Phytoplankton community composition derived from optics and remote sensing: Approaches, challenges, and next steps

Ali Chase, Applied Physics Laboratory – University of Washington, USA
IOCCG Summer Lecture Series, 26 July 2022, Villefranche-sur-Mer, France

Contact: alichase@uw.edu

Why Phytoplankton Community Composition?

Dierssen et al., 2021

Lecture motivation…

From the NASA PACE website homepage:

…& inspiration

Slide content inspired by and borrowed from Jeremy Werdell (NASA), Julia Uitz (LOV), Dylan Catlett (WHOI), & many papers (see tables & references)

Lecture outline & key points

→ Previous studies to estimate phytoplankton community composition from optics & remote sensing

→ Recent work and expansion to include new approaches and data types

→ Where do we go from here? (hint: you tell me!)

Go to **www.menti.com** and use the code **8534 4169**

What comes to mind when you hear "Phytoplankton Community Composition"?

Mentimeter

Phytoplankton Community Composition (PCC) - some definitions

PSC = Phytoplankton Size Classes (note: also Photosynthetic Carotenoids…)

- pico, nano, and micro (what should the size cutoffs be?)

PG = Phytoplankton Groups

- a catch-all terms for species and size classes?

PFT = Phytoplankton Functional Types

- biogeochemical function?

Beware: The meanings of ***all*** *of these terms may change based on the user*

Bottom line: we want to define the phytoplankton present in the water by some metric that differs/moves beyond total biomass (most commonly approximated via estimates of chlorophyll *a* concentration)

And what about units???

Absolute

- Concentrations (cells/L)
- Biovolume (mg/m^3)
- Biomass, carbon (mg/m^3)
- Chl *a* (micrograms/L, mg/m^3)

Relative

- Fraction (%) of total Chl *a*
- Fraction (%) of total biovolume
- Fraction of some subset of the total community (e.g., % of all microplankton)
- "Dominant" group (in what units?)

Probability of occurrence (at some threshold?)

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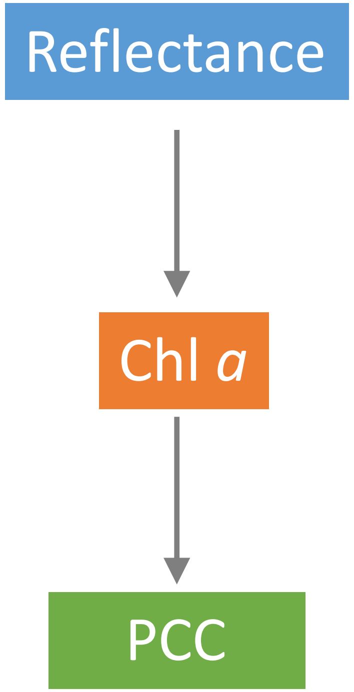
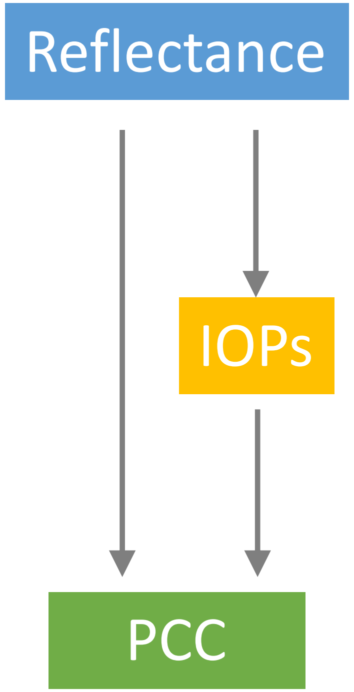
Science is an incremental continuum; we build and grow from past efforts. We should think critically about both what has been done, and what we are currently doing (and why)

Previously developed algorithms: two main categories

<u>Abundance-based</u>



<u>Spectral-based</u>



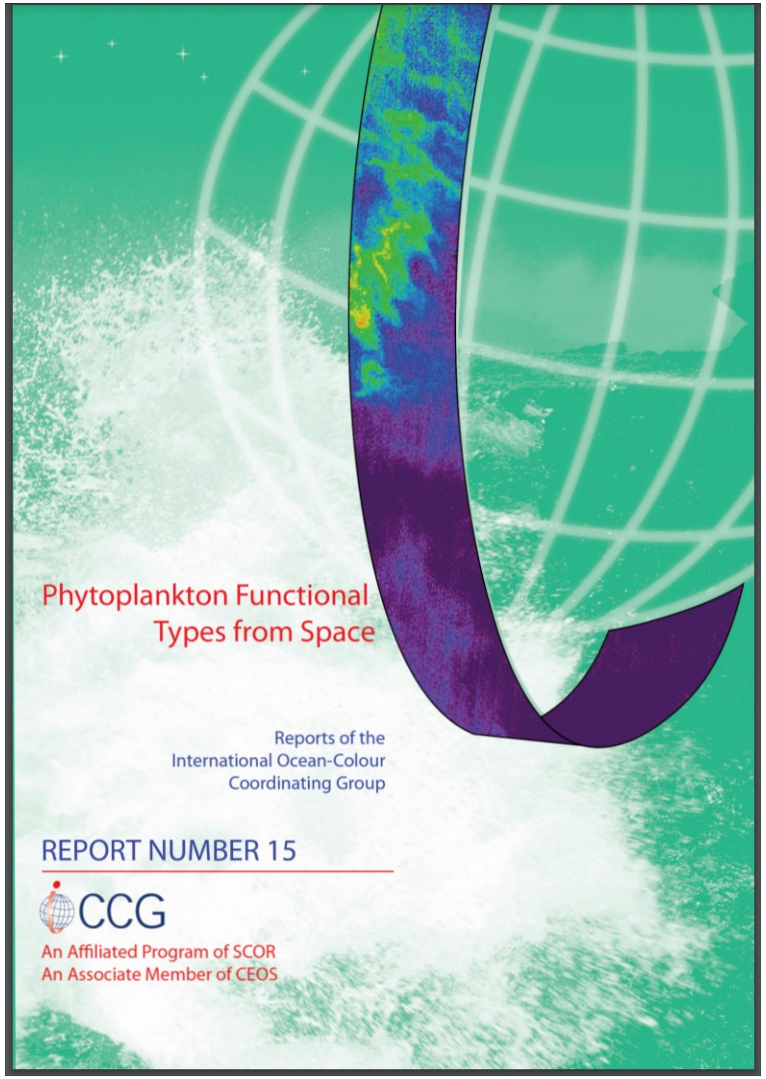
IOCCG Report Number 15, 2014

Phytoplankton Functional Types from Space

Edited by:
Shubha Sathyendranath (Plymouth Marine Laboratory)

Report of an IOCCG working group on Phytoplankton Functional Types, chaired by Shubha Sathyendranath and based on contributions from (in alphabetical order):

Jim Aiken, Séverine Alvain, Ray Barlow, Heather Bouman, Astrid Bracher, Robert J. W. Brewin, Annick Bricaud, Christopher W. Brown, Aurea M. Ciotti, Lesley Clementson, Susanne E. Craig, Emmanuel Devred, Nick Hardman-Mountford, Takafumi Hirata, Chuanmin Hu, Tihomir S. Kostadinov, Samantha Lavender, Hubert Loisel, Tim S. Moore, Jesus Morales, Cyril Moulin, Colleen B. Mouw, Anitha Nair, Dionysios Raitsos, Collin Roesler, Shubha Sathyendranath, Jamie D. Shutler, Heidi M. Sosik, Inia Soto, Venetia Stuart, Ajit Subramaniam and Julia Uitz.



https://ioccg.org/wp-content/uploads/2018/09/ioccg_report_15_2014.pdf

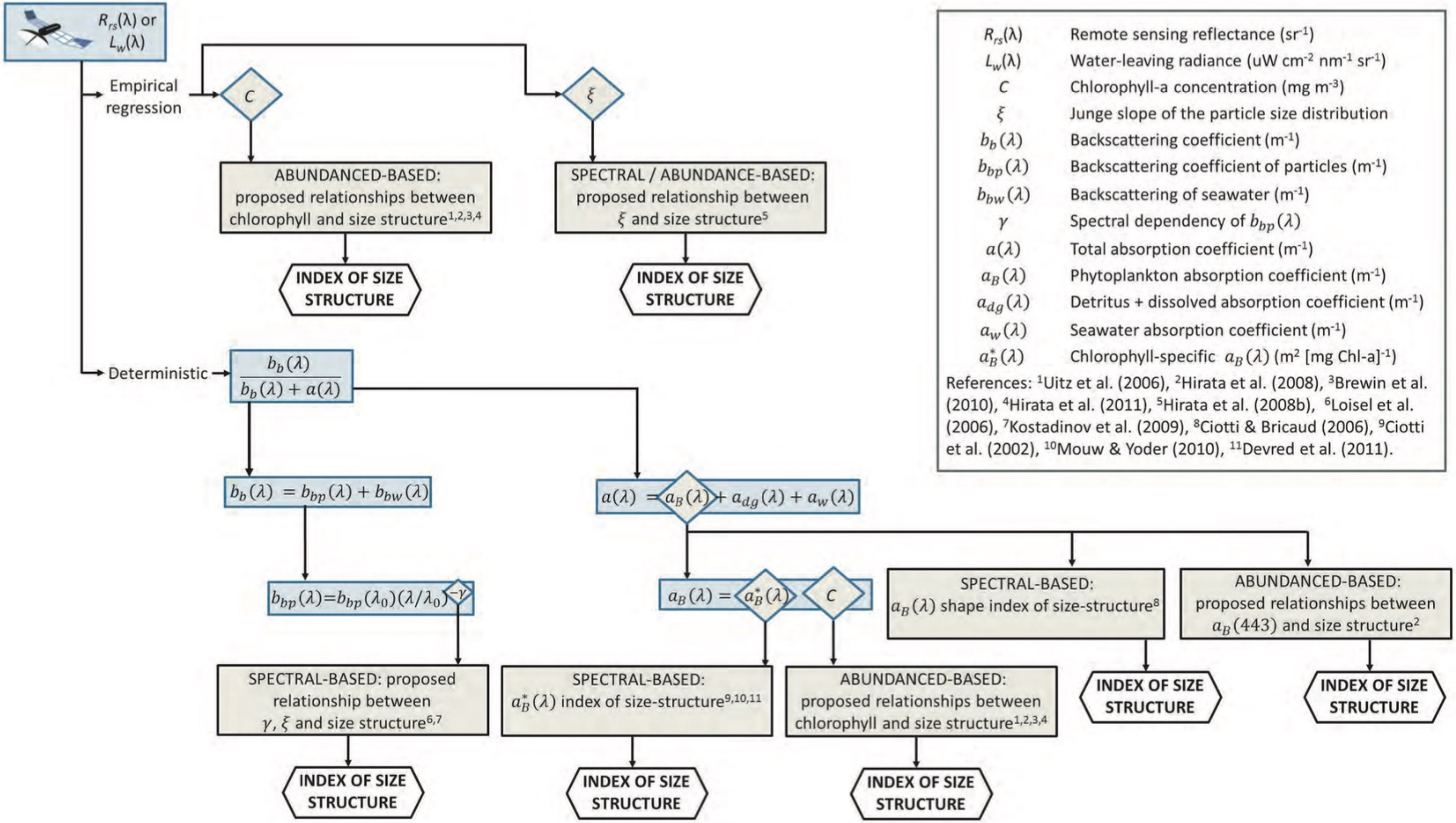


Figure 4.11 A hierarchical classification of models used for phytoplankton size-class detection. The models become progressively more complex and complete as we move from the upper to the lower level of the flow diagram.

https://ioccg.org/wp-content/uploads/2018/09/ioccg_report_15_2014.pdf

A Consumer's Guide to Satellite Remote Sensing of Multiple Phytoplankton Groups in the Global Ocean

Colleen B. Mouw[1], Nick J. Hardman-Mountford[2], Séverine Alvain[3], Astrid Bracher[4,5], Robert J. W. Brewin[6,7], Annick Bricaud[8], Aurea M. Ciotti[9], Emmanuel Devred[10], Amane Fujiwara[11], Takafumi Hirata[12,13], Toru Hirawake[14], Tihomir S. Kostadinov[15], Shovonlal Roy[16] and Julia Uitz[8]*

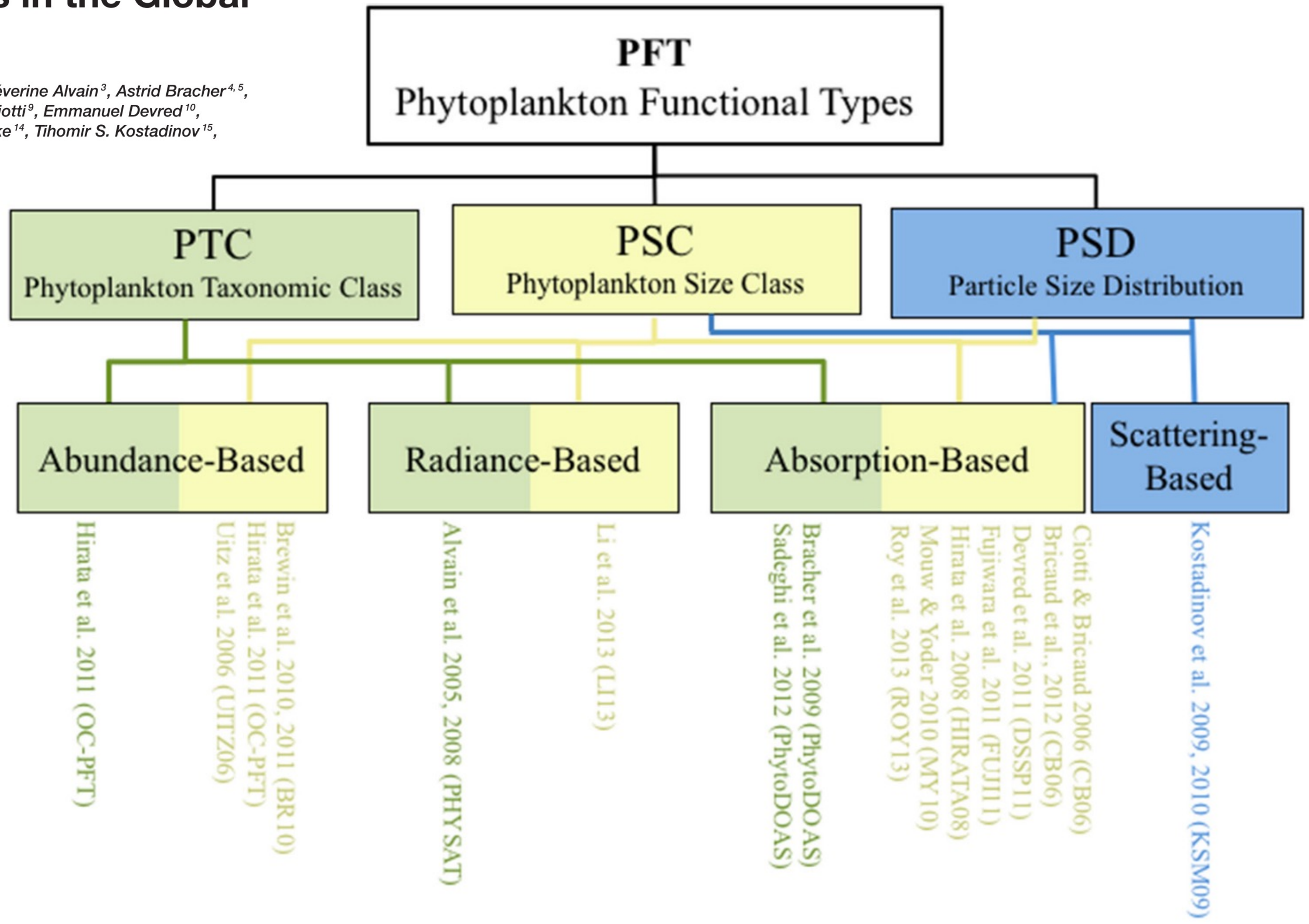


FIGURE 1 | Schematic of various phytoplankton functional type (PFT) algorithms grouped according to their output classification (PTC, PSC, or PSD) and algorithm development types (abundance-, radiance-, absorption-, and scattering-based). Color indicates the output classification of phytoplankton taxonomic class (PTC, green), phytoplankton size class (PSC, yellow) or particle size distribution (PSD, blue).

TABLE 2 | Summary of satellite inputs and outputs.

Type	Algorithm references	Algorithm abbreviation	Development inputs								Satellite inputs						Satellite Outputs							
			nLw/Rrs	*[Chl]*	a_{ph}	a_{cdm}	b_{bp}	η	*S*	HPLC pigments	*nLw/Rrs*	*[Chl]*	*at*	a_{ph}	a_{cdm}	b_{bp}	*Micro*	*Nano*	*Pico*	*Hapto (cocco)*	*Dino*	*Cyano (Pro/Syn)*	*Diatom*	*Phaeo*
Abundance	Brewin et al., 2010	BR10		x						x		x					x	x	x					
	Brewin R. J. et al., 2011	BR10		x	x					x		x					x	x	x					
	Hirata et al., 2011	OC-PFT		x						x		x					x	x	x	x	x	x	x	
	Uitz et al., 2006	UITZ06								x		x					x	x	x					
Radiance	Alvain et al., 2005, 2008	PHYSAT	x	x						x	x	x						x		x		x	x	x
	Li et al., 2013	LI13	x							x	x						x	x	x					
Absorption	Bracher et al., 2009	PhytoDOAS			x						x											x	x	
	Sadeghi et al., 2012a	PhytoDOAS	x		x						x									x	x		x	
	Ciotti and Bricaud, 2006; Bricaud et al., 2012	CB06	x	x	x	x			x			x	x				(x)		x					
	Devred et al., 2011	DSSP11	x	x	x	x	x		x	x	x						x	x	x					
	Fujiwara et al., 2011	FUJI11	x	x	x			x			x			x			x		(x)					
	Hirata et al., 2008	HIRATA08		x	x					x				x			x	x	x					
	Mouw and Yoder, 2010a	MY10	x	x	x	x	x			x	x	x			x		x		(x)					
	Roy et al., 2013	ROY13		x	x					x		x		x			x	x	x					
Scattering	Kostadinov et al., 2009, 2010	KSM09					x	x			x					x	x	x	x					

The four algorithm types are indicated by color: abundance (green), radiance (red), absorption (yellow), scattering (blue). The development inputs, satellite inputs, and satellite outputs are indicated with "x" for each algorithm. Instances where other size classes could be inferred but are not directly retrieved are indicated with "(x)". Notation for column headers can be found in ***Table 1****.*

Inputs ≠ Outputs is a fundamental algorithm limitation

Mouw et al., 2017

Obtaining Phytoplankton Diversity from Ocean Color: A Scientific Roadmap for Future Development

Astrid Bracher[1,2]*, Heather A. Bouman[3], Robert J. W. Brewin[4,5], Annick Bricaud[6,7], Vanda Brotas[8], Aurea M. Ciotti[9], Lesley Clementson[10], Emmanuel Devred[11], Annalisa Di Cicco[12], Stephanie Dutkiewicz[13], Nick J. Hardman-Mountford[14], Anna E. Hickman[15], Martin Hieronymi[16], Takafumi Hirata[17,18], Svetlana N. Losa[1], Colleen B. Mouw[19], Emanuele Organelli[4], Dionysios E. Raitsos[4], Julia Uitz[6,7], Meike Vogt[20] and Aleksandra Wolanin[1,2,21]

- Gap 1: Information Mismatch between Satellite-Derived Phytoplankton Composition Products and User Group Target Variables
- Gap 2: Lack of Traceability of Uncertainties in PG Algorithms
- Gap 3: Missing Capabilities of Current Ocean Color Satellite Measurements
- Gap 4: Lack of Regional Capability of PG Algorithms

TABLE 2 | A compilation of global algorithms to retrieve phytoplankton composition from satellite data.

And regional

Approach		Phytoplankton composition product		References
ABUNDANCE		Size classes		Uitz et al., 2006; Brewin et al., 2010, 2015 Soppa et al. 2014 Losa et al. 2017 (combined abundance and spectral) Chase et al. 2022 (diatom carbon)
		Size classes and multiple taxa		Hirata et al., 2011
SPECTRAL	REFLECTANCE	Multiple taxa		Alvain et al., 2005, 2008; Li et al., 2013; Ben Mustapha et al., 2014 Rêve-Lamarche et al. 2017; Xi et al. 2020
		Single taxon	Coccolithophores	Brown and Yoder, 1994; Moore et al., 2012 Sathyendranath et al. 2004 Kramer et al. 2018
			Trichodesmium	Subramaniam et al., 2002; Westberry et al., 2005
	ABSORPTION	Size index		Ciotti and Bricaud, 2006; Mouw and Yoder, 2010; Bricaud et al., 2012
		Size classes		Devred et al., 2006, 2011; Hirata et al., 2008; Fujiwara et al., 2011; Roy et al., 2013
		Multiple taxa		Bracher et al., 2009; Sadeghi et al., 2012a; Werdell et al., 2014
	BACK-SCATTERING	Size classes		Kostadinov et al., 2009, 2016; Fujiwara et al., 2011
ECOLOGICAL		Taxonomic groups		Palacz et al., 2013 Raitsos et al., 2008

Lecture outline & key points

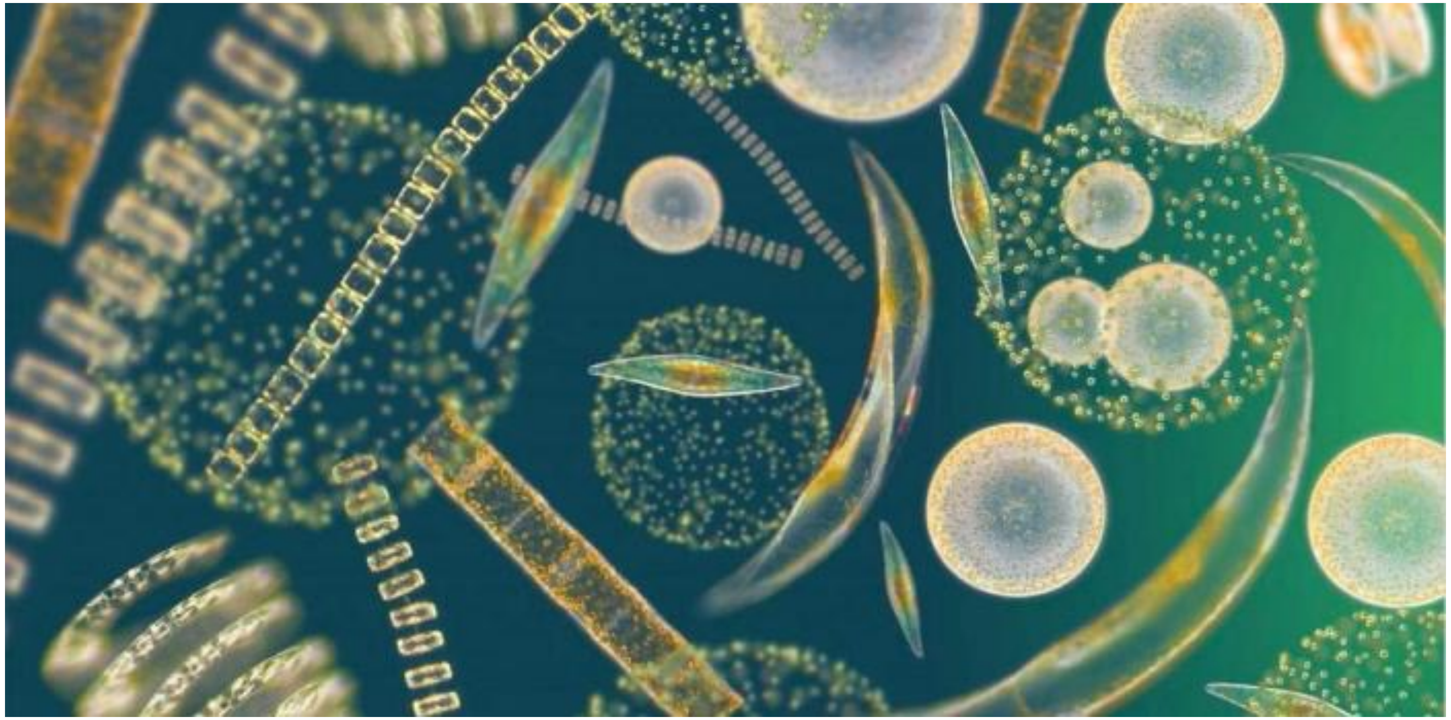
→ **Previous studies to estimate phytoplankton community composition from optics & remote sensing**

→ **Recent work and expansion to include new approaches and data types**

→ **Where do we go from here? (hint: you tell me!)**

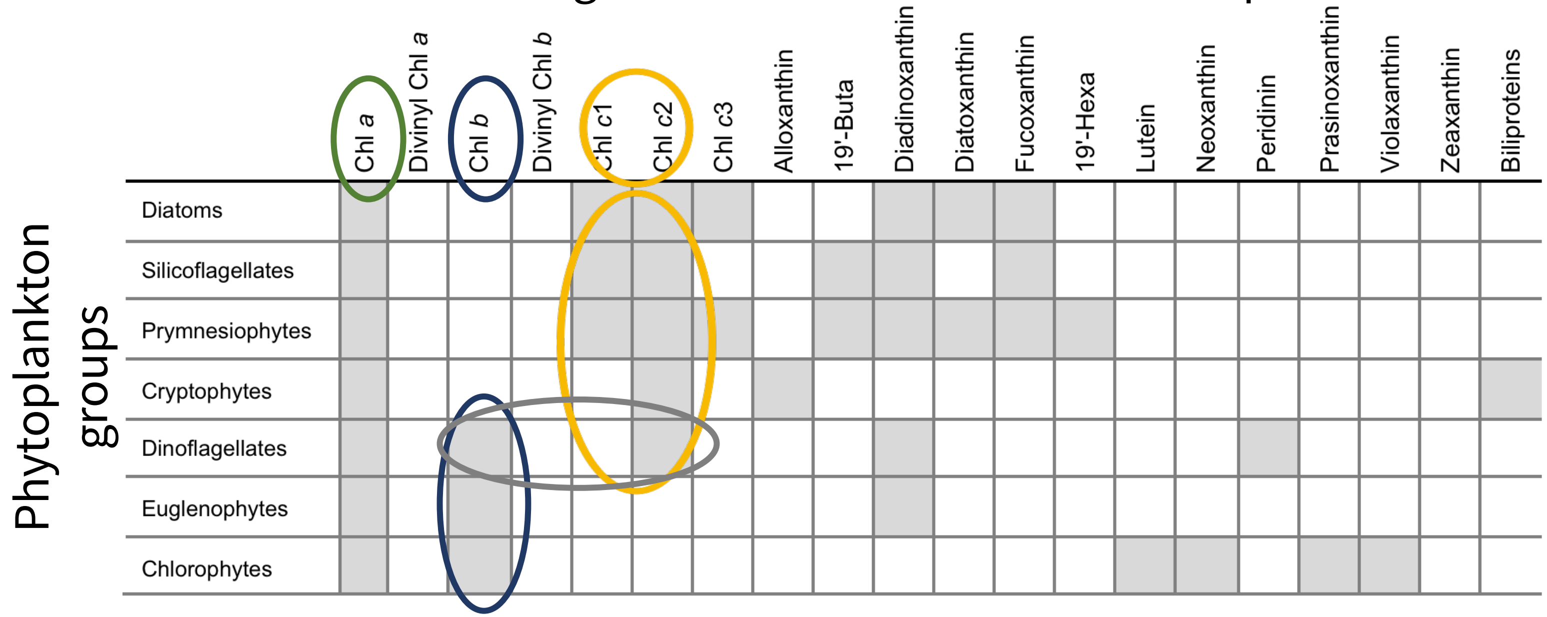
How is phytoplankton community composition defined in situ?

- Microscopy
- Pigments
- Flow cytometry
- Automated imagery
- Merged size spectra
- Genetic information



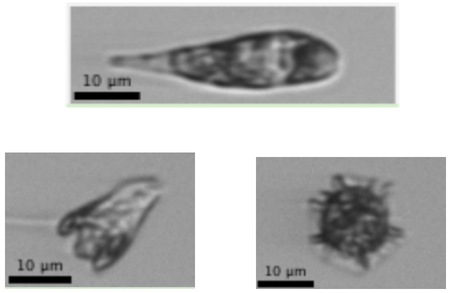
Phytoplankton pigments attributed to different groups

Pigments from discrete water samples



Chlorophyll *b*

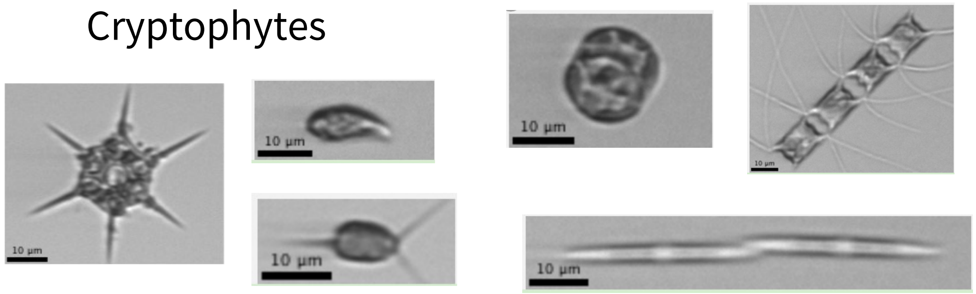
Chlorophytes, Euglenoids



Chlorophyll *c*

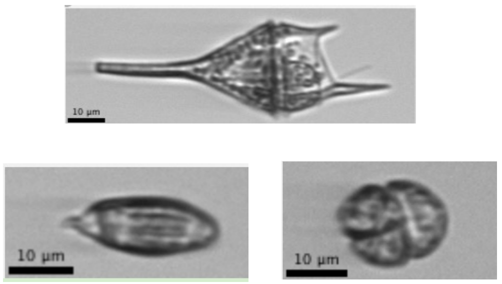
Silicoflagellates
Prymnesiophytes
Cryptophytes

Diatoms



Chlorophylls *b* & *c*

Dinoflagellates



CHEMTAX method applied using pigments concentrations

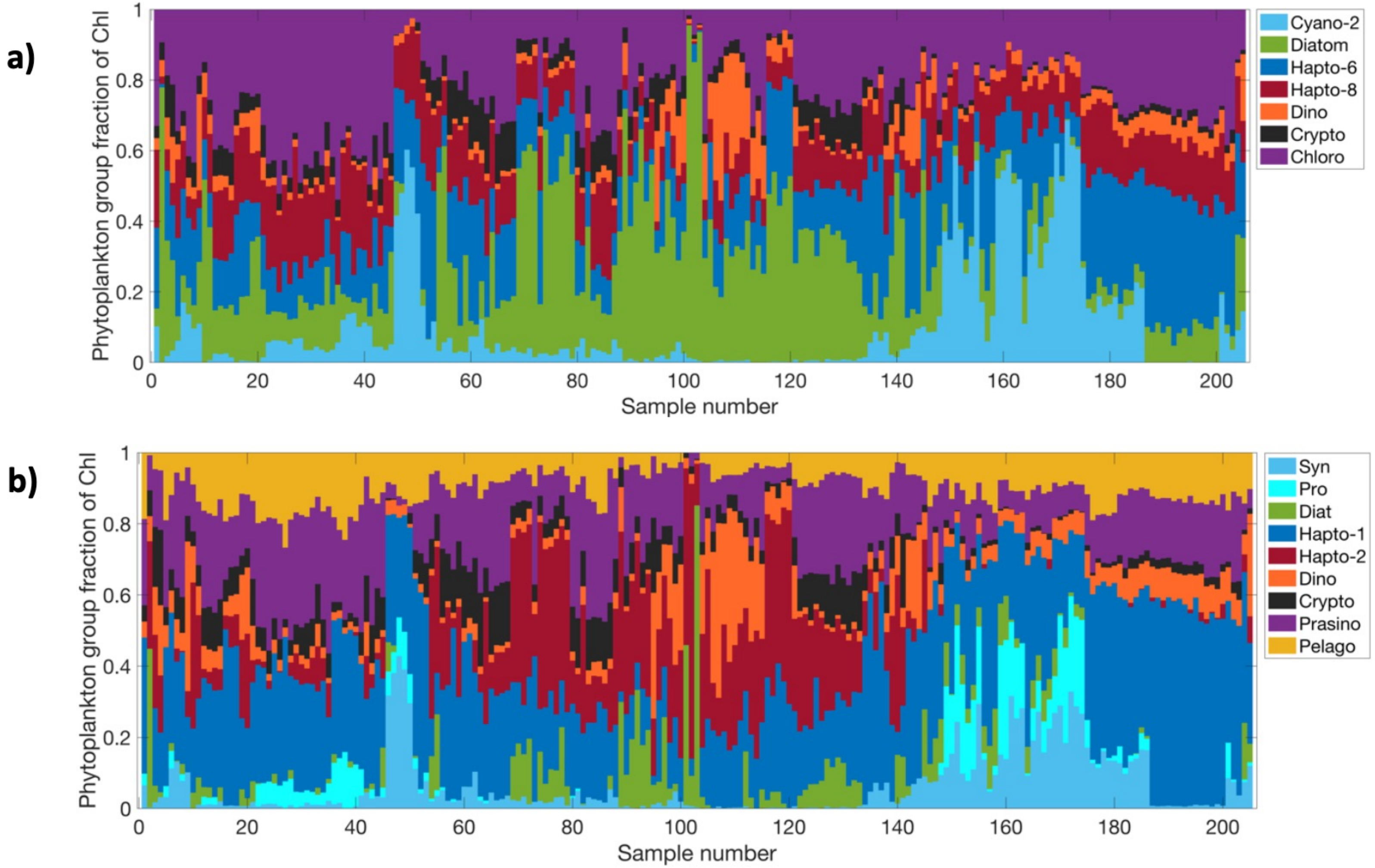
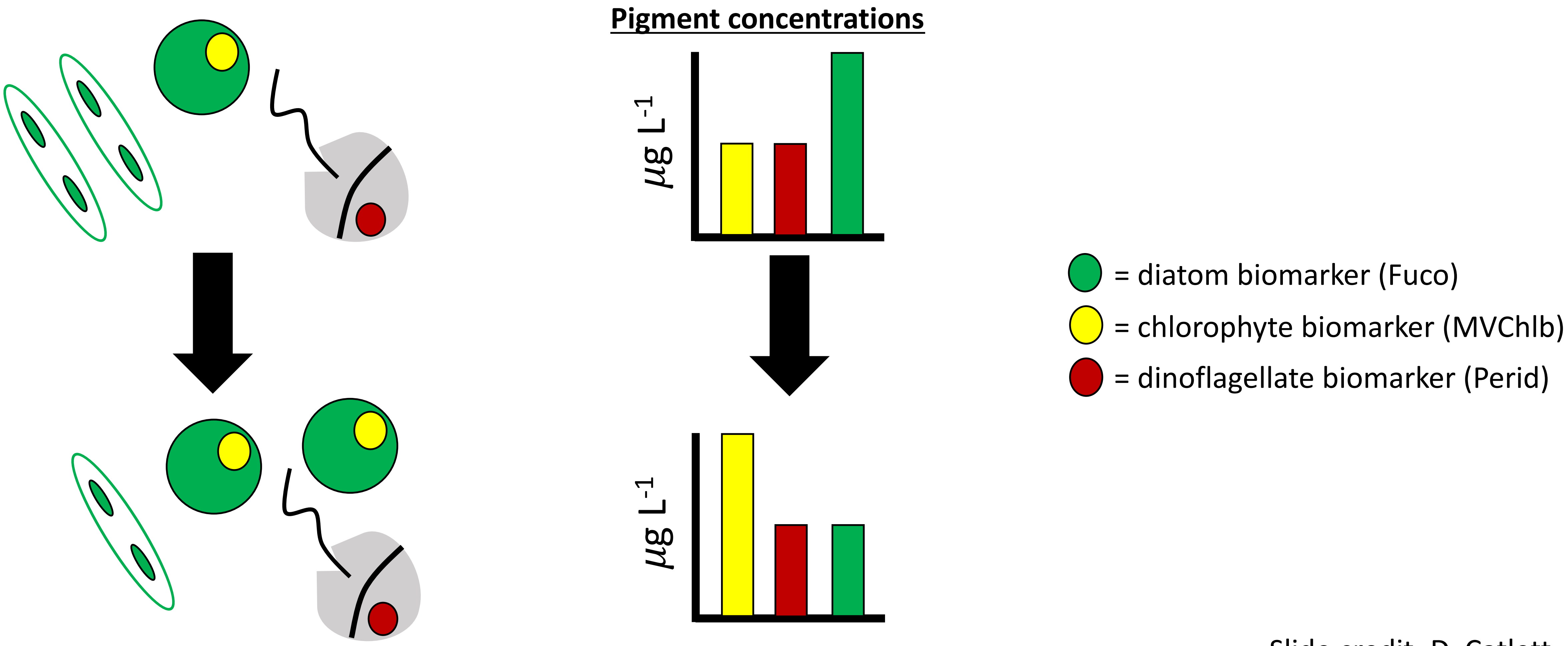


Figure S2. a) Phytoplankton group contribution to Chl *a* from CHEMTAX analysis with inputs from Swan et al. 2016. **b)** Phytoplankton group contribution to Chl *a* from CHEMTAX analysis with Inputs from van de Poll et al. 2013.

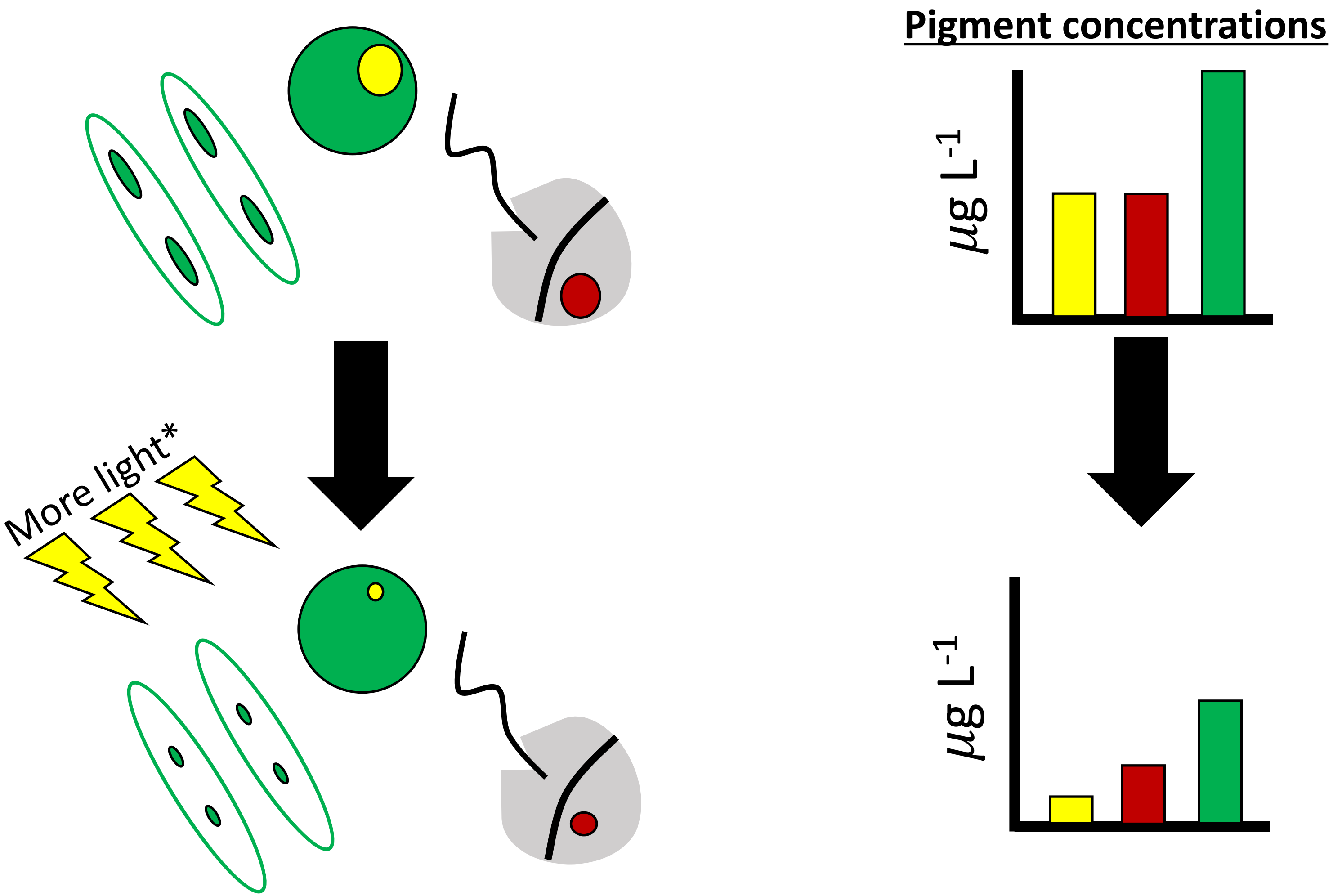
Chase et al., 2022, supp. Info.

The assumption: biomarker pigment concentration changes reflect changes in PCC



Slide credit: D. Catlett

Problem 1: Phytoplankton physiological responses to environmental changes



= diatom biomarker (Fuco)

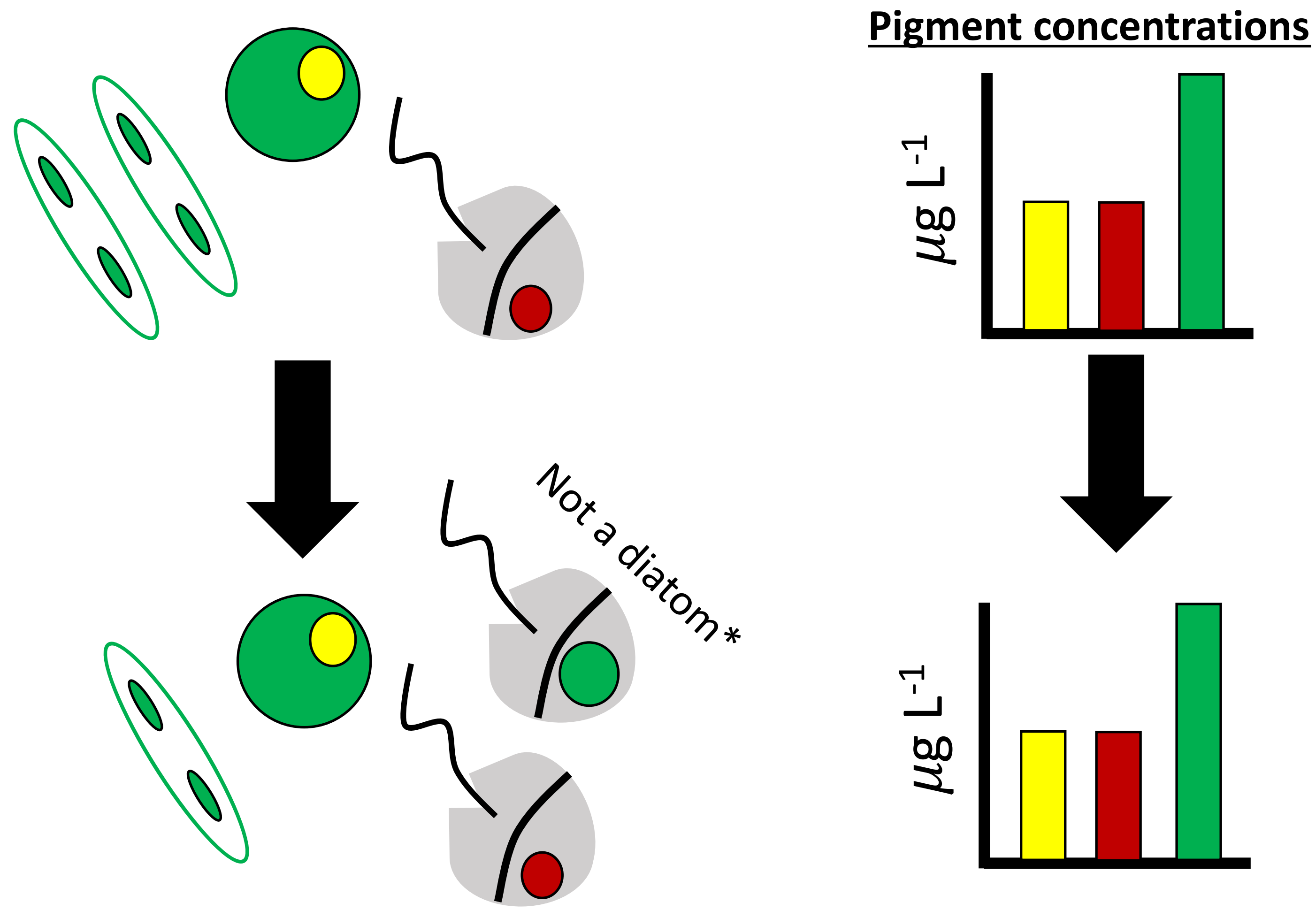
= chlorophyte biomarker (MVChlb)

= dinoflagellate biomarker (Perid)

*Other stimuli that impact pigment expression include nutrient availability, temperature, others. Responses to specific stimuli vary across species and groups

Slide credit: D. Catlett

Problem 2: Many biomarker pigments lack specificity to a single phytoplankton group



= diatom biomarker (Fuco)

= chlorophyte biomarker (MVChlb)

= dinoflagellate biomarker (Perid)

*Other sources of inter- and intra-group variability in biomarker pigment expression are known

Slide credit: D. Catlett

Globally Consistent Quantitative Observations of Planktonic Ecosystems

Fabien Lombard[1,2], Emmanuel Boss[3]*, Anya M. Waite[4], Meike Vogt[5], Julia Uitz[1],*

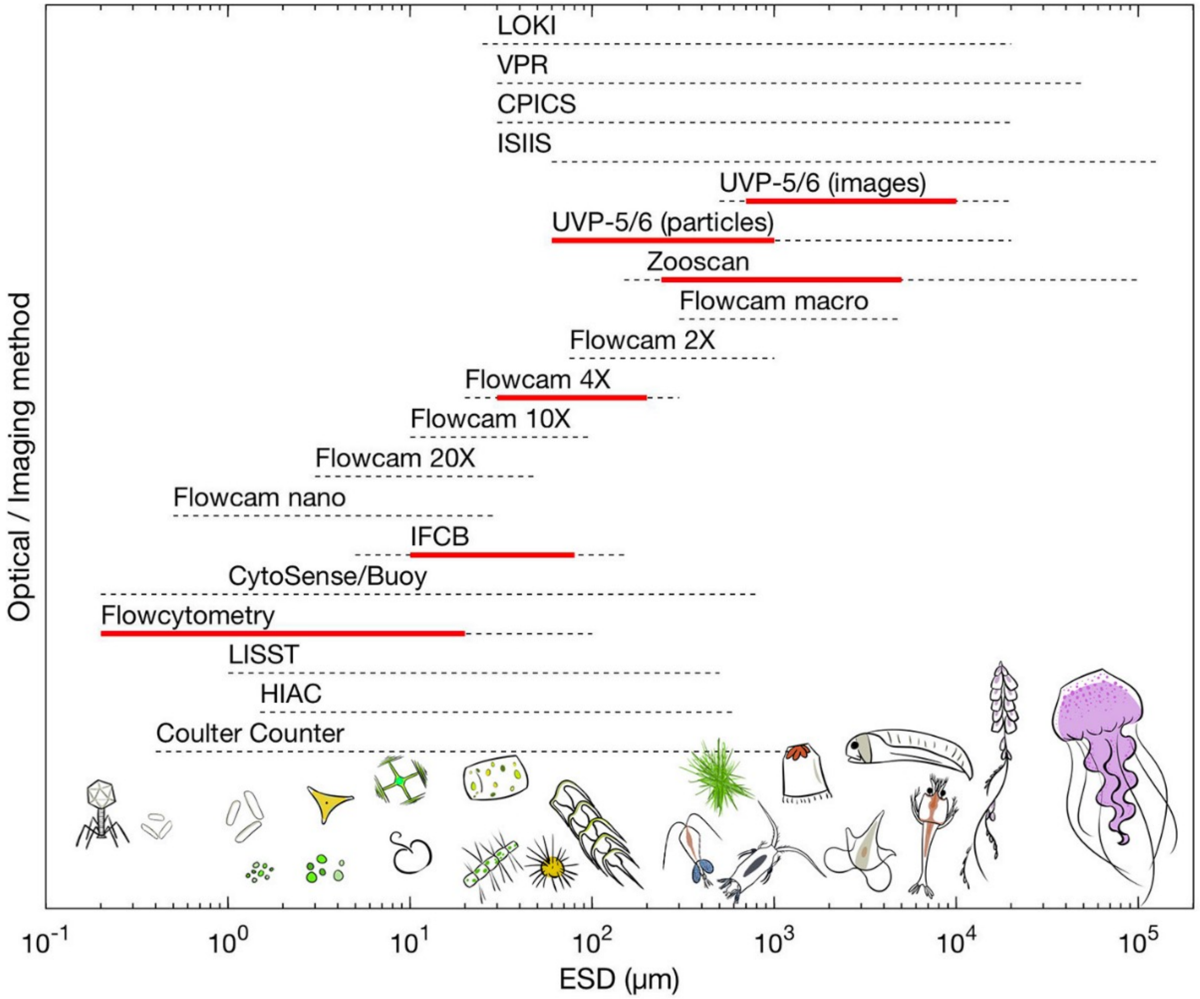
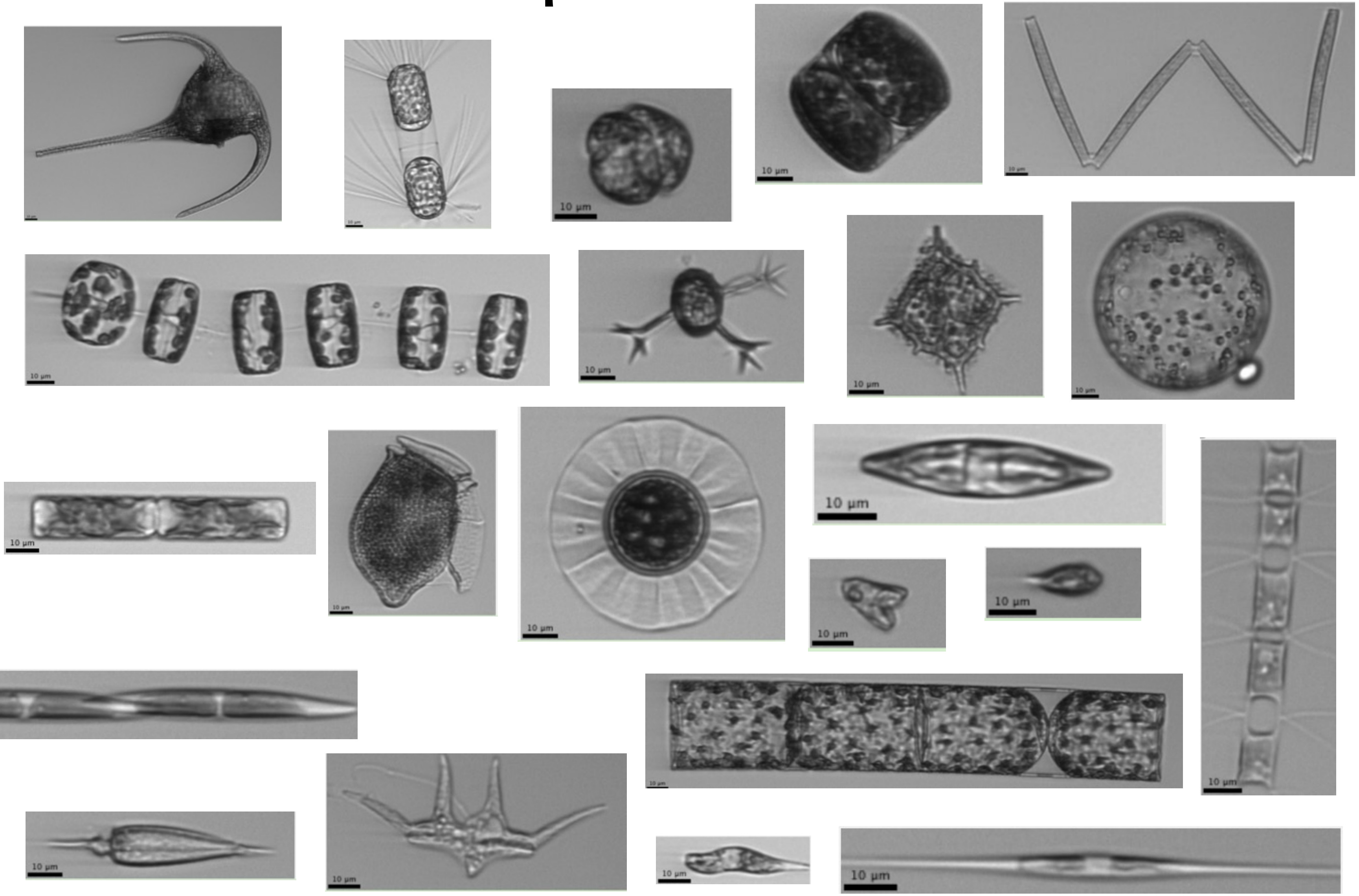
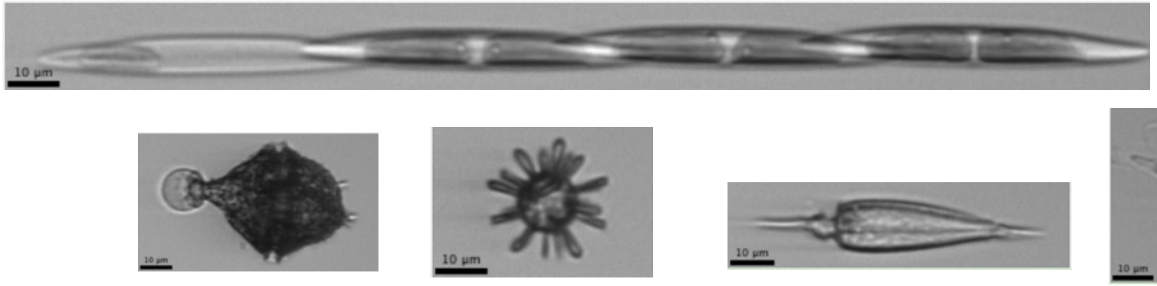


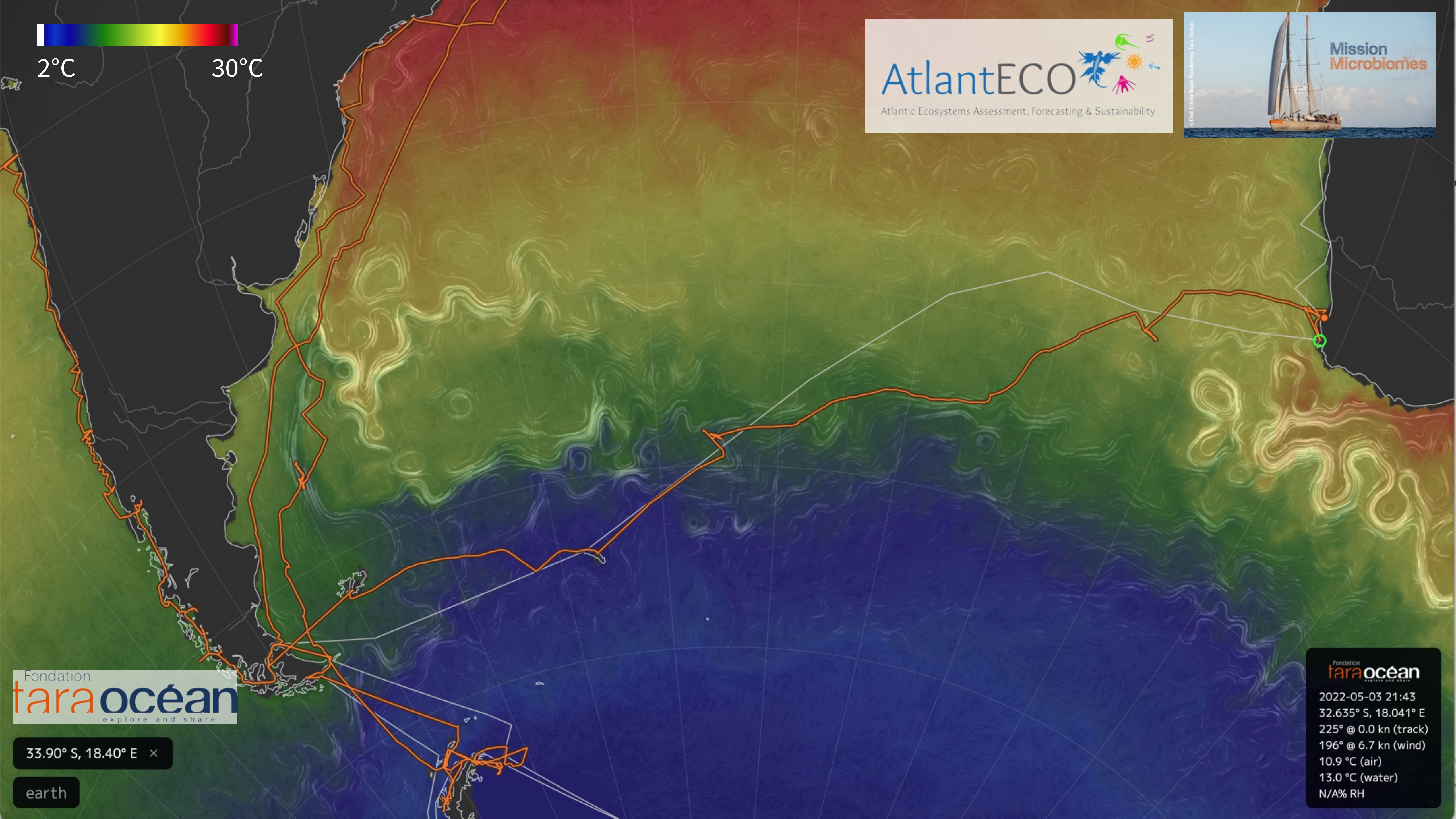
FIGURE 1 | Comparison of the total size range of plankton (in equivalent spherical diameter; ESD) that available optical and imaging methods can sample. Dashed lines represent the total operational size range from commercial information while the red line represent the practical size range which is efficient to obtain quantitative information, for an example see **Figure 2**. Drawings by Justine Courboules.

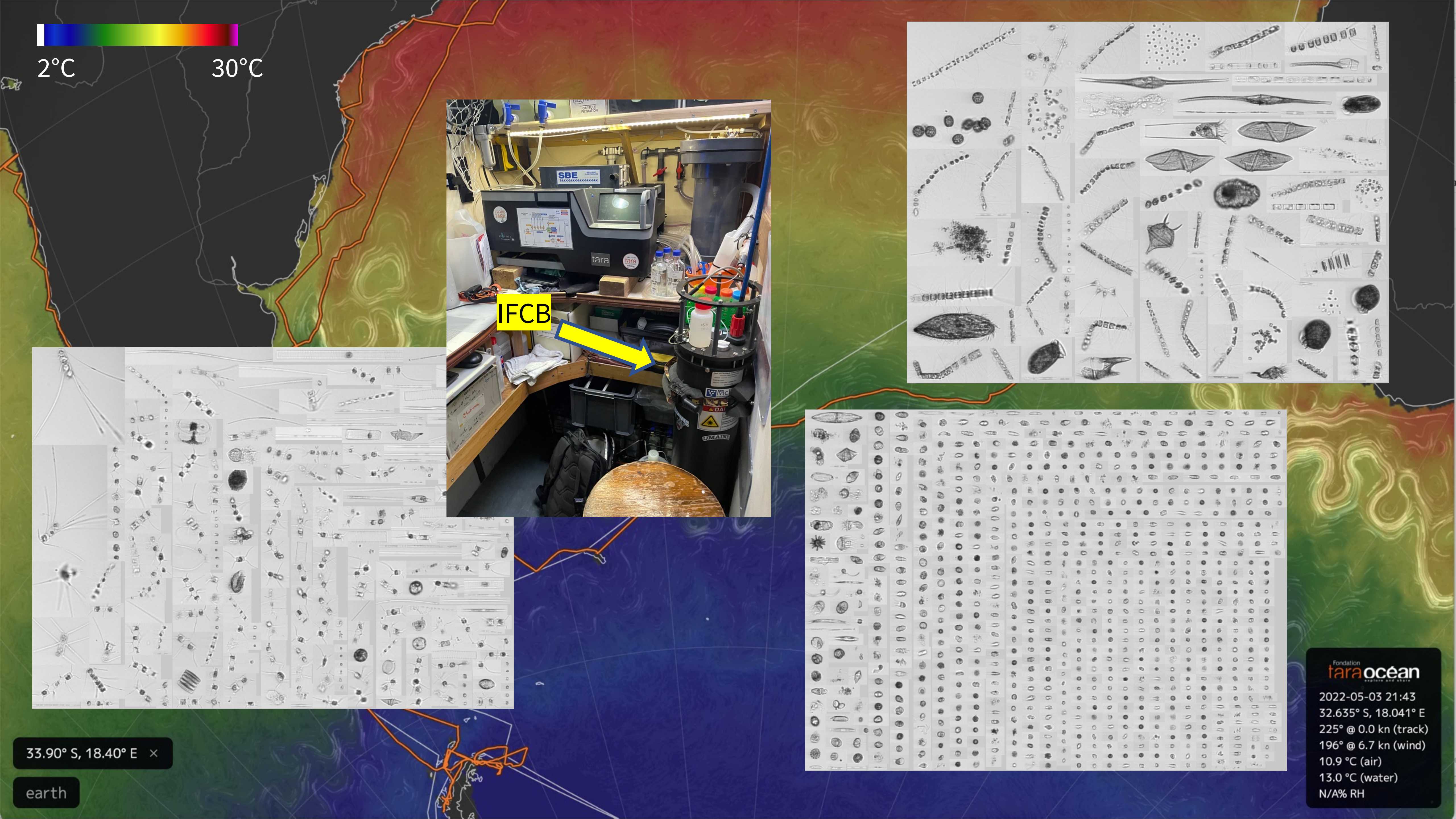
Plankton imagery used to determine community composition of cells ~8-150 µm

Imaging FlowCytobot (IFCB)






2°C
30°C
AtlantECO
Atlantic Ecosystems Assessment, Forecasting & Sustainability
Mission Microbiomes
Fondation tara océan explore and share
33.90° S, 18.40° E ×
earth
Fondation tara océan
2022-05-03 21:43
32.635° S, 18.041° E
225° @ 0.0 kn (track)
196° @ 6.7 kn (wind)
10.9 °C (air)
13.0 °C (water)
N/A% RH



2°C
30°C
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2022-05-03 21:43
32.635° S, 18.041° E
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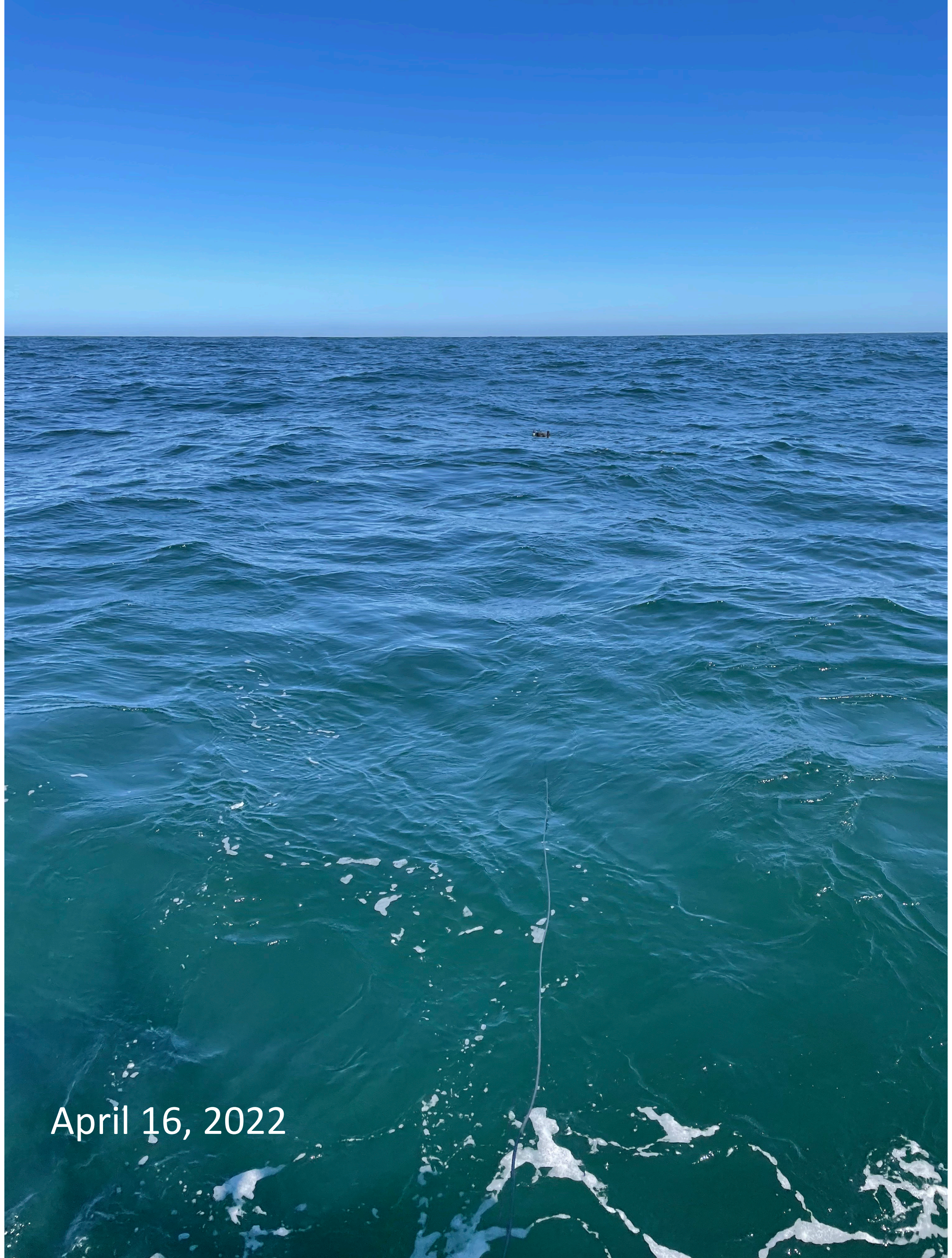
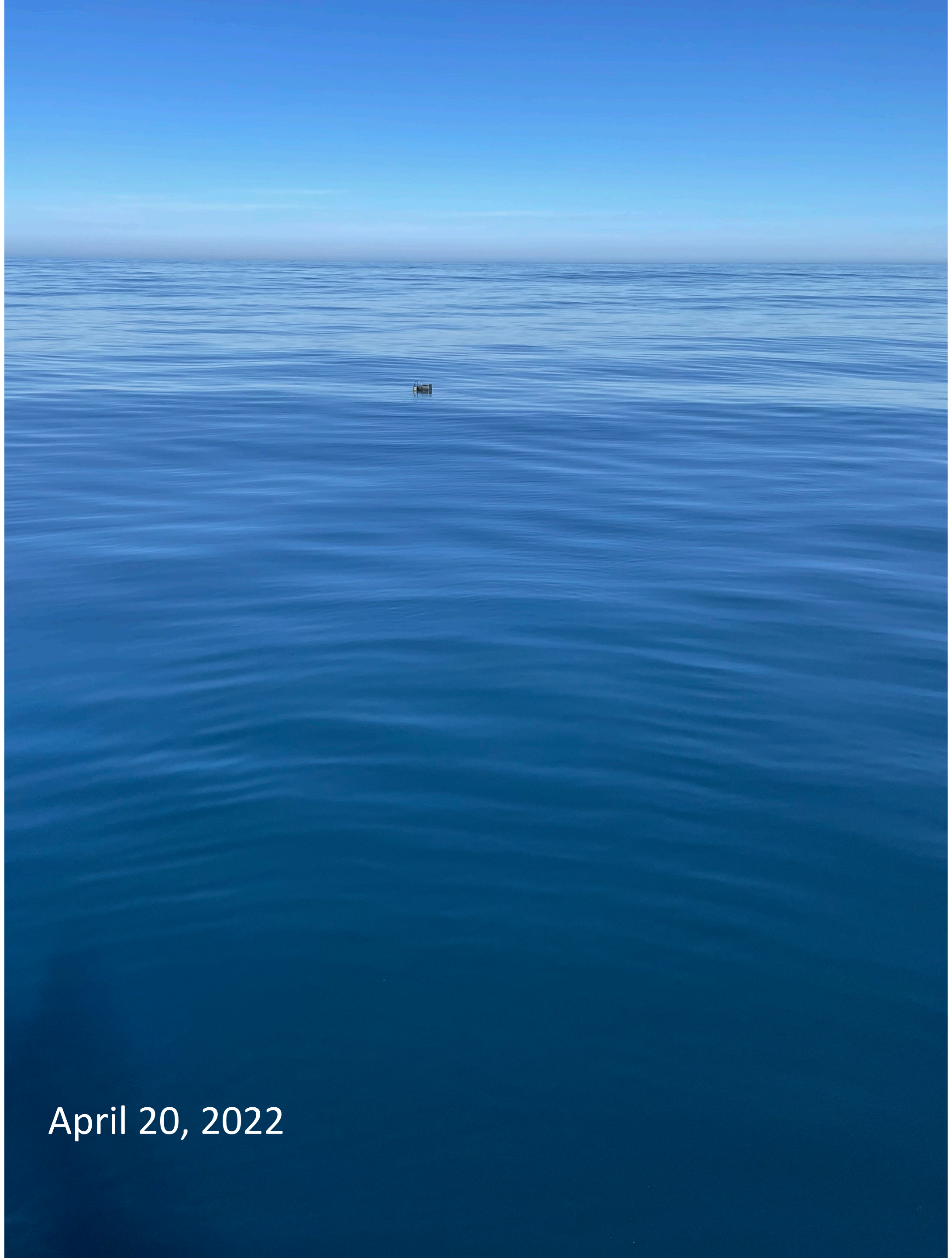
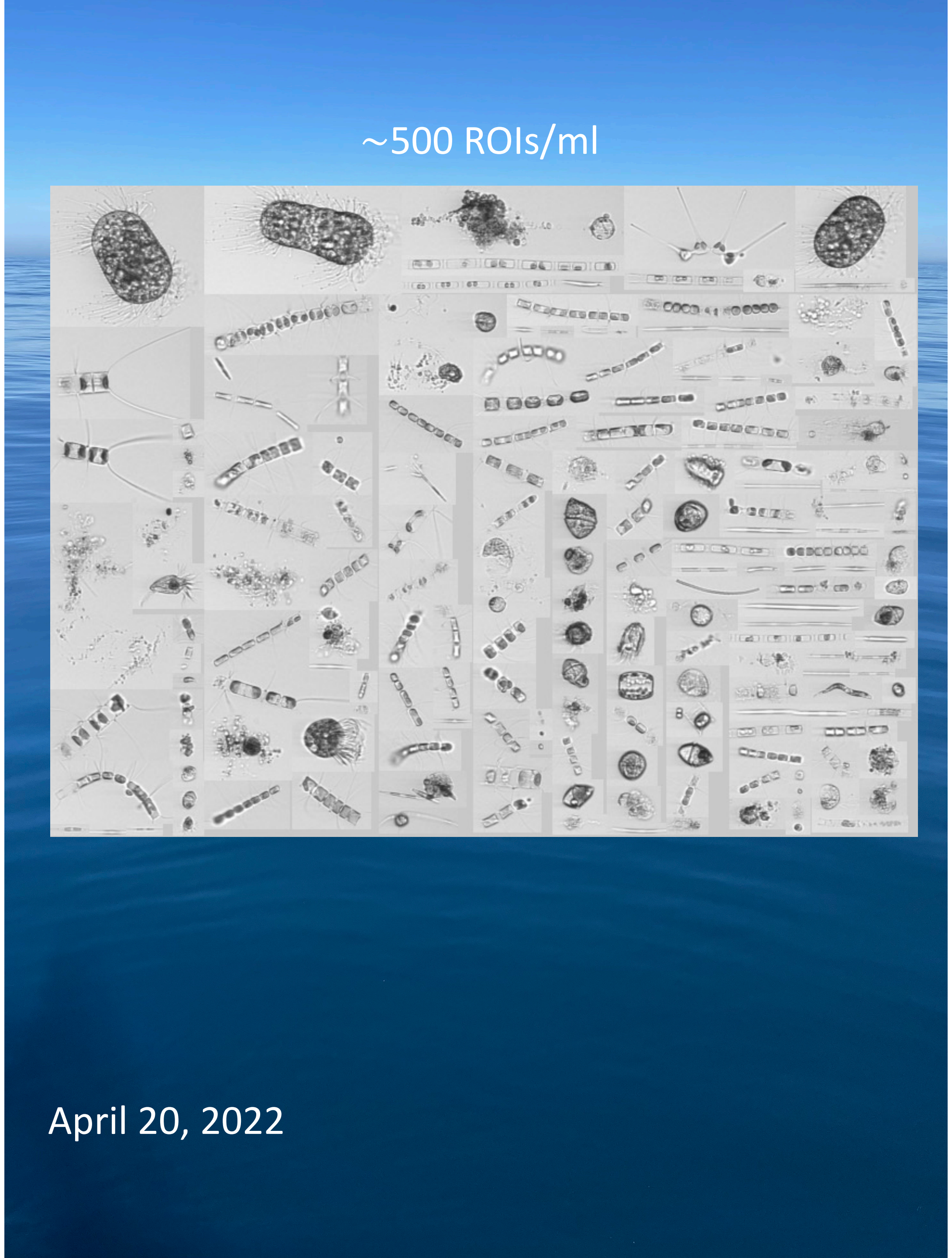

April 16, 2022

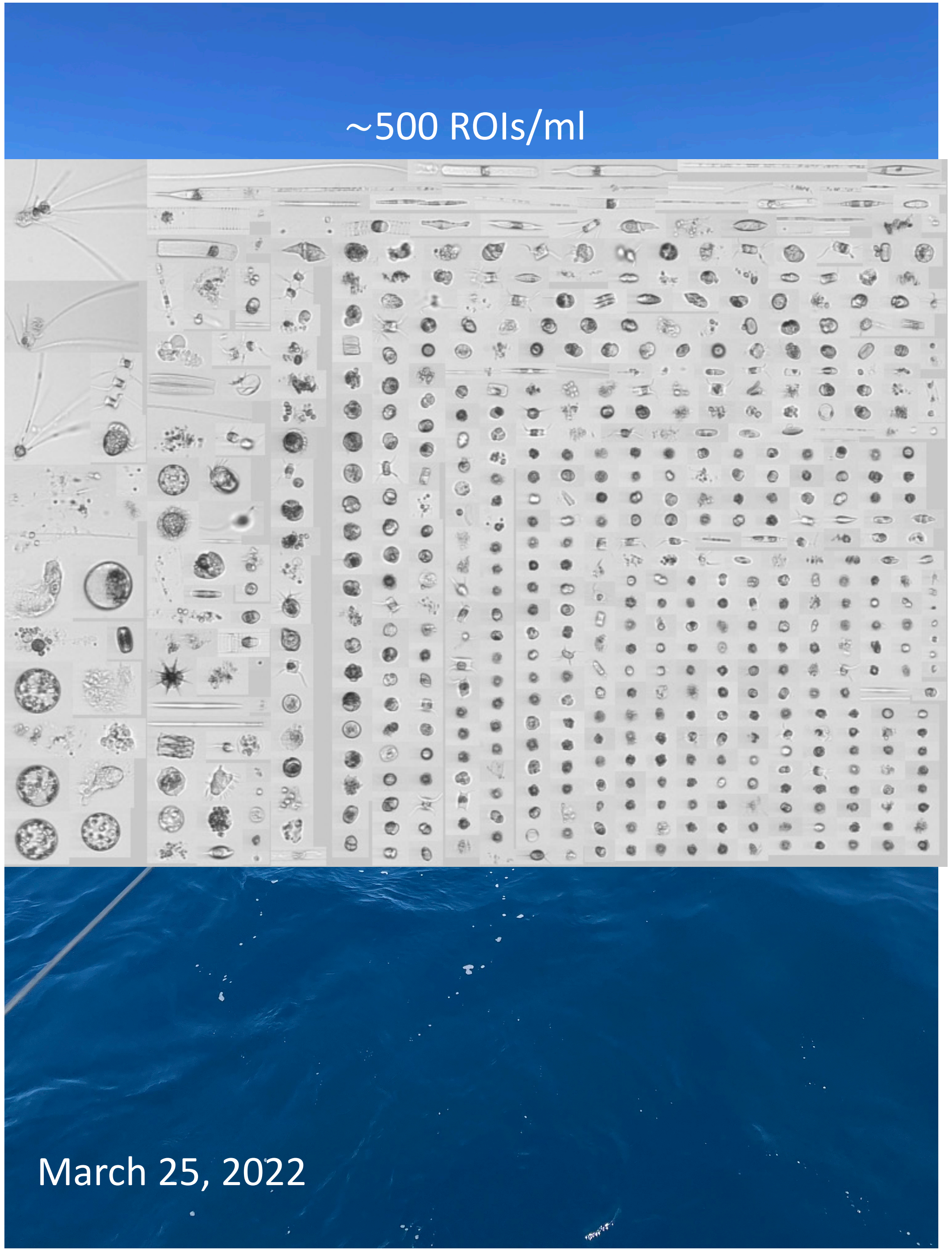

April 20, 2022

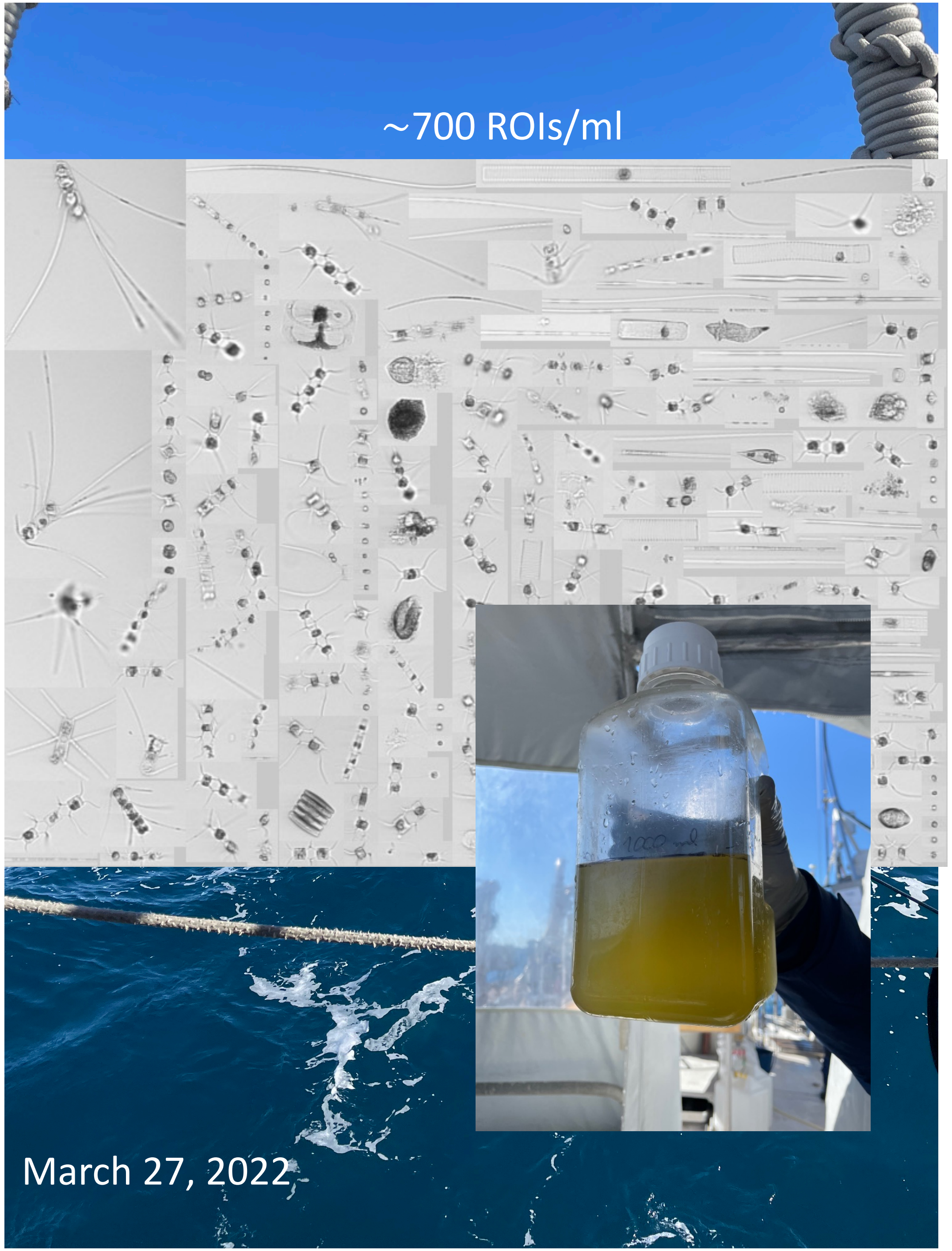

~3,000 ROIs/ml
April 16, 2022


~500 ROIs/ml
April 20, 2022

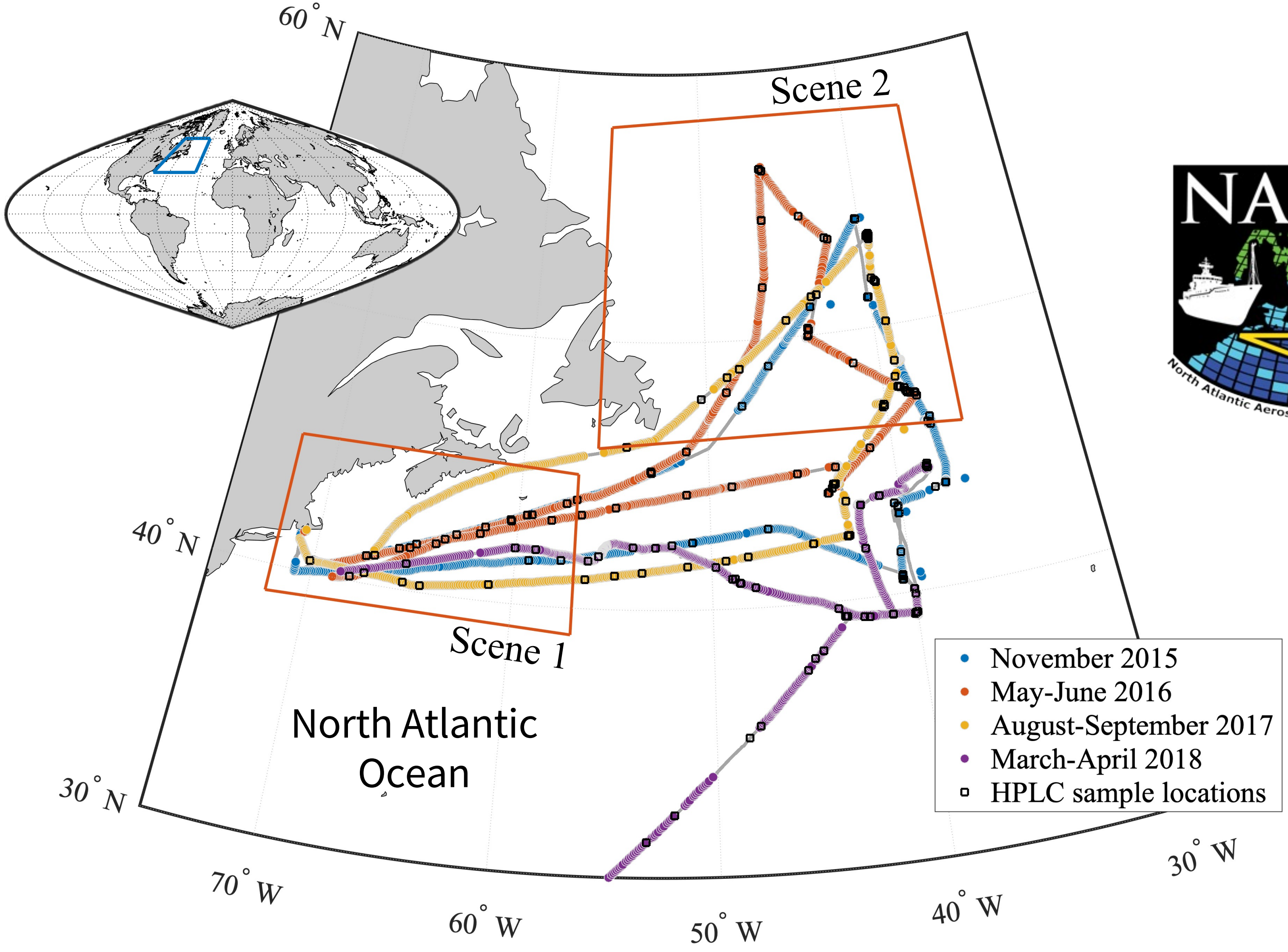

March 25, 2022

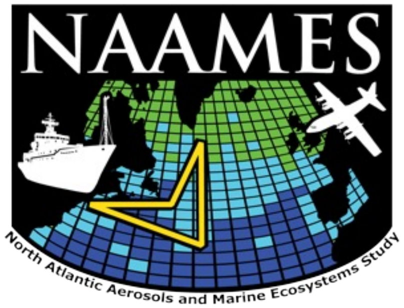

March 27, 2022


~500 ROIs/ml
March 25, 2022

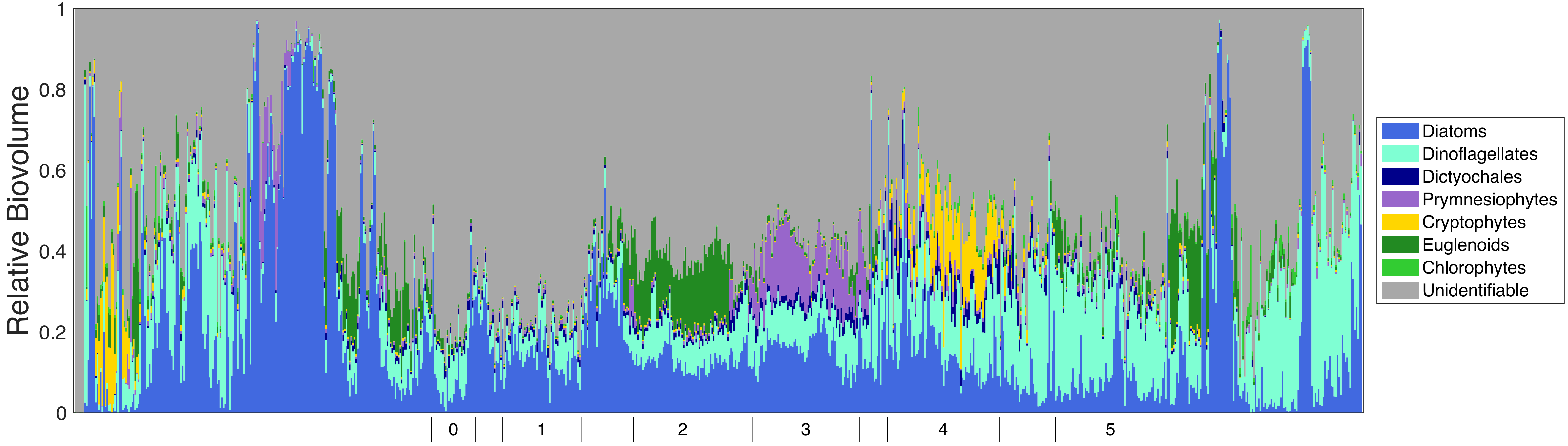

~700 ROIs/ml
March 27, 2022

~5 million IFCB images spanning four seasons



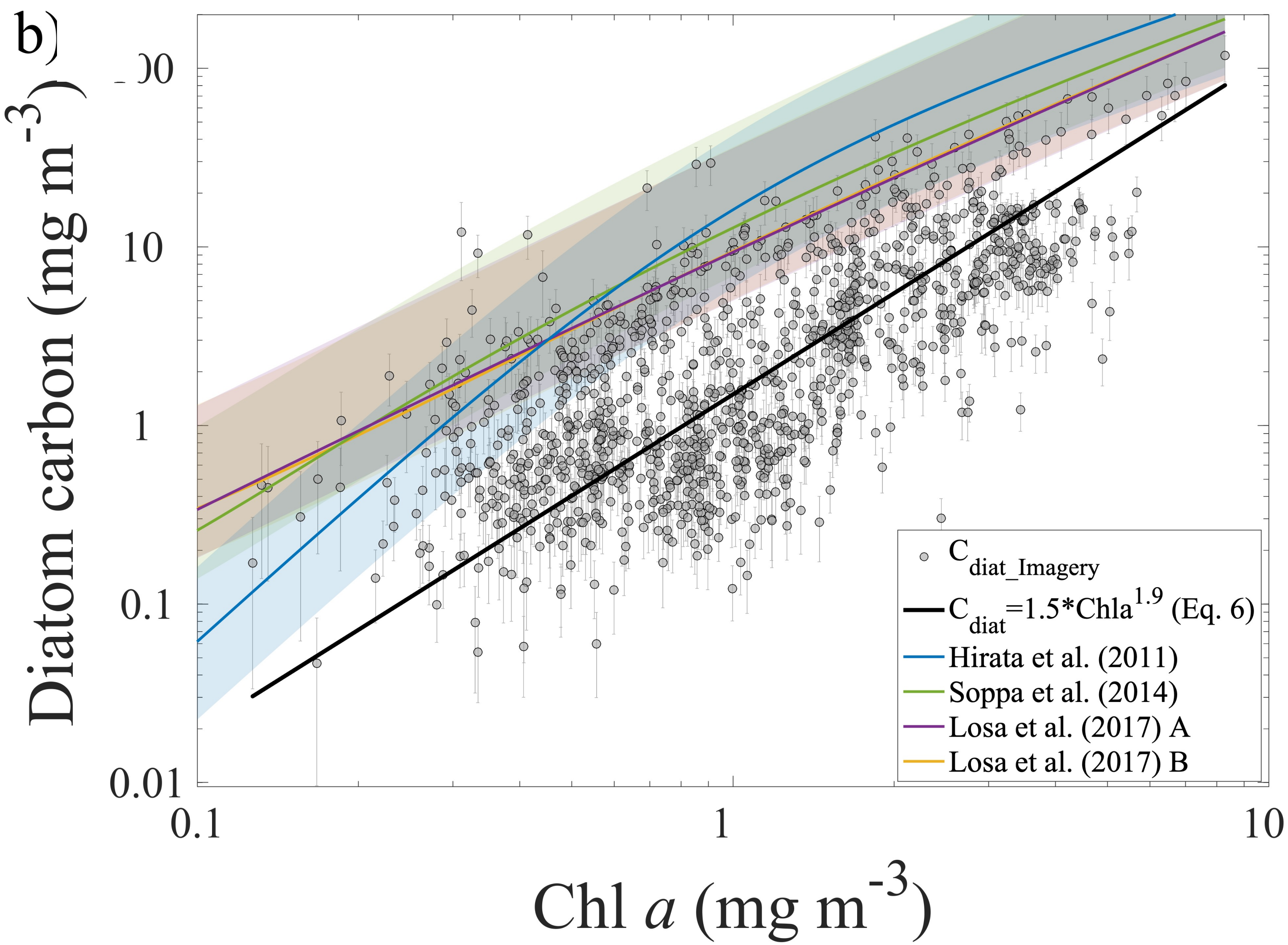


High spatial resolution measurements of phytoplankton taxonomic groups



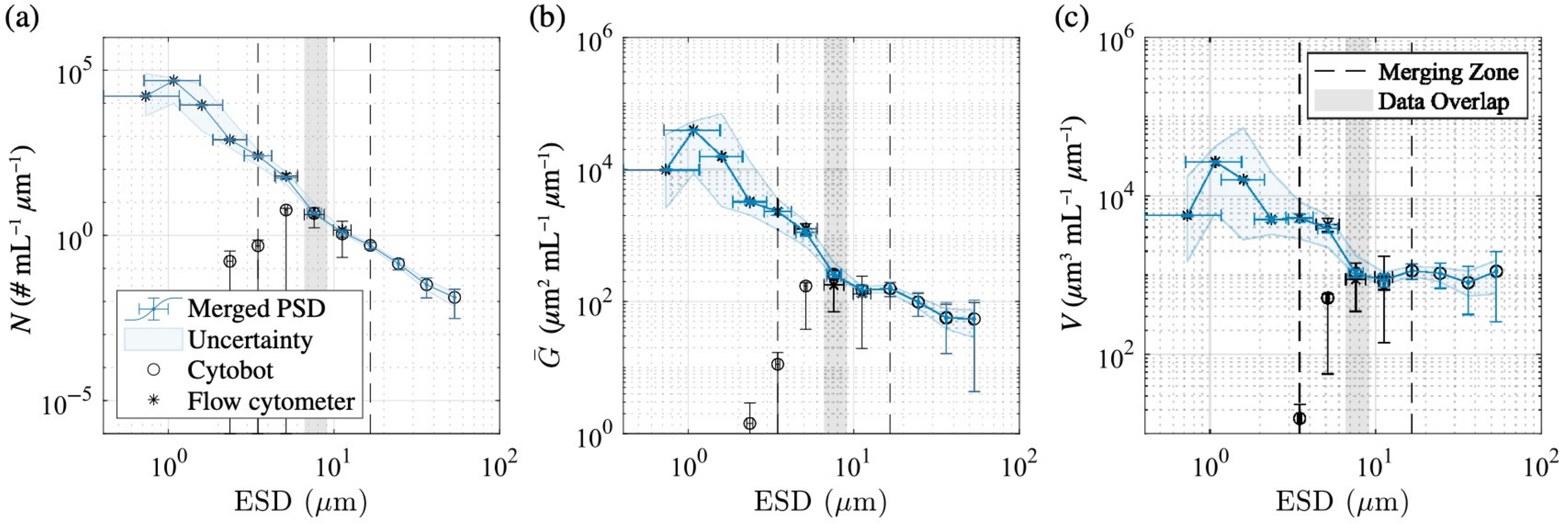
NAAMES
North Atlantic Aerosols and Marine Ecosystems Study

Variability in diatom carbon across chlorophyll *a*



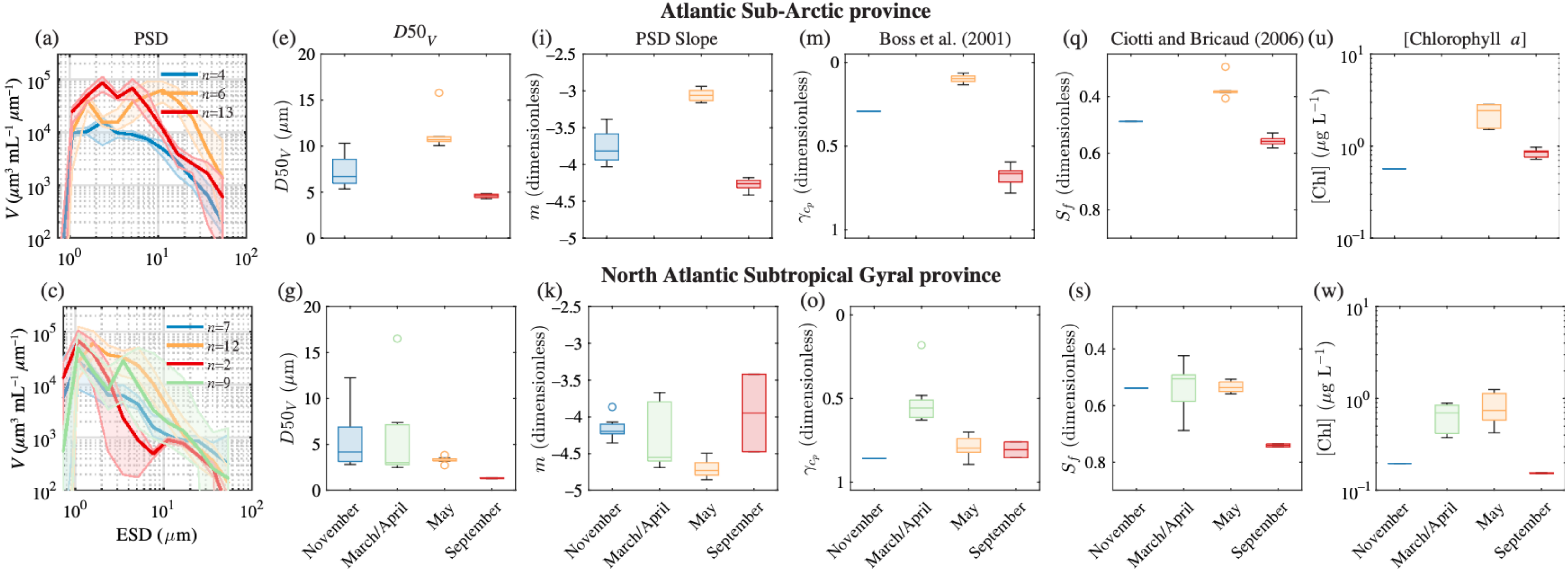
Chase et al., 2022

Merged cytometry-based phytoplankton size distributions



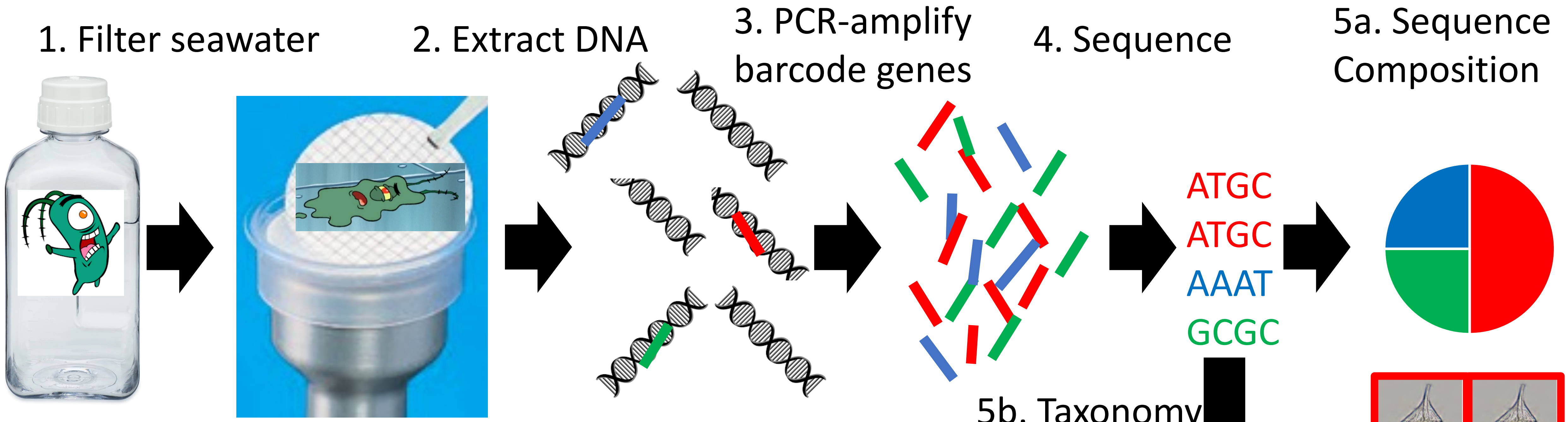
Haëntjens et al., 2022

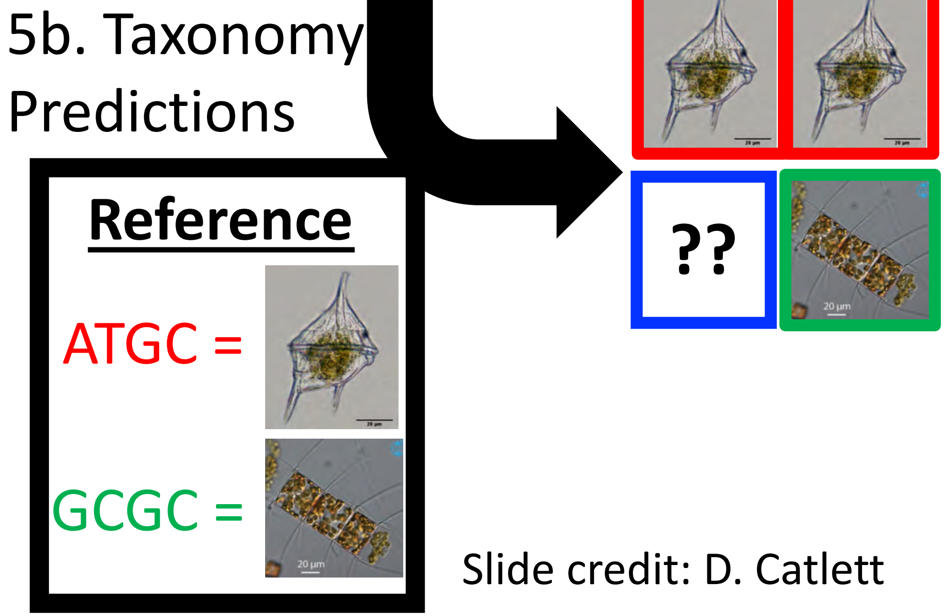
PSDs and optical size proxies



Haëntjens et al., 2022

DNA meta-barcoding





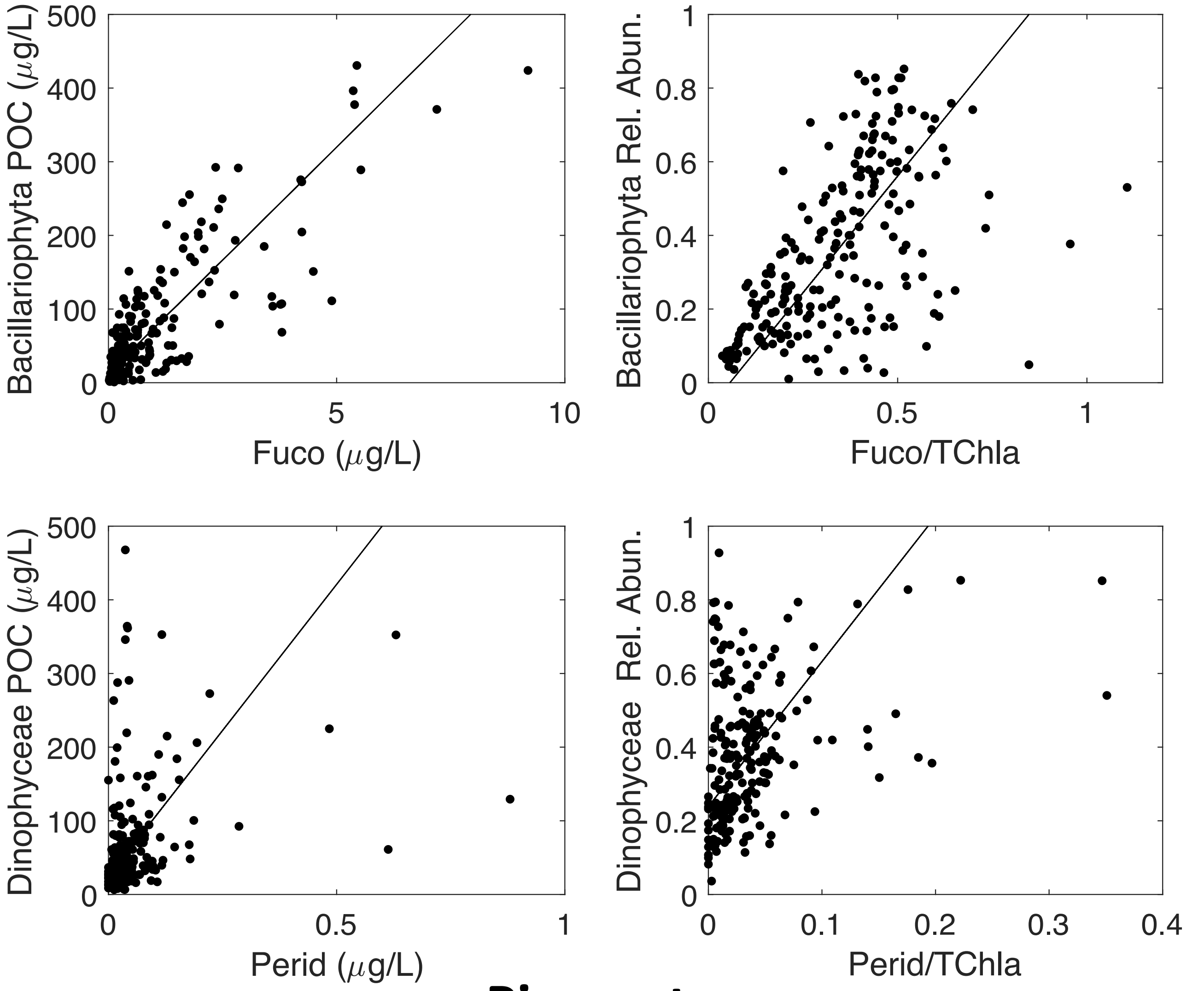
- DNA meta-barcoding "measures" the relative sequence abundances of amplicon sequence variants (ASVs ≈ species)
- Compare ASVs to reference seqs with known origin to assign taxonomy, get relative abundances of species/groups

Slide credit: D. Catlett

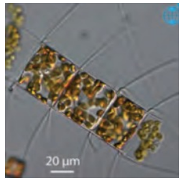
Phytoplankton group comparisons

Concentrations **Compositions**

DNA Meta-barcoding



Pigments



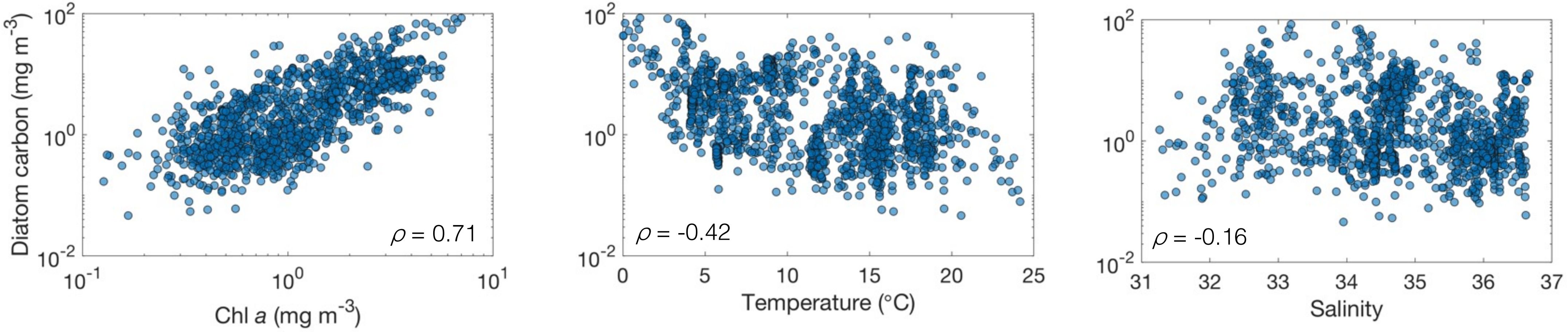
Diatoms

(Phytoplanktonic) Dinoflagellates

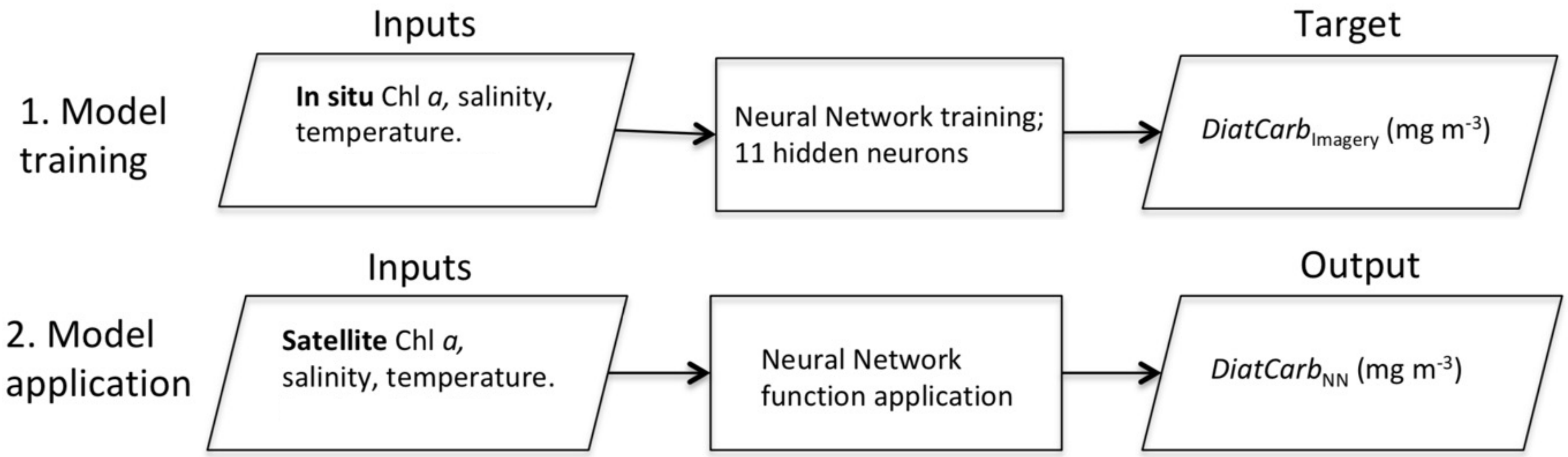
Slide credit: D. Catlett

*Catlett et al., in review at *L&O*

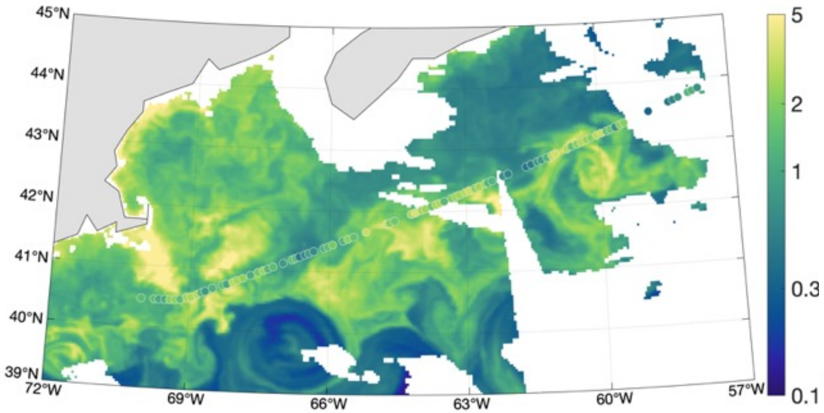
Shallow neural networks trained using plankton imagery data



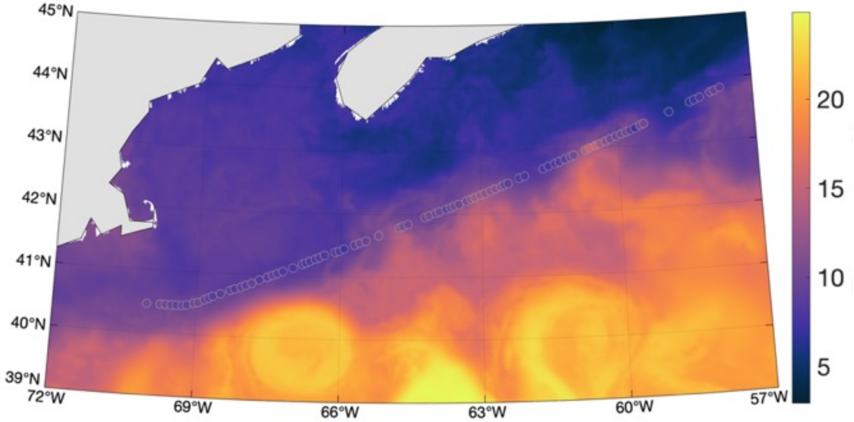
→ Diatom carbon and environmental variables are correlated but with high variability



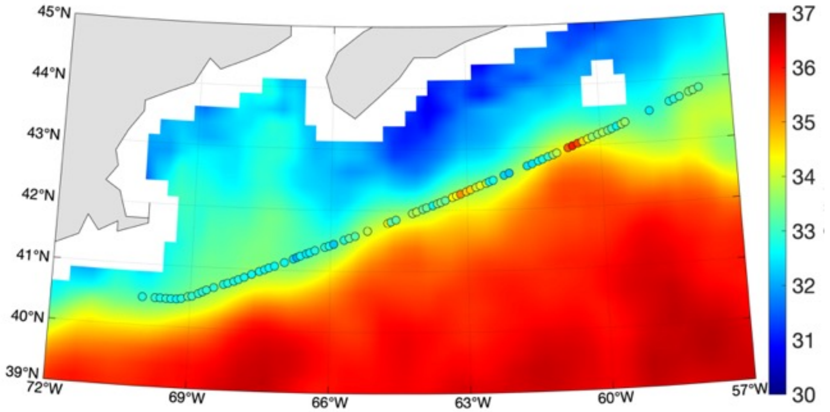
Merging satellite products from multiple platforms



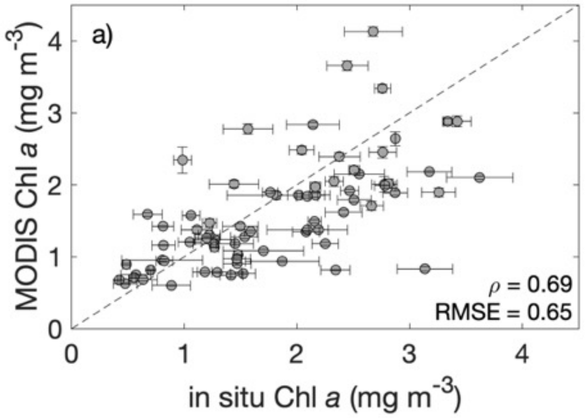
Daily MODIS Aqua Chl *a*

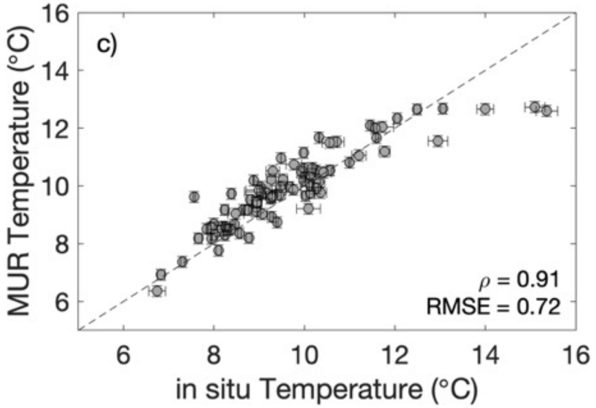


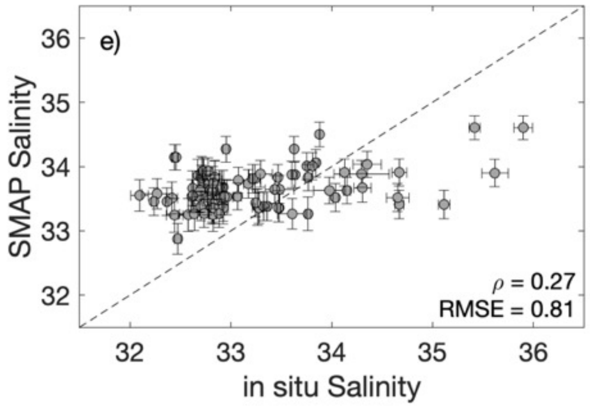
Daily MUR SST product



Monthly SMAP SSS





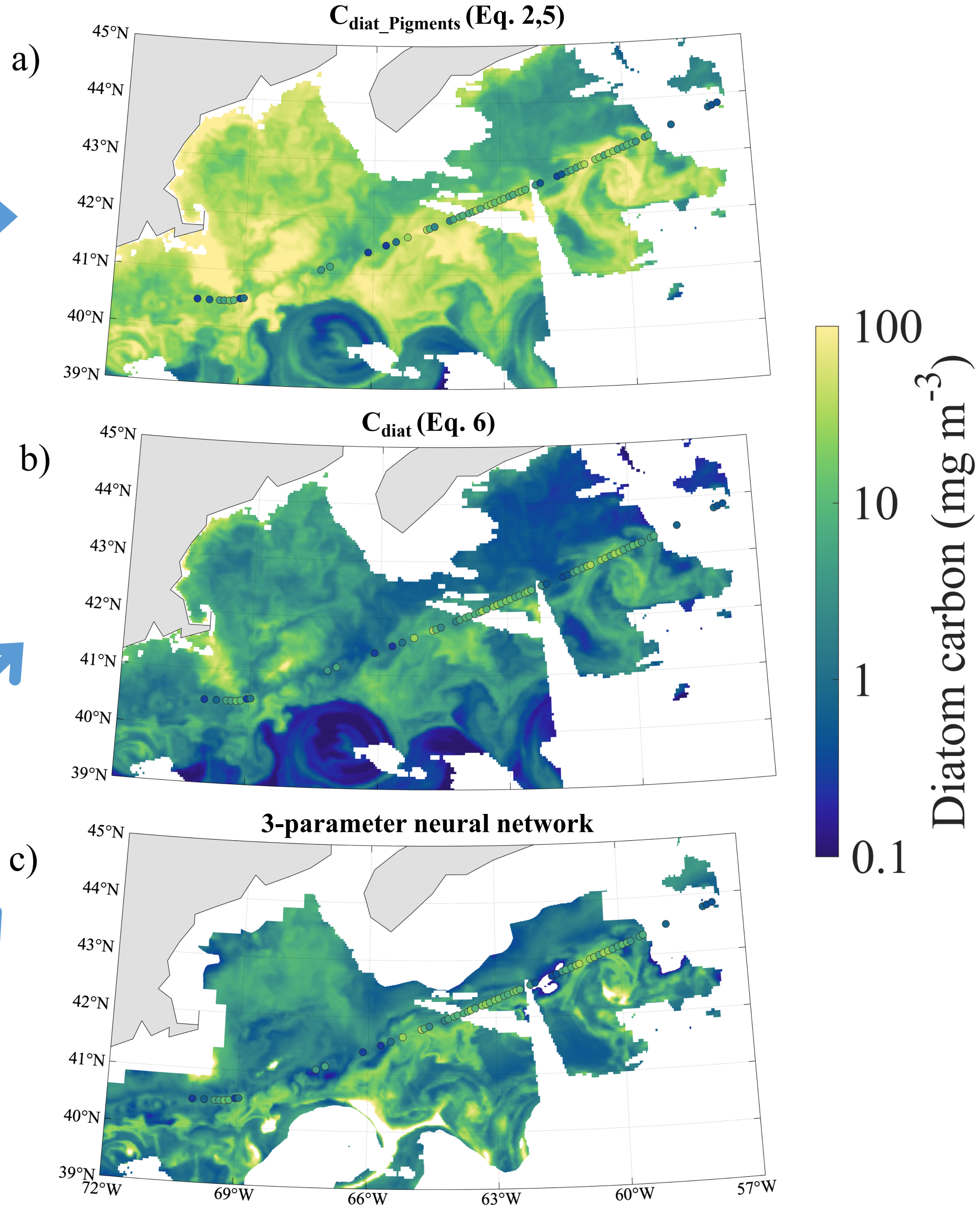


Chase et al., 2022

Comparison of satellite-based estimates of diatom carbon

Diatoms defined by pigment proxy

Diatoms defined by plankton imagery



Previous Chl a-based method (Hirata et al., 2011)

Updated Chl a-based method

Neural network-based method

Chase et al., 2022

Uncertainty calculations are necessary!

Cell biovolume estimate

Diatom ID accuracy

$$\mathbf{Unc_{data}} = \sqrt{\mathbf{0.17^2 + 0.18^2 + 0.1^2 + 0.29^2}} = \mathbf{0.39},$$

Statistical counting error

Chl *a* uncertainty

$\mathbf{Unc_{data}}$

Neural network uncertainty

$$\mathbf{Unc_{NN}} = \sqrt{\mathbf{0.39^2 + 0.52^2}} = \mathbf{0.65},$$

At low estimated diatom carbon values, the absolute error dominates over the relative error, and thus Unc_{NN} = max(1.05 mg m^{-3}, 65%)

Is it good enough???

Machine learning techniques to characterize functional traits of plankton from image data

Eric C. Orenstein,[1] Sakina-Dorothée Ayata,[1,2*] Frédéric Maps,[3,4] Érica C. Becker,[5] Fabio Benedetti,[6]

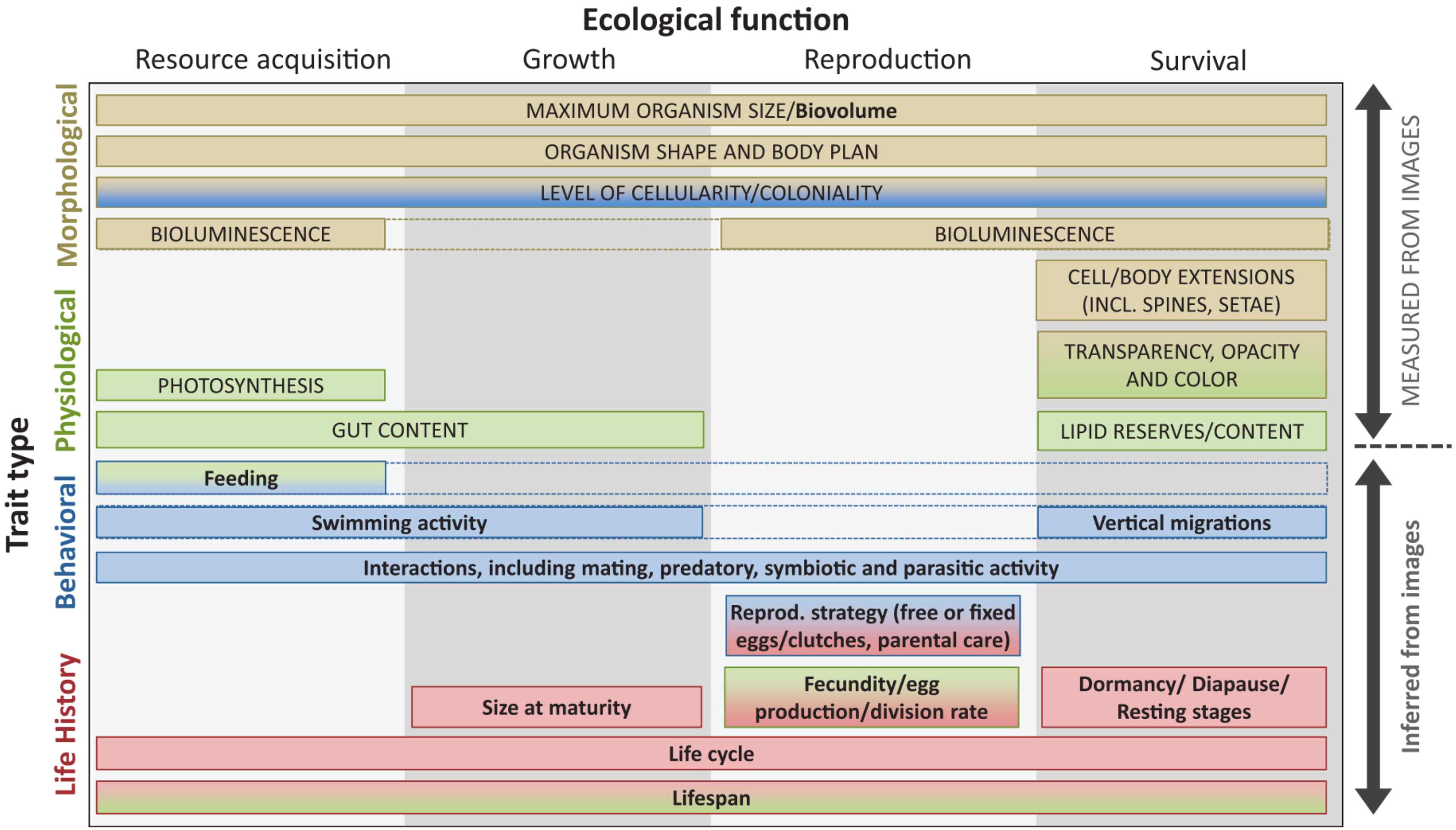
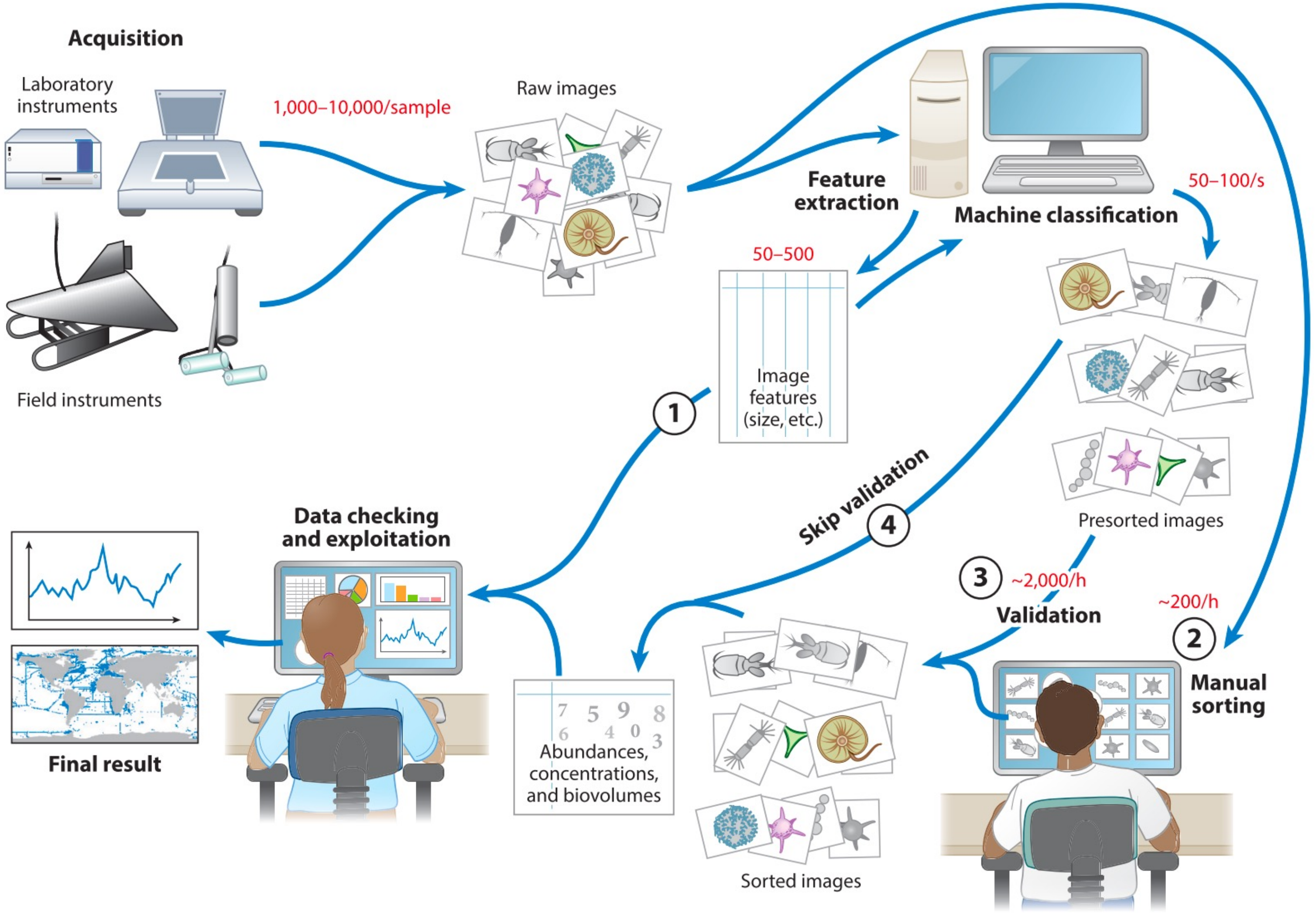


Fig. 1. Plankton functional traits that can be estimated from images, following the unified typology of Martini et al. (2021). Trait types along the *y*-axis follow the order of the "Plankton traits from images" section. Measured traits, ones that can be quantified solely from images, are in capital letters. Inferred traits, which require additional information beyond raw pixels, are written in bold text.

Annual Review of Marine Science

Machine Learning for the Study of Plankton and Marine Snow from Images

Jean-Olivier Irisson,[1] Sakina-Dorothée Ayata,[1] Dhugal J. Lindsay,[2] Lee Karp-Boss,[3] and Lars Stemmann[1]



→ Note that deep learning networks do not necessarily require a separate feature extraction step

LIMNOLOGY AND OCEANOGRAPHY
Methods

ASLO
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Machine and Deep Learning Approaches to Methodological Challenges

Virtual Issues | First published: **1 May 2022** | Last updated: **2 May 2022**

→ 9 of 20 manuscripts related to various types of plankton imaging

Define and train a convolutional neural network (CNN) model

- Define and compile the layers of the CNN model
- Train the model and save the history object

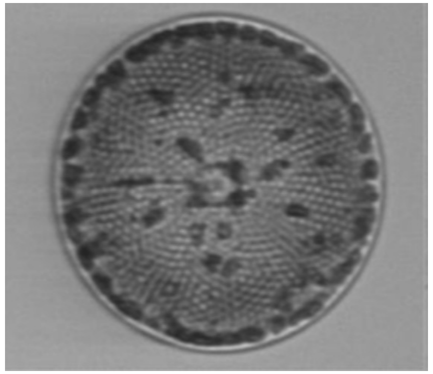
```
def create_cnn_model_A1(width, height, depth, filters=(32, 16, 64, 32, 128, 128, 64, 256, 256, 128),
regress=False):
    inputShape = (height, width, depth)
    chanDim = -1
    inputs = Input(shape=inputShape)
    for (i, f) in enumerate(filters):
        if i == 0:
            x = inputs
        x = Conv2D(f, (3, 3), padding="same")(x)
        x = Activation("relu")(x)
        x = BatchNormalization(axis=chanDim)(x)
        if i in [1, 3, 6, 9]:
            x = MaxPooling2D(pool_size=(3, 3))(x)
    x = Flatten()(x)
    x = Dense(512)(x)
    x = Activation("relu")(x)
    x = BatchNormalization(axis=chanDim)(x)
    x = Dropout(rate=0.2)(x)
    x = Dense(1000)(x)
    x = Activation("relu")(x)
    if regress:
        x = Dense(1, activation="linear")(x)
    model = Model(inputs, x)
    return model
```

```
H = model.fit(
      trainGen,
      steps_per_epoch=totalTrain // batch_size,
      validation_data=validationGen,
      validation_steps=totalVal // batch_size,
      #epochs=2,
      epochs=10,
      callbacks=[tensorboard_callback])
```

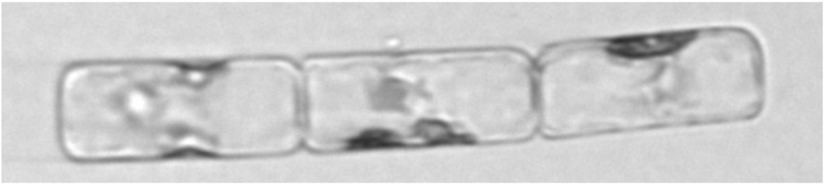
Considerations for model runs in plankton image classification

<u>Preprocessing</u>

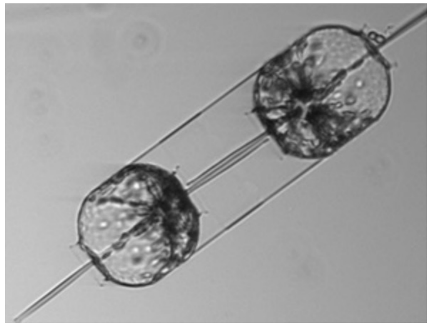
- Data augmentation, rotations, replicates
- Preserve the length/width ratio when data are prepared?
- Model tests to evaluate impact of image augmentation
- Background color and normalization to one shade of gray (concerns of varying instruments and users)
- Adjust darkness as a form of augmentation
- Position of image within the field of view



Mouw Lab, URI



Sosik Lab, WHOI



Kudela Lab, UCSC

Lecture outline & key points

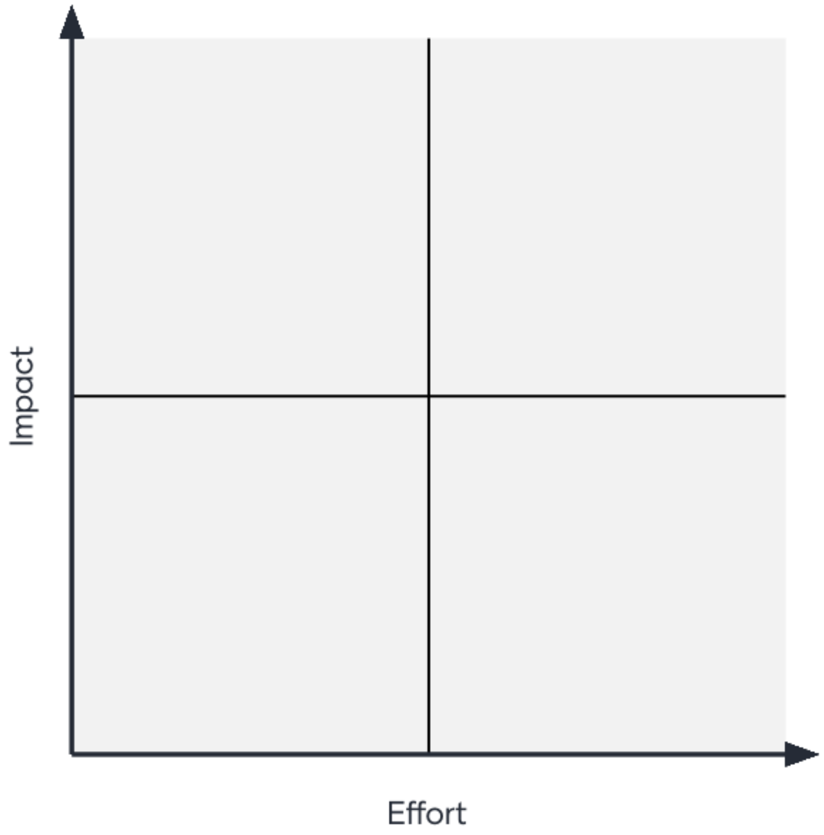
→ **Previous studies to estimate phytoplankton community composition from optics & remote sensing**

→ **Recent work and expansion to include new approaches and data types**

→ **Where do we go from here? (hint: you tell me!)**

Go to **www.menti.com** and use the code **8534 4169**

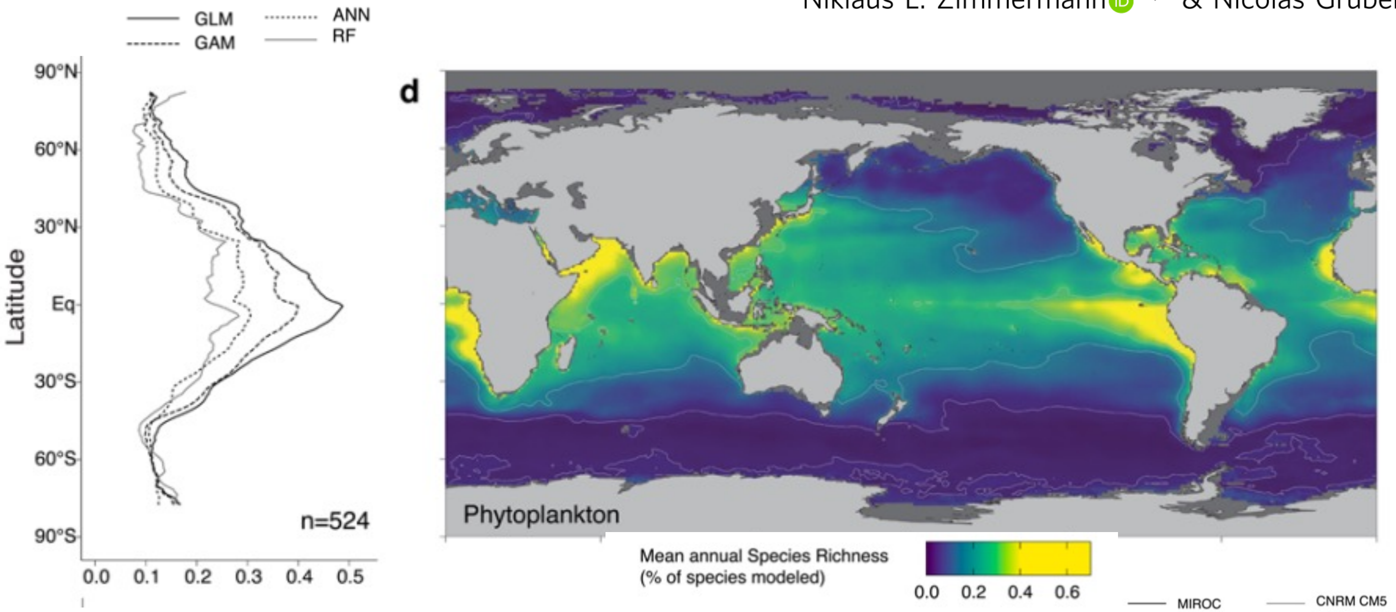
In your opinion, rate the impact and effort of four facets of PCC algorithm development



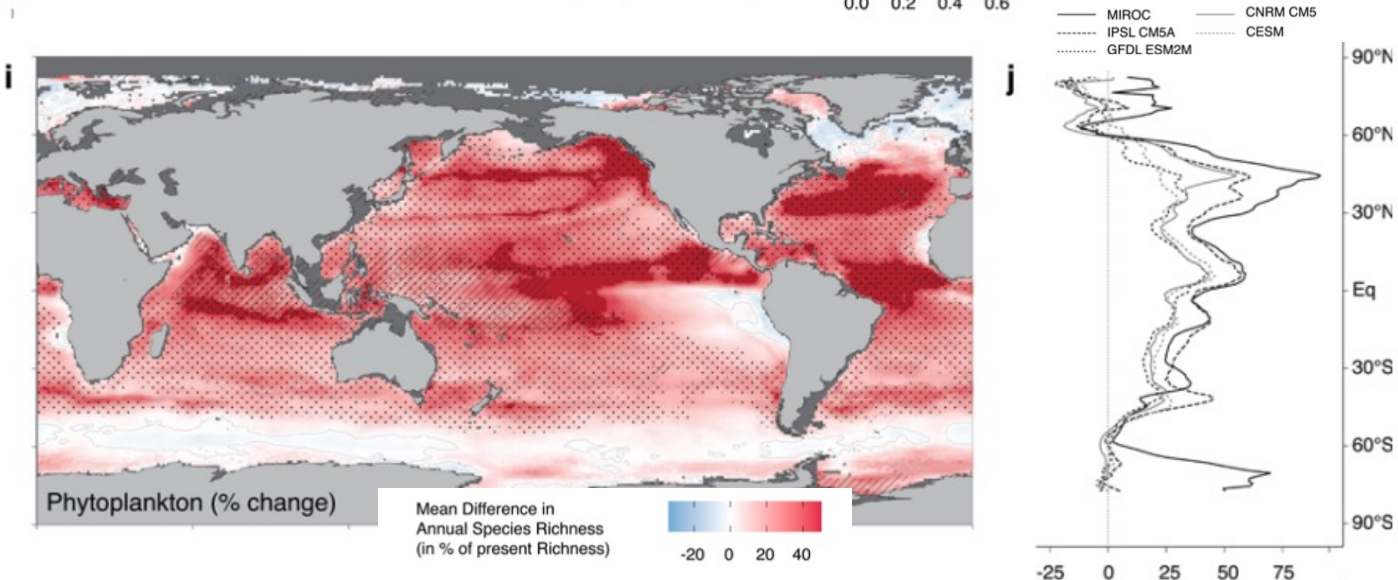
1. Absolute (vs relative) quantities
2. Broad applicability
3. Closure w/independent methods/models
4. End user needs

Major restructuring of marine plankton assemblages under global warming

Fabio Benedetti[1✉], Meike Vogt[1], Urs Hofmann Elizondo[1], Damiano Righetti[1], Niklaus E. Zimmermann[2,3] & Nicolas Gruber[1]



Annual mean species richness in the contemporary surface ocean

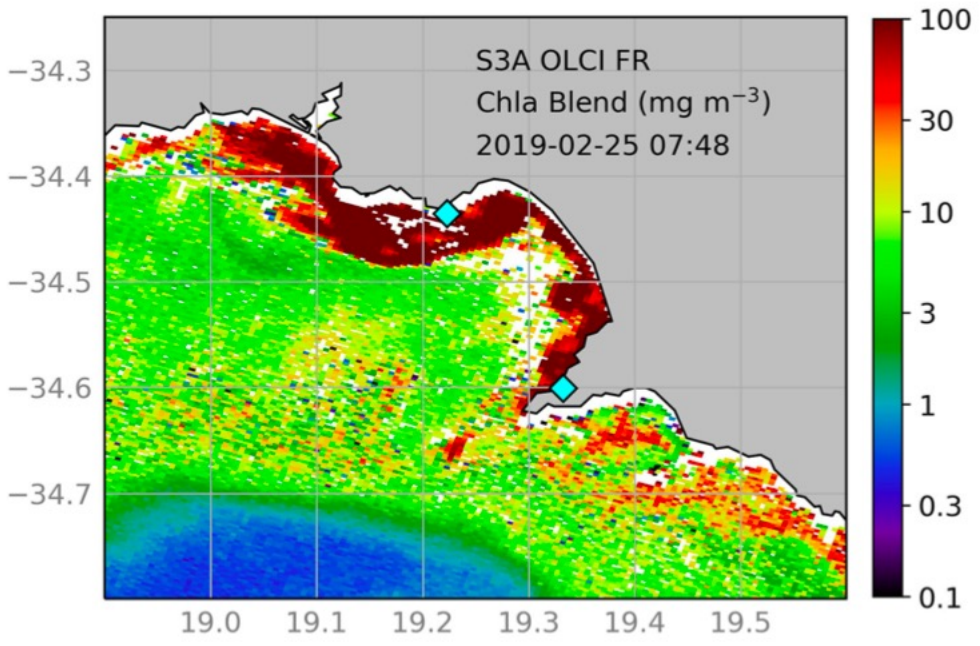


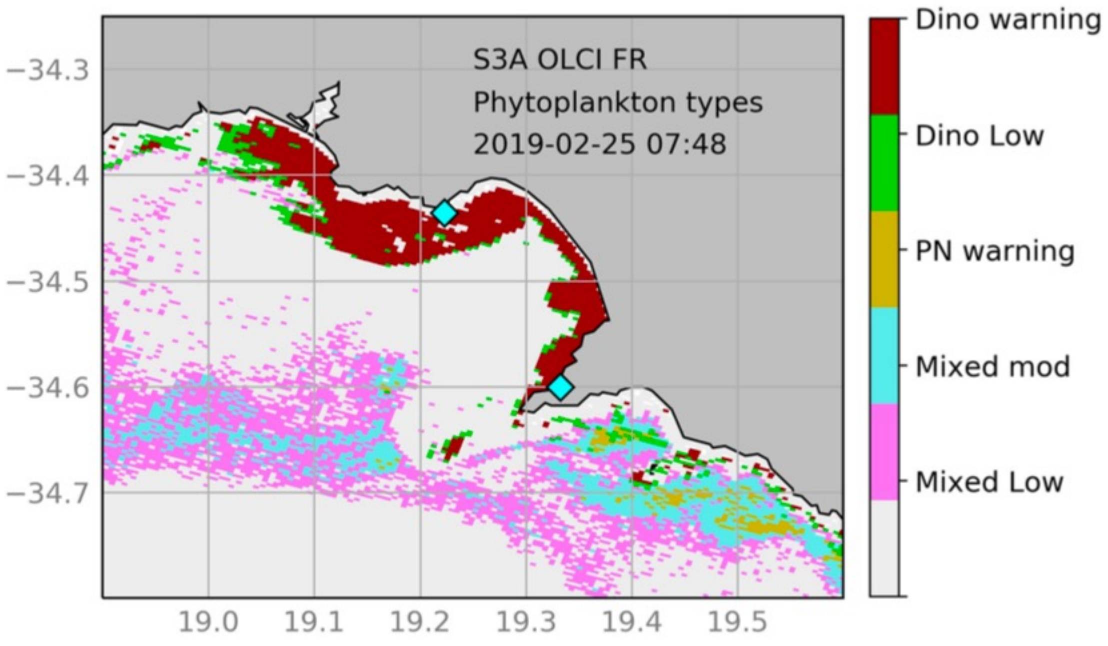
Projected change in species richness for 2081-2100 period

Benedetti et al. 2021

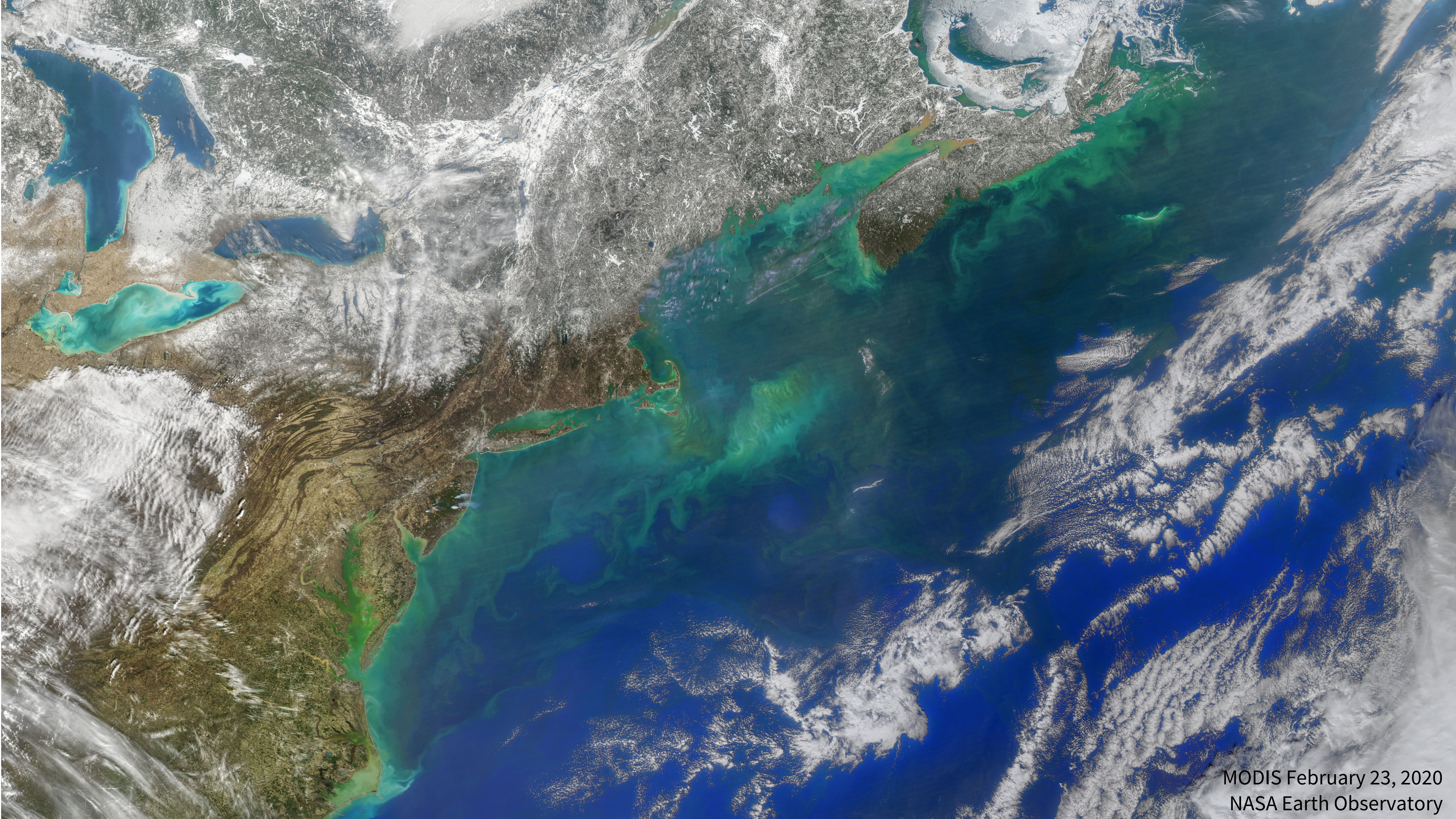
Satellite Ocean Color Based Harmful Algal Bloom Indicators for Aquaculture Decision Support in the Southern Benguela

Marié E. Smith [1] and Stewart Bernard [1,2]*





Smith and Bernard, 2020


MODIS February 23, 2020
NASA Earth Observatory

How can we navigate the push-pull of untapped potential in PCC algorithms, and the inherent challenges?

*Different questions will have different data needs. Consider when a given data product is applicable, and when it is not. **What** do you want to know, and **why**?*

→ Consider scales of spatial and temporal variability
→ Remember that uncertainties “complete the data”

Overcoming the Challenges of Ocean Data Uncertainty

In oceanography, as in any scientific field, the goal is not to eliminate uncertainty in data, but instead to better quantify and clearly communicate its size and nature.

By **Shane Elipot**, **Kyla Drushka**, **Aneesh Subramanian**, and **Mike Patterson** 12 January 2022

> *An ocean data set may otherwise be of the highest scientific quality, but if quantified uncertainties do not accompany it, it will not be useful to scientists or other stakeholders.*

> *Some concepts that are applicable to bench measurements are difficult to translate to the oceanographer's laboratory—the ocean—because the ocean and the climate system in which it is embedded are constantly changing.*

This view from the International Space Station shows sea ice floes and eddy currents near the coast of Russia's Kamchatka Peninsula. Credit: NASA JSC Earth Science and Remote Sensing Unit

https://eos.org/opinions/overcoming-the-challenges-of-ocean-data-uncertainty

From Orenstein et al., 2022:

“…we would like to advocate for two goals that we should pursue as a community: (1) more open and efficient sharing of trait-annotated datasets, and (2) development of educational programs at the interface of computer science and ecology.”

Open science

- Guidelines
- Repositories
- Trainings
- Tools

PANGEO

A community platform for Big Data geoscience

https://pangeo.io/index.html

GO FAIR

FAIR data principles, making data **F**indable, **A**ccessible, **I**nteroperable and **R**eusable (**FAIR**).

https://www.go-fair.org/

zenodo

https://zenodo.org/

Simons CMAP

Collaborative Marine Atlas Project

an open-source data portal interconnecting data sets across Oceanography disciplines

https://simonscmap.com/

TOPS

TRANSFORM TO OPEN SCIENCE

Transform to Open Science (TOPS)

https://science.nasa.gov/open-science/transform-to-open-science

Cloud Computing Platforms

Microsoft Azure

Microsoft Data Science Virtual Machine (DSVM)

amazon web services

Google Cloud

→ Many have free resources for students/academic users

A few favorite resources for GitHub, python, and machine learning

Git – the simple guide:
https://rogerdudler.github.io/git-guide/

Data Analysis in python for oceanographers:
https://currents.soest.hawaii.edu/ocn_data_analysis/index.html

Recommendation from Patrick:
https://www.pythonlikeyoumeanit.com/

Tools for satellite data analysis designed by Patrick:
https://github.com/patrickcgray/open-geo-tutorial

Set of four videos that explain neural networks and deep/shallow learning:
https://www.youtube.com/watch?v=aircAruvnKk&list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi

This website lets you play around with number of layers and neurons in a neural network and visualize the effects:
https://playground.tensorflow.org

General resource for clear explanations of math terms and concepts:
https://betterexplained.com/

What are the major challenges in PCC algorithm work?

- Sensitivity of methods to the uncertainties in measured products and/or intermediate derived products

- Target variables (PCC groups) are often defined by proxy, ultimately limiting algorithm refinement

- Sufficient datasets for model development and testing are not trivial to collect

- Linking what is needed by end users (e.g., climate & ecosystem modelers, water quality management & HAB detection)

What are the exciting opportunities in PCC algorithm work?

- Advancements in data collection technology for assessing in situ PCC
- Hyperspectral satellite remote sensing & UAV data
- Increased application of machine learning and computing power advancements
- Incorporation of additional/ancillary data, both in situ and via combing data from multiple satellite platforms
- Improved models and data collection that in turn provide insights into finer spatial and temporal scale properties of ocean dynamics

Thank you!

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