PACE Science & Applications Team
Heidi Dierssen

10/21/2021

PACE

Plankton, Aerosol, Cloud, ocean Ecosystem

Heidi Dierssen

University of Connecticut

Science and Applications Team Lead

“A lack of spectral information **at key wavelengths** has limited many of the approaches for evaluating ocean biodiversity and biogeochemistry, particularly in coastal and inland waters.”

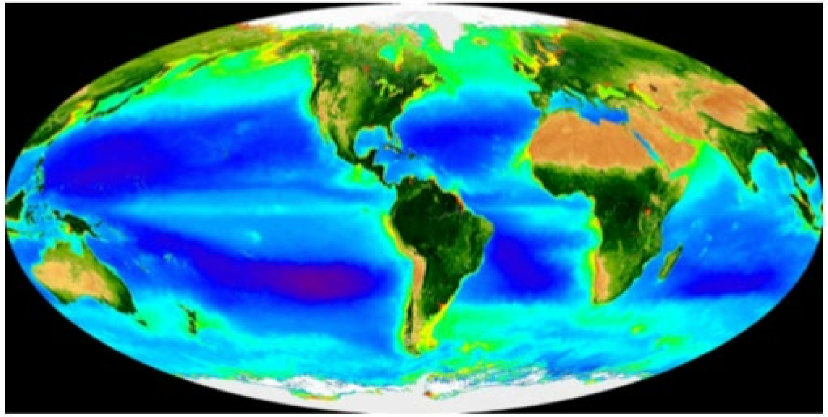
150 shades of green (and brown) *(Vandermeulen et al. 2020)*

Figure 1.1 Different colours of water (images courtesy of CSIRO) depending on their concentration of optical water quality variables

CEOS report 2018

Overarching Science Questions

Pre-Aerosol, Clouds, and ocean Ecosystem (PACE) Mission Science Definition Team Report



October 16, 2012

Courtesy: Eric Gorman, OCI Instrument Systems Engineer

How & why are ocean biogeochemical cycles & standing stocks changing? How do they influence the Earth system?

How do physical ocean processes affect ocean ecosystems? How do ocean biological processes influence ocean physics?

What is the distribution of both harmful & beneficial algal blooms & how is their appearance & demise related to environmental forcing?

What are the long-term changes in aerosol & cloud properties & how are these properties correlated with inter-annual climate oscillations?

What are the magnitudes & trends of direct radiative forcing components?

How do aerosols influence ocean ecosystems & biogeochemical cycles? How do ocean biological & chemical processes affect the atmosphere?

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

*Select types may be differentiated.

** using lidar techniques

Routine	Demon-strated	Unproven	Ecosystem Model

frontiers in Environmental Science

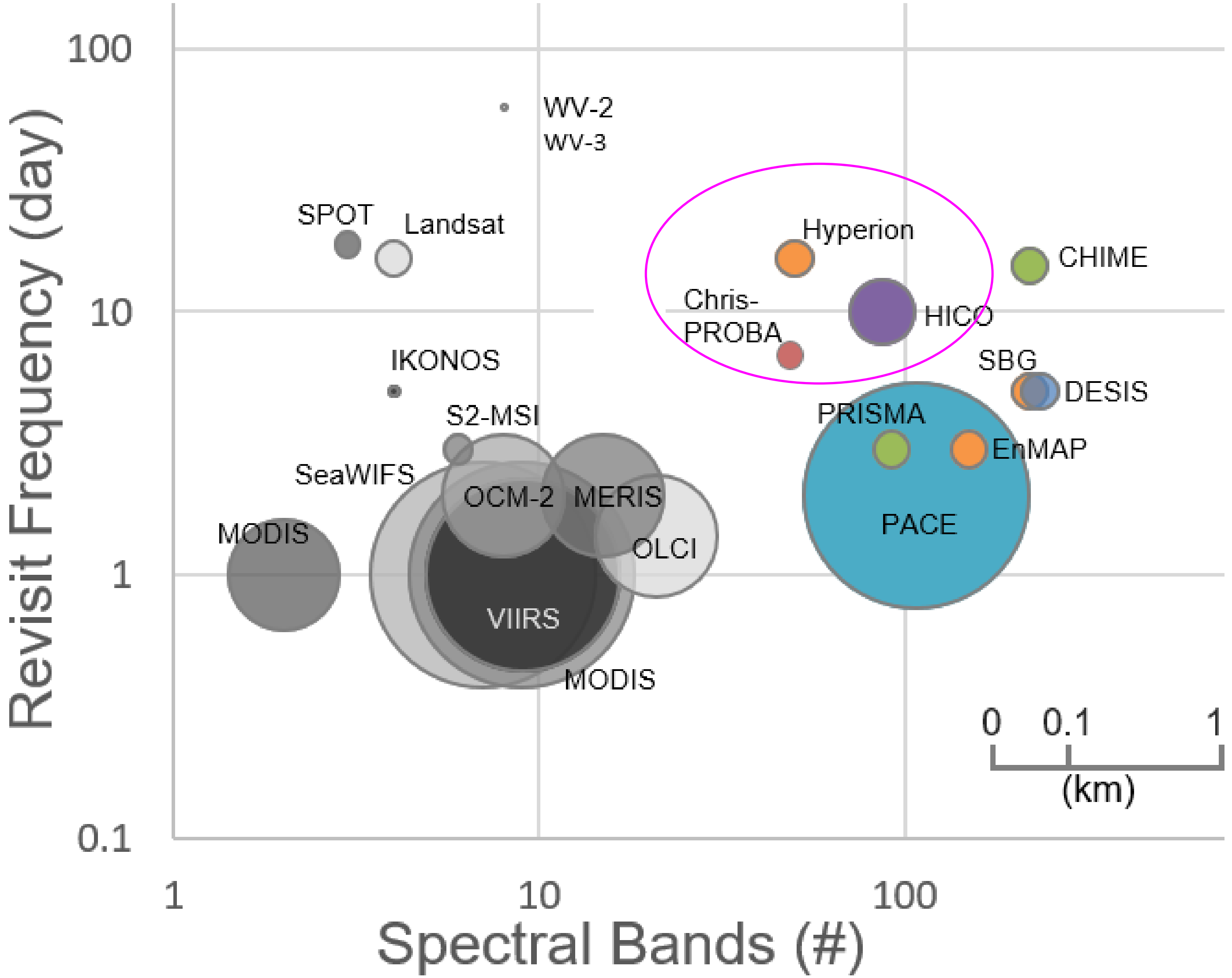
REVIEW
published: 07 June 2021
doi: 10.3389/fenvs.2021.649528

Check for updates

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

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

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

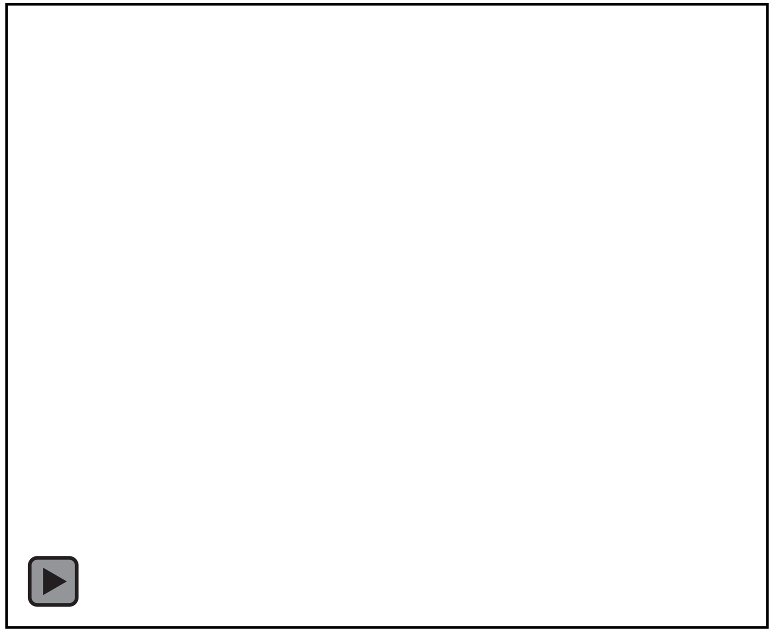


Dierssen et al. Frontiers. 2021

PACE Instrument(s) Critical Parameters

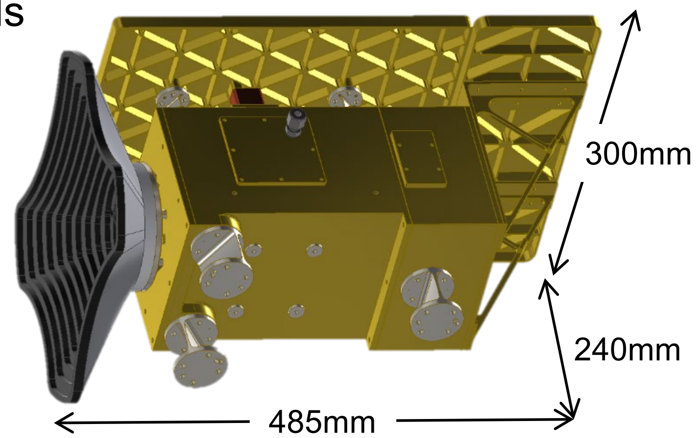
Ocean Color Instrument (GSFC):

- 340nm – 890nm at 5nm bands
- SWIR bands 940, 1038, 1250, 1378, 1615, 2130, 2260 nm
- Wide swath ±56° cross
- 1km GSD
- Avg Data Rate: 20 Mbps
- Mass ~ 260 kg CBE (includes portion of tilt structure)
- ±20 deg tilt for Sun glint avoidance



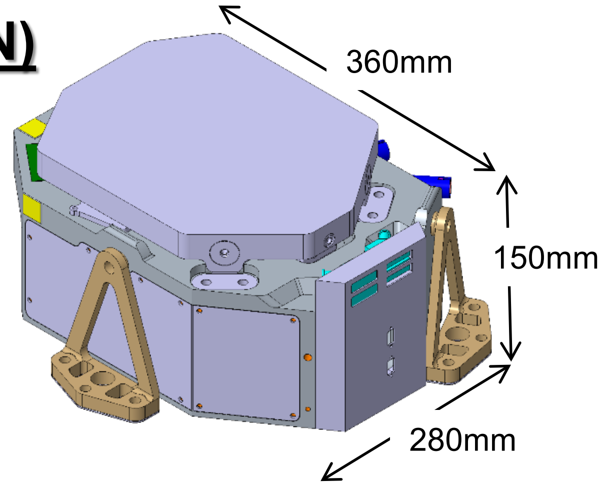
HARP2 Polarimeter (UMBC)

- 440, 550, 670 & 870nm Bands
- 10-60 viewing angles
- Wide swath ±47° cross-track
- GSD 700m binned to 3km
- Avg Data Rate 10 Mbps
- Mass ~10 kg CBE



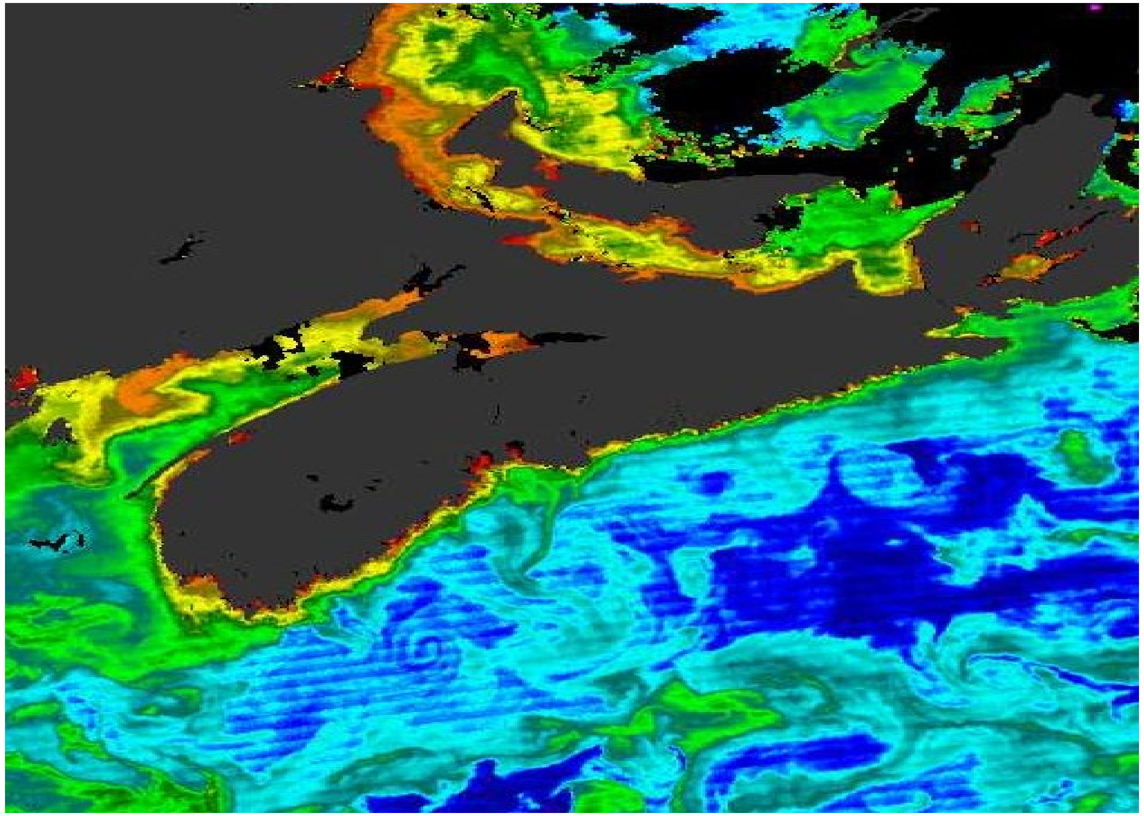
SPEXone: Polarimeter (SRON)

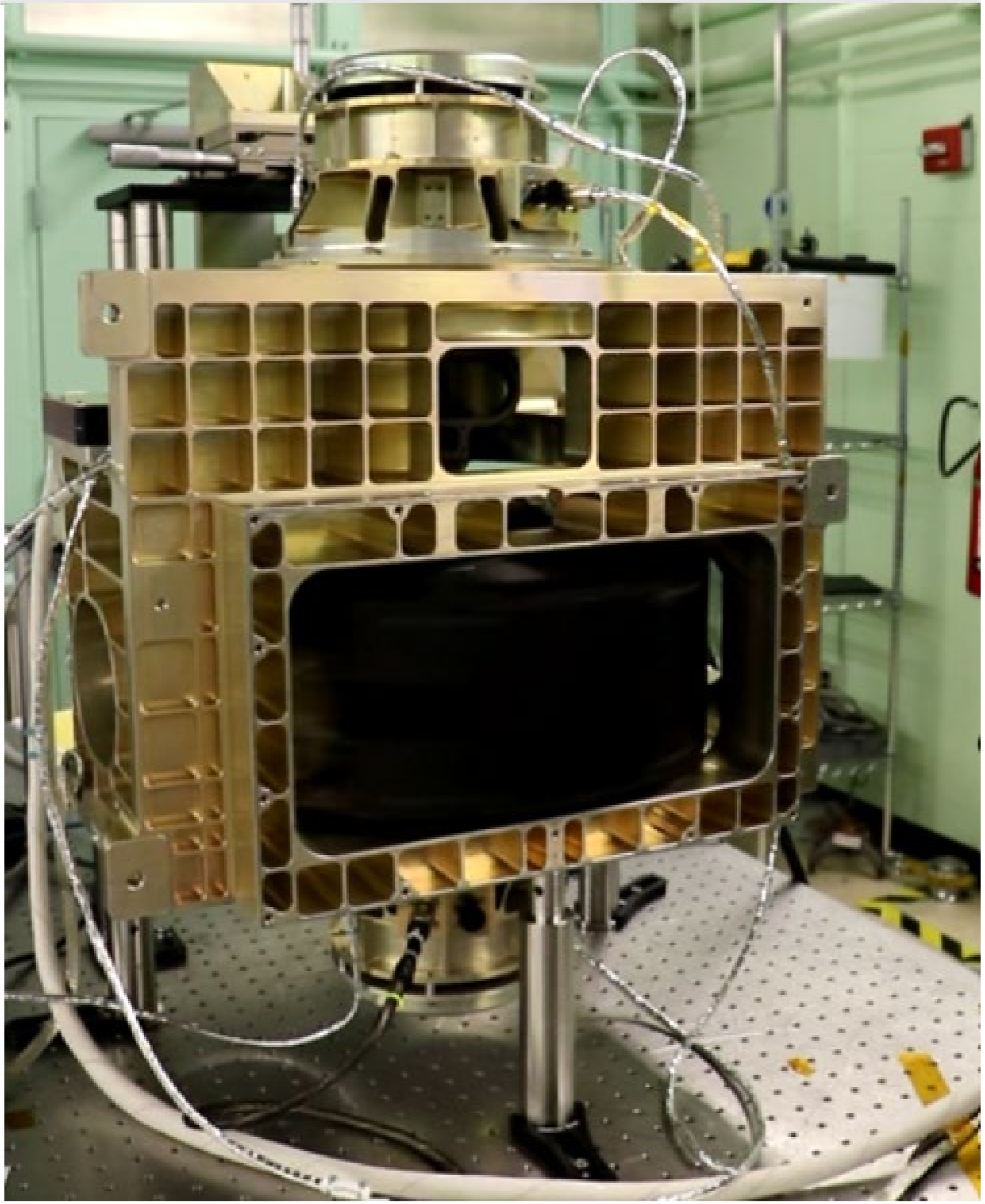
- 385 to 770nm at 2nm Bands
- 5 viewing angles
- Narrow swath ±4.5° cross
- GSD approx. 2.5km
- Avg Data Rate 5.3 Mbps
- Mass ~ 11 kg CBE



Whiskbroom imager

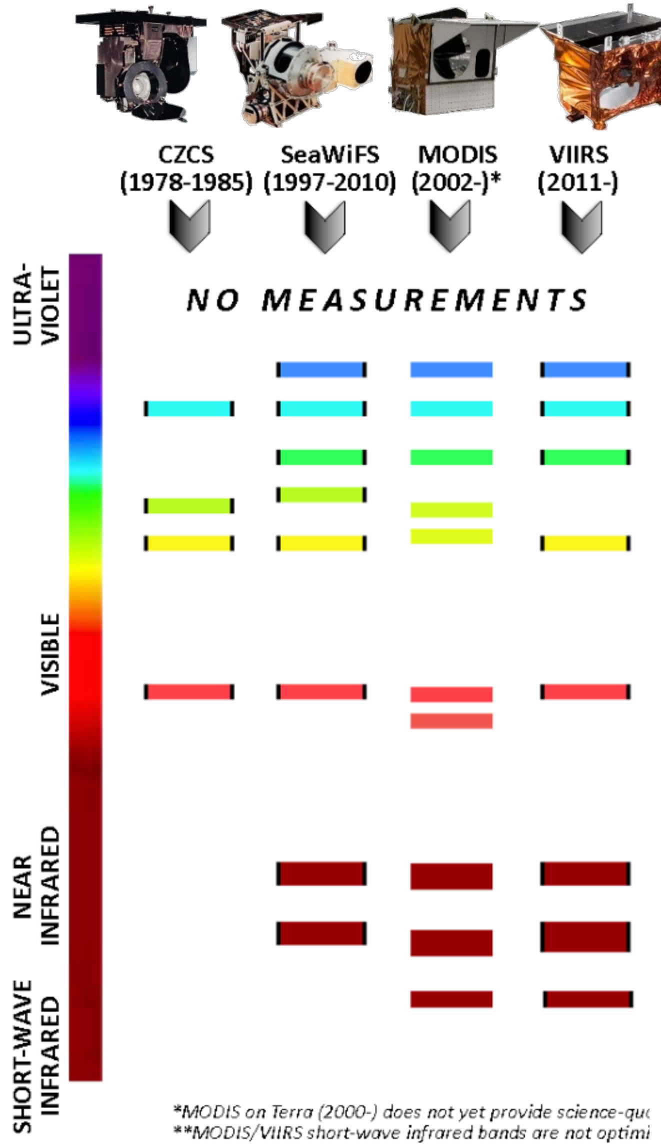
- SeaWiFS heritage
- Avoid stripes

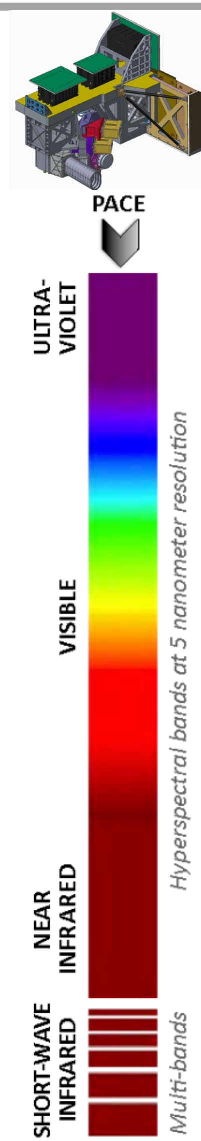




Courtesy Eric Gorman, PACE OCI Systems Engineer

Moving from Multi-spectral to Hyperspectral





Core ocean data products

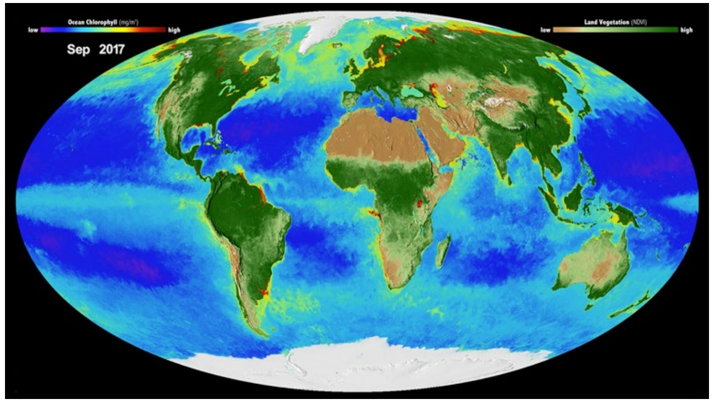
concentration of chlorophyll-a
diffuse attenuation coefficients
phytoplankton absorption
non-algal + CDOM absorption
particulate backscattering
photosynthetic available radiation
concentration of particulate carbon

Advanced ocean data products

phytoplankton community structure & biomass
phytoplankton physiological parameters
photosynthetic pigments
primary/community production
dissolved carbon pools
particle abundances & size distributions
carbon fluxes & export
water quality & clarity

Courtesy Eric Gorman, PACE OCI Systems Engineer

PACE Timeline



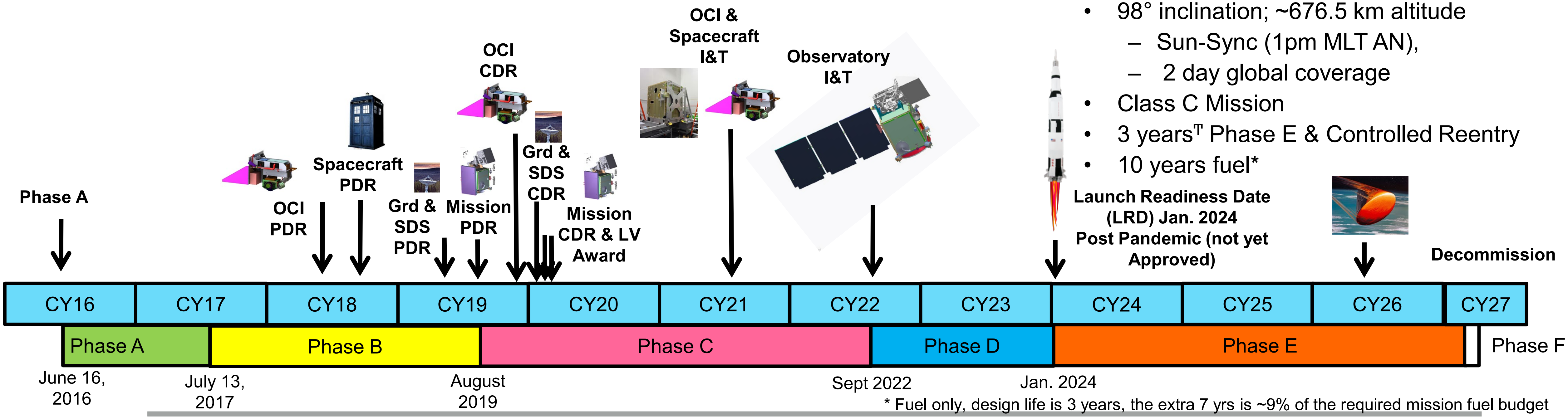
PACE Science
New opportunities to monitor fisheries and respond to toxic algae blooms, and key ocean and atmosphere data for forecasting air quality and weather that will improve our understanding of Earth's climate.

Mission Elements (Organization)

- Competed Science Team (NASA ESD)
- Vicarious Calibration (NASA ESD)
- Science Data Analysis (GSFC)
- Ocean Color Instrument (GSFC)
- Spacecraft – (GSFC)
- Polarimeters – (SRON, UMBC)
- Mission Operations – (GSFC)
- Launch services (LSP-SpaceX)

Key Mission Parameters

- 98° inclination; ~676.5 km altitude
  - Sun-Sync (1pm MLT AN),
  - 2 day global coverage
- Class C Mission
- 3 years^T Phase E & Controlled Reentry
- 10 years fuel*



* Fuel only, design life is 3 years, the extra 7 yrs is ~9% of the required mission fuel budget

^{T} Baseline Requirement

PACE Science and Applications Team (SAT)

GOALS of Team

Algorithm development

- **Algorithm production** implemented as Standard, Provisional, Test or Special
- **Algorithm documentation** to be available online
- **Algorithm implementation** with project team

Algorithm performance

- **Algorithm performance** including propagation of **system-level uncertainties**.
- Protocols and strategies for science **data product validation**

Outreach

- **Partnerships with end-users** through Early Adopters Program.
- **Communication** to the public with news and updates on PACE research.

Mission Requirements

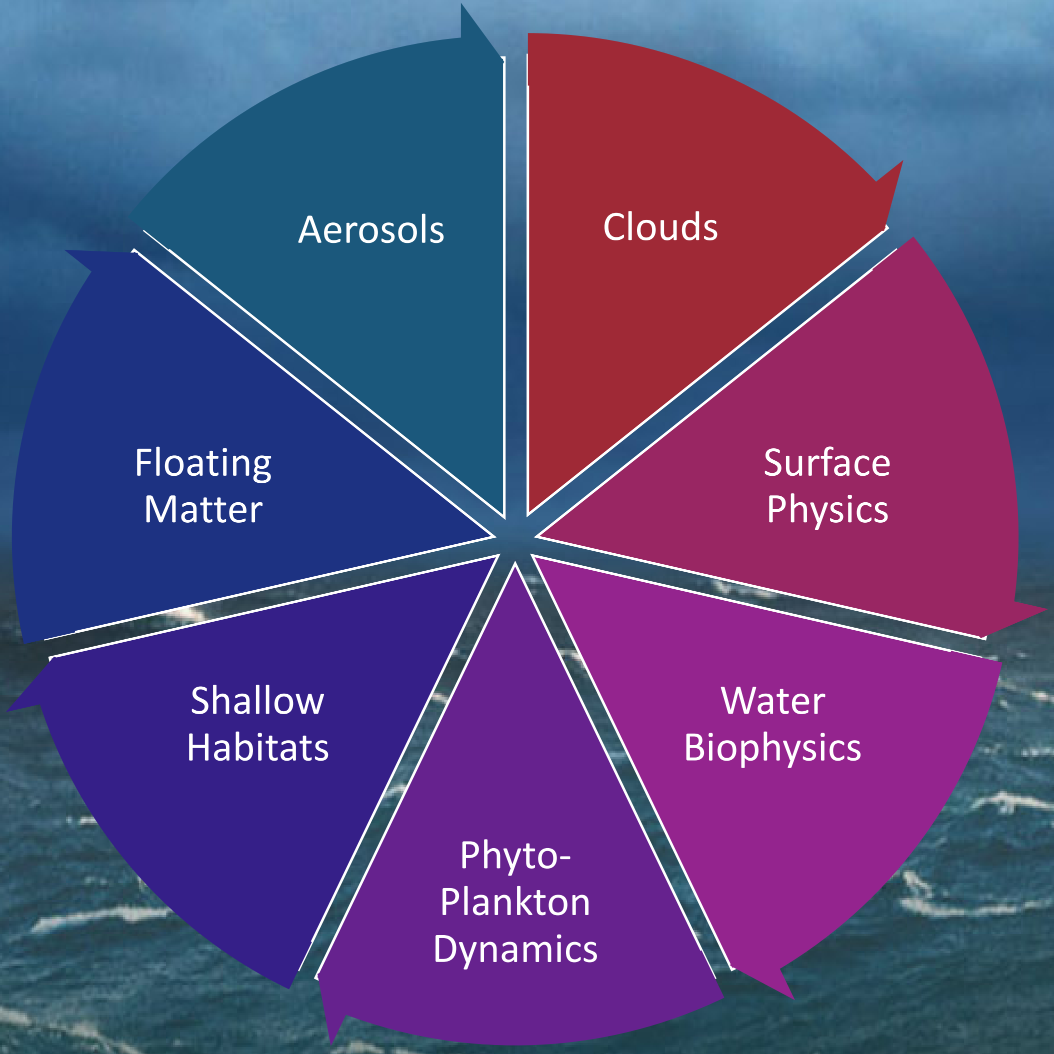
Table 1. Required Ocean Color Instrument (OCI) ocean color data products.

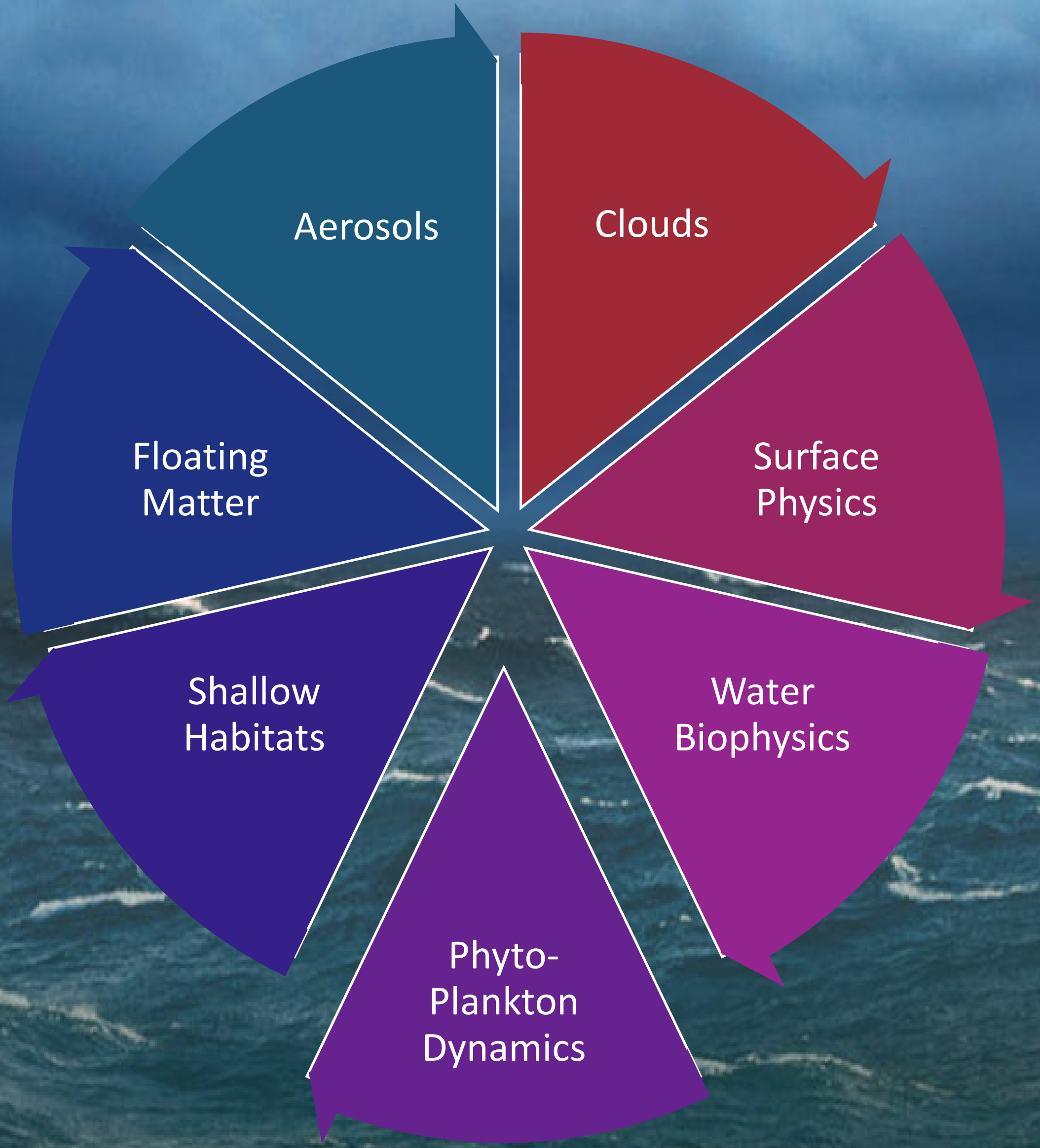
Data Product	Baseline Uncertainty
Water-leaving reflectances centered on (±2.5 nm) 350, 360, and 385 nm (15 nm bandwidth)	0.0057 or 20%
Water-leaving reflectances centered on (±2.5 nm) 412, 425, 443, 460, 475, 490, 510, 532, 555, and 583 (15 nm bandwidth)	0.0020 or 5%
Water-leaving reflectances centered on (±2.5 nm) 617, 640, 655, 665 678, and 710 (15 nm bandwidth, except for 10 nm bandwidth for 665 and 678 nm)	0.0007 or 10%
Ocean Color Data Products to be Derived from Water-leaving Reflectances	
Concentration of chlorophyll-a	
Diffuse attenuation coefficients 400-600 nm	
Phytoplankton absorption 400-600 nm	
Non-algal particle plus dissolved organic matter absorption 400-600 nm	
Particulate backscattering coefficient 400-600 nm	
Fluorescence line height	

Table 2. Required OCI aerosol and cloud data products.

Data Product	Range	Baseline Uncertainty
Total aerosol optical depth at 380 nm	0.0 to 5	0.06 or 40%
Total aerosol optical depth at 440, 500, 550 and 675 nm over land	0.0 to 5	0.06 or 20%
Total aerosol optical depth at 440, 500, 550 and 675 nm over oceans	0.0 to 5	0.04 or 15%
Fraction of visible aerosol optical depth from fine mode aerosols over oceans at 550 nm	0.0 to 1	±25%
Cloud layer detection for optical depth > 0.3	NA	40%
Cloud top pressure of opaque (optical depth > 3) clouds	100 to 1000 hPa	60 hPa
Optical thickness of liquid clouds	5 to 100	25%
Optical thickness of ice clouds	5 to 100	35%
Effective radius of liquid clouds	5 to 50 µm	25%
Effective radius of ice clouds	5 to 50 µm	35%
Atmospheric data products to be derived from the above		
Water path of liquid clouds		
Water path of ice clouds		
Short-wave Radiative Effect		

PACE SCIENCE 24 TEAMS BY TOPIC



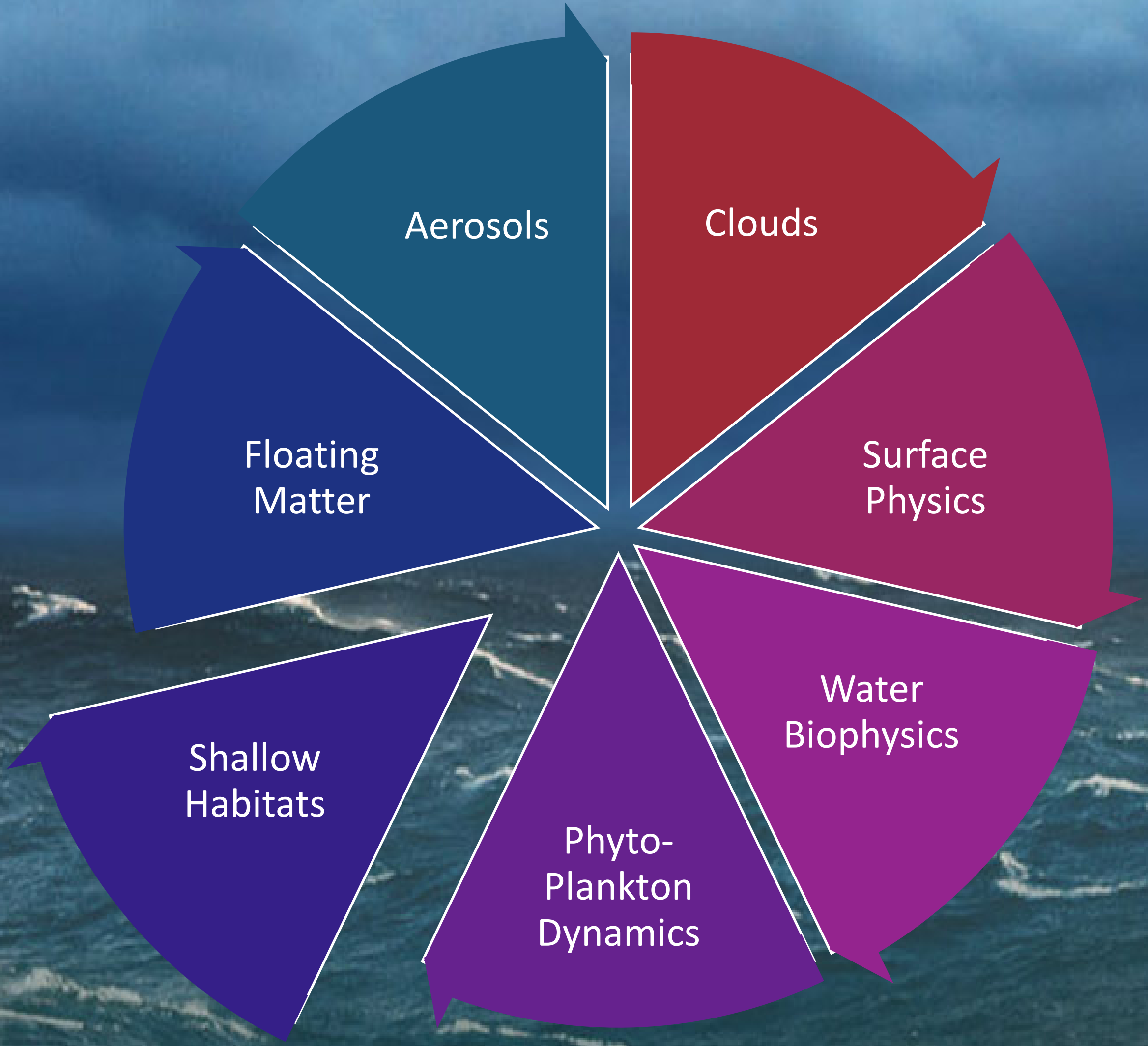


Science Team

Gaube
Pahlevan
Rousseaux
Shuchman
Siegel
Westberry

Properties

- Phytoplankton Pigment Concentration/Marker
  - Chlorophyll-a
  - Phycocyanin
  - Etc..
- Phytoplankton Composition
- Net Primary Productivity
- Fluorescence Line Height
- Adaptive Maximum Chlorophyll Index



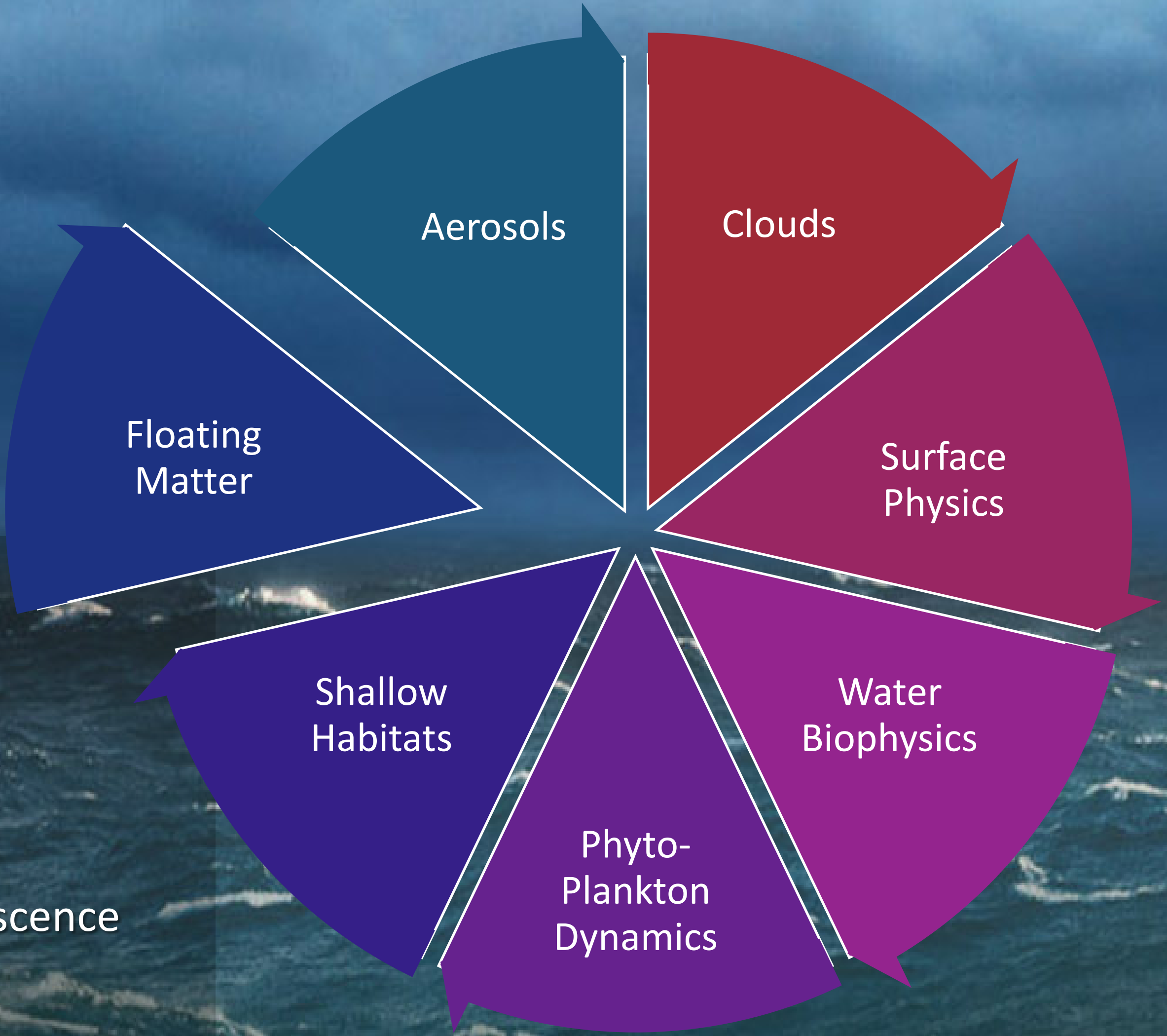
Science Team

Barnes

Properties

- Benthic Classification
  - Coral
  - Seagrass
  - Shallow Algae
  - Sediment
- Benthic Condition
  - Change over time

__Science Team__
Hu
Ottaviani
Shuchman



__Properties__

- Sargassum Dynamics
  - Density
  - Depth
  - Carbon, nitrogen, phosphorous
  - Sun-induced fluorescence
- Oil Detection
- Surface Scum Index

PACE SAT Algorithms

Presentation		Last Name
Unified algorithm for aerosol characterization from OCI		Remer
Radiative Transfer Simulator and Polarimetric Inversion for PACE		Zhai
Retrievals of the Ocean Surface Refractive Index		Ottaviani
Joint polarimetric aerosol and ocean color retrievals with deep learning	FastMAPOL	Gao
Algorithms to obtain inherent optical properties of seawater		Stramski
The PACE-MAPP collaborative algorithm project		Stamnes
Freshwater Hyperspectral HABs Algorithms		Shuchman
Retrieving water quality indicators via MDNs		Pahlevan
Chi factor and BRDF		Zhang
PACE UV Retrieval of Oceanic and Atmospheric Data products		Chowdhary
Spectral Derivative Methods for Quantifying Phytoplankton Pigments for PACE		Siegel

Inversion algorithm for PACE	ZTT Model	Twardowski
MAIAC Processing of OCI Over Land: Aerosol Chemical Speciation		Go (Lyapustin)
HARP2 Level 1 Data Processing Plan		Xu
Remote sensing of cloud properties using PACE SPEXone and HARP-2		van Diedenhoven
Phytoplankton Algorithms and Data Assimilation: Preparing a Pre-launch Path to Exploit PACE Spectral Data		Rousseaux
PACE implementations for optically shallow waters		Barnes
A toolbox for the diagnostic assessment of spectral behavior	AVW	Vandermeulen
Radiative products for PACE		Boss
Support for PACE OCI Cloud Products		Meyer
Hyperspectral algorithms for OCI atmospheric correction and UV penetration		Krotkov
Net Primary Production for PACE OCI	NPP PACE, PhytoC	Westberry
Machine learning approaches for predicting phytoplankton community composition from ocean color		Craig
SpexONE - Aerosols	remoTAP	Hasekamp

Standard Semi-analytical Formulation

$$r_{rs,\infty} = \sum_{i=1}^{2} g_i \left(\frac{b_b}{a + b_b}\right)^i$$

Backscattering over absorption

Proportionality factor bidirectionalality of Incoming and reflected light

$$b_b = b_{b,water} + b_{b,large\ part.} + b_{b,small\ part.}$$

$$a = a_{water} + a_d + a_g + a_{ph}$$

ZTT (Zaneveld-Twardowski-Tonizzo) model

water Raman contribution (Westberry et al. 2013)

$$r_{rs}(\theta_s, \theta_v, \phi, V, a, b_b, \beta) \cong \boxed{r_{rs,Raman}(\theta_s{}', a, b_b)}$$

$$+ \frac{1}{\bar{\mu}_d(\theta_s', V, \frac{b_b}{a})} \boxed{\frac{\beta(\psi)}{b_b}} \boxed{\frac{a}{b_b}} \left(1 - \cos(\theta_v)\, \Psi_{K_{Lu}}(\psi) \bar{\mu}_\infty \left(\frac{b_b}{a}\right)^{-1}\right) + f_L(\psi, \lambda) \left(1 - \boxed{\tilde{b}_b}^{-1}\right) + \boxed{\tilde{b}_b}^{-1} \Big]^{-1}$$

average cosine of downwelling light field (E_d/E_{od})

phase function in backward direction

absorption over backscattering

coefficients related to diffuse attenuation of radiance in viewing direction

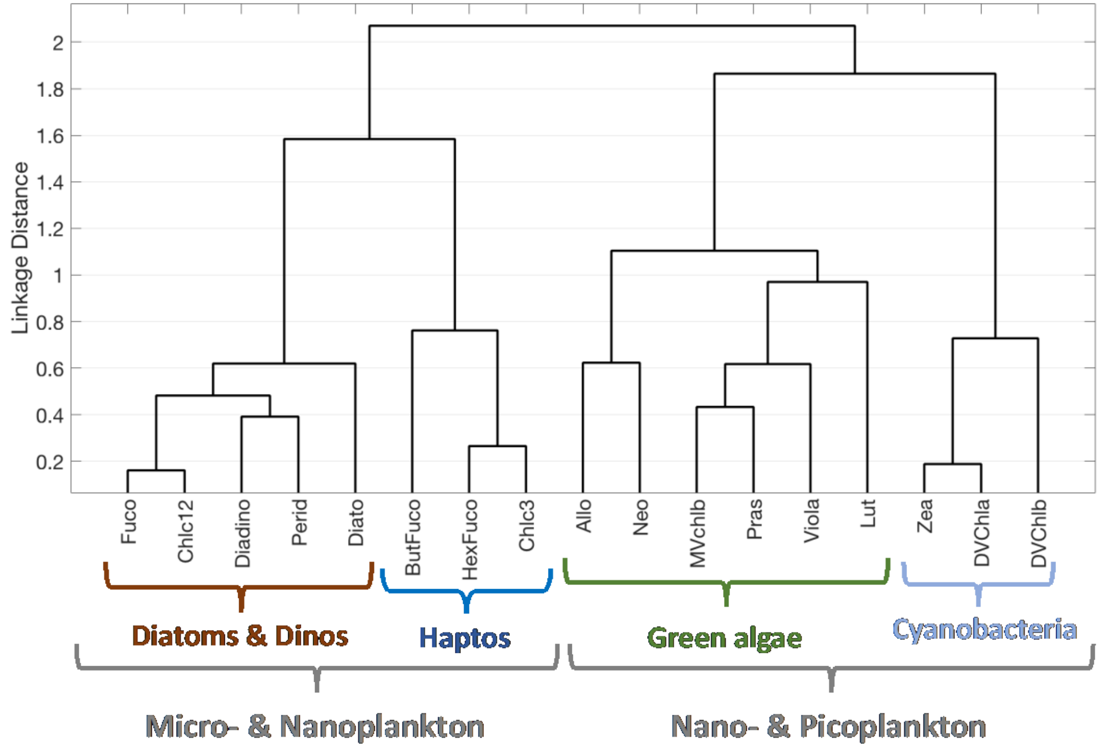
(Twardowski and Tonizzo 2017)

shape function for upwelling component of path radiance

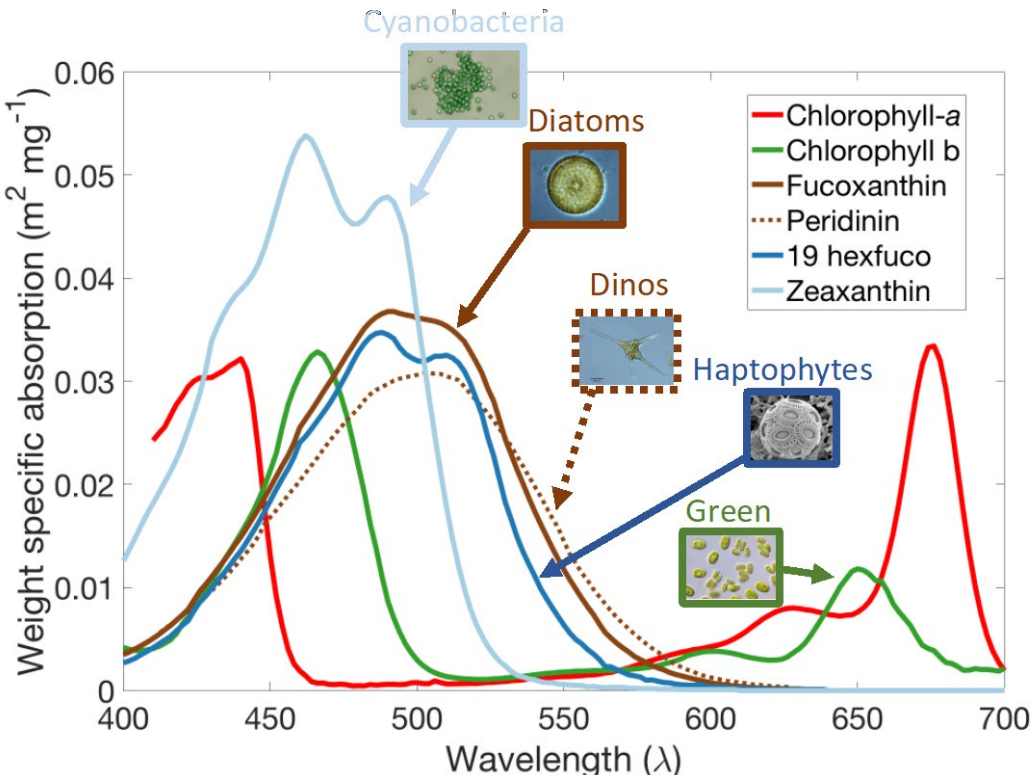
backscattering ratio b_b/b

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

Spectral derivative methods for estimating phytoplankton pigment concentrations

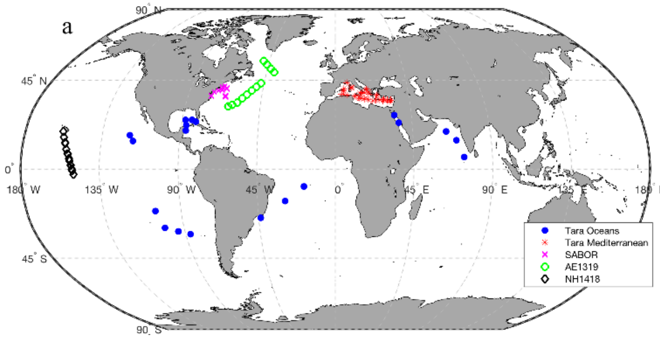


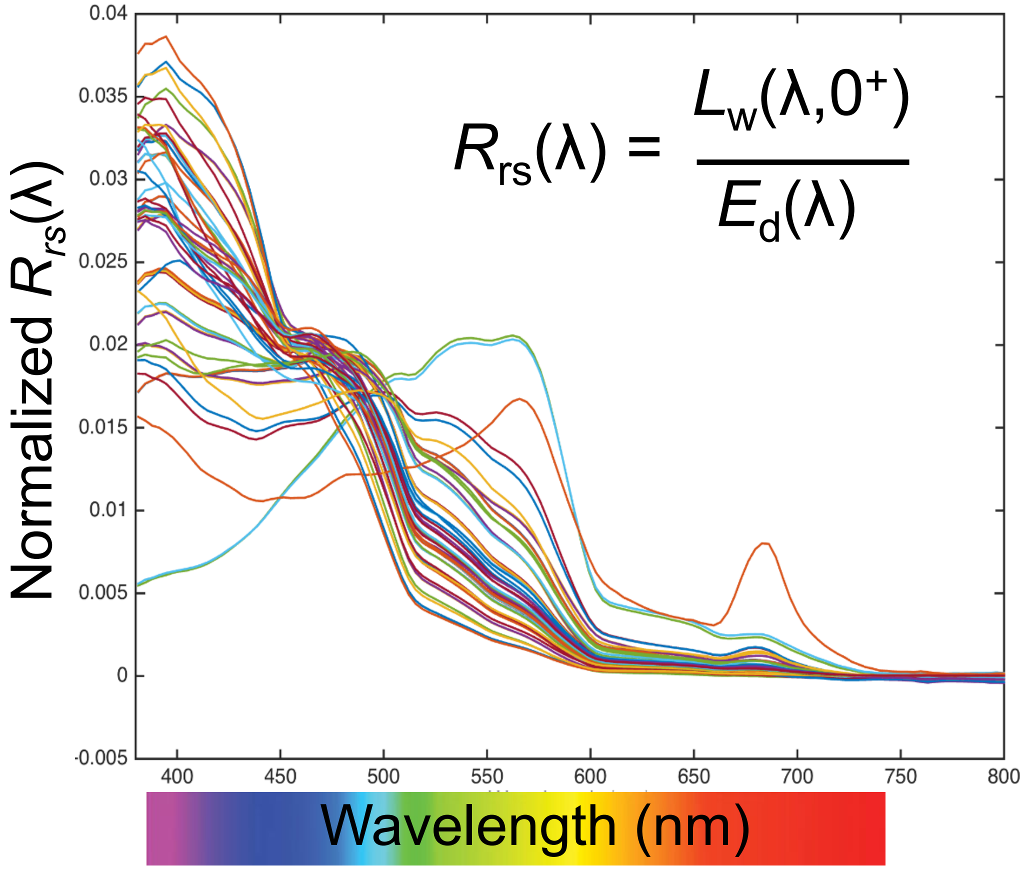
Kramer & Siegel JGR-Oceans [2019]



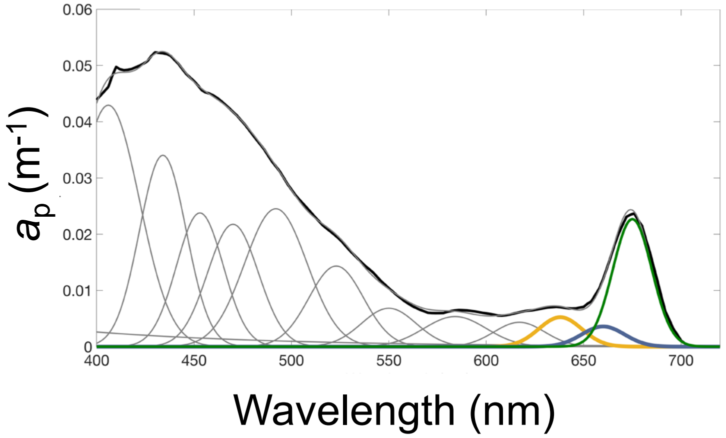
- Large degree of covariability among pigments
- Limits number of PFT groups can be retrieved using **HPLC pigments**

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





$$R_{rs}(\lambda) = \frac{L_w(\lambda, 0^+)}{E_d(\lambda)}$$



Chase et al. 2017, JGR-Oceans

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

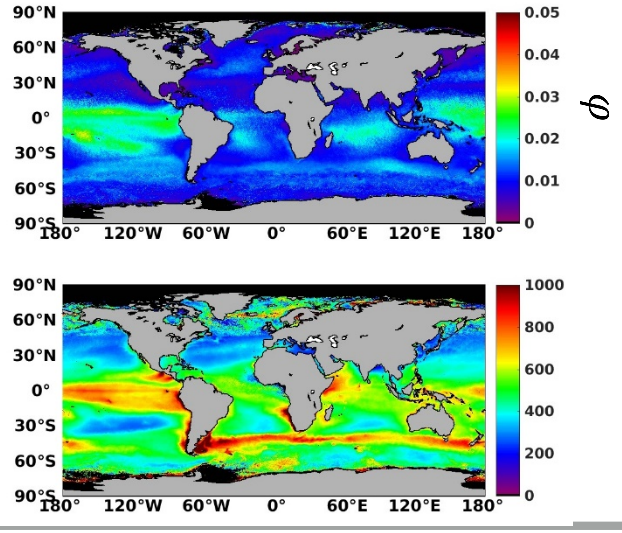
<u>Team members:</u>

Toby Westberry (PI)

Mike Behrenfeld (Co-I)

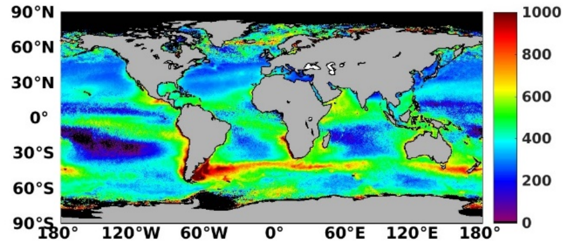
Jason Graff (Co-I)

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



$$\Delta NPP = \left(\frac{\varphi}{\varphi_{thresh}} - 1\right)$$

∫ΔNPP = 10.9 Pg C



Testing PACE Terrestrial Ecosystem Productivity Algorithms Using HICO

K. Fred Huemmrich, Petya P.K. Campbell, University of Maryland Baltimore County - kfhuemm@gmail.com

Used HICO data to test potential PACE terrestrial algorithms for productivity

Require robust algorithms that work across vegetation types due to PACE's large pixels

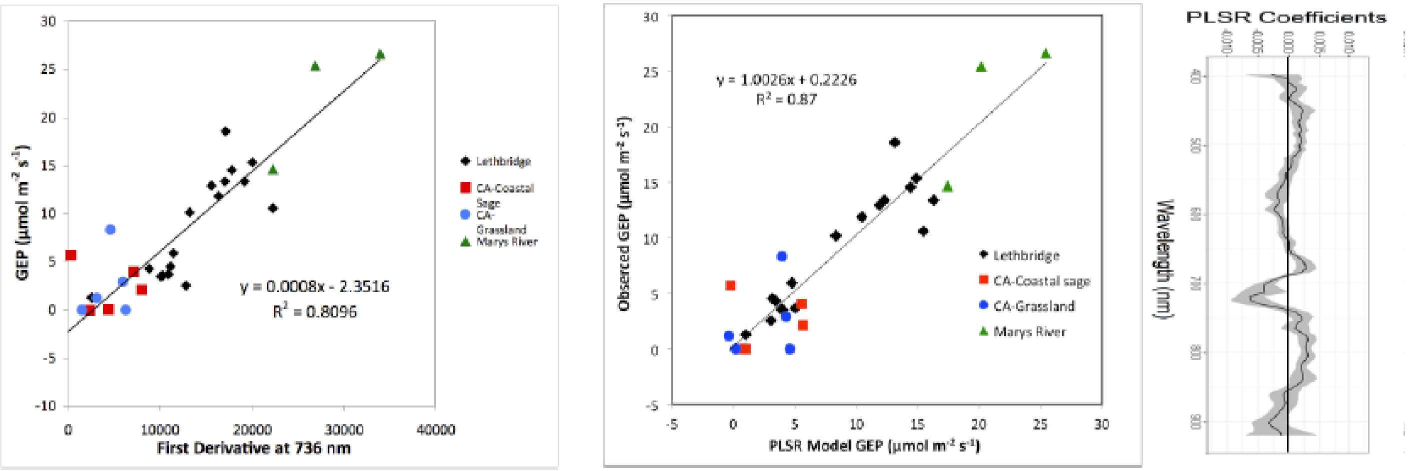
- most land pixels will likely be mixtures

Examined four different sites with flux towers measuring productivity. Sites included grass, shrubs, and forest covers

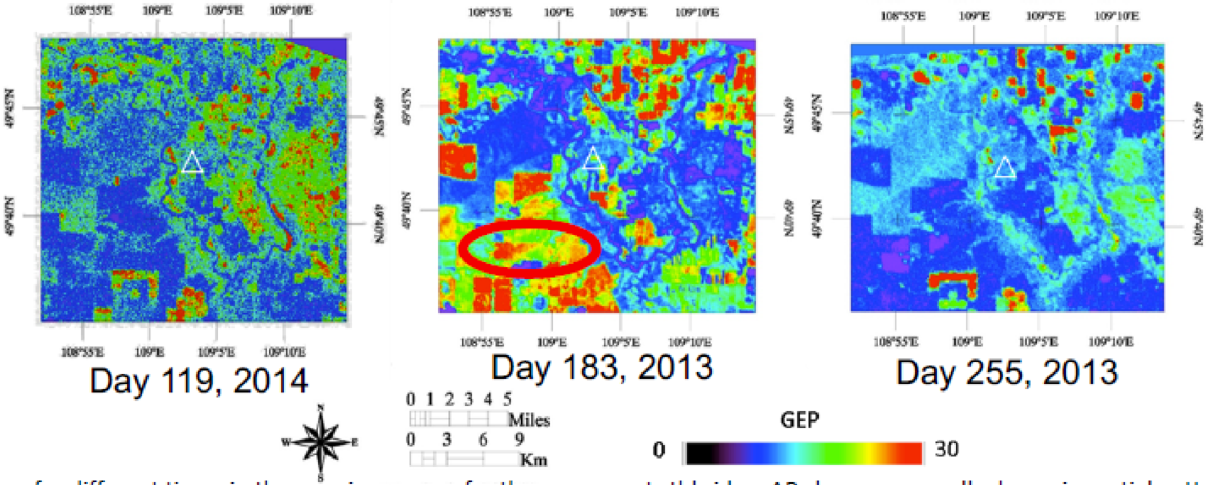
Multiple approaches were successful

Further studies are required to determine optimal approaches for PACE that describe diverse vegetation types

This work may be advanced by leveraging SBG activities such as the reprocessed imaging spectrometer data by SISTER project (SBG Space-based Imaging Spectroscopy and Thermal PathfindER)



Two examples of successful approaches to retrieve GEP from HICO reflectances are: left figure uses descriptions of spectral shape, in this case first derivatives of spectral reflectance at 736 nm, and right figure uses statistical approaches such as Partial Least Squares Regression (PLSR) (the figure to the far right shows the coefficients for each spectral bands from the PLSR calculation).

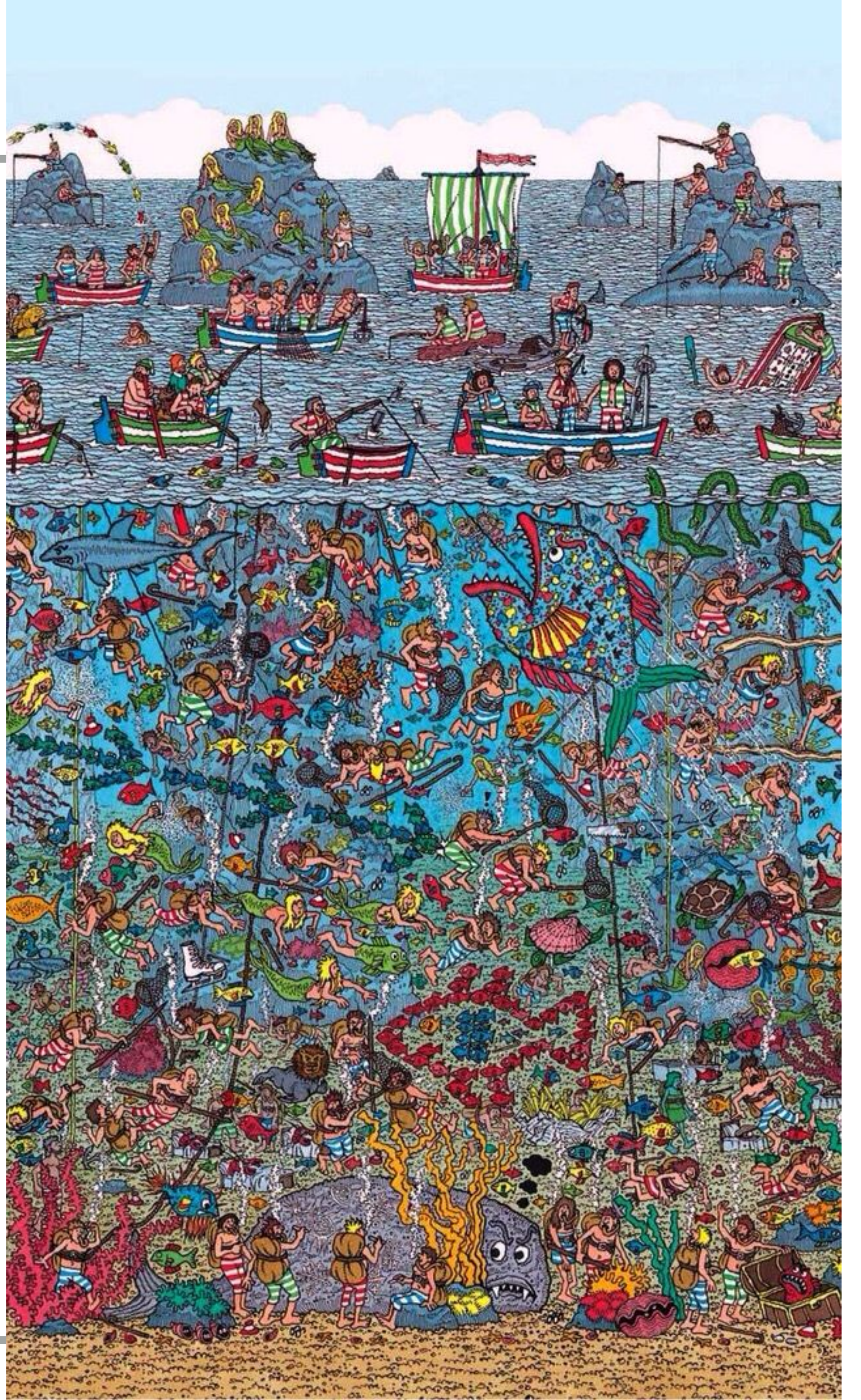


HICO imagery for different times in the growing season for the area near Lethbridge, AB shows seasonally dynamic spatial patterns of GEP. Further, the reflectance-based algorithm describes both between and within field variability in GEP as indicated by the variability in the circled field in the midsummer (center) image. In visible color images this field is uniformly green. The triangle marks the location of the flux tower.

Reference: Huemmrich, et al. (2017) ISS as a Platform for Optical Remote Sensing of Ecosystem Carbon Fluxes: A Case Study Using HICO." IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing 10(10) : 4360-4375, DOI 10.1109/JSTARS.2017.2725825

PACE SAT and Validation

- Draft Validation Plan is currently being updated
- Validation:
  - hyperspectral radiometry and polarimetry
  - atmospheric and aquatic products
  - within 12 months of launch
- Variety of sub-orbital validation data
  - Aeronet/Aeronet-OC moorings
  - Ship-based cruises
  - Airborne campaigns
- SAT will provide recommendations to the PACE Validation Science Team.
- Innovative ideas about how to best validate satellite missions – biggest bang for buck



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

Field and Culture Data		
Casey, K. A., Rousseaux, C. S., Gregg, W. W., Boss, E., Chase, A. P., Craig, S. E., et al. (2020). *Earth System Science Data*, *12*(2), 1123–1139. https://doi.org/10.5194/essd-12-1123-2020. https://doi.pangaea.de/10.1594/PANGAEA.902230.	Field, Global	A global compilation of in situ aquatic high spectral resolution inherent and apparent optical property data for remote sensing applications
Carpenter, Dierssen, Hochberg, Lee. 2014-2017. The Coral Reef Airborne Laboratory (CORAL) database. https://doi.org/10.5067/SeaBASS/CORAL/DATA001 https://airbornescience.jpl.nasa.gov/campaign/coral	Field, Pacific Reefs	In situ IOP and AOP data collected over Pacific coral reefs in conjunction with PRISM hyperspectral imagery
Knaeps et al. (2018). The SeaSWIR dataset. https://doi.org/10.1594/PANGAEA.886287	Field, Regional	Hyperspectral marine reflectances, total suspended matter, and turbidity measurements gathered at three turbid estuarine sites.
Behrenfeld et al., 2014-2017. North American Aerosol and Marine Ecosystem Study (NAAMES). https://doi.org/10.5067/SeaBASS/NAAMES/DATA001	Field, North Atlantic	Four cruises in North Atlantic with AOPS, IOPs, associated with phytoplankton and aerosol data.
Siegel et al. 2018-2020. Ocean EXPORTS https://doi.org/10.5067/SeaBASS/EXPORTS/DATA001	Field, Pacific & Atlantic	Data on export and fate of upper ocean net primary production coupled to IOP and AOP measurements.
Marine Biodiversity Observation Network (MBON) Data Portal. https://mbon.ioos.us/	Field, Regional	Biodiversity time series of flora and fauna along coastal zones with ancillary data.
Mortelmans et al. (2019). Lifewatch Flanders Marine Institute Observatory Data. In prep for Reflectance https://doi.org/10.14284/393	Field, Coastal North Sea	Monthly phytoplankton pigment, suspended matter, turbidity, and recently hyperspectral radiometry
Vanderwoude et al. (2020). NOAA GLERL Great Lakes Harmful Algal Bloom Database Doi: In prep	Field, Great Lakes	Monthly sampling of Great Lakes phytoplankton composition and hyperspectral optics
Bracher et al. 2020. Coupled phytoplankton composition and radiometry from Atlantic Ocean. https://doi.org/10.1594/PANGAEA.913536	Field, Atlantic	Phytoplankton pigment concentration, groups, and radiometric measurements in the Atlantic Ocean.
Bagniewski, W. et al. (2010). North Atlantic Bloom Experiment 2008. https://www.bco-dmo.org/project/2098	Field, Atlantic	Phytoplankton dynamics, profiled hyperspectral reflectance with autonomous optical backscatter, attenuation, radiance
Dekker, Anstee, In prep. Digital Earth Australia. Australian Shallow Waters Spectral Library https://ozcoasts.org.au/management/library/	Field, Australia	Spectral library repository for aquatic ecosystem substratum and substratum cover types
Clementson and Wojtasiewicz (2019). Australian National Algae Culture Collection https://doi.org/10.1016/j.dib.2019.104020	Culture	Dataset on the in vivo absorption characteristics and pigment composition of various phytoplankton species
Voss et al. NOAA Marine Optical Buoy (MOBY) https://www.star.nesdis.noaa.gov/socd/moby/filtered_spec/	Field, Hawaii	Hyperspectral water-leaving reflectance
Joyce, K. 2020. Shared Drone Spectroscopy https://www.geonadir.com/	Field, Global	Public repository for drone data including hyperspectral datasets

Dierssen et al. Frontiers (2021)

Simulated Databases

Simulated and Derived Data		
Craig, Susanne E; Lee, Zhongping; Du, Keping (2020). National Aeronautics and Space Administration, PANGAEA, https://doi.org/10.1594/PANGAEA.915747.	Simulated, Global	Top of Atmosphere, Hyperspectral Synthetic Dataset for PACE (Phytoplankton, Aerosol, and ocean Ecosystem) Ocean Color Algorithm Development.
Gregg, W. W., & Rousseaux, C. S. (2017). Simulating PACE Global Ocean Radiances. *Frontiers in Marine Science, 4*. https://doi.org/10.3389/fmars.2017.00060	Simulated, Global	Dynamic simulation of global water-leaving radiances at 1 nm spectral resolution using an ocean model containing multiple ocean phytoplankton groups, etc.
Bracher et al. 2017. Phytoplankton composition from 2002-2012 in world ocean https://doi.org/10.1594/PANGAEA.870486	Derived, Global	Global monthly mean surface chlorophyll a for diatoms, coccolithophores and cyanobacteria from SCIAMACHY data

Loisel and Stramski Developing a new simulated dataset for PACE.

Simulated Imagery on PACE website

Simulated Ocean Color Imagery

Simulated OCI Instrument Model

Simulated GMAO

Simulated PyToast

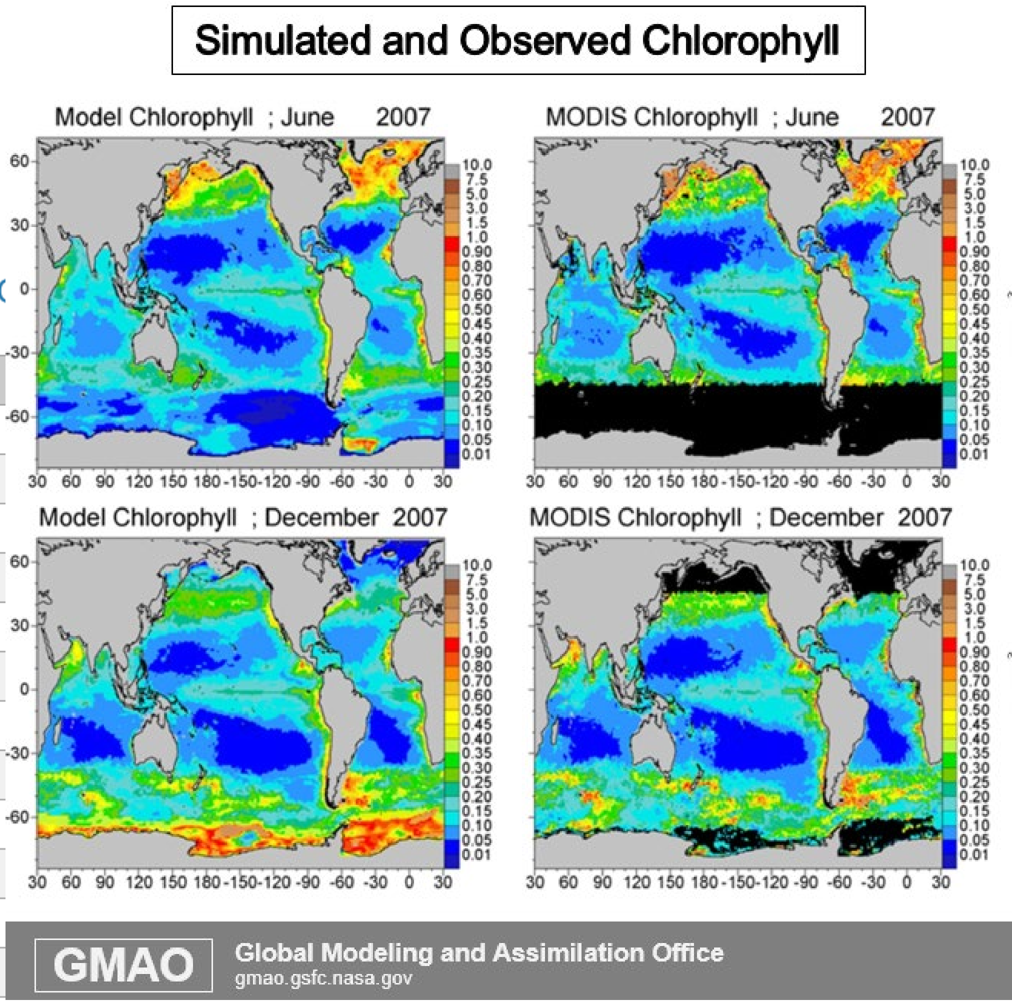
Simulated Polarimetry Imagery

Simulated SPEXone data

AirHARP Proxy Data

OceanData Home ▸ directaccess ▸ PACE ▸ (

Filename
PACE_OCI_SIM.20190321T000000.L1B.V7.nc
PACE_OCI_SIM.20190321T000500.L1B.V7.nc
PACE_OCI_SIM.20190321T001000.L1B.V7.nc
PACE_OCI_SIM.20190321T001500.L1B.V7.nc
PACE_OCI_SIM.20190321T002000.L1B.V7.nc
PACE_OCI_SIM.20190321T011000.L1B.V7.nc
PACE_OCI_SIM.20190321T011500.L1B.V7.nc
PACE_OCI_SIM.20190321T012000.L1B.V7.nc
PACE_OCI_SIM.20190321T012500.L1B.V7.nc
PACE_OCI_SIM.20190321T013000.L1B.V7.nc
PACE_OCI_SIM.20190321T013500.L1B.V7.nc
PACE_OCI_SIM.20190321T014000.L1B.V7.nc
PACE_OCI_SIM.20190321T014500.L1B.V7.nc



PACE Applications & Early Adopter Program

Leveraging Science to Advance Society

Erin Urquhart[1,2], Natasha Sadoff [1,2]

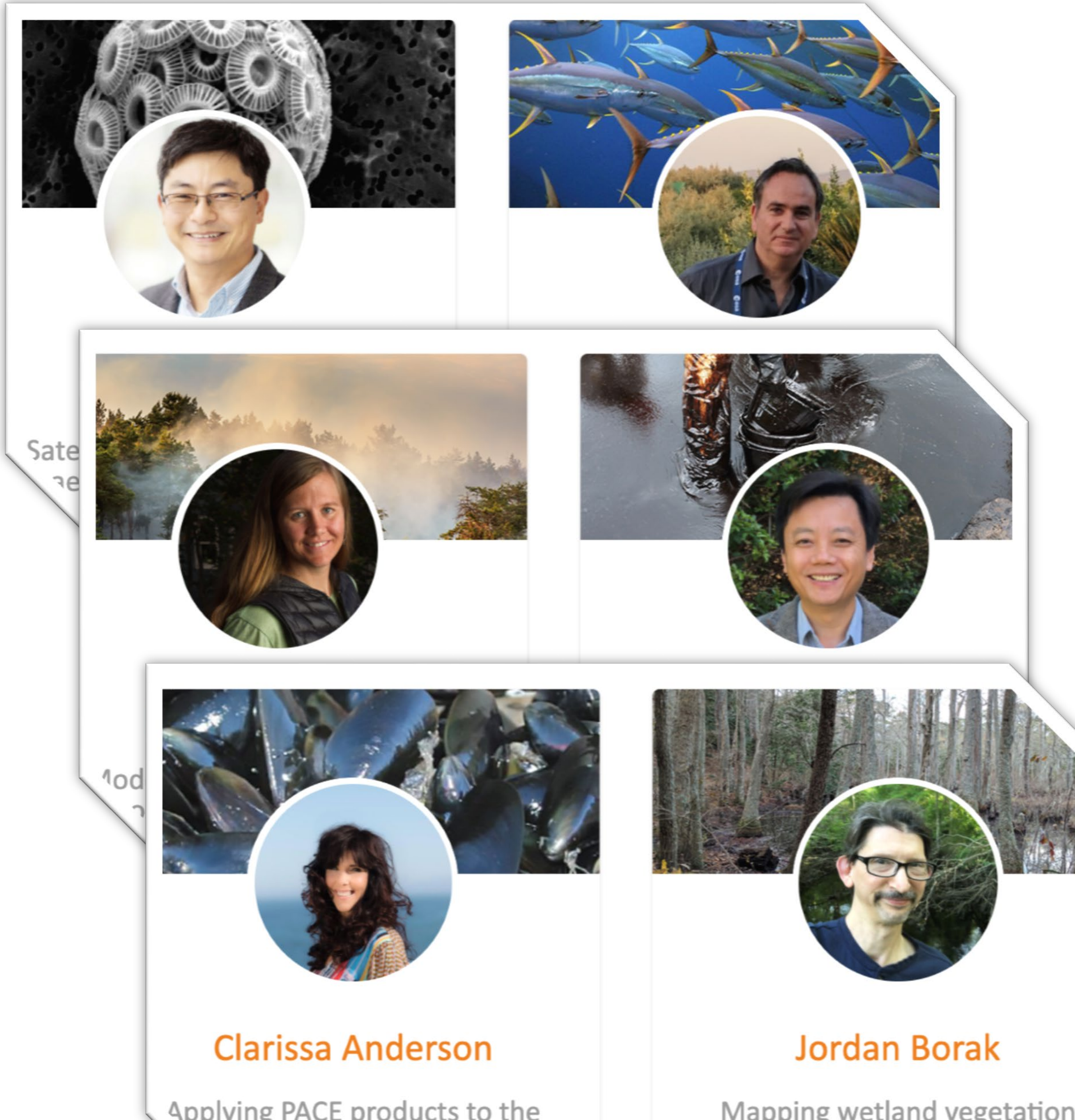
[1]NASA GSFC, [2]SSAI

PACE Early Adopter Program

The PACE Early Adopter program promotes applied science and applications research designed to scale and integrate PACE data into policy, business, and management activities that benefit society and inform decision making.

Goals:

- Expand the user communities with tangible and potential applications that would benefit from the use of PACE data
- Facilitate feedback on PACE data products pre-launch
- Accelerate the use and integration of PACE products into applications post-launch by providing specific support to Early Adopters who commit to engage in pre-launch applied research



PACE Early Adopter Program

PACE Applications Program (*a year in review*)

https://pace.oceansciences.org/app_workshops_02.htm

Not too late to become an Early Adopter!

science community engagement

Current Science & Applications Team (SAT#2) intact through mid-2023
Next team (SAT#3) expected to be competed via NASA ROSES-23

PACE Validation Science Team (PVST) to be assembled ~6 months prior to launch (as of today, this would be ~mid-2023)

- Preliminary focus on validation of threshold products (ocean color radiometry, AOT, clouds)
- Evolution into validation of derived/advanced products, including polarimetry, & closure experiments
- Mission interested in collaborations / synergies / advanced planning with international partners
- **Separate but complementary PACE Post-launch Airborne eXperiment (PACE-PAX)**

System Vicarious Calibration team down-select planned for late 2022

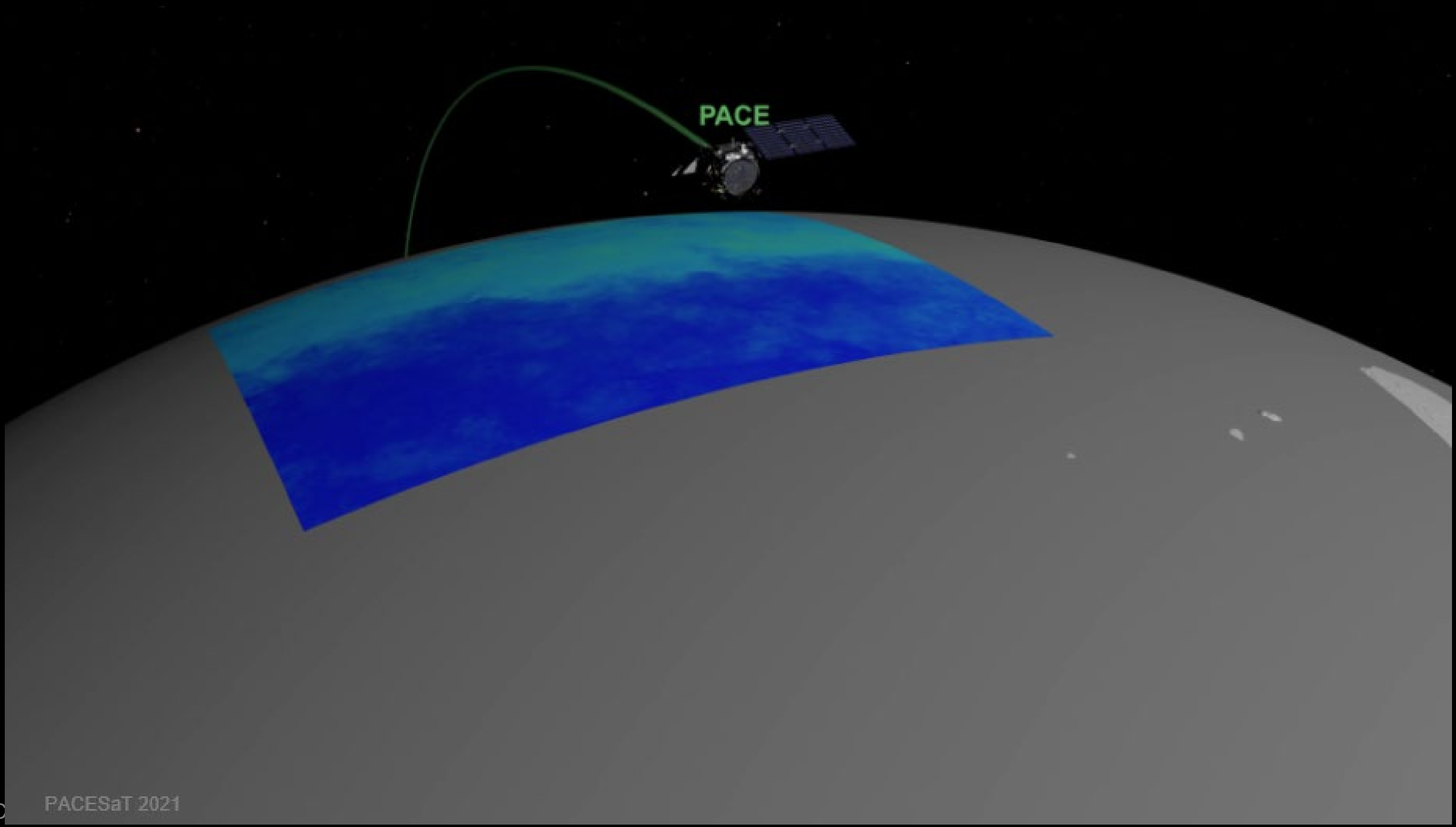
- Two teams to one
- Coincides with end of 2^{nd} project years
- Originally planned for mid-late 2021 after 1^{st} project years

Participate in Applications Program & Early Adopters

PACE Science Data Product Selection Plan pace.oceansciences.org/docs/PACE_Validation_Plan_14July2020.pdf

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



Questions