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# PACE Science and Application Team Updates

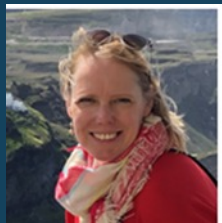
# Plankton, Aerosol, Cloud and ocean Ecosystem (PACE) :



## Synergies in Data, Science, and Applications

PACE

Plankton, Aerosol, Cloud, ocean Ecosystem  
Science and Applications Team



Heidi Dierssen, Jeremy Werdell and Lorraine Remer

University of Connecticut

Science and Applications Team Lead

# Hyperspectral Revolution

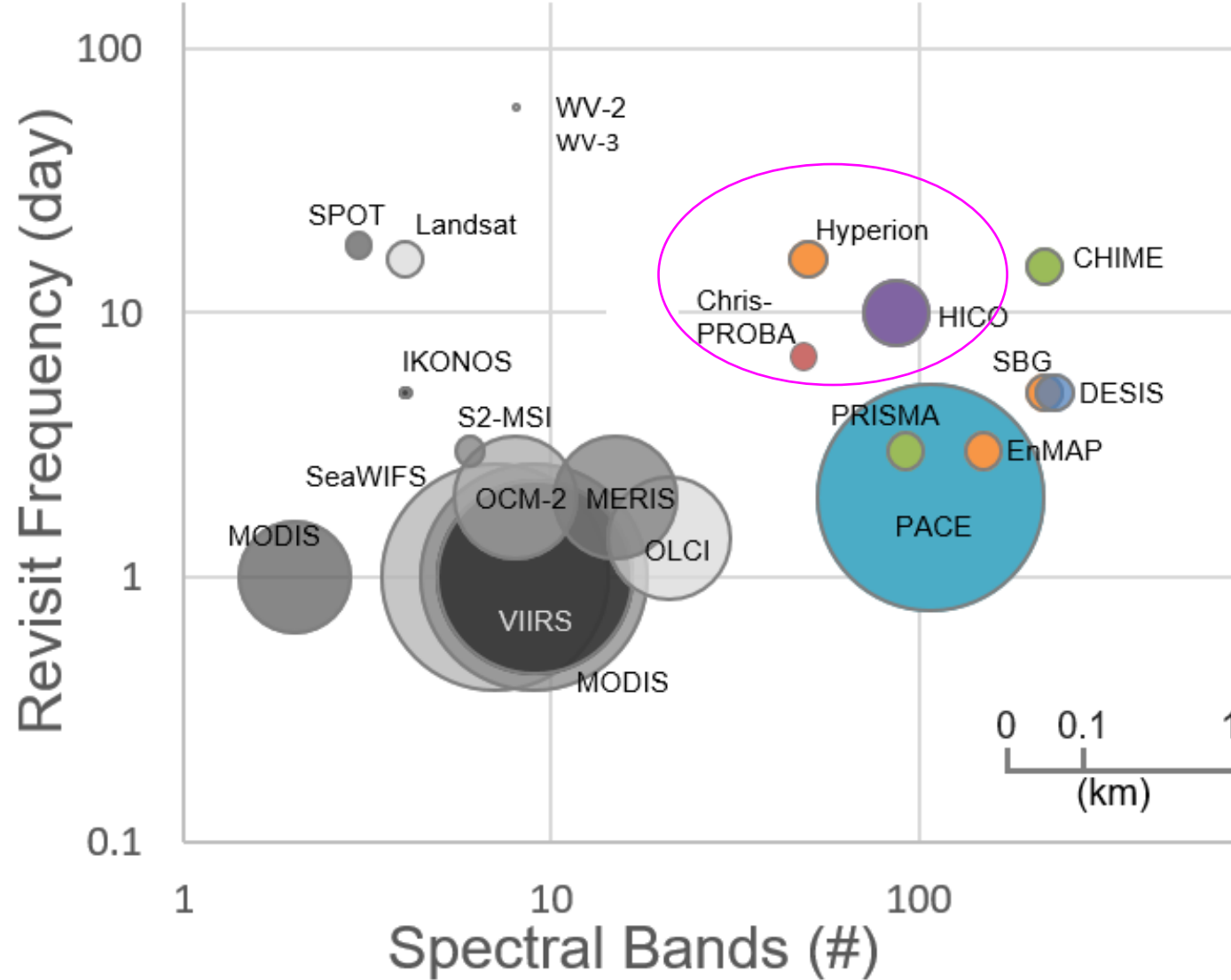




Fig. 7. A host of new applications will be available with better discrimination of pelagic and benthic biodiversity promised by hyperspectral imagery.

Dierssen et al. 2021



Class	Essential Biodiversity Variable (EBV)	Wetlands	Benthic communities		Pelagic		
		Mangrove/Salt marsh	Macrophytes & Macroalgae	Coral	Phytoplankton	Fish, Zooplankton	Apex Predator
Genetic Composition	Population genetic diversity						
Species Populations	Distribution						
	Abundance						
	Size/vertical distribution					**	
Species Traits	Pigments*					NA	NA
	Phenology						
Community Composition	Taxonomic diversity*						
Ecosystem Structure	Functional type*						
	Fragmentation/heterogeneity						
Ecosystem Function	Net primary production					NA	NA
	Net ecosystem production					NA	NA

# Living up to the Hype of Hyperspectral Aquatic Remote Sensing: Science, Resources and Outlook

Heidi M. Dierssen<sup>1\*</sup>, Steven G. Ackleson<sup>2</sup>, Karen E. Joyce<sup>3</sup>, Erin L. Hestir<sup>4</sup>, Alexandre Castagna<sup>5</sup>, Samantha Lavender<sup>6</sup> and Margaret A. McManus<sup>7</sup>

<sup>1</sup>Department of Marine Sciences, University of Connecticut, Groton, CT, United States, <sup>2</sup>Naval Research Laboratory, Washington, DC, United States, <sup>3</sup>College of Science and Engineering / TropWATER, James Cook University Nguma-bada Campus, Cairns, QLD, Australia, <sup>4</sup>Civil & Environmental Engineering, University of California Merced, Merced, CA, United States, <sup>5</sup>Protistology and Aquatic Ecology, Ghent University, Ghent, Belgium, <sup>6</sup>Pixalytics Ltd., Plymouth, United Kingdom, <sup>7</sup>Department of Oceanography, University of Hawai'i at Mānoa, Honolulu, HI, United States

\*Select types may be differentiated. \*\* using lidar techniques

Routine	Demonstrated	Unproven	Ecosystem Model
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# PACE Science and Applications Team (SAT)

Monthly meetings to discuss mission/algorithm synergies, new papers & opportunities , gaps,



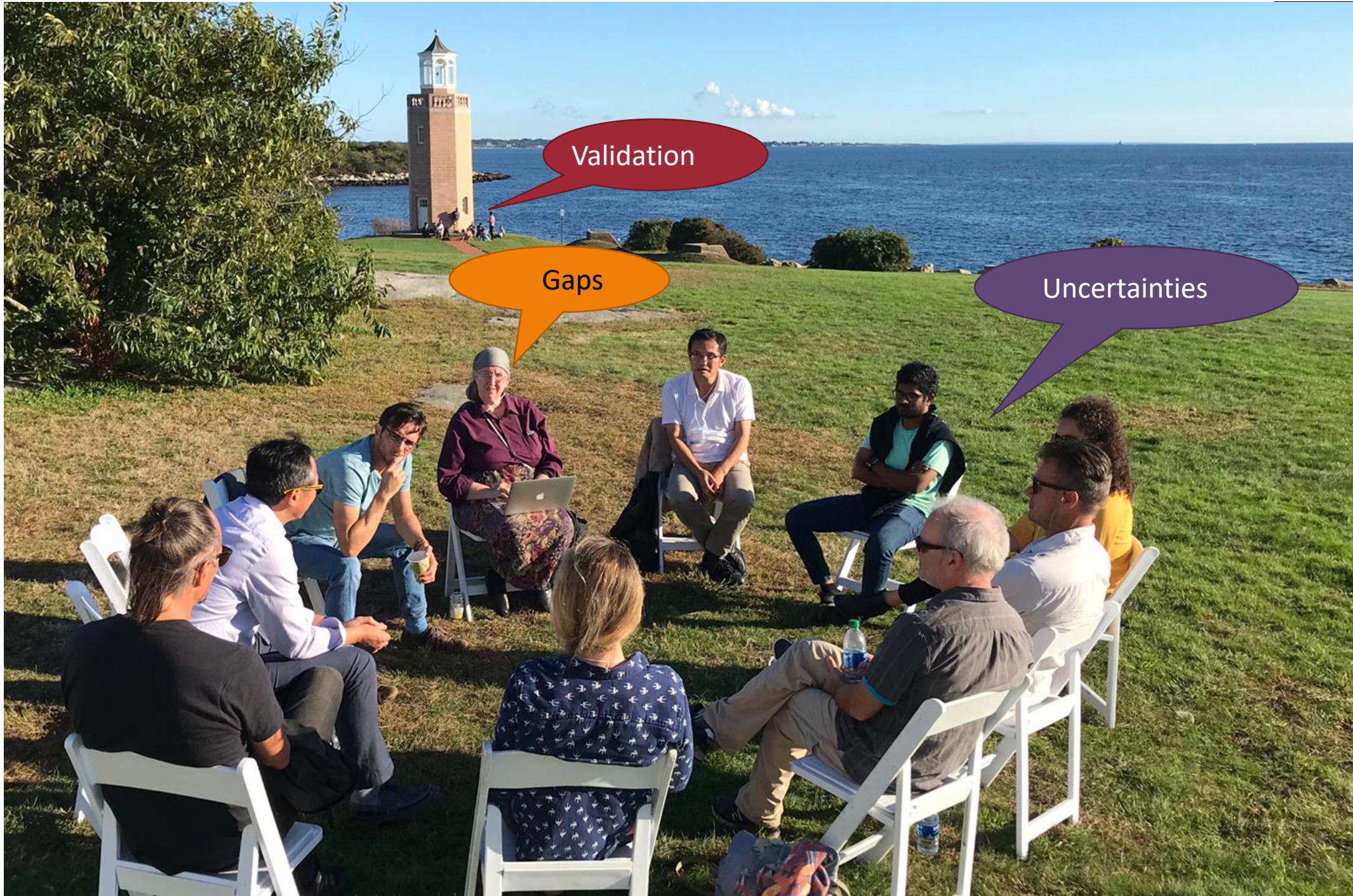
Credit OskarLandi

6-8 October 2021 Team Meeting UCONN Avery Point  
Plus Streaming Totals: 75 Cities 195 Unique IP Addresses



# GOALS of Team





Validation

Gaps

Uncertainties



# Standard Product Suites So Far...

## Suite OC\_AOP

1. Rrs 350-720 @ 2.5nm
2. Rrs\_unc 350-720 @ 2.5 nm
3. aot 865
4. angstrom 443/865 relative
5. ipar
6. PAR 400-700nm integrated
7. nflh
8. AVW
9. QWIP (TBD, but likely)
10. l2flags

## Suite OC\_IOP

1. a SeaWiFS wavelengths or more
2. bb SeaWiFS wavelengths or more
3. aph SeaWiFS wavelengths or more
4. aph\_443\_unc
5. adg\_443
6. adg\_443\_unc
7. adg\_s
8. bbp\_443
9. bbp\_443\_unc
10. bbp\_s
11. Kd SeaWiFS wavelengths or more

## Suite OC\_BGC

1. chlor\_a
2. POC
3. PIC
4. PhytoC

# APPARENT VISIBLE WAVELENGTH (APV) USING HYPERSPECTRAL DATA



Remote Sensing of Environment

journal homepage: [www.elsevier.com/locate/rse](http://www.elsevier.com/locate/rse)



150 shades of green: Using the full spectrum of remote sensing reflectance to elucidate color shifts in the ocean

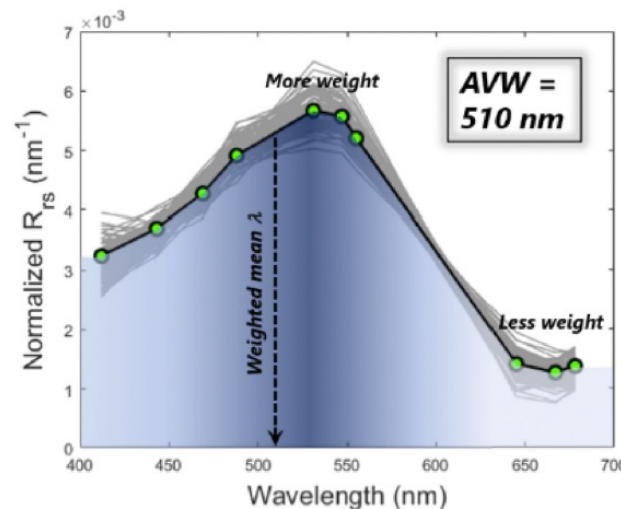
Ryan A. Vandermeulen<sup>a,b,\*</sup>, Antonio Mannino<sup>b</sup>, Susanne E. Craig<sup>b,c</sup>, P. Jeremy Werdell<sup>b</sup>

<sup>a</sup> Science Systems and Applications, Inc., Lanham, MD, 20706, USA

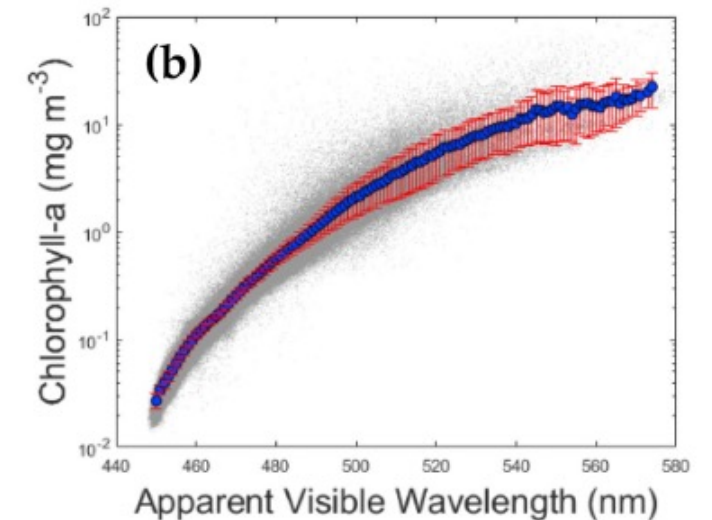
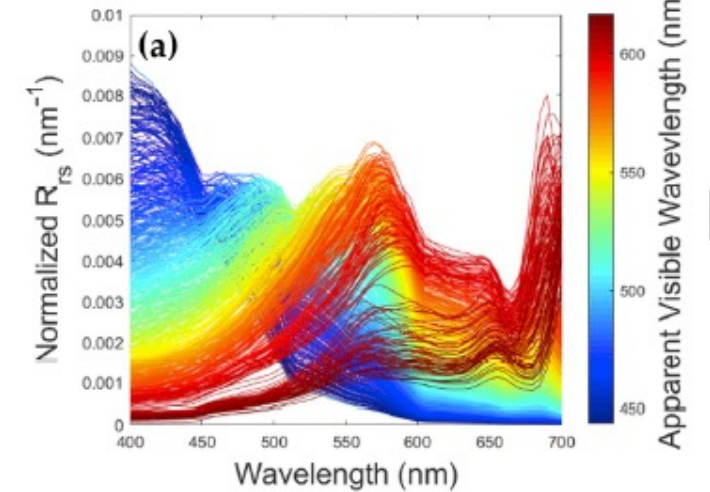
<sup>b</sup> NASA Goddard Space Flight Center, Greenbelt, MD, 20771, USA

<sup>c</sup> University Space Research Association, Columbia, MD, 21046, USA

$$AVW = \frac{\sum_{i=\lambda_1}^{\lambda_n} R_{rs}(\lambda_i)}{\sum_{i=\lambda_1}^{\lambda_n} \frac{R_{rs}(\lambda_i)}{\lambda_i}} = \left( \frac{\sum_{i=\lambda_1}^{\lambda_n} \lambda_i^{-1} R_{rs}(\lambda_i)}{\sum_{i=\lambda_1}^{\lambda_n} R_{rs}(\lambda_i)} \right)^{-1}$$



Synthetic Dataset





# QWIP: A Quantitative Metric for Quality Control of Aquatic Reflectance Spectral Shape Using the Apparent Visible Wavelength

Heidi M. **Dierssen**<sup>1\*</sup>, Ryan A. **Vandermeulen**<sup>2,3</sup>, Brian B. **Barnes**<sup>4</sup>, Alexandre **Castagna**<sup>5</sup>, Els **Knaeps**<sup>6</sup> and Quinten **Vanhellemont**<sup>7</sup>

## OPEN ACCESS

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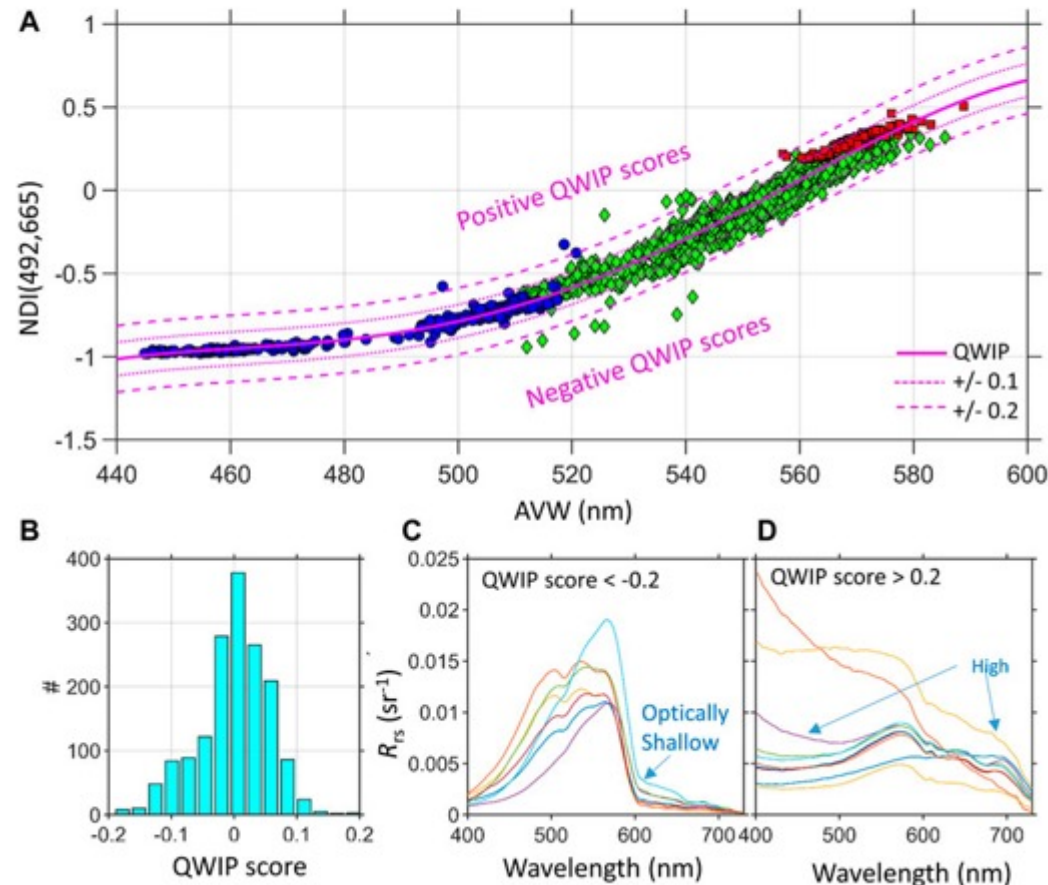
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<sup>1</sup>Department of Marine Sciences, University of Connecticut, Groton, CT, United States, <sup>2</sup>Ocean Ecology Laboratory, Goddard Space Flight Center, National Aeronautics and Space Administration, Greenbelt, MD, United States, <sup>3</sup>Science Systems and Applications Inc., Lanham, MD, United States, <sup>4</sup>College of Marine Science, University of South Florida, St. Petersburg, FL, United States, <sup>5</sup>Protistology and Aquatic Ecology, Department of Biology, Ghent University, Ghent, Belgium, <sup>6</sup>Flemish Institute for Technological Research (VITO), Mol, Belgium, <sup>7</sup>Royal Belgian Institute of Natural Sciences, Brussels, Belgium

The colors of the ocean and inland waters span clear blue to turbid brown, and the corresponding spectral shapes of the water-leaving signal are diverse depending on the various types and concentrations of phytoplankton, sediment, detritus and colored dissolved organic matter. Here we present a simple metric developed from a global dataset spanning blue, green and brown water types to assess the quality of a measured or derived aquatic spectrum. The Quality Water Index Polynomial (QWIP) is founded on the Apparent Visible Wavelength (AWW), a one-dimensional geophysical metric of color that is inherently correlated to spectral shape calculated as a weighted harmonic mean across visible wavelengths. The QWIP represents a polynomial relationship between the hyperspectral AWW and a Normalized Difference Index (NDI) using red and green

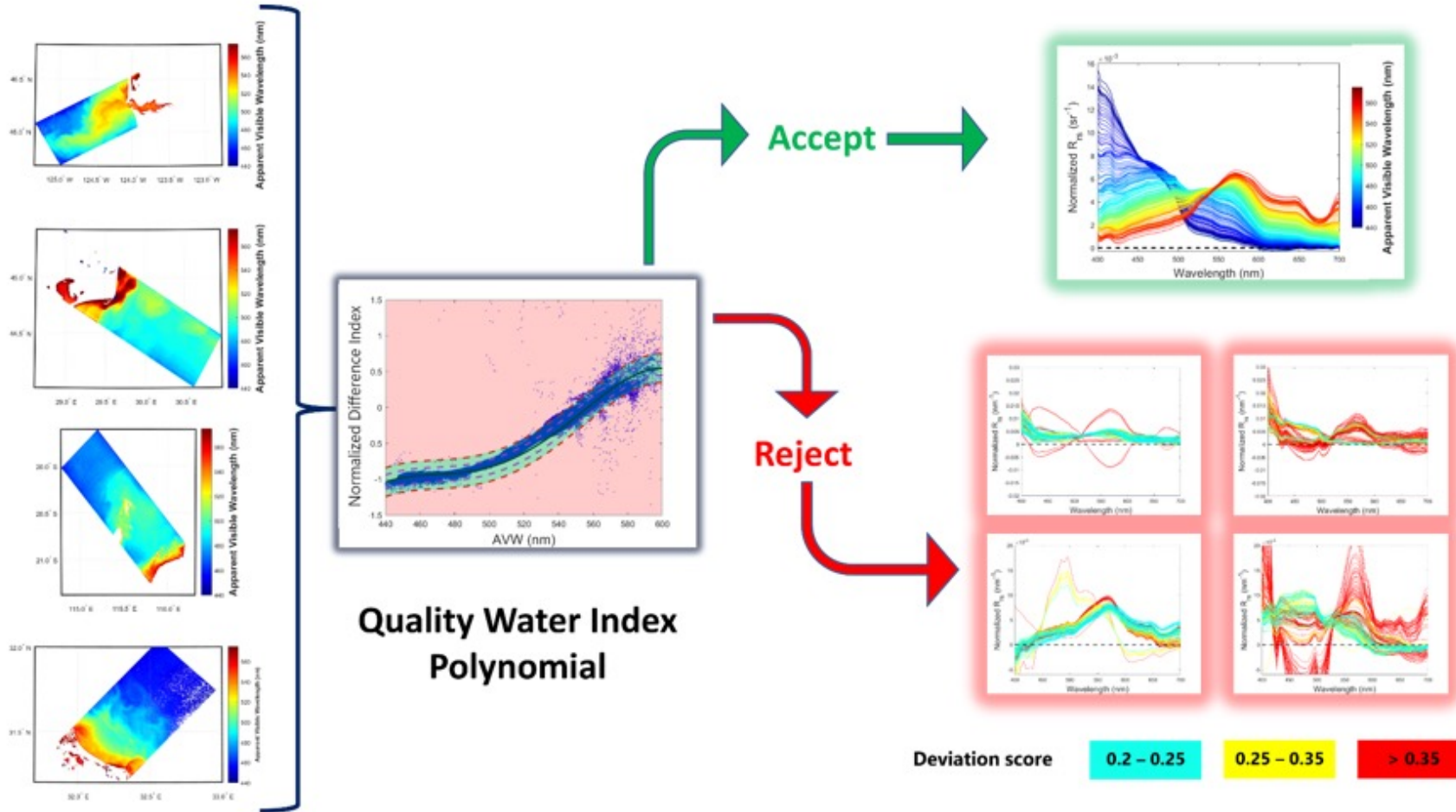
# QWIP

**Algorithm Development:** The method was developed using a large global dataset of remote sensing reflectance ( $n = 1,629$ ) compiled from different studies (CASCK-P dataset, see Dierssen et al. 2022).



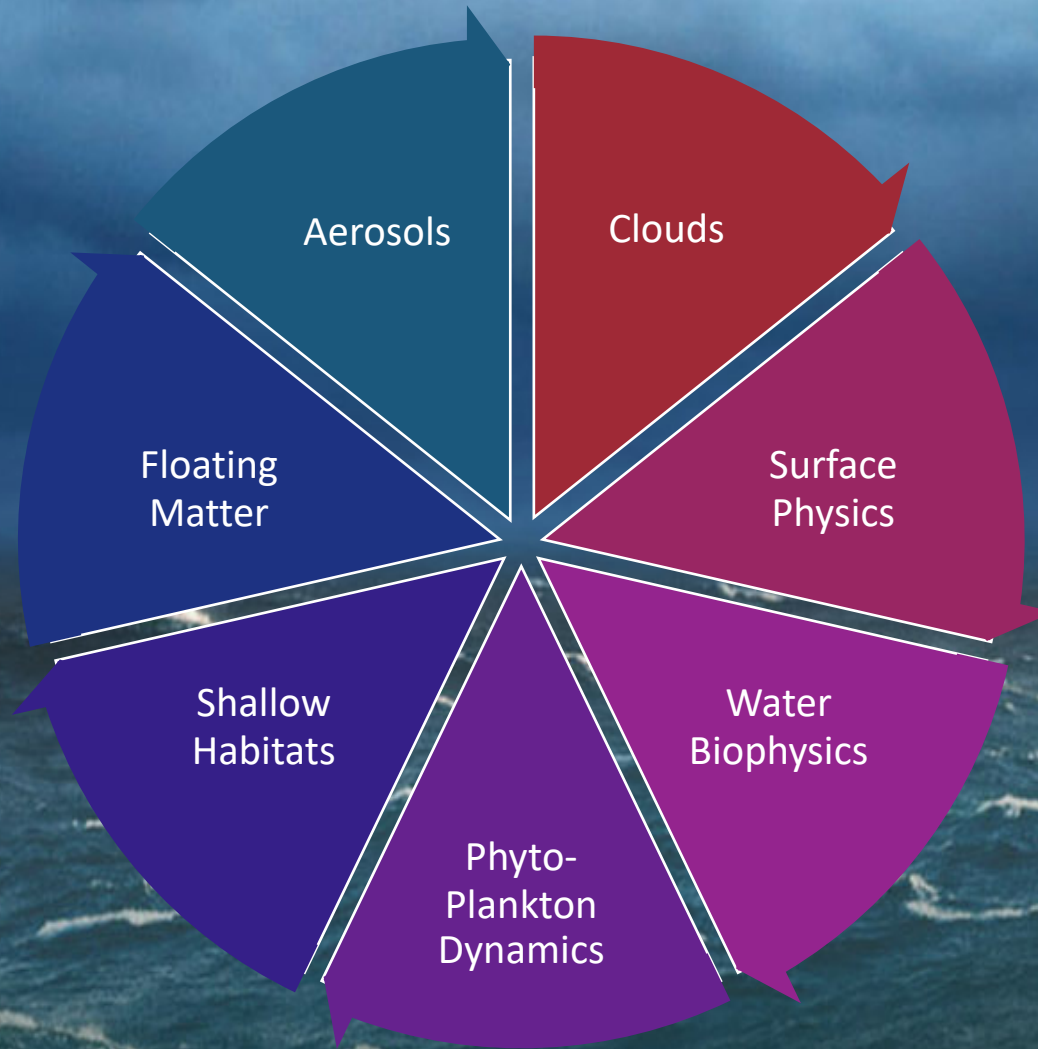
(A) The QWIP relationship between Apparent Visible Wavelength (AVW) and the Normalized Difference Index (NDI) with the CASCK-P training dataset showing the final tuned QWIP polynomial (thick magenta line) with different levels of QWIP scores ( $\pm 0.1$  dotted magenta and  $\pm 0.2$  dashed magenta). Water types include: Blue-green (blue circles), Green (green diamonds) and Brown (red squares). (B) Histogram of the QWIP scores from (A) are predominantly within  $\pm 0.1$  for the training data. (C) The remote sensing reflectance ( $R_{rs}$ ) of outliers with negative QWIP scores  $< -0.2$  were associated with optically shallow water features. (D) Outliers with QWIP scores  $> 0.2$  exhibited higher blue associated with surface reflected skylight and higher overall magnitude spectra.

## Satellite verification:



*Comparing full spectral information against empirical indices enables a quick and efficient means of assessing the relative quality of satellite and/or in situ data. Mapped HICO scenes are passed through the QWIP procedure, and spectra are accepted/rejected based on a nominal acceptance threshold. As spectral data increasingly deviate from the polynomial relationship between AVW and NDI (490,665), the anomalous spectral features become more prominent.*

# PACE SCIENCE 24 TEAMS BY TOPIC



# PACE SAT Provisional Algorithms Upcoming

<a href="#">Unified algorithm for aerosol characterization from OCI</a>	Unified Aerosol	Remer
<a href="#">Radiative Transfer Simulator and Polarimetric Inversion for PACE</a>	Simulation Delivered	Zhai
<a href="#">Inverse retrieval of the ocean surface refractive index</a>	OSIRIS	Ottaviani
<a href="#">Joint polarimetric aerosol and ocean color retrievals with deep learning</a>	FastMAPOL	Gao
<a href="#">Algorithms to obtain inherent optical properties of seawater</a>	3SAA (aph,ad,ag,bbp,Kd)	Stramski
<a href="#">The PACE-MAPP collaborative algorithm project</a>	PACE-MAPP	Stamnes
<a href="#">Freshwater Hyperspectral HABs Algorithms</a>		Shuchman
<a href="#">Retrieving water quality indicators via MDNs</a>	Water Quality	Pahlevan
<a href="#">Chi factor and BRDF</a>		Zhang
<a href="#">PACE UV Retrieval of Oceanic and Atmospheric Data products</a>		Chowdhary
<a href="#">Spectral Derivative Methods for Quantifying Phytoplankton Pigments for PACE</a>	Pigments	Siegel

<a href="#">IOP Inversion and BRDF algorithms for PACE</a>	ZTT Model IOP, BRDF	Twardowski
<a href="#">MAIAC Processing of OCI Over Land: Aerosol Chemical Speciation</a>	MAIAC	Lyapustin, Go
<a href="#">HARP2 Level 1 Data Processing Plan</a>		Xu
<a href="#">Remote sensing of cloud properties using PACE SPEXone and HARP-2</a>	RSP Heritage	van Diedenhoven
<a href="#">Phytoplankton Algorithms and Data Assimilation: Preparing a Pre-launch Path to Exploit PACE Spectral Data</a>		Rousseaux
<a href="#">PACE implementations for optically shallow waters</a>		Barnes
<a href="#">A toolbox for the diagnostic assessment of spectral behavior</a>	AVW	Vandermeulen
<a href="#">Radiative products for PACE</a>	All things radiative	Boss, Frouin
<a href="#">Support for PACE OCI Cloud Products</a>		Meyer
<a href="#">Hyperspectral algorithms for OCI atmospheric correction and UV penetration</a>		Krotkov
<a href="#">Net Primary Production for PACE OCI</a>	NPP, FLH, PhytoC	Westberry
<a href="#">HARP2</a>		Vanderlei
<a href="#">SPEXONE - Aerosols</a>	remoTAP	Hasekamp
<a href="#">Spectral Decomposition: Chl b, Chl c, and grouped photoprotective carotenoids</a>	Pigments	Chase, Gaube

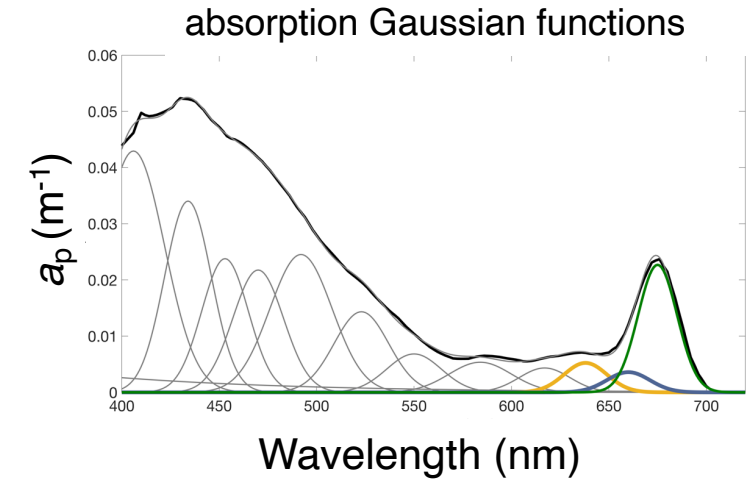
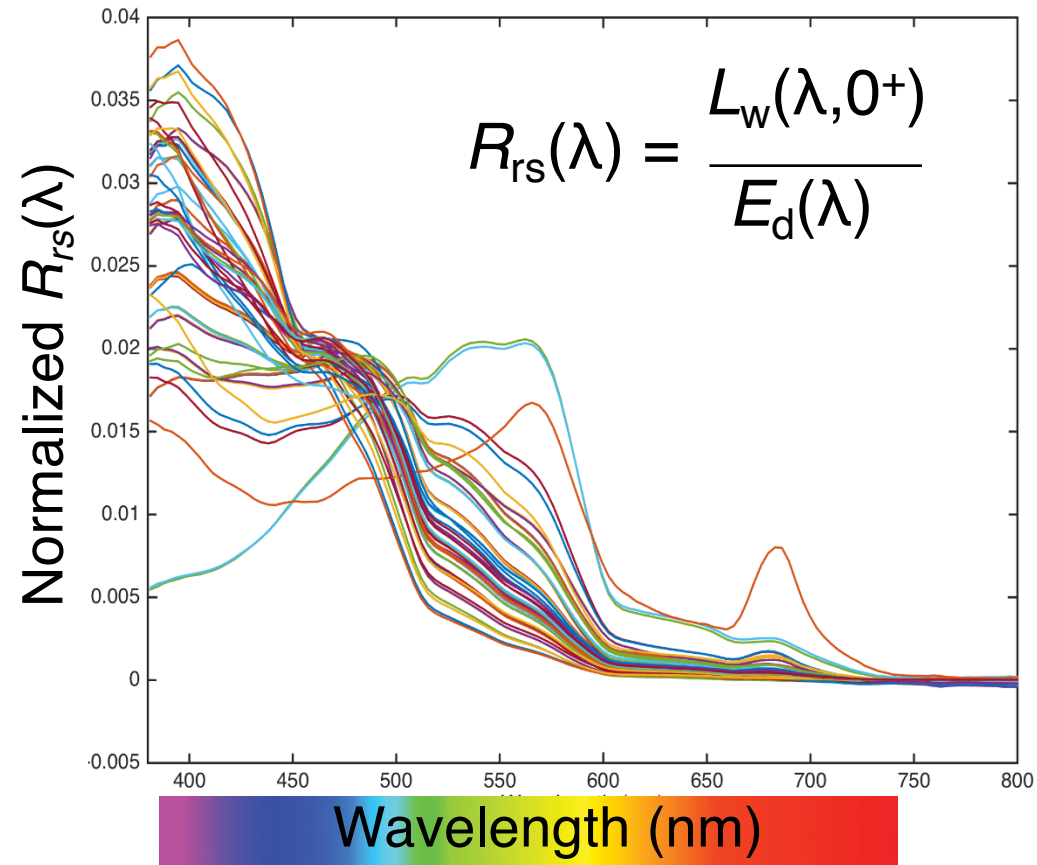
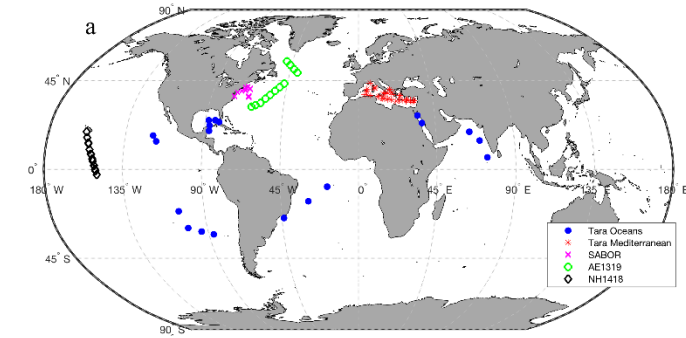


# PACE SAT Review of Phytoplankton Community Composition from Space

Led by Ivona Cetinić and Cecile Rousseaux

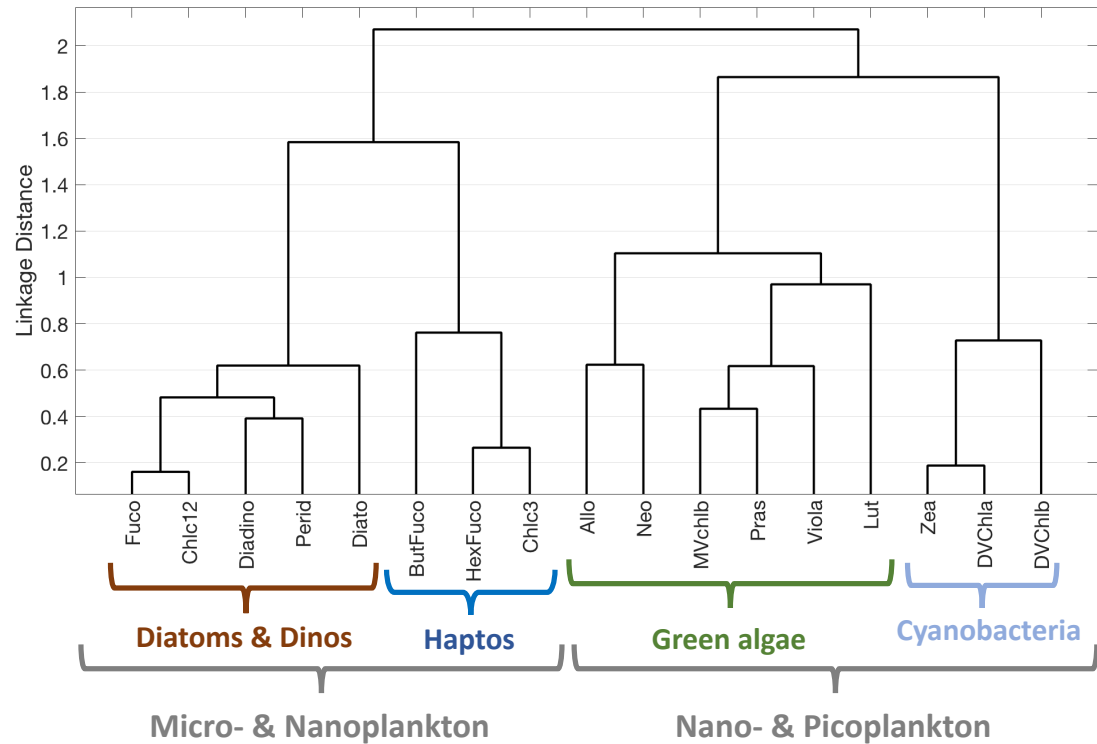


# Chase, Gaube et al. using Gaussian Functions to estimate Phytoplankton Pigments

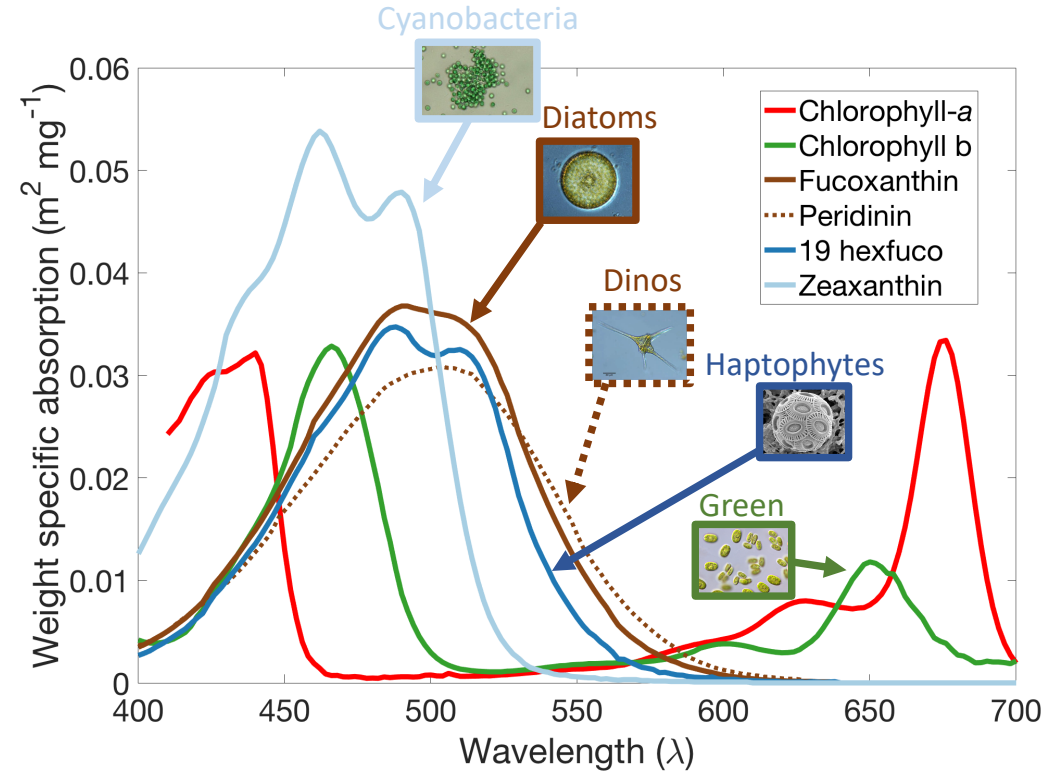


# Kramer & Siegel Modeling Pigments and Phytoplankton Community Composition (PCC)

Spectral derivative methods for estimating phytoplankton pigment concentrations



Kramer & Siegel JGR-Oceans [2019]



- Large degree of covariability among pigments
- Limits number of PFT groups can be retrieved using **HPLC pigments**

# A Net Primary Production (NPP) algorithm for application to PACE OCI



## Team members:

Toby Westberry (PI)

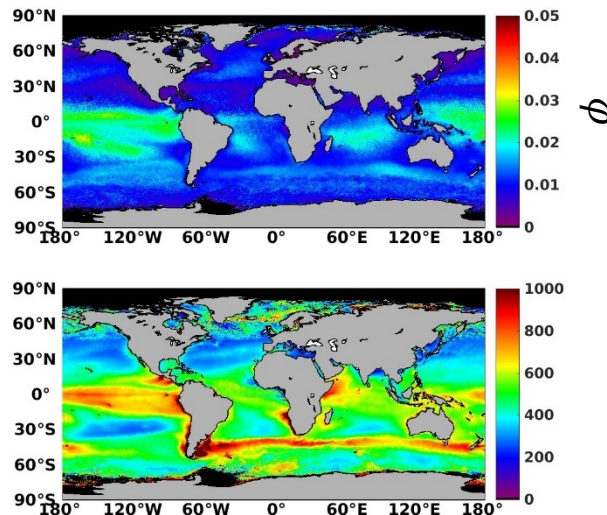
Mike Behrenfeld (Co-I)

Jason Graff (Co-I)

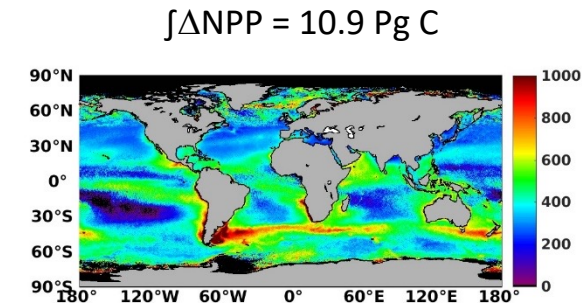


**Oregon State**  
University

Keywords: Phytoplankton, photosynthesis, primary production, biomass, physiology, photoacclimation, fluorescence, growth rate



$$\Delta NPP = \left( \frac{\phi}{\phi_{thresh}} - 1 \right)$$



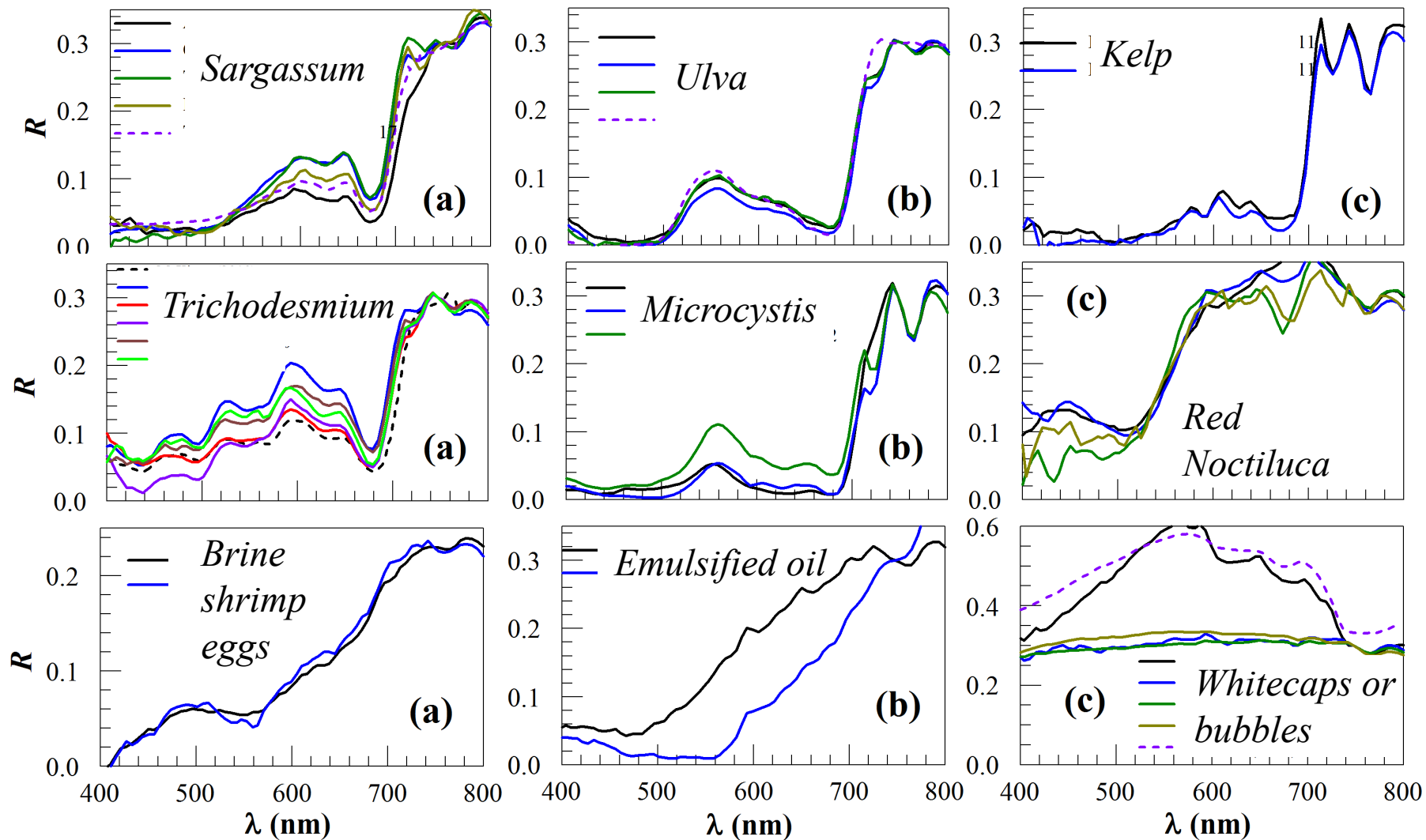


# PACE measurements of *Sargassum* macroalgae

Project PI: Chuanmin Hu, University of South Florida

Co-PIs: Brian Lapointe (FAU) and Gustavo Goni (NOAA)

## Examples with HICO





# Hyperspectral Data is *critically needed* for algorithm development and validation

Earth Syst. Sci. Data, 12, 1123–1139, 2020

<https://doi.org/10.5194/essd-12-1123-2020>

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ESSD | Articles | Volume 12, issue 2

Article

Assets

Peer review

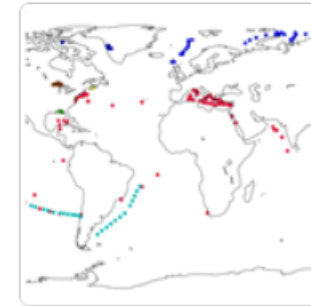
Metrics

Related articles

Data description paper

19 May 2020

## A global compilation of in situ aquatic high spectral resolution inherent and apparent optical property data for remote sensing applications



Kimberly A. Casey<sup>1,2</sup>, Cecile S. Rousseaux<sup>1,3,4</sup>, Watson W. Gregg<sup>1,3</sup>, Emmanuel Boss<sup>5</sup>, Alison P. Chase<sup>5</sup>, Susanne E. Craig<sup>4,6</sup>, Colleen B. Mouw<sup>7</sup>, Rick A. Reynolds<sup>8</sup>, Dariusz Stramski<sup>8</sup>, Steven G. Ackleson<sup>9</sup>, Annick Bricaud<sup>10</sup>, Blake Schaeffer<sup>11</sup>, Marlon R. Lewis<sup>12</sup>, and Stéphane Maritorena<sup>13</sup>

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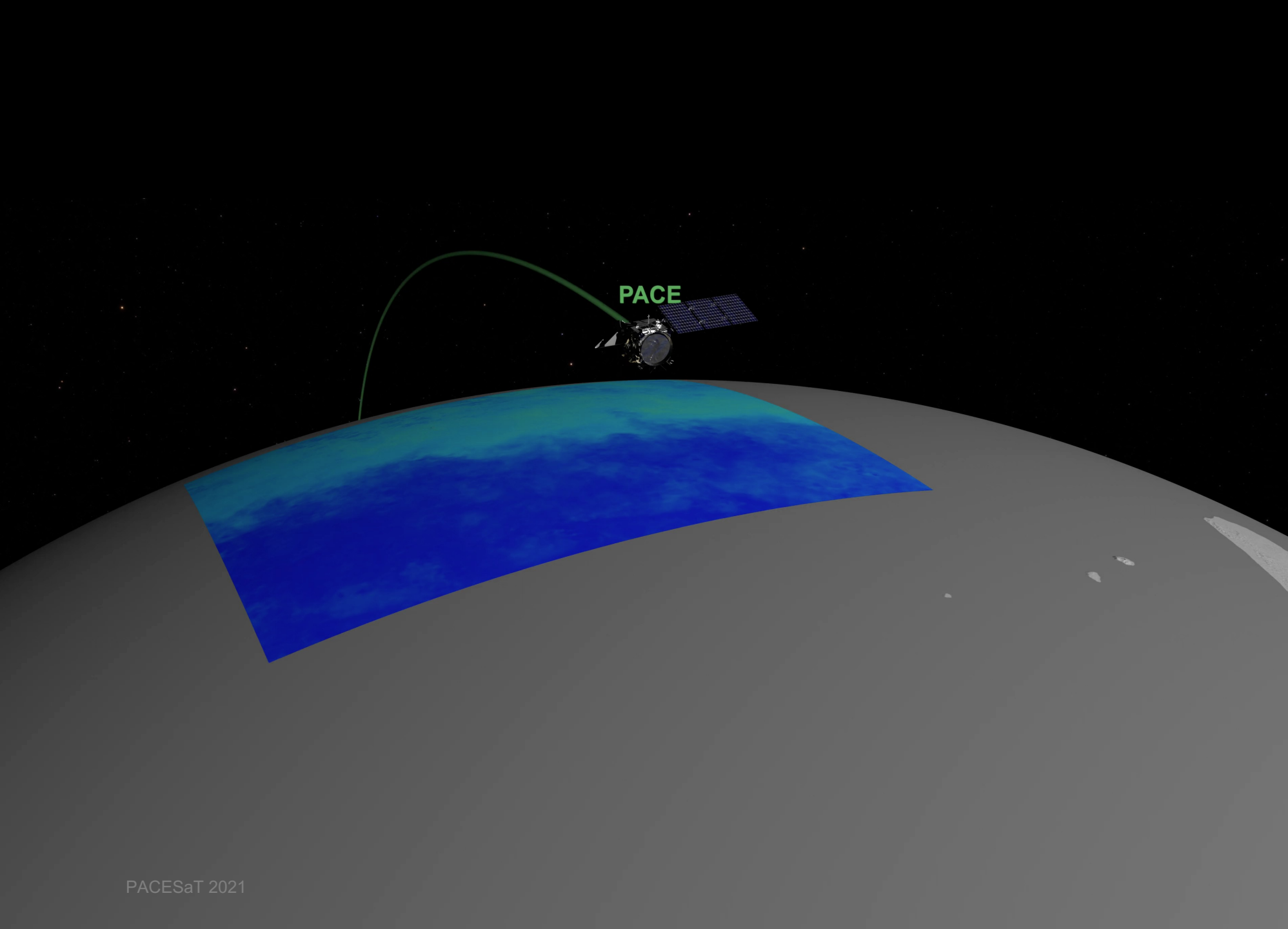
Received: 17 Jun 2019 – Discussion started: 22 Jul 2019 – Revised: 05 Dec 2019 – Accepted: 23 Jan 2020 – Published: 19 May 2020

## What are the **Opportunities** for Synergies between Missions **Pre-launch (2022-2024)**?



- Collection of **new hyperspectral datasets** shared across missions
  - Simulated data with more realistic assumptions
  - Field and airborne campaigns proposed for all missions
- Development of **common algorithms and data products** across three science teams
- Shared working groups to better characterize aquatic biodiversity in terms of **phytoplankton community composition**
- Shared methods for calculating and distributing **Uncertainties** for products
- Development of **Coupled Ocean-Atmosphere Modeling** to achieve better joint retrievals
- Joint efforts to conduct **Vicarious Calibration and Product Validation**





## Questions