Retrieval of phytoplankton pigments from underway spectrophotometry in the Fram Strait

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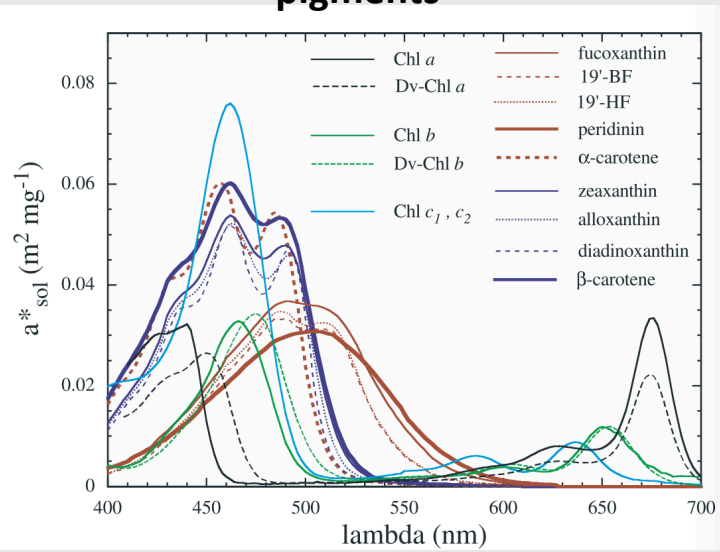
Phytoplankton pigments

- ✓ Help Snacking on SUNLIGHT — photosynthesis
- ✓ Protect against SUN BURNT — photoprotection

Source: Ocean Optics Web Book

Light absorption spectra of various pigments

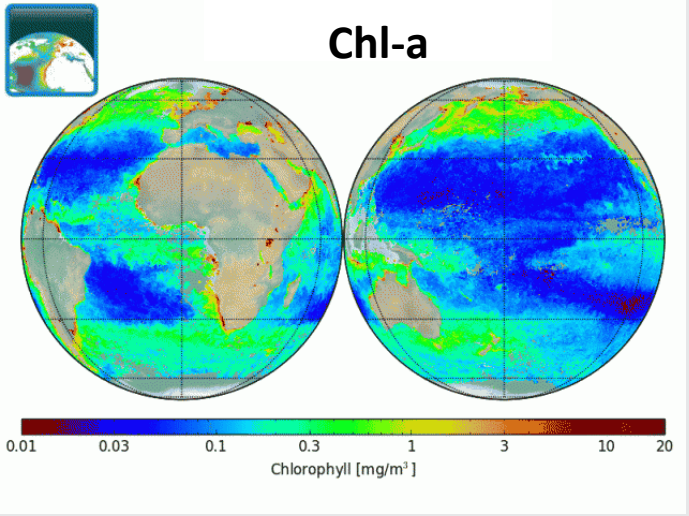


Source: Bricaud et al., 2004

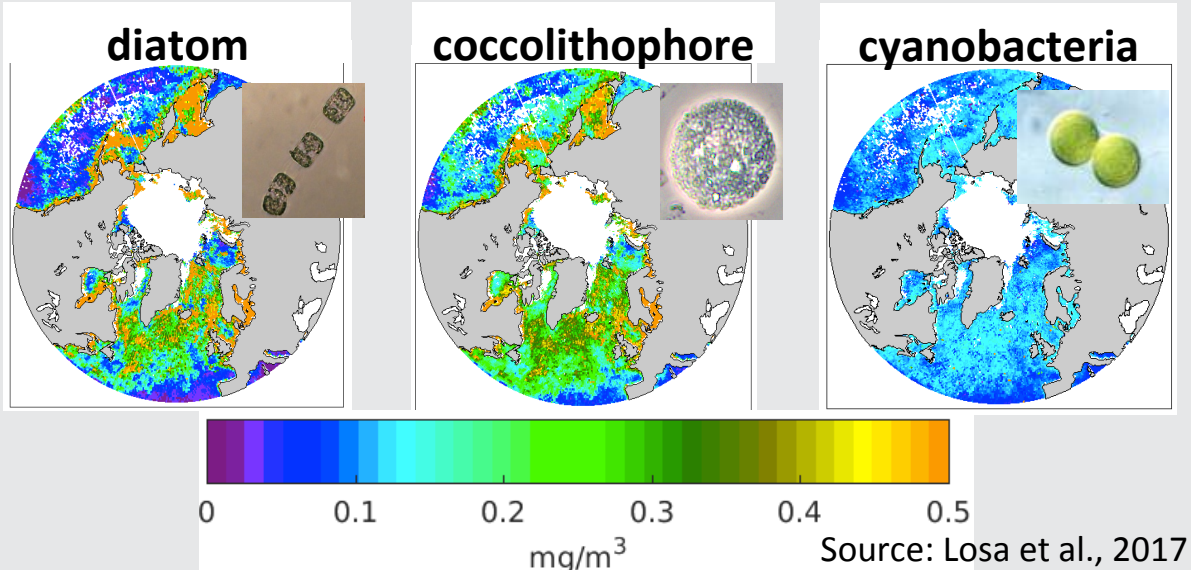
Phytoplankton pigments in remote sensing applications

develop, validate or refine bio-optical algorithms

- ✓ Phytoplannkton biomass
- ✓ Functional types:



Source: ESA Ocean Color CCI



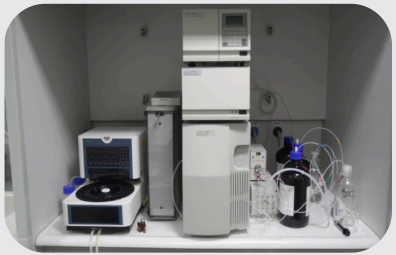
Source: Losa et al., 2017

Quantify phytoplankton pigments

1. Measure them using High Performance Liquid Chromatography (HPLC)


Discrete water sampling


---> Filtration


---> HPLC

2. Retrieve them from optical measurements (e.g. absorption, reflectance)

- ✓ **Spectral decomposition:**
  phytoplankton absorption = absorption of (pigment 1 + pigment 2 + …)
- ✓ **Spectral reconstruction:**
  absorption of (pigment 1 + pigment 2 + …) = phytoplankton absorption
- ✓ …

Esp. from *in situ* Optical sensors!

This study

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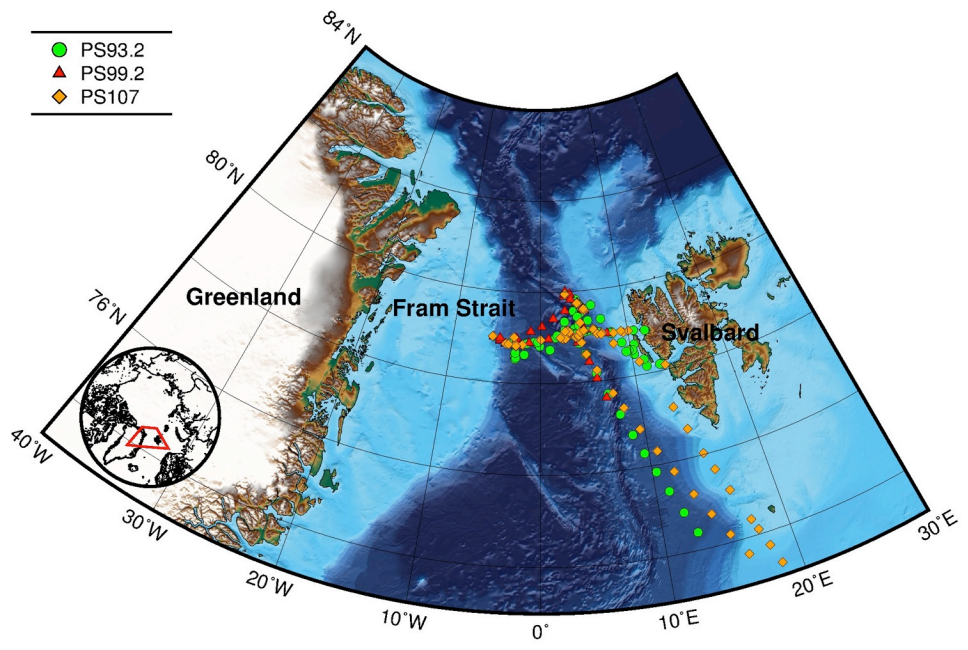
Fram Strait

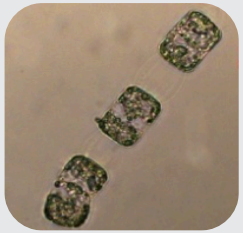


- ✓ Mass (75%), heat (90%) exchanges
- ✓ Sea ice mass export (10%)

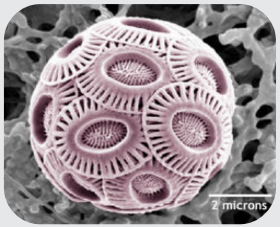
- ○ Climate change
- ○ Light & nutrient conditions change
- ○ **phytoplankton community change**

Satellite data: poor spatial-temporal resolution; lack of assessment of the applicability of global bio-optical algorithms

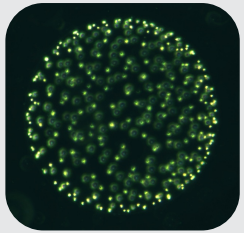
***In situ* data**: insufficient HPLC data, even less optical measurements



diatom

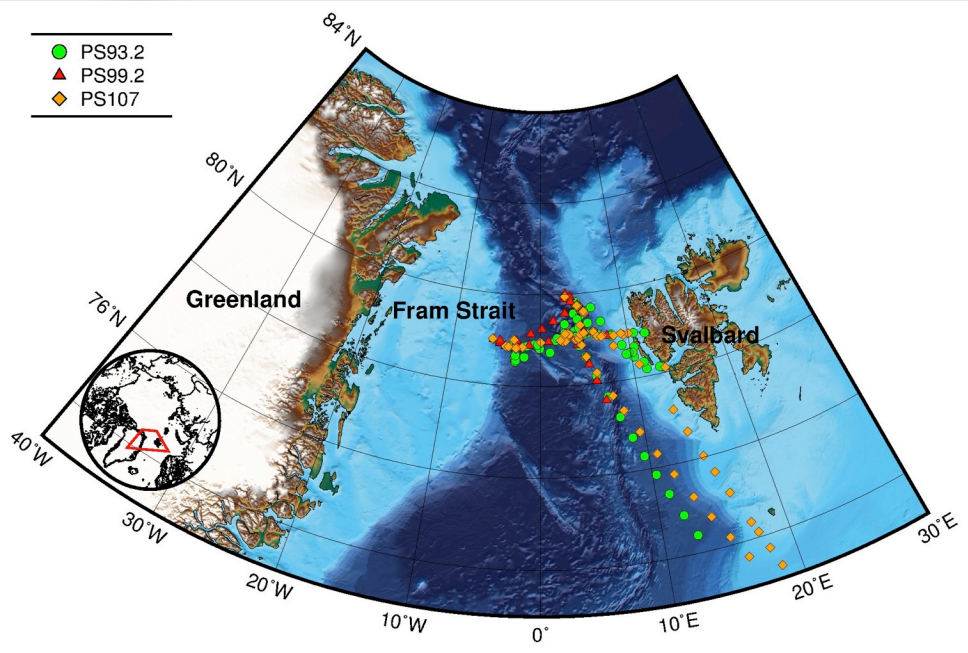


coccolithophore



phaeocystis

Data set



Expedition: icebreaker *R/V Polarstern*

- PS93.2 (Jul - Aug 2015)
- PS99.2 (Jun - Jul 2016)
- PS107 (Jul - Aug 2017)

✓ HPLC pigments (18 types) from 299 discrete samples

✓ Collocated particle absorption a_p from underway spectrophotometry

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Objectives

01 Adapt the 2 pigment retrieval algorithms to the Fram Strait: Gaussian decompostion (Chase et al., 2013) and matrix inversion technique (Moisan et al., 2011).

02 Retrieve pigments from continuous *in situ* particulate absorption data measured by underway spectrophotometry.

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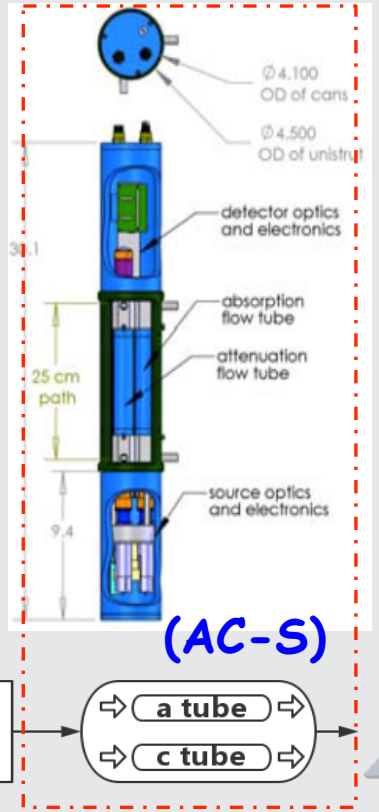
Underway spectrophotometry

AC-S spectrophotometer



- Hyperspectral: 400-735 nm, > 80 wavelengths outputs
- spectral resolution: 10 nm
- Sampling frequency: 4 Hz

Final output: particle absorption a_p

Diagram of the underway AC-S flow-through system

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AC-S data quality control

01

Spikes removal

air bubbles

02

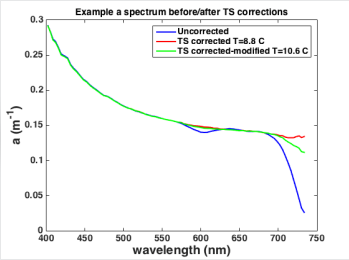
1-min interval bin

4 measurements per sec.

03

T & S correction

Temperature and salinity dependency of pure water abs.



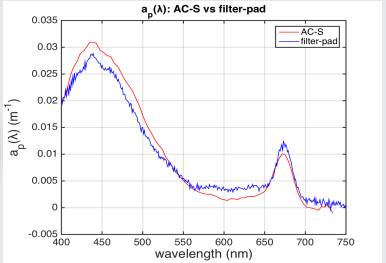
04

a_p calculation

Linear interpolation

05

Scattering & Residual T correction



06

Validated with filter-pad data

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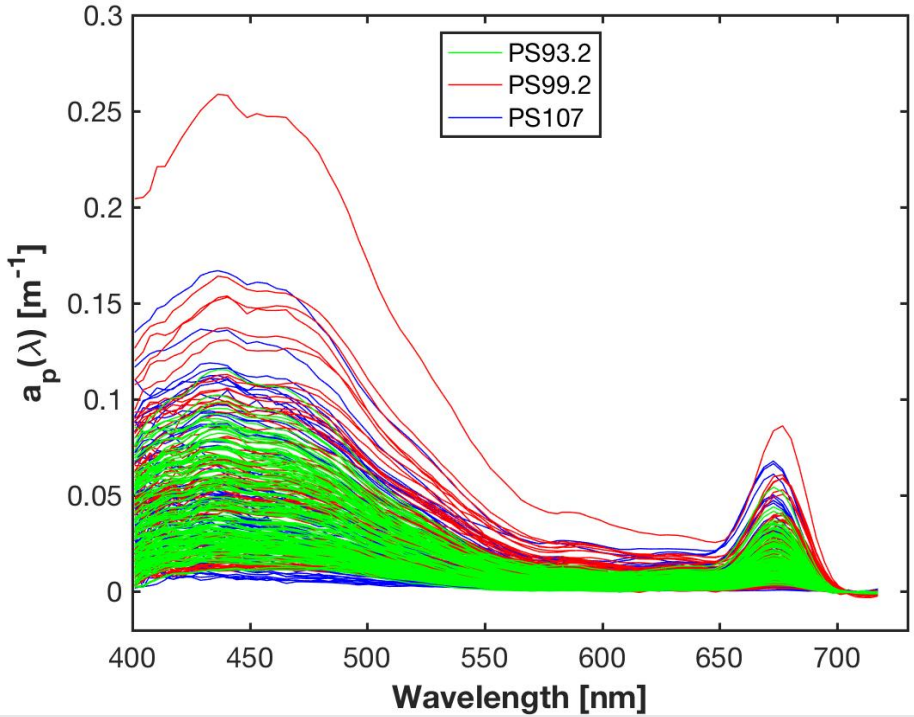
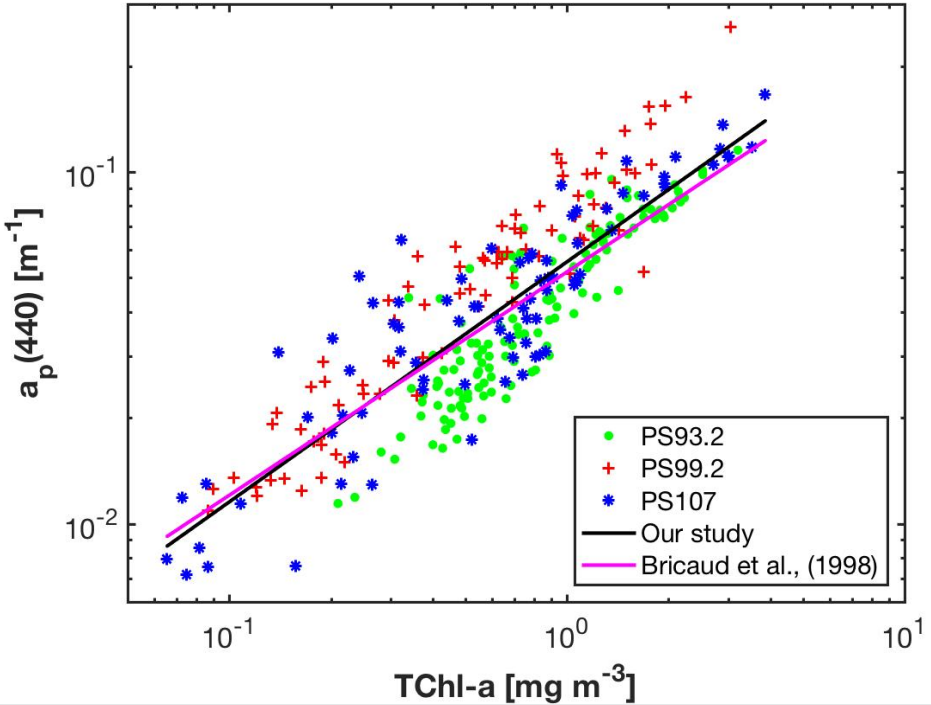
Collocated $a_p(\lambda)$-pigment data set





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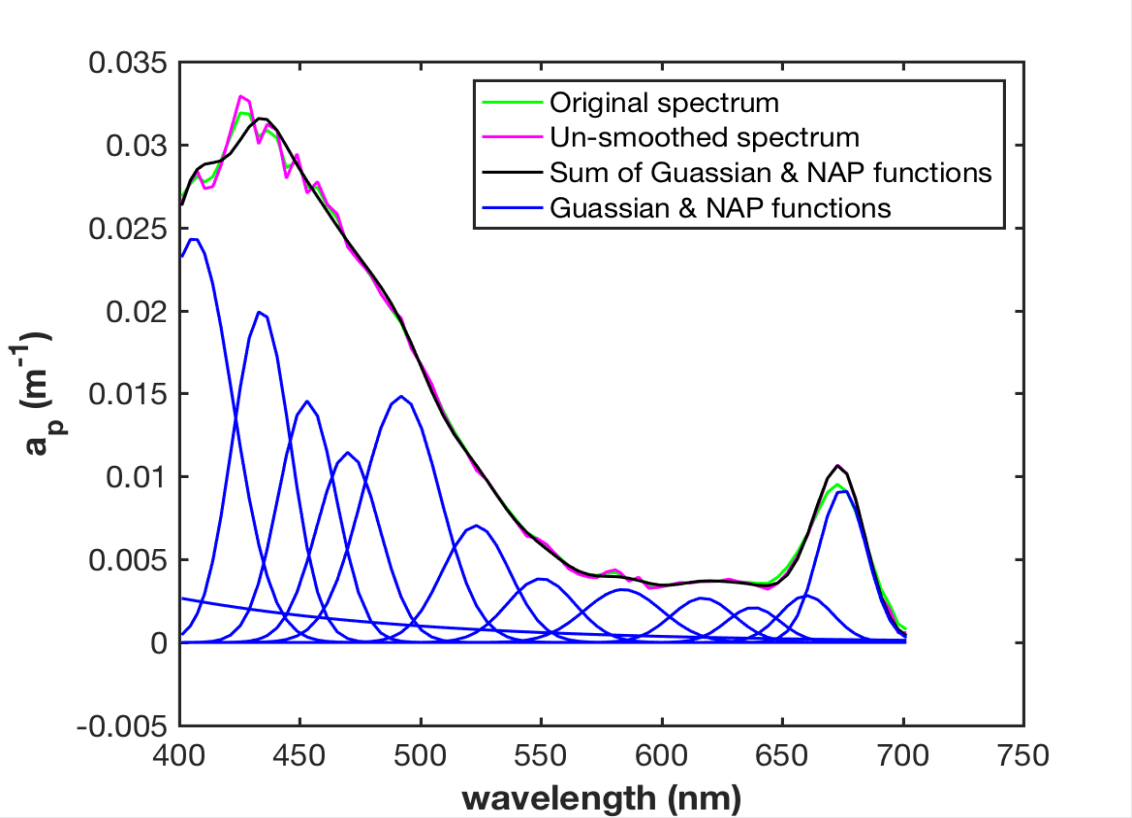
Gaussian decomposition (Spectral decomposition)



- ✓ First proposed by:

Hoepffner and Sathyendranath (1993)

- ✓ Adapted by:

Chase et al. (2013)

- ✓ 12 Gaussian functions representing pigments' absorption
- ✓ 1 non-algal particle (NAP) absorption

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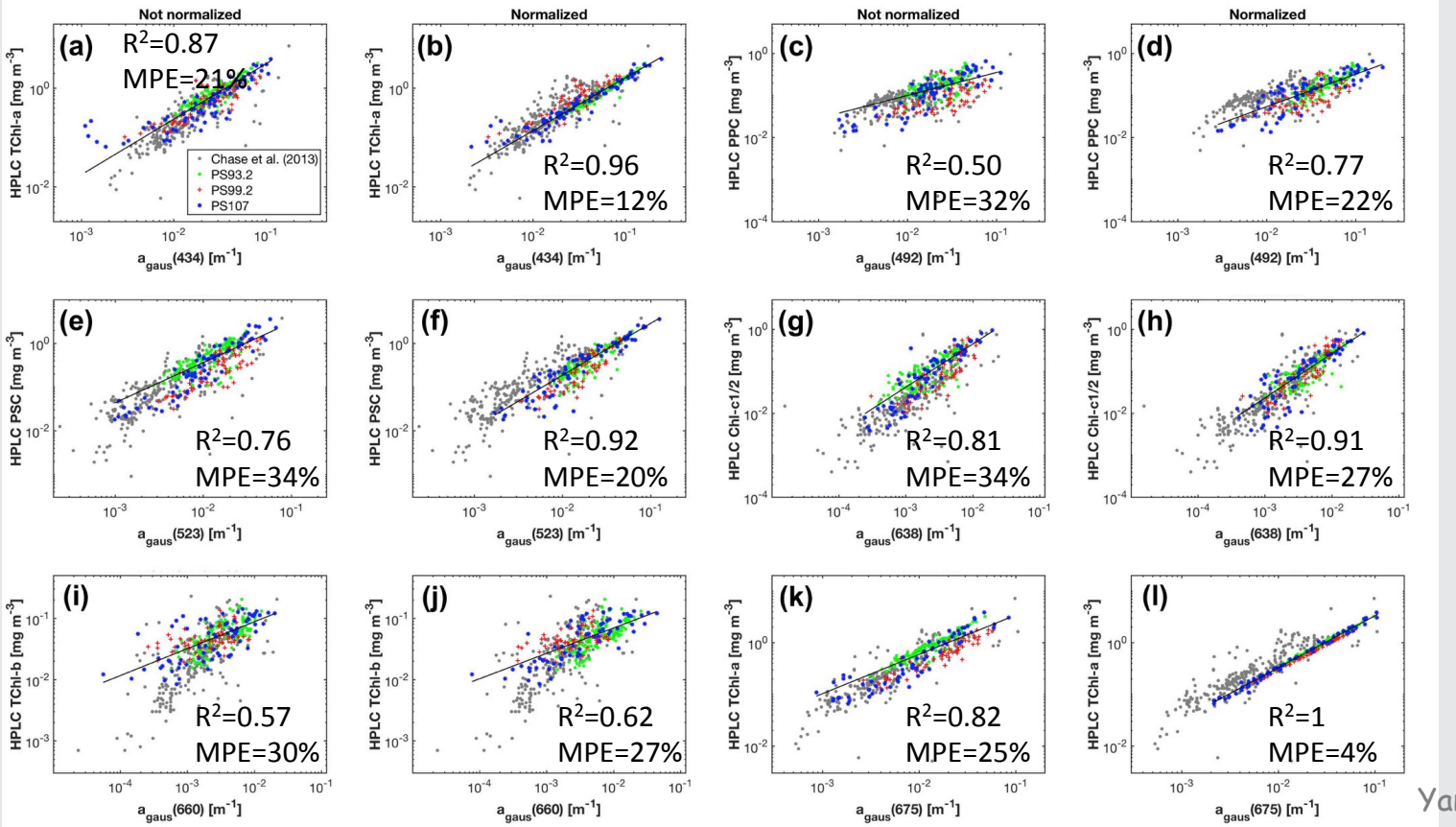
Guassian decomposition (Spectral decomposition)

Our improvement to this method: pigment package effect normalization



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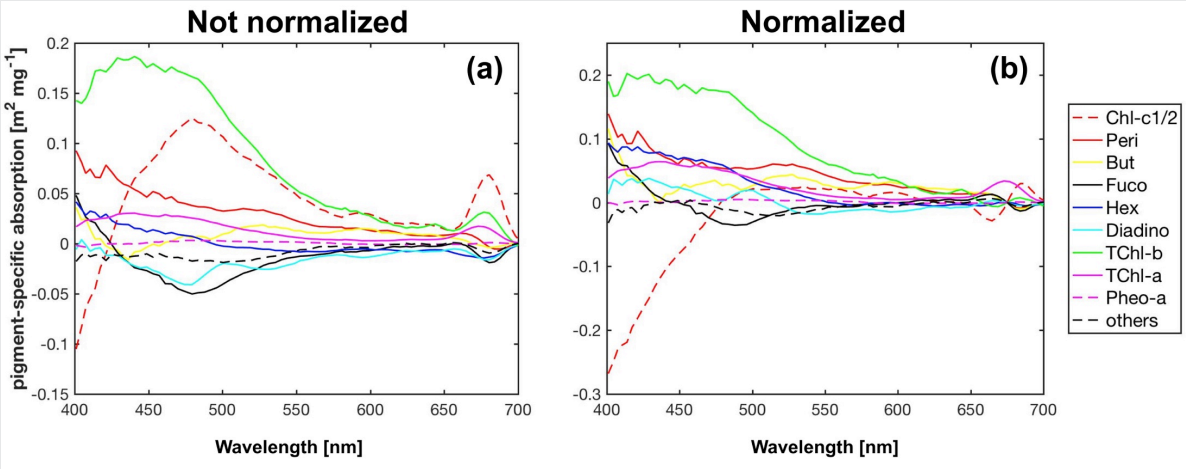
Matrix Inversion Technique (Spectral reconstruction)

Moisan et al. (2011)

- ✓ Reconstruction model: $a_1^*(\lambda)\, c_1 + a_2^*(\lambda)\, c_2 + \ldots + a_3^*(\lambda)\, c_3 = a_{ph}(\lambda)$
- ✓ $a^*(\lambda)$ – pigment-specific absorption spectra (shape)
- ✓ c – pigment concentration (magnitude)



Normalization ---> Increase the differences between a* (λ) ---> Reduce model sensitivity

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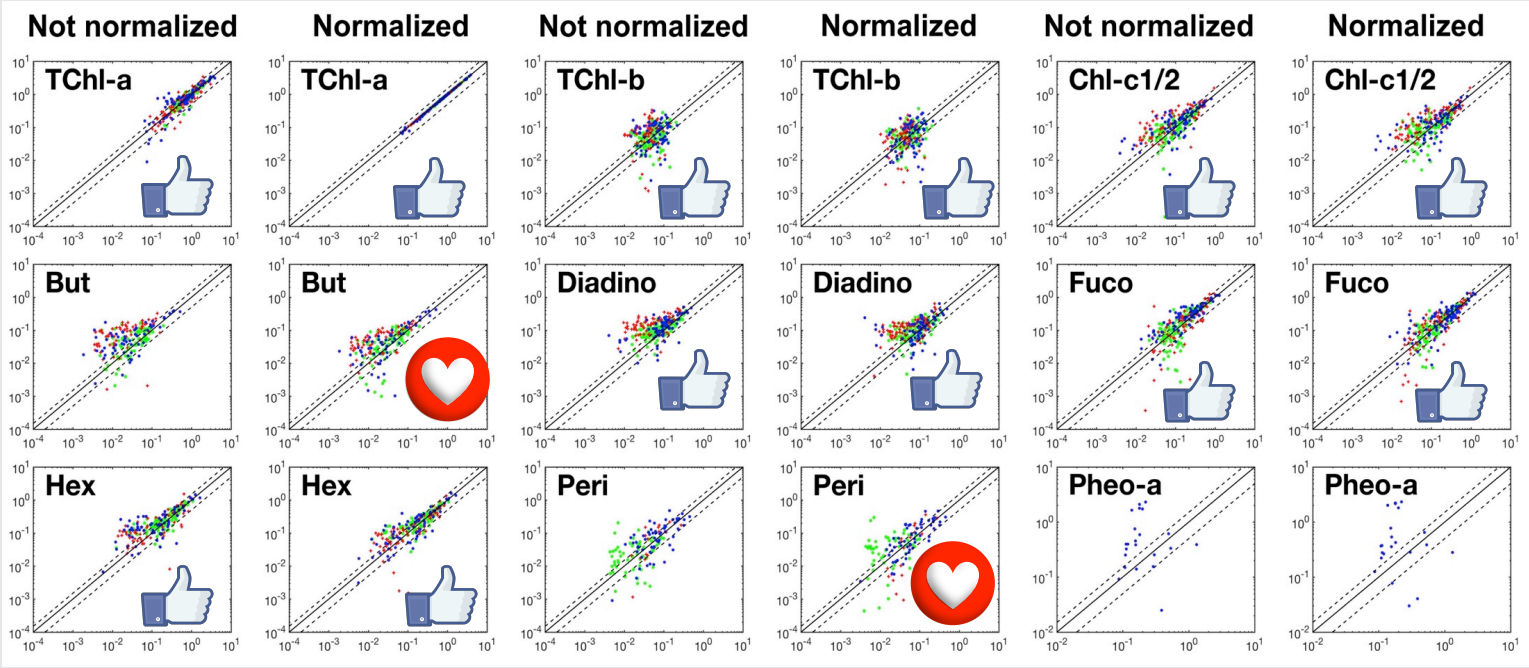
Select 9 pigments

Our improvement to this method: reduce model sensitivity by

- ✓ Develop a scheme for selecting pigments involved
- ✓ Data perturbations based cross validation



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Compare 2 methods: estimation errors

pigments	Gaussian decomposition		Matrix inversion technique	
	Not normalized	Normalized	Not normalized	Normalized
TChl-a	21%	4%	16-22%	1-4%
TChl-b	30%	27%	53-60%	53-61%
Chl-c1/2	34%	27%	41-45%	45-53%
Fuco	-	-	35-45%	40-53%
Hex	-	-	37-44%	36-42%
Diadino	-	-	62-65%	60-66%
But	-	-	-	67-70%
Peri	-	-	-	68-75%
PSC	34%	20%	-	-
PPC	32%	22%	-	-

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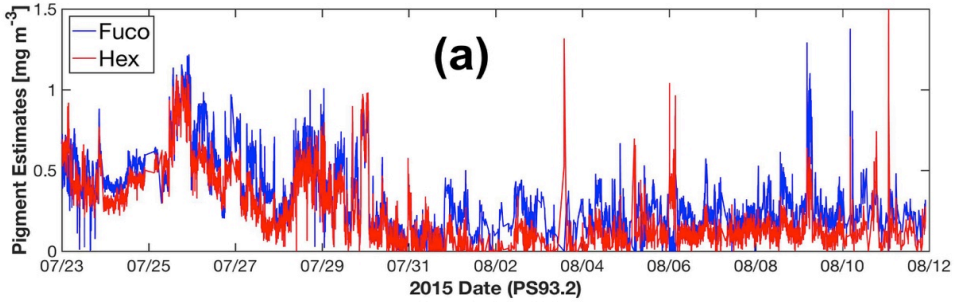
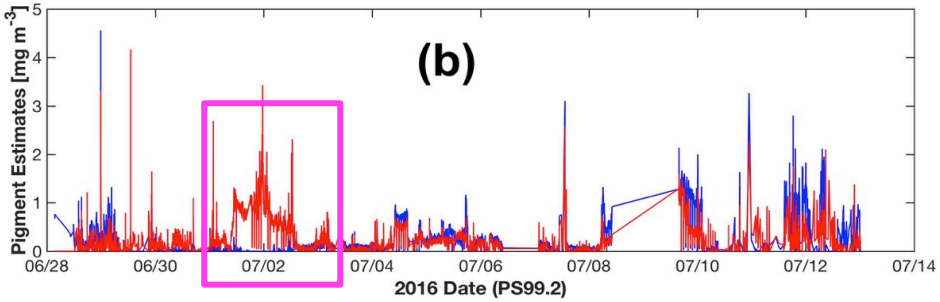
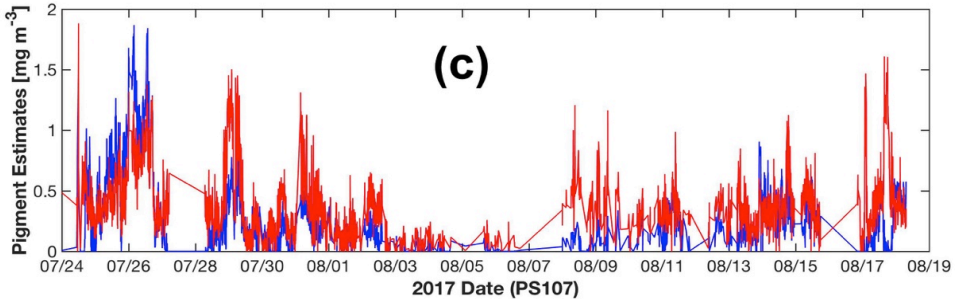
Leave-one-out cross validation

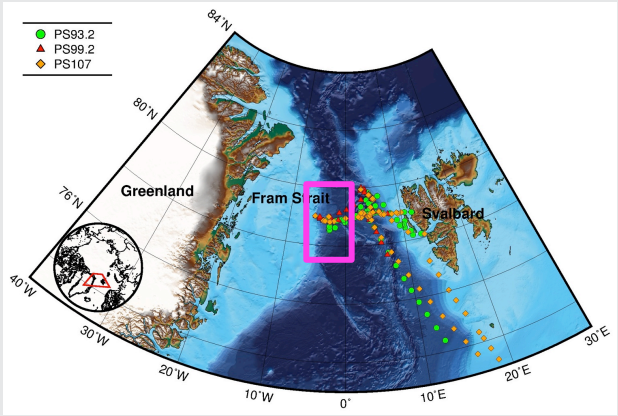
Phytoplankton pigments time series







- ✓ Estimated using matrix inversion.
- ✓ Fuco (fucoxanthin): diatoms.
- ✓ Hex (19'-hexanoyloxyfucoxanthin): prymnesiophytes.



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Conclusions

01

Adapt the 2 pigment retrieval algorithms to the Fram Strait: Gaussian decompostion (Chase et al., 2013) and matrix inversion technique (Moisan et al., 2011).

Gaussian decomposition: TChl-a, TChl- b, Chl-c1/2, PSC and PPC. (20-34%)

✓ Normalization: estimation errors reduced. (12-27%)

matrix inversion technique: TChl-a, TChl-b, Chl-c1/2, Fuco, Hex, Diadino. (37-65%)

✓ Normalization: +But, Peri (67-76%)

✓ Sensitivity reduction routine

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Conclusions

02

Retrieve pigments from continuous *in situ* particulate absorption data measured by underway spectrophotometry.

✓ High resolution phytoplankton marker pigment data in the Fram Strait were obtained.

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Outlook

Retrieve key phytoplankton groups in the Fram Strait.

A

B

coupling of phytoplankton composition and distribution to physical and biogeochemical properties.

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