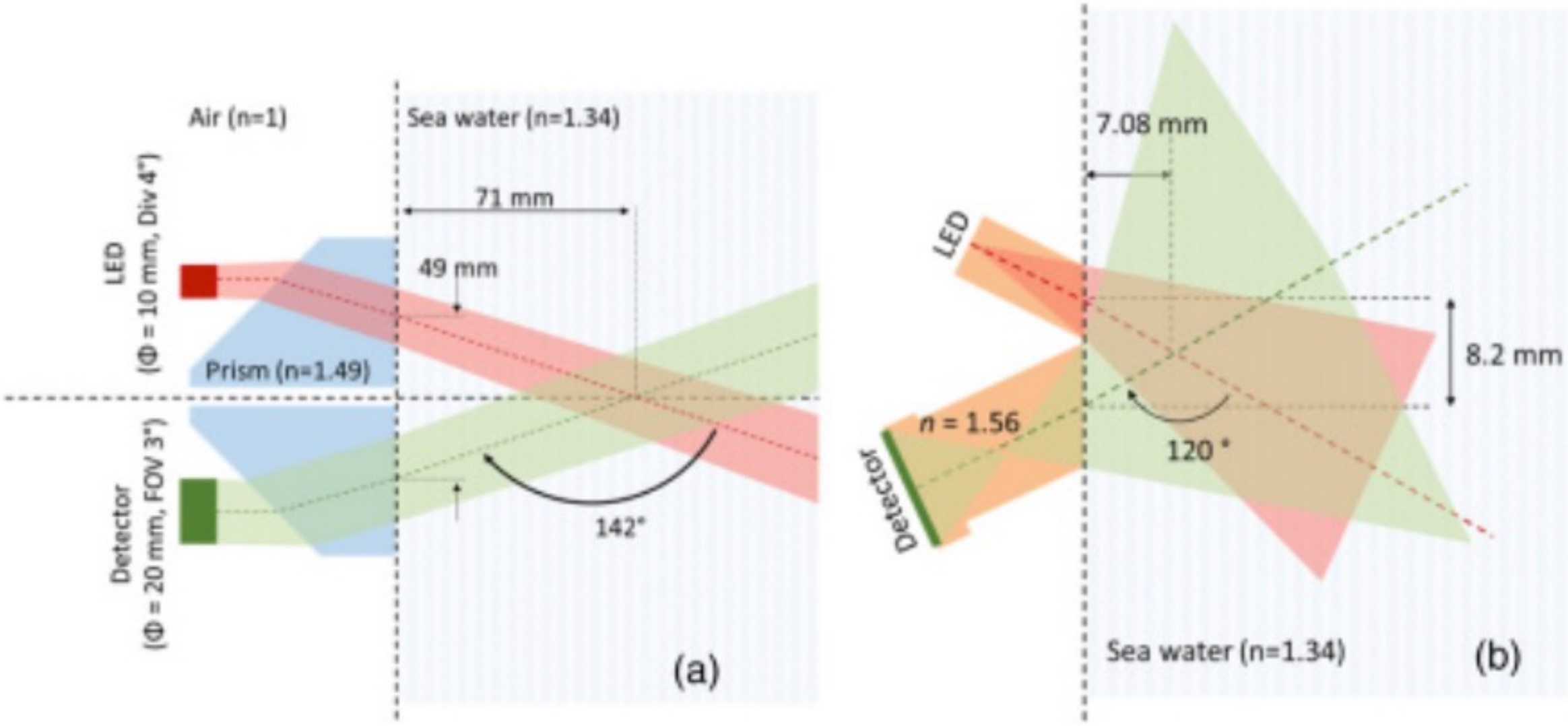
Huot and Antoine, 2016

Single (wide) angle backscattering sensors (recap from Mike)





Angular distribution HS-6 vs. Eco-BB:



Zhang et al., 2021

Different ways to calibrate these sensors: beads & reflective plaque

In case of plaque, need to know:

1. distance of plaque.
2. reflectivity of plaque (as function of wavelength).

In case of bead calibration, need to know:

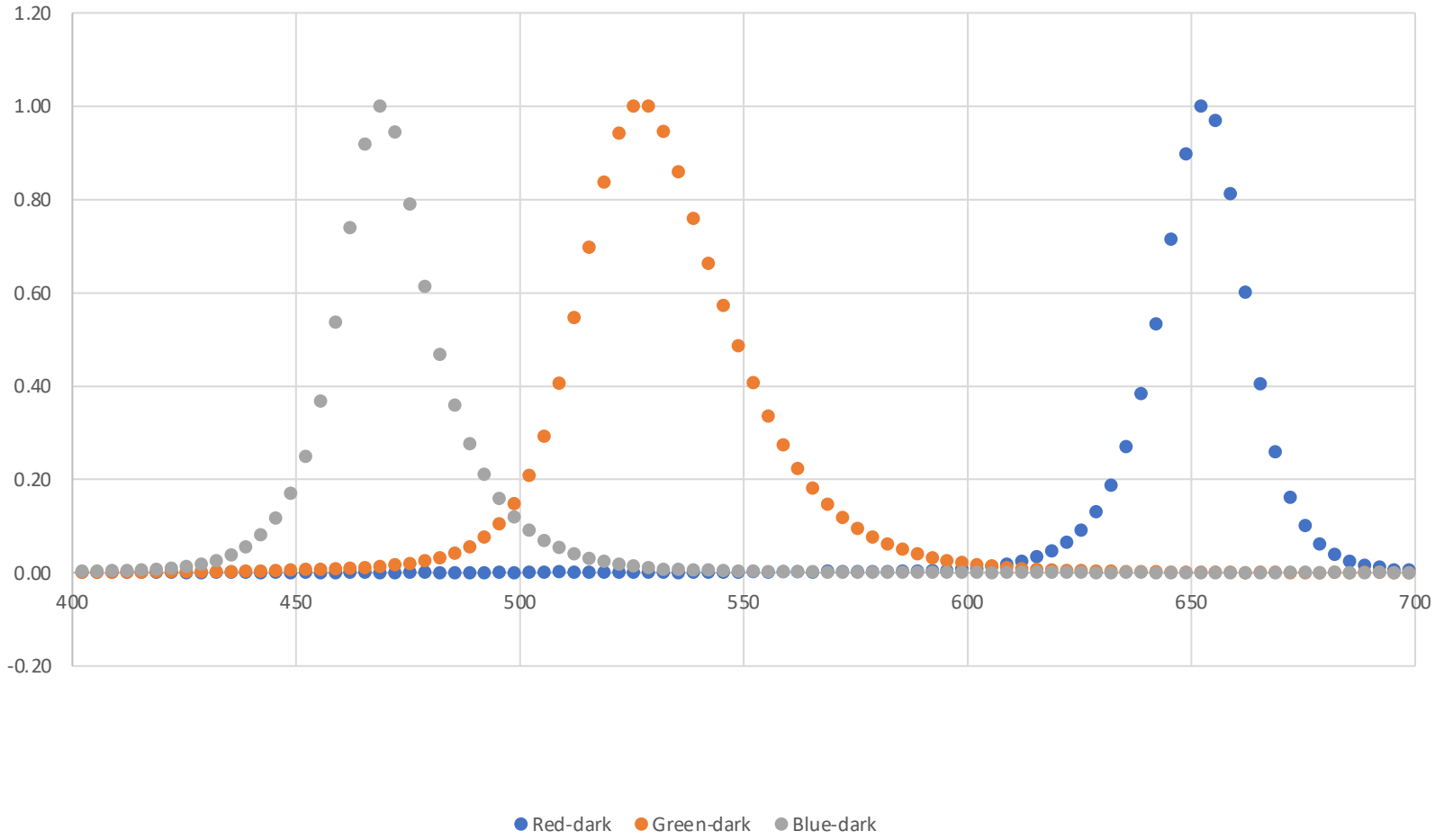
1. Angular response (centroid + dispersion).
2. Bead size and its dispersion.
3. Bead index of refraction.
4. Wavelength and its dispersion.

Comparison between both in the field – a way to evaluate ***uncertainties***.

Example: What wavelengths is your sensor?

Nominal wavelengths:

470
532
650



Matters when you do bead calibrations

You are given a backscattering sensor.

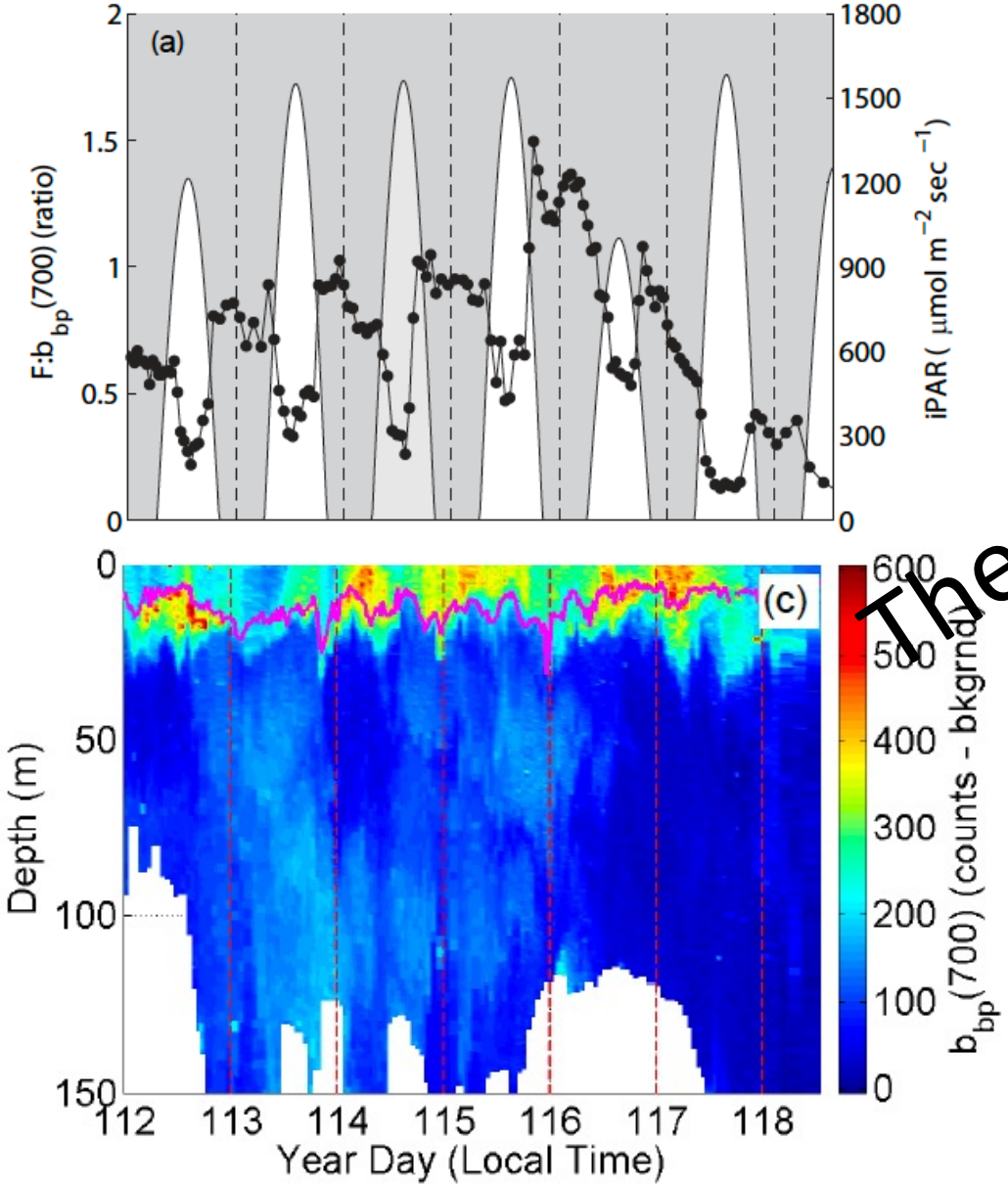
- You put it in water. What do you expect the signal to be?
- You leave it for a whole day on a mooring. How do you expect the signal to vary?
- Would you expect a change in signal if you changed the frequency of sampling?

You are given a fluorescence sensor.

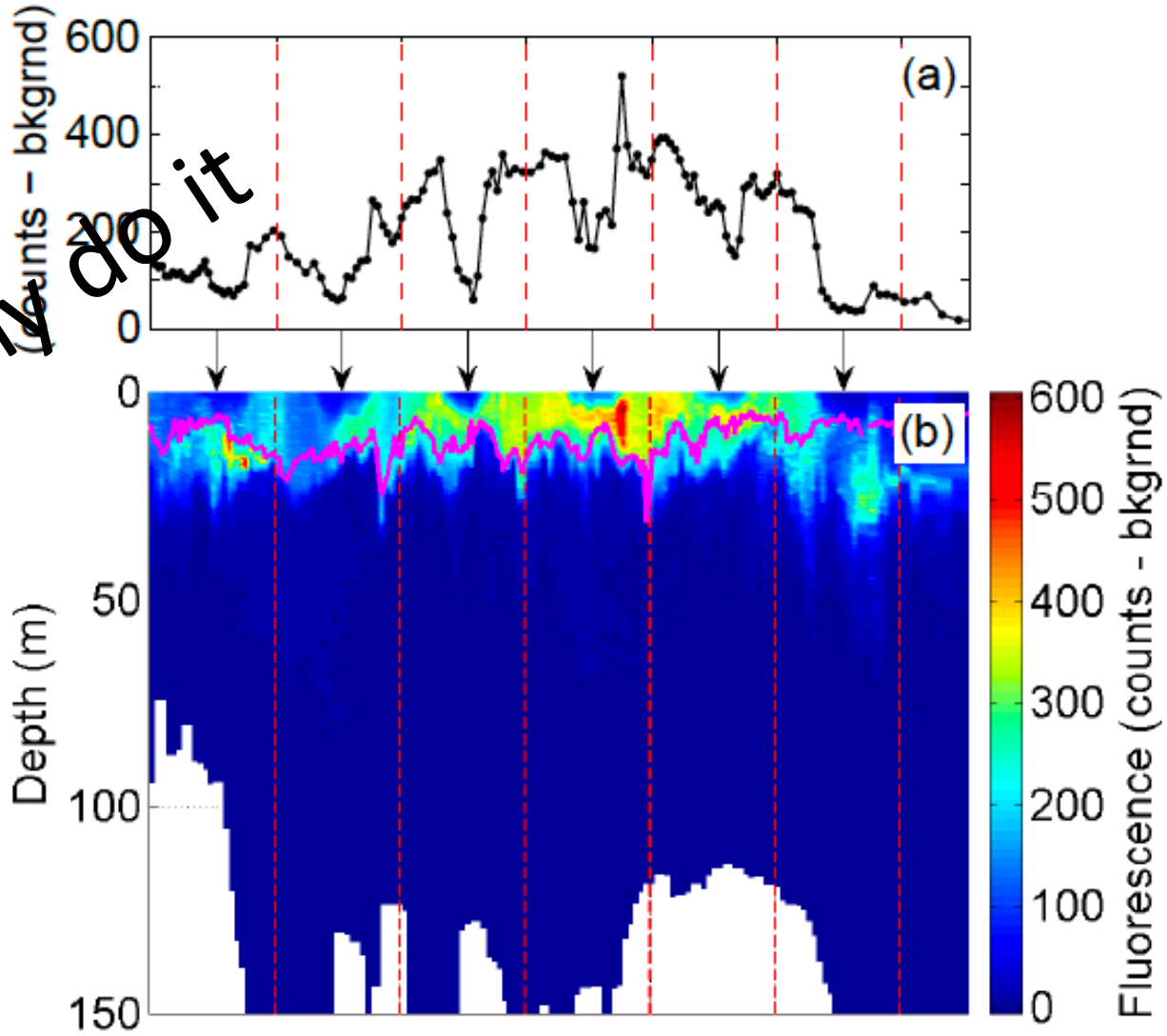
- You put it in water. What do you expect the signal to be?
- You leave it for a whole day on a mooring. How do you expect the signal to vary?
- Would you expect a change in signal if you changed the frequency of sampling?

Glider data: diel signal in F_{chl}

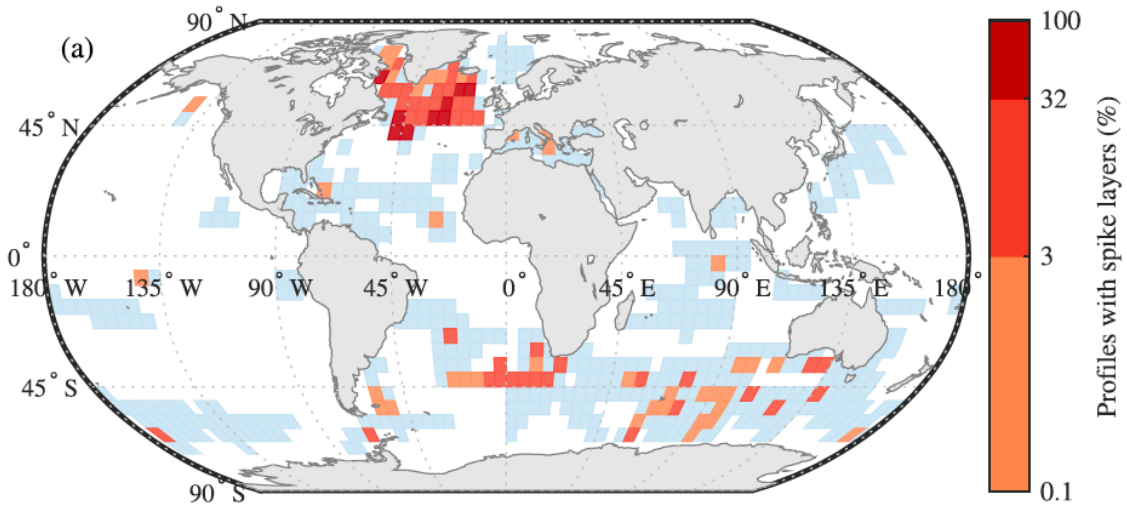
Sackman et al., 2008

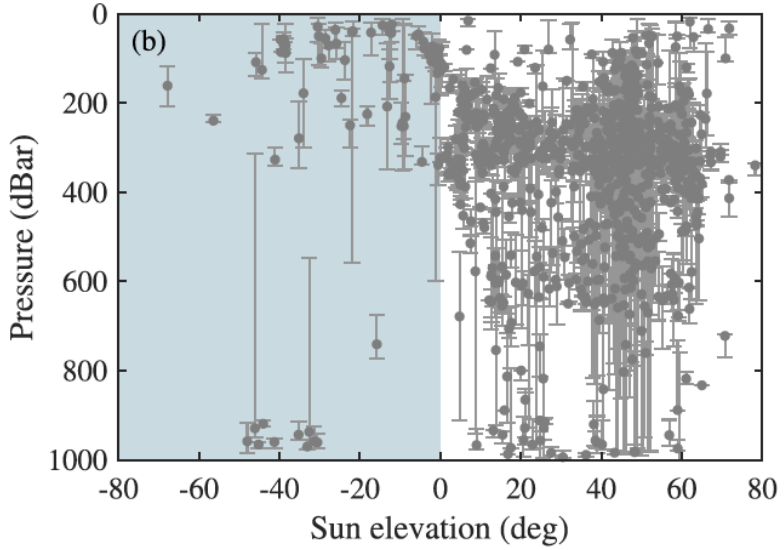


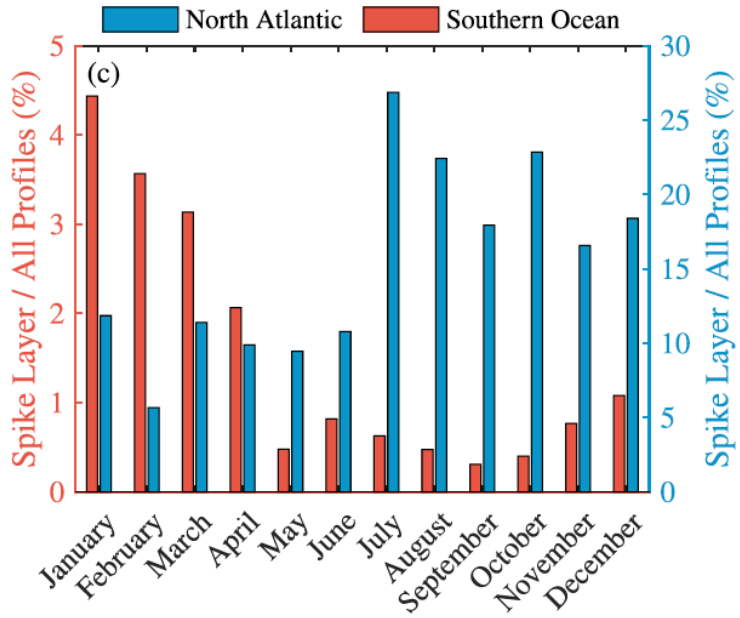
Then, why do it

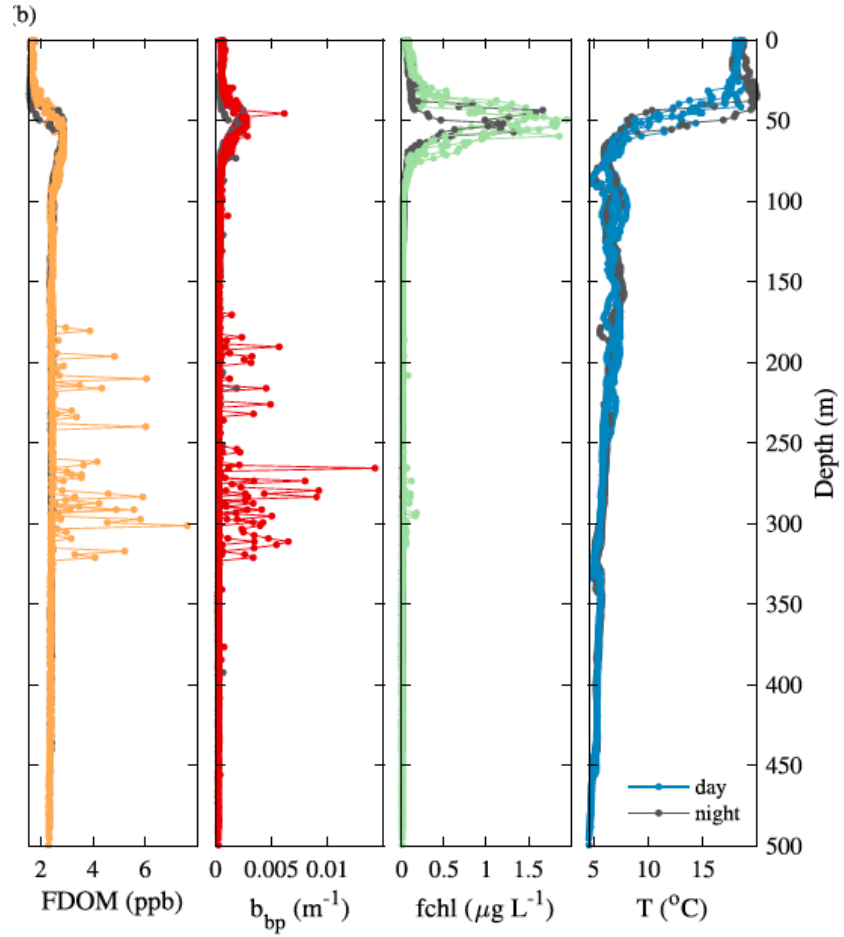


Argo float data: spikes in F_{cdom}



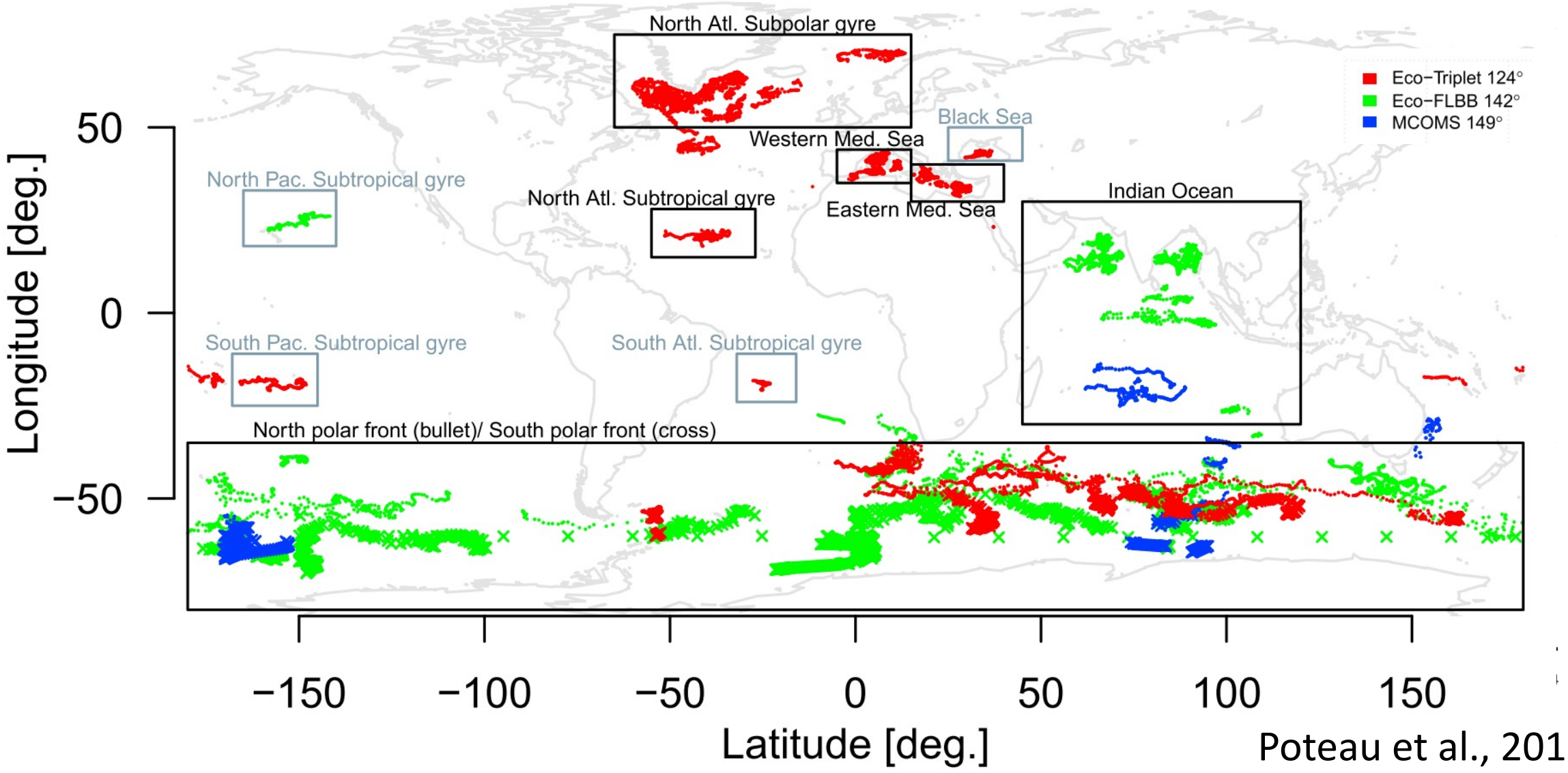






Haentjens et al., 2017

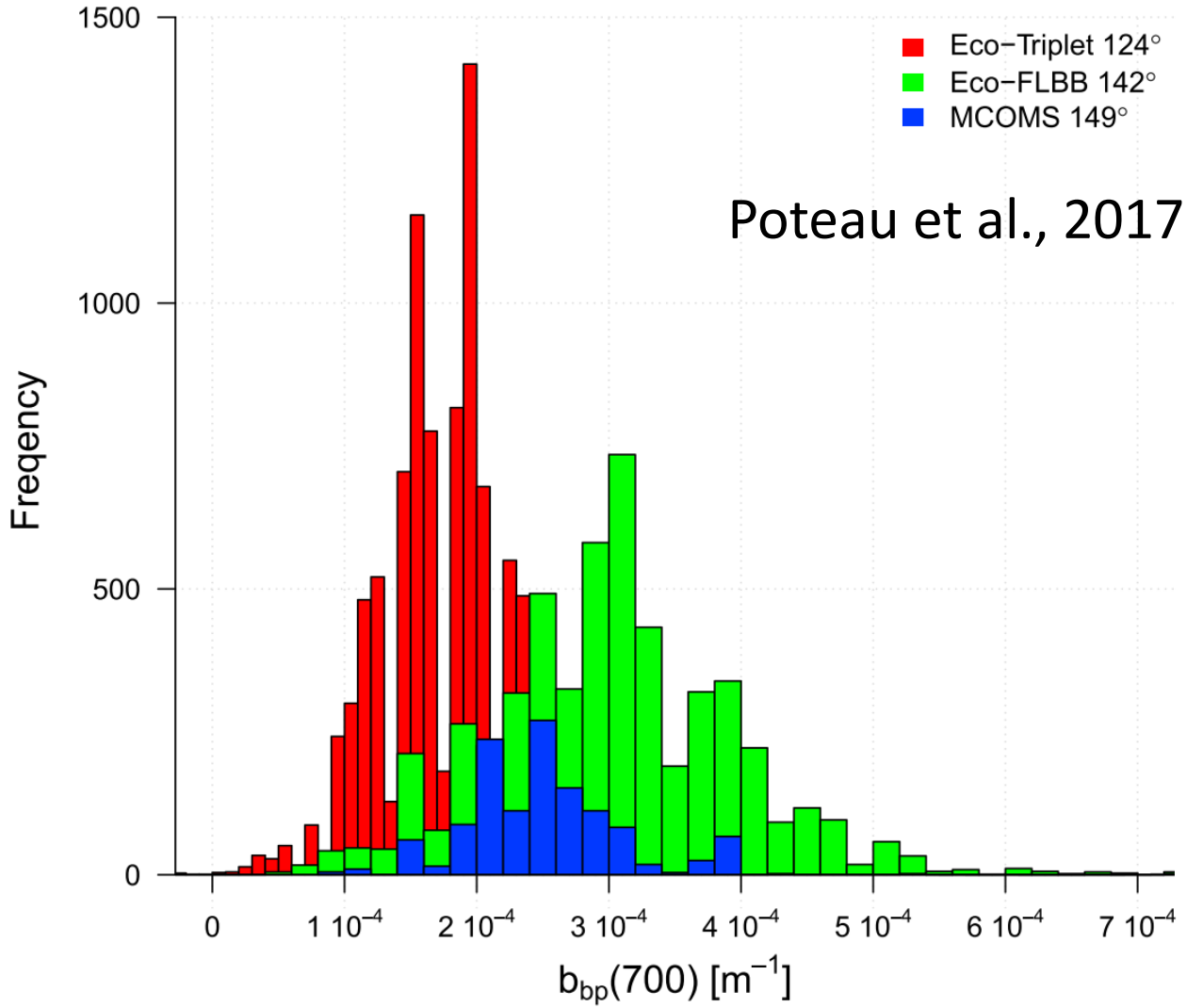
Closure: at great depth(>900m) we expect IOPs to be consistent.



Poteau et al., 2017

Always have at least two ways to get to the quantity of interest.

Closure: at great depth(>900m) we expect IOPs to be consistent.



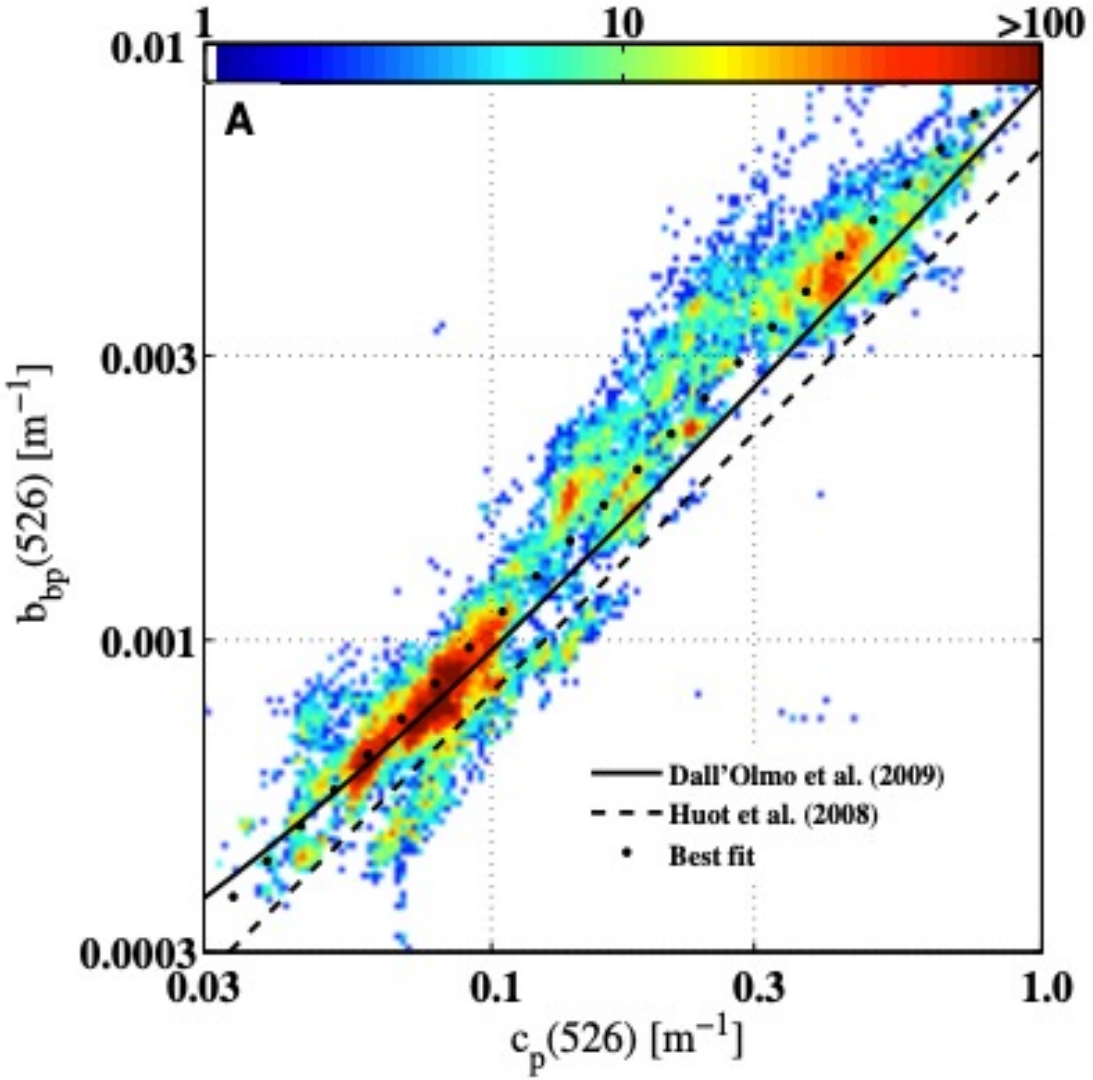
Poteau et al., 2017

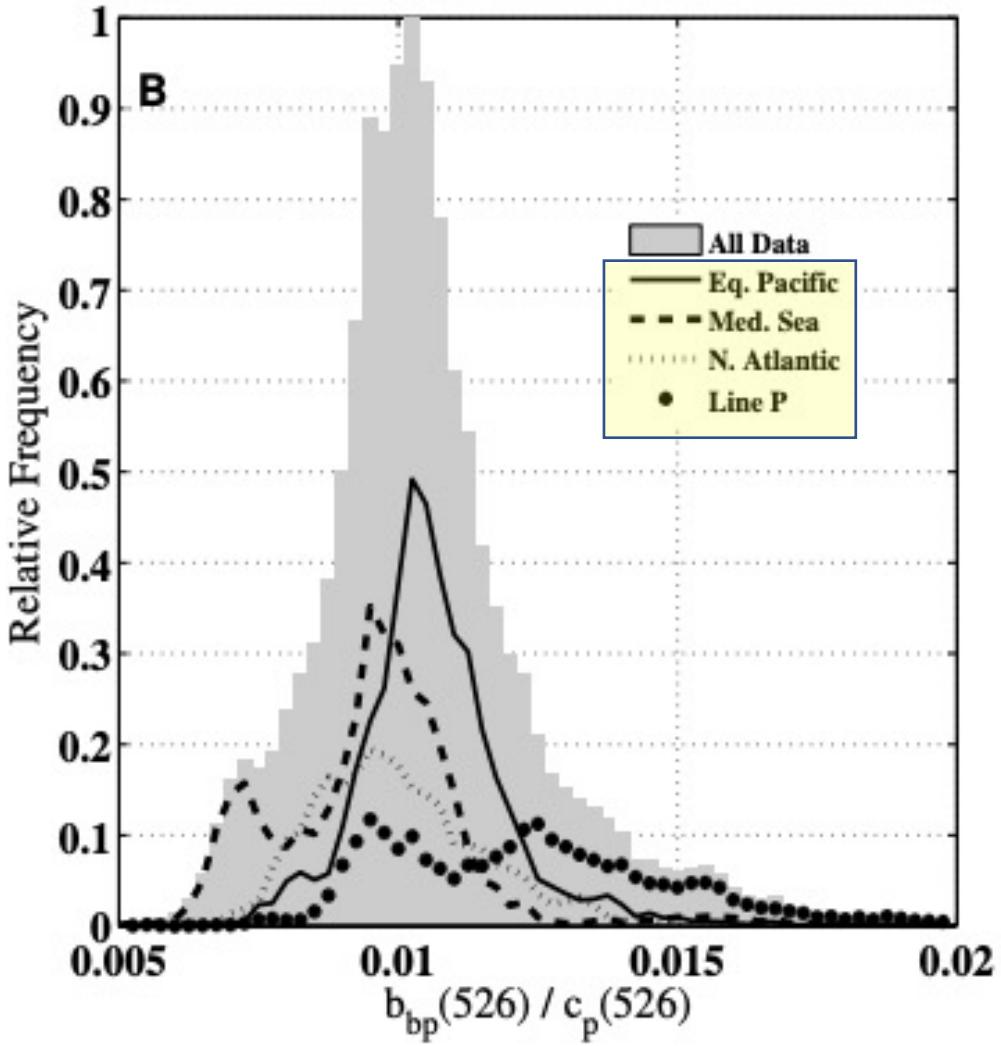
Resulted in the manufacturer looking back in their procedures and updating calibration coefficients.

Looking at distributions is a very powerful means to compare quantities.

Always have at least two ways to get to the quantity of interest.

Closure: Optical properties are correlated – respond first to concentration.





Always have at least two ways to get to the quantity of interest.

Westberry et al., 2010

Challenges to obtain IOPs of aquatic environments

Take home messages:

- What is your reference/blank?
- We almost NEVER measure what we want.
- Do not trust data unless convinced otherwise (closure).
- Know well every instrument you work with data from so ***you*** can recognize when data is reasonable.
- Think about information content.