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
Overarching Science Questions

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?

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

October 16, 2012

Courtesy: Eric Gorman, OCI Instrument Systems Engineer
# Living up to the Hype of Hyperspectral Aquatic Remote Sensing: Science, Resources and Outlook

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## Table of Essential Biodiversity Variable (EBV) Classifications

<table>
<thead>
<tr>
<th>Class</th>
<th>Wetlands</th>
<th>Benthic communities</th>
<th>Pelagic</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Essential</td>
<td>Macrophytes &amp;</td>
<td>Coral</td>
</tr>
<tr>
<td></td>
<td>Biodiversity</td>
<td>Macroalgae</td>
<td>Phytoplankton</td>
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<tr>
<td></td>
<td>Variable (EBV)</td>
<td></td>
<td>Fish Zooplankton</td>
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<td></td>
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<td></td>
<td>Apex Predator</td>
</tr>
</tbody>
</table>

**Species Composition**
- Population genetic diversity

<table>
<thead>
<tr>
<th>Species Populations</th>
<th>Mangrove/Salt marsh</th>
<th>Macrophytes &amp; Macroalgae</th>
<th>Coral</th>
<th>Phytoplankton</th>
<th>Fish Zooplankton</th>
<th>Apex Predator</th>
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</thead>
<tbody>
<tr>
<td>Distribution</td>
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<tr>
<td>Abundance</td>
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<tr>
<td>Size/vertical</td>
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<tr>
<td>distribution</td>
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</tr>
</tbody>
</table>

**Species Traits**
- Pigments*
- Phenology
- Taxonomic diversity*
- Functional type*
- Fragmentation/heterogeneity
- Net primary production
- Net ecosystem production

<table>
<thead>
<tr>
<th>Species Traits</th>
<th>Mangrove/Salt marsh</th>
<th>Macrophytes &amp; Macroalgae</th>
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<th>Fish Zooplankton</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Pigments*</td>
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<tr>
<td>Phenology</td>
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<tr>
<td>Taxonomic diversity*</td>
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<tr>
<td>Functional type*</td>
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<td>heterogeneity</td>
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<td>Net primary</td>
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<tr>
<td>production</td>
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<tr>
<td>Net ecosystem</td>
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<tr>
<td>production</td>
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</tr>
</tbody>
</table>

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

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## Figures

- PACE
• hyperspectral scanning radiometer
• 340–890 nm, 5 nm resolution, 2.5 nm steps
• plus, 940, 1038, 1250, 1378, 1615, 213 and 2250 nm
• 1 day global coverage
• ground pixel size of 1 km² at nadir
• ± 20° fore/aft tilt to avoid Sun glint
• twice monthly lunar calibration
• daily on-board solar calibration
• built at NASA Goddard Space Flight Center

PACE Ocean Color Instrument
PACESaT 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
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

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*MODIS on IRS (2000-2002) does not yet provide calibrated data.
**MODIS/VIIRS short-wave infrared bands are not optimal.

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* Phase E & Controlled Reentry
- 10 years fuel*

Launch Readiness Date (LRD) Jan. 2024
Post Pandemic (not yet Approved)

Decommission

PACE Mission Status
Oct. 6, 2021

Courtesy Andre Dress PACE Project Manager
PACE Science and Applications Team (SAT)

Plus Streaming Totals: 75 Cities 195 Unique IP Addresses

Credit Oskar Landi
## 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
Table 1. Required Ocean Color Instrument (OCI) ocean color data products.

<table>
<thead>
<tr>
<th>Data Product</th>
<th>Baseline Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water-leaving reflectances centered on (±2.5 nm) 350, 360, and 385 nm (15 nm bandwidth)</td>
<td>0.0057 or 20%</td>
</tr>
<tr>
<td>Water-leaving reflectances centered on (±2.5 nm) 412, 425, 443, 460, 475, 490, 510, 532, 555, and 583 (15 nm bandwidth)</td>
<td>0.0020 or 5%</td>
</tr>
<tr>
<td>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)</td>
<td>0.0007 or 10%</td>
</tr>
</tbody>
</table>

**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.

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

Aerosols
Clouds
Surface Physics
Water Biophysics
Floating Matter
Shallow Habitats
Phyto-Plankton Dynamics

Clouds
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Floating Matter
Shallow Habitats
Phyto-Plankton Dynamics
Aerosols
Science Team
Hu
Ottaviani
Shuchman

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

Aerosols
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Shallow Habitats
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Aerosols
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<thead>
<tr>
<th>Presentation</th>
<th>Last Name</th>
</tr>
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<tr>
<td>Unified algorithm for aerosol characterization from OCI</td>
<td>Remer</td>
</tr>
<tr>
<td>Radiative Transfer Simulator and Polarimetric Inversion for PACE</td>
<td>Zhai</td>
</tr>
<tr>
<td>Retirevals of the Ocean Surface Refractive Index</td>
<td>Ottaviani</td>
</tr>
<tr>
<td>Joint polarimetric aerosol and ocean color retrievals with deep learning</td>
<td>Gao</td>
</tr>
<tr>
<td>Algorithms to obtain inherent optical properties of seawater</td>
<td>Stramski</td>
</tr>
<tr>
<td>The PACE-MAPP collaborative algorithm project</td>
<td>Stamnes</td>
</tr>
<tr>
<td>Freshwater Hyperspectral HABs Algorithms</td>
<td>Shuchman</td>
</tr>
<tr>
<td>Retrieving water quality indicators via MDNs</td>
<td>Pahlovan</td>
</tr>
<tr>
<td>Chi factor and BRDF</td>
<td>Zhang</td>
</tr>
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<td>PACE UV Retrieval of Oceanic and Atmospheric Data products</td>
<td>Chowdhary</td>
</tr>
<tr>
<td>Spectral Derivative Methods for Quantifying Phytoplankton Pigments for PACE</td>
<td>Siegel</td>
</tr>
<tr>
<td>Topic</td>
<td>Authors</td>
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<td>----------------------------------------------------------------------</td>
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<tr>
<td>Inversion algorithm for PACE</td>
<td>Twardowski</td>
</tr>
<tr>
<td>MAIIAC Processing of OCI Over Land: Aerosol Chemical Speciation</td>
<td>Go (Lyapustin)</td>
</tr>
<tr>
<td>HARP2 Level 1 Data Processing Plan</td>
<td>Xu</td>
</tr>
<tr>
<td>Remote sensing of cloud properties using PACE SPEXone and HARP-2</td>
<td>van Diedenhoven</td>
</tr>
<tr>
<td>Phytoplankton Algorithms and Data Assimilation: Preparing a Pre-launch Path to Exploit PACE Spectral Data</td>
<td>Rousseaux</td>
</tr>
<tr>
<td>PACE implementations for optically shallow waters</td>
<td>Barnes</td>
</tr>
<tr>
<td>A toolbox for the diagnostic assessment of spectral behavior</td>
<td>Vandermeulen</td>
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<tr>
<td>Radiative products for PACE</td>
<td>Boss</td>
</tr>
<tr>
<td>Support for PACE OCI Cloud Products</td>
<td>Meyer</td>
</tr>
<tr>
<td>Hyperspectral algorithms for OCI atmospheric correction and UV penetration</td>
<td>Krolkov</td>
</tr>
<tr>
<td>Net Primary Production for PACE OCI</td>
<td>Westberry</td>
</tr>
<tr>
<td>Machine learning approaches for predicting phytoplankton community composition from ocean color</td>
<td>Craig</td>
</tr>
<tr>
<td>SpexONE - Aerosols</td>
<td>remoTAP</td>
</tr>
<tr>
<td>NPP PACE, PhytoC</td>
<td>Hasekamp</td>
</tr>
</tbody>
</table>
Standard Semi-analytical Formulation

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

Proportionality factor
Bidirectionalality of
Incoming and reflected light

\[ b_b = b_{b,\text{water}} + b_{b,\text{large part}} + b_{b,\text{small part}} \]

\[ a = a_{\text{water}} + a_d + a_g + a_{\text{ph}} \]

ZTT (Zaneveld-Twardowski-Tonizzo) model

\[ r_{RS}(\theta_s, \theta_v, \phi, V, a, b_b, \beta) \equiv r_{RS,\text{Raman}}(\theta_s', a, b_b) \]

- Average cosine of downwelling light field
- Absorption over backscattering
- Phase function in backward direction
- Shape function for upwelling component of path radiance
- Backscattering ratio \( b_d/b_b \)

Water Raman contribution
(\textit{Westberry et al. 2013})

Coefficients related to diffuse attenuation of radiance in viewing direction
(\textit{Twardowski and Tonizzo 2017})
Spectral derivative methods for estimating phytoplankton pigment concentrations

• 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

Team members:
Toby Westberry (PI)
Mike Behrenfeld (Co-I)
Jason Graff (Co-I)

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

\[ \Delta NPP = \frac{\varphi}{\varphi_{thresh}} - 1 \]

\[ \int \Delta NPP = 10.9 \text{ Pg C} \]
Testing PACE Terrestrial Ecosystem Productivity Algorithms Using HICO

K. Fred Huemmrich, Petya P.K. Campbell, University of Maryland Baltimore County - kfhuemmm@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.

• 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 in Development and Validation

#### Field and Culture Data

|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|--------------|--------------------------------------------------------------------------------|

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Dierssen et al. Frontiers (2021)

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

<table>
<thead>
<tr>
<th>Simulated and Derived Data</th>
<th>Simulated, Global</th>
<th>Top of Atmosphere, Hyperspectral Synthetic Dataset for PACE (Phytoplankton, Aerosol, and ocean Ecosystem) Ocean Color Algorithm Development</th>
</tr>
</thead>
<tbody>
<tr>
<td>Craig, Susanne E; Lee, Zhongping; Du, Keping (2020). National Aeronautics and Space Administration, PANGAEA, <a href="https://doi.org/10.1594/PANGAEA.915747">https://doi.org/10.1594/PANGAEA.915747</a></td>
<td>Simulated, Global</td>
<td>Top of Atmosphere, Hyperspectral Synthetic Dataset for PACE (Phytoplankton, Aerosol, and ocean Ecosystem) Ocean Color Algorithm Development</td>
</tr>
<tr>
<td>Bracher et al. 2017. Phytoplankton composition from 2002-2012 in world ocean <a href="https://doi.org/10.1594/PANGAEA.870486">https://doi.org/10.1594/PANGAEA.870486</a></td>
<td>Derived, Global</td>
<td>Global monthly mean surface chlorophyll a for diatoms, coccolithophores and cyanobacteria from SCIAMACHY data</td>
</tr>
</tbody>
</table>

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 • (GMAO) Global Modeling and Assimilation Office gmao.gsfc.nasa.gov
PACE Applications & Early Adopter Program

*Leveraging Science to Advance Society*

Erin Urquhart\textsuperscript{1,2}, Natasha Sadoff \textsuperscript{1,2}

\textsuperscript{1}NASA GSFC, \textsuperscript{2}SSAI
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 Applications Program (a year in review)

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 2nd project years
• Originally planned for mid-late 2021 after 1st project years

Participate in Applications Program & Early Adopters

PACE Science Data Product Selection Plan pace.oceansciences.org/docs/PACE_Validation_Plan_14July2020.pdf
<table>
<thead>
<tr>
<th>Global change</th>
<th>Biogeochemical modeling</th>
<th>Ecological processes</th>
<th>Ecological indicators</th>
<th>Environmental reporting</th>
<th>Hazard Monitoring</th>
<th>Food Security</th>
</tr>
</thead>
<tbody>
<tr>
<td>• latitudinal distributional shifts</td>
<td>• phytoplankton community composition</td>
<td>• rates of primary production</td>
<td>• hypoxia</td>
<td>• meeting thresholds</td>
<td>• detection and tracking of harmful algal blooms</td>
<td>• finding pelagic and benthic habitats for fisheries</td>
</tr>
<tr>
<td>• phenology shifts</td>
<td>• nutrient cycling</td>
<td>• nitrogen fixers, DMS producers, silicifiers, calcifiers</td>
<td>• eutrophication</td>
<td>• species composition</td>
<td>• assessing storm impacts</td>
<td>• locations/monitoring for aquaculture</td>
</tr>
<tr>
<td>• bloom dynamics</td>
<td>• export of particles</td>
<td>• trophic dynamics &amp; food web efficiency</td>
<td>• informed monitoring and assessment</td>
<td>• detecting anomalies</td>
<td>• monitoring oil spill extent and cleanup</td>
<td>• food safety &amp; toxin production</td>
</tr>
</tbody>
</table>

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