PACE Water Resources

Demonstrating the Use of NASA's PACE Hyperspectral Ocean Color Instrument Data for Enhanced Coastal Management

DEVELOP Technical Report
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1. Abstract

This project developed tools to support the future use of Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) hyperspectral imagery in water resource monitoring and research by NASA DEVELOP teams and members of the PACE applications community. We sought to address a need to aid processing and visualizing hyperspectral PACE Ocean Color Instrument (OCI) data by researchers and decision-makers involved with coastal water quality management and harmful algal bloom (HAB) monitoring. To supplement the day of simulated PACE imagery available, we used Aqua MODIS earth observations with Level 3 processing from March 2022 to help build a Python graphical user interface (GUI) for visualizing ocean biogeochemical parameters relevant to the early detection and monitoring of HABs. We used simulated PACE OCI Level 2 data derived from the Python Top of Atmosphere Simulation Tool (PyTOAST) to build Jupyter Notebooks for band subset and selection. The Level 3 PACE Viewer components support users with quick visualizations as well as the creation of geoTIFFs and time-series. The Level 2 Jupyter Notebooks address user concerns over the volume and complexity of hyperspectral imagery. The PACE Viewer is useful for visual inspection and netCDF data processing but should not be used for geospatial analysis. This tool can be used to alleviate the technical burdens of working with hyperspectral data and support the early detection and monitoring of HABs using PACE satellite imagery.

Key Terms

PACE hyperspectral imagery, Aqua MODIS, graphical user interface, chlorophyll-a, harmful algal blooms, Python Top of Atmosphere Simulation Tool

2. Introduction

2.1 Background Information

Sustainable coastal management and ocean ecosystem monitoring are critical as the impacts of anthropogenic climate change intensify. Rising sea levels, coastal flooding and erosion, changes in the biogeochemical conditions of our waters, and extreme coastal weather events increasingly threaten human health, infrastructure, and economic activity, as well as the diverse ecosystems in oceans and coastal areas. (Griggs & Reguero, 2021). Evidence suggests that future climate scenarios will, among a multitude of other impacts, worsen the frequency and intensity of harmful algal blooms (HABs) in both marine and freshwater environments. In coastal waters, sea temperature rise, an overabundance of nutrient inputs, increased atmospheric carbon dioxide concentrations, changes in salinity, intensified coastal upwelling, and sea level rise all favor the growth of HABS (United States Environmental Protection Agency Office of Water, 2013). HABs can lead to economic losses (e.g., fish kills) and threats to public health (e.g., shellfish & drinking water contamination and aerosolized toxin exposure; Woods Hole Oceanographic Institution, 2019). HABs pose significant threats to coastal community wellbeing and HAB research is critical to ocean ecosystem monitoring and sustainable management (Figure 1).

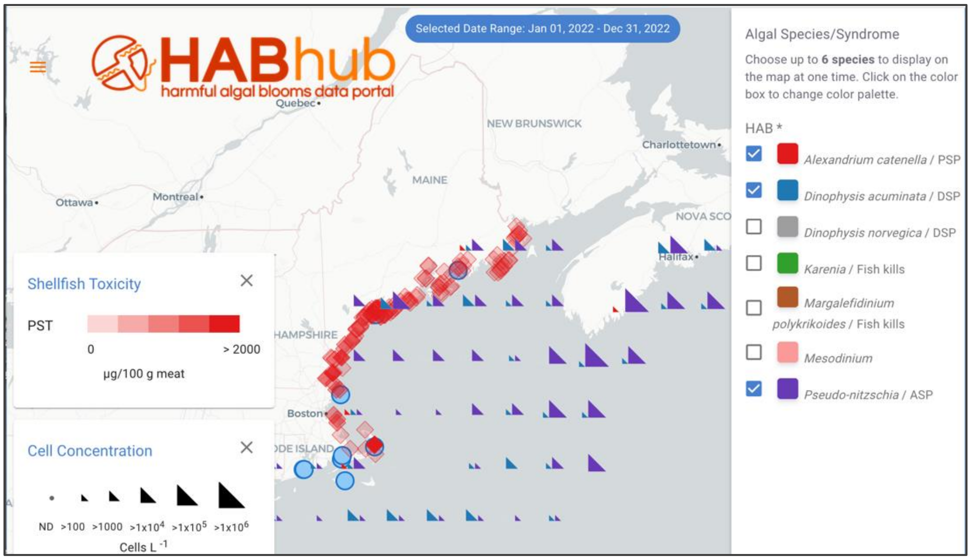

Figure 1. The Woods Hole Oceanographic Institute's HABHub portal is one example of a tool used by water quality managers and policymakers. It displays shellfish toxicity and phytoplankton concentrations in the Gulf of Maine. HABHub data were collected from a combination of in situ water sampling, automated submersible microscopes known as Imaging FlowCytobots, and shellfish toxicity closures.

Satellite remote sensing is a powerful tool for effective ocean water quality monitoring and management. Earth observations enable consistent, accurate monitoring of indicators, such as water temperature, ocean color, salinity, sea level fluctuation, and concentration of organic materials, across a large study area (Le Traon et al., 2015). Since the deployment of the Coastal Zone Color Scanner (CZCS) on the Nimbus 7 satellite for water remote sensing in 1978, many subsequent satellites have been launched with the intent to further marine research (Blondeau-Patissier et al., 2014). Over time, new instruments for coastal monitoring improved in terms of spectral and temporal resolution. Multispectral ocean color imagery from satellite instruments such as NASA's Aqua Moderate Resolution Imaging Spectroradiometer (MODIS) and NOAA's Visible Infrared Imaging Radiometer Suite (VIIRS) have been used as a means of estimating marine chlorophyll-a concentrations, an indicator of primary production and phytoplankton biomass (O'Dowd et al., 2008; Quinn & Bates, 2011). In some cases, sensors have even been used to help determine what dominant phytoplankton groups— coccolithophores, diatoms, or dinoflagellates—might be in the water, using methods such as the PHYSAT model (Navarro et al., 2014). Considering the contributions that multispectral imagery has made to our understanding of the ocean, the numerous wavelengths of light detected by hyperspectral sensors are useful for informing marine ecological forecasts and verifying *in situ* field measurements. As such, a new and exciting addition to the ocean color satellite fleet is NASA's Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) mission. PACE launched in February 2024, five months after the completion of this project.

While in orbit, PACE measures atmospheric and oceanic properties using three instruments. The Ocean Color Instrument (OCI) will measure ocean color to estimate marine biogeochemical indicators such as Chlorophyll-a; it is the most advanced remote sensing tool for ocean color monitoring in NASA's history. Most ocean color sensors used today perform multispectral imaging that measures the reflectance of light at a small number of bands along the electromagnetic spectrum — typically fewer than fifteen (Purkis & Chirayath, 2022). Instead, the PACE OCI is hyperspectral, meaning it measures hundreds of bands in the UV, visible, and near-infrared ranges of the electromagnetic spectrum, as well as several bands in the shortwave infrared range, with 5 nm band widths and spectral steps of 2.5 nm ("NASA PACE", 2023). Hyperspectral imaging (HSI) provides a higher spectral resolution than multispectral imaging. The main obstacle to using HSI for applications in coastal management and ocean monitoring, aside from the relative lack of HSI data available, is the size and complexity of hyperspectral data. Adjacent bands in HSI are highly correlated, and often do not provide significantly different information; therefore, it is difficult to discern which bands are redundant for image classification and which are most appropriate for generating usable insights (Dierssen et al., 2021). Processing and visualizing hyperspectral data are not intuitive tasks – even for users experienced working with multispectral imagery.

2.2 Project Partners & Objectives

For this project, we partnered with the PACE Applications Program, a team that aims to engage end users, such as scientists, policy makers, public health practitioners, and industry professionals, to work with PACE data. We developed applications for PACE data processing and visualization with a diverse group of end users in mind, accounting for varying needs and interests. One key group of end users we considered are researchers: future NASA DEVELOP project teams, other teams within NASA, and other academics in the remote sensing field who want to use PACE ocean color data for research purposes. These users most likely have some familiarity with satellite data, although they may only have experience working with multispectral imagery. We aimed to provide them with advanced functionality, while at the same time easing their transition from multispectral data to hyperspectral data. Equally important, however, were users outside the scientific research community: those in the coastal management industry such as water managers, restoration ecologists, nonprofit coordinators, and public health officials. We aimed to provide this group of end users with an intuitive, human-friendly interface and easy access to science products relevant to their work, such as chlorophyll-a concentration threshold maps.

We conducted this project to aid future DEVELOP teams in the incorporation of PACE OCI hyperspectral data in their projects, as well as to integrate PACE OCI hyperspectral data in applied science research efforts. Higher levels of spectral detail in hyperspectral images provides scientists the ability to distinguish between different dominant phytoplankton community compositions, identify types of minerals, and detect microplastics solely through remote sensing and image analysis. We created a variety of Python applications to make processing and visualizing PACE data more user-friendly and intuitive, particularly for users unfamiliar with hyperspectral data.

3. Methodology

3.1 Data Acquisition

We sourced Earth observations from simulated PACE hyperspectral and multispectral proxy datasets. The PACE mission generated a complete simulated day-in-the-life collection of Ocean Color Instrument (OCI) images for March 21, 2022. We accessed these PACE Simulated OCI images of chlorophyll-a, sea surface temperature (SST), particulate inorganic carbon (PIC), particulate organic carbon (POC), total suspended solid (TSS), backscattering coefficient of particles (bbp_443), phytoplankton absorption at 443 nm (aph_443), and the absorption coefficient of colored dissolved organic matter (adg_443) from the Level 3 mapped collection via NASA's Ocean Color Data website. NASA's Ocean Ecology Laboratory created the simulated PACE OCI data using the Python Top of Atmosphere Simulation Tool (PyTOAST) and Aqua MODIS data. We also used Aqua MODIS Level 3 image data from March 2022 to build our Python scripts. We used an extended record of Aqua MODIS data to ensure data values are available for all pixels because unfavorable measurement conditions, such as clouds and sun glint, can limit the quality of available data over short time periods. We acquired all images at the 4 km spatial resolution in the EPSG:4326 coordinate reference system. These PACE and Aqua MODIS datasets are available at the NASA Ocean Biology Distributed Active Archive Center (OB.DAAC).

3.2 Tool Development

We designed and utilized a Python tool and Jupyter Notebooks to process both the simulated PACE imagery and observed Aqua MODIS imagery, ensuring seamless data integration and analysis. Our Python graphical user interface (GUI) tool ingests PACE Level 3 netCDF files from a specified file path on the user's desktop and applies a range of data processing and visualization functions to the user's chosen PACE Level 3 netCDF files. Level 3 PACE files contain geophysical data retrievals that have been temporally and spatially aggregated onto a geo-referenced Earth grid, but Level 2 files remain in the native satellite swath coordinate system, without temporal compositing or projection. While the Jupyter Notebooks apply similar data processing and visualization functions to both Level 2 and Level 3 imagery, the GUI is designed to work with Level 3 imagery only. Both the GUI and notebooks apply water quality thresholds to the imagery to make the data useful for water resources research and management.

After establishing a working directory of OCI data, we read the netCDF files into the Python script. Each day-in-the-life PACE netCDF file contains an OCI variable (e.g., chlorophyll-a Concentration) and the dimensions: latitude, longitude, 8-bit color, and RGB. Other OCI variables incorporated into the tool, as noted above, include SST, PIC, POC, TSS, bbp_443, aph_443, and adg_443. We had the tool layer user-selected variables on top of an ocean basemap, specifically using "naturalearth_lowres" from geopandas, and clip the variables to the areas of interest using the set_xlim and set_ylim functions, which are part of the matplotlib axes module. We chose the Gulf of Maine between 46.14° N and 36.3° N and 64.69° W and 75.23° W (Figure 2).

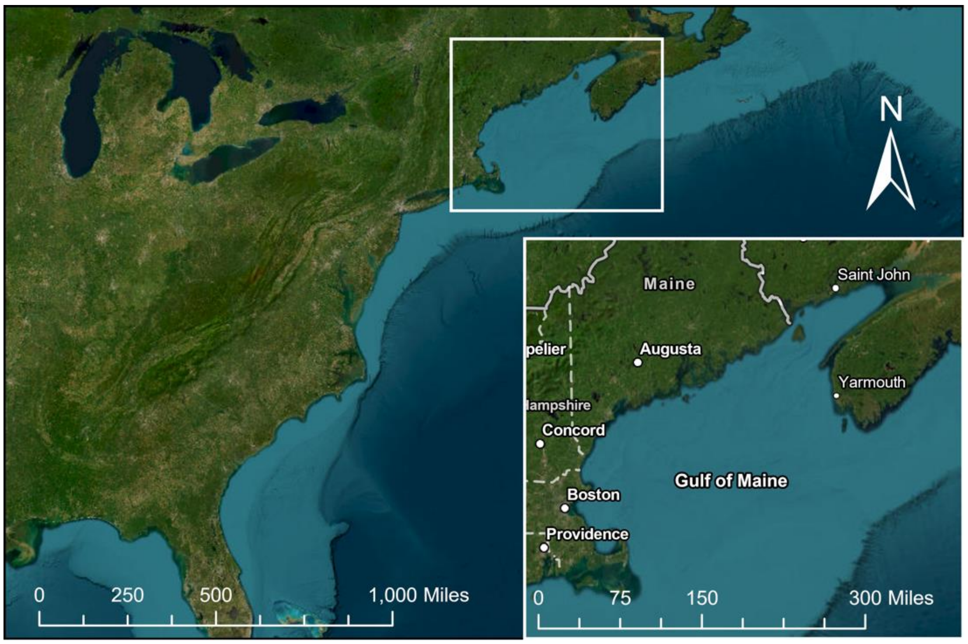

Figure 2. This is a study area map showing world imagery of the East Coast of America with a subset map highlighting the Gulf of Maine. (World Imagery: Earthstar Geographics, ESRI, HERE, Garmin, FAO, NOAA, USGS, EPA, NRCan, Parks Canada).

We used the netCDF4 library to process the netCDF files as well as geopandas and matplotlib libraries to generate visualizations. We reprojected all images to EPSG:3857 for web visualization. We chose a logarithmic scale to display the color palette representing chlorophyll-a concentrations because a logarithmic scale adjusts for relatively low base chlorophyll-a concentrations compared to relatively extreme concentrations during blooms (Figure 3). After downloading, processing, and visualizing, we merged the netCDFs into a single netCDF file using netCDF4 for improving ease of further processing. Code from the NOAA Center for Satellite Applications and Research aided the processing of netCDF files using netCDF4. NetCDFs can be merged along a user-specified dimension, aggregated by time or OCI variable, through the xarray library's "combine_by_coords". Level 3 earth observation files at the same resolution, containing different variables of interest, can be merged. Finally, once the netCDF merger was complete, we employed rioxarray and gdal (gdal.Open and gdal.GetDriverByName) to create GeoTIFF files from the processed images for GIS software capability. NetCDFs can also be saved as a PNG or a JPEG for visualization.
The script's main objective is to automate most of these processes, requiring the user to simply click easy-to-interpret buttons in the GUI to extract the metadata, subset the region of interest, and choose the variables of interest. To accomplish this, we utilized the Python tkinter package to create the GUI. The GUI allows ocean

biogeochemical variables such as chlorophyll-a, PIC, POC, and SST to be selected through a pop-up menu. The tool allows one to derive a subset image for an area of interest by entering the coordinates. In addition, a user can select a specific point on the map and be provided with key statistics for that area, such as chlorophyll-a concentration. Statistics such as mean, maximum, and minimum for an area of interest can also be generated, including for very small areas. The various statistics that the tool produces could particularly benefit water quality and resource managers. Finally, users can enter a threshold value in the GUI, so a variable is only mapped for a certain intensity level, ensuring only levels of concern for a particular variable are mapped. Datasets are typically opened using xarray for further processing, while numpy is vital for generating statistics.

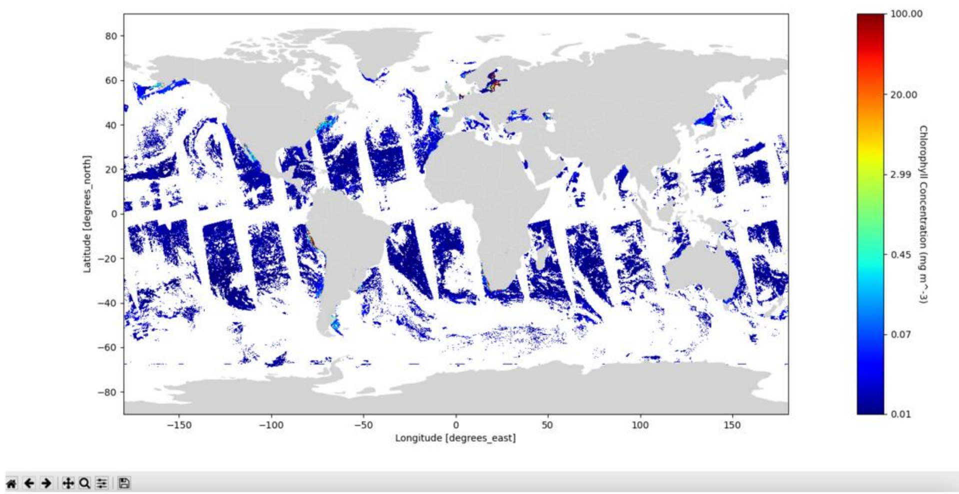

Figure 3. This image of the user interface displays global chlorophyll-a concentrations in milligrams per cubic meter from March 21, 2022 simulated PACE imagery.

4. Results & Discussion

4.1 Analysis of Results

The PACE Viewer visualizes global Level 3 products, converts netCDFs into raster data layers for geospatial analysis, subsets by region, calculates statistics of interest, and subsets surface reflectance values of interest. The visualizations in Figure 3 show a patchy display of chlorophyll-a concentrations because it is visualizing simulated data from March 21, 2022. The visualizations will work best with monthly or annual composite images once PACE is in orbit and collecting science quality data. In addition to visualizations, the PACE Viewer can generate pixel statistics. Statistical analysis can be conducted to obtain a mean, maximum, and minimum value across a small area of water for a given variable, as well as to obtain standard deviation values. In addition to spatial analysis, temporal analysis can also be performed simply by downloading and processing multiple netCDF files across time periods, allowing end users to better understand changes over time. While the simulated PACE data may be limited in terms of dates available, a temporal analysis can still be demonstrated with the help of Aqua MODIS data.

The Level 3 functionalities of the PACE Viewer can be applied to Level 3 products from any sensor, not just PACE. The Jupyter Notebooks can also be used for processing and visualizing Level 3 ocean and atmospheric properties acquired by many sensors, including but not limited to PACE. While there is flexibility in the PACE Viewer, the Level 3 functionalities do not address hyperspectral data volume because Level 3 data comes pre-processed through the OB.DAAC. In contrast to the Level 3 data, Level 2 files require sensor-specific processing, and in this case the PACE Viewer is calibrated specifically for PACE. Level 2 file Remote Sensing Reflectance (Rrs) band selection and subsetting are only available through Jupyter Notebooks without geolocation, but these Level 2 functionalities have not been built into the GUI.

One major limitation of this tool is that it was developed using one day of PACE simulated imagery. As a result, it is unknown whether the Jupyter Notebooks will integrate real PACE imagery in the same way they integrate simulated imagery. While simulated PACE imagery is structured to reflect how the PACE satellite images will be stored, there is still possibility for discrepancies between the two data structures once the satellite launches and data becomes available. Furthermore, the tool is designed to process multiple days', or months', worth of data, but it was developed with a single days' worth of simulated imagery. Due to the limited temporal resolution of our simulated data, as well as the lack of testing with data obtained while in orbit, the PACE Viewer should not be used for in-depth geospatial analysis. Tool availability is an additional limitation to making the PACE Viewer useful to our partners. Prior to software release, the tool will not be available to end users external to NASA. While DEVELOP teams will be able to use the PACE Viewer right away, some of our target audience, such as users who want to familiarize themselves with PACE hyperspectral data prior to launch, will not be able to do so using the PACE Viewer.

4.2 Feasibility Assessment

The PACE Viewer will enable a broader community of users to interact with PACE data because it reduces the time and technical expertise needed in order to visualize and process PACE images. Similar to SeaDAS, a software package from NASA that is commonly used for the processing and analysis of ocean color data, the tool can show information about chlorophyll-a and various OCI parameters on a pixel-by-pixel basis as well as subset the data to regions of interest. The tool's GUI is more user-friendly than SeaDAS, which will help the PACE applications community and future DEVELOP teams interact with PACE data in a time-efficient manner and provide a practical, simpler alternative to SeaDAS. For future DEVELOP teams working on 10-week feasibility studies with PACE data, the tool will reduce the time spent on data processing so that they can focus on data analysis.

Both the PACE Applications Program and DEVELOP intend to engage users with a variety of backgrounds in using PACE data, so access to a simple GUI interface to visualize and handle the data without extensive code or data processing skills is particularly valuable. Affordable technological support in the early detection and monitoring of HABs is important because they pose a threat to public health and economies in coastal communities. The tool was designed with a diverse array of end users in mind, including researchers, policymakers, and community members in coastal communities. As such, some functionalities and aspects of the tool are less useful to some partners and end users than others. The dashboard may be useful to researchers like DEVELOP teams but will likely be less useful to water quality managers and end users seeking to apply PACE data to their decision-making. These end users in the water resource management community will likely benefit more from aggregating statistics by region and mapping chlorophyll-a thresholds with related uncertainty values.

4.3 Future Work

Going forward, the PACE Viewer can be improved by adding more functionalities for processing and visualizing hyperspectral imagery. Refining the user interface would make the tool easier to use for a variety of end users, especially those who are beginners to hyperspectral imagery. The tool was developed pre-launch and now that observed PACE OCI data is publicly available, the tool's capabilities should be tested with observed data and integrated with the OB.DAAC PACE Application Programming Interface (API) for real time updating to streamline data accessibility. Since the Level 2 imagery is geolocated in sections, the ability to "stitch" together or mosaic user selected Level 2 granules would improve tool functionality and ease visualization. Additionally, updating the land mask in the GUI to a higher-resolution global map would improve the detailed land characteristics, specifically in coastal regions of interest. Now that imagery has been released from the PACE satellite in orbit, a time series to visualize daily, monthly, and annual changes would be useful to many end users. The tools to work with Level 2 data in the PACE Viewer are limited, and further development would serve future end users in accessing the full power of PACE's hyperspectral imagery.
In the future, adding analysis capabilities to the PACE Viewer would benefit future DEVELOP teams or varying professional end users. Incorporating spectral signatures of different phytoplankton community compositions could aid in detecting species that frequently occur within a study area of interest. Additional

development of the processing tool could improve analysis by adding regression analysis and trend line features as well as covariance tools to the software for predictive capabilities whenever data is limited in time and space. Water quality managers would benefit from a threshold tool that detects chlorophyll-a concentrations above a user-defined threshold and applies a user-selected uncertainty algorithm to estimate the uncertainty levels of any given chlorophyll-a concentration exceeding the threshold. For example, the tool would be able to tell users that a region of interest is above the threshold of 10 milligrams per cubic meter of chlorophyll-a with a 60% uncertainty margin. This capability would serve water quality managers or public health officials in improving and maintaining optimal water quality for an area of interest. In the future, the PACE Viewer could include simple geospatial analysis capabilities, such as a raster calculator, reclassify tool, or quick processing of user-selected indices. For example, the Normalized Difference Chlorophyll Index (NDCI) is widely used to accurately identify chlorophyll-a for algal bloom identification in freshwater systems (Mishra & Mishra, 2012) so building out the tool with the capacity for users to build and execute expressions would improve the tool's utility.

5. Conclusions

Half a year after the completion of this project, PACE's ocean color data is now valuable to many people for multiple purposes, especially Level 3 mapped data. The GUI tool created through this project enables easy use of PACE's data by a variety of end users that may include water managers, fishermen, public health officials, researchers, boaters, and the public. Coding and sophisticated data analysis skills are not required to access and understand the data once such is in an open access geospatial data viewer, making the data accessible to a wide audience. End users can use the PACE Viewer for their tailored needs, especially for enhancing public safety and health. Inclusive access would help users in avoiding HABs in the water, ensuring swimmers' safety from dangerous pathogens, monitoring ecological health, and highlighting algal bloom conditions that may diminish air quality. To help achieve such objectives, the tool provides the ability to subset regions of interest and derive user queried point statistics, such as for Chlorophyll-a concentrations and other variables linked to bioactivity and overall water conditions. The data complements in situ measurements to provide a more comprehensive image-based water quality visualization. Merging different variables into composite images and converting netCDFs to GeoTIFFs for easier use further simplifies the visualization and interpretation of the data. Finally, analysis of Level 2 data ensures the PACE data viewing tool can provide more sophisticated information for end users who do wish to use it for research purposes, making it an easy to access valuable and straightforward science tool for visualizing highly complex geospatial data. Altogether, the GUI tool can be used to increase the public utility of PACE data and maximizes the public benefit of the mission.

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7. Glossary

API – Application Programming Interface
CZCS – Coastal Zone Color Scanner

Earth observations – Satellites and sensors that collect information about the Earth's physical, chemical, and biological systems over space and time
GUI – graphical user interface; visual environment that uses windows, icons, and menus to carry out commands, such as opening and exporting files. This allows users to perform any action without having to have programming knowledge
HAB – harmful algal bloom
HSI – hyperspectral imaging
MODIS –Moderate Resolution Imaging Spectroradiometer
OB.DAAC - Ocean Biology Distributed Active Archive Center
OCI – Ocean Color Instrument
PACE – Plankton, Aerosol, Cloud, ocean Ecosystem
PIC – particulate inorganic carbon
POC – particulate organic carbon
PyTOAST – Python Top of Atmosphere Simulation Tool
SST – sea surface temperature
TSS – total suspended solid
VIIRS – Visible Infrared Imaging Radiometer Suite

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