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Review



Phytoplankton composition from sPACE: Requirements, opportunities, and challenges

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ABSTRACT

Ocean color satellites have provided a synoptic view of global phytoplankton for over 25 years through near surface measurements of the concentration of chlorophyll *a*. While remote sensing of ocean color has revolutionized our understanding of phytoplankton and their role in the oceanic and freshwater ecosystems, it is important to consider both total phytoplankton biomass and changes in phytoplankton community composition in order to fully understand the dynamics of the aquatic ecosystems. With the upcoming launch of NASA's Plankton, Aerosol, Clouds, ocean Ecosystem (PACE) mission, we will be entering into a new era of global hyperspectral data, and with it, increased capabilities to monitor phytoplankton diversity from space. In this paper, we analyze the needs of the user community, review existing approaches for detecting phytoplankton community composition in situ and from space, and highlight the benefits that the PACE mission will bring. Using this three-pronged approach, we highlight the challenges and gaps to be addressed by the community

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going forward, while offering a vision of what global phytoplankton community composition will look like through the “eyes” of PACE.

1. Background

Phytoplankton are microscopic photosynthetic organisms that inhabit all sunlit waters and represent the first level of the aquatic food web. They play a vital role in the global ecosystem where phytoplankton convert carbon dioxide into carbohydrates and oxygen through the process of photosynthesis. The primary photosynthetic pigment in most phytoplankton species is Chlorophyll *a* (*Chl a*), and its concentration has been commonly used as a proxy for phytoplankton biomass in oceanographic research and monitoring programs for almost 100 years (first chlorophyll measurements collected in 1934 by Harvey (1934)). Ocean color satellites (SeaWiFS, MODIS, VIIRS) have provided continuous global datasets of aquatic *Chl a* since 1997 (O'Reilly et al., 1998), generating insight into spatial and temporal changes in phytoplankton biomass (Behrenfeld et al., 2006; Gregg and Rousseaux, 2014; Gregg et al., 2017; McClain et al., 2022; Siegel et al., 2013). Despite the ubiquity of *Chl a*, taxonomic diversity in phytoplankton is wide-ranging, spanning across eukaryotic and eubacterial domains. This taxonomic diversity underpins vast morphological diversity among phytoplankton (e.g., Beardall et al., 2009), including variation in pigment composition (e.g., Jeffrey et al., 2011), environmental requirements (e.g., for light, nutrients, and temperature), trophic strategies (e.g., Mitra et al., 2016), and in the roles phytoplankton play in aquatic biogeochemistry (e.g., Dutkiewicz et al., 2020).

Knowledge of phytoplankton community composition (PCC) and its spatial and temporal variability is vital for our understanding of the many aspects of aquatic ecosystems, as well as the services those ecosystems provide. It is critical to assess water quality (including harmful algal blooms - HABs) and functioning of the higher trophic levels including fisheries worldwide. Knowledge about PCC can be used to manage and support the aquaculture industry, including to infer optimal site selection and sustainable aquaculture development³ (Anderson et al., 2009, 2019; Johnson et al., 2019; Snyder et al., 2017), to prevent economic losses due to the impact of HABs (Smith and Bernard, 2020; Wolny et al., 2020), or to support monitoring of potential impacts that aquaculture might have on aquatic ecosystems (e.g., eutrophication; Gowen, 1994) or on natural phytoplankton population estimates (Schaeffer et al., 2015; Frieder et al., 2022). Furthermore, to understand the effects of climate variability on aquatic biogeochemistry, the role of the oceans as a sink of anthropogenic carbon, and the various effects of human pressure on water resources, it is imperative that we improve our characterization of the food web's foundation—the phytoplankton community—across the continuum of aquatic ecosystems. Understanding the role that different phytoplankton groups play in the export of carbon, specifically in regard to ballasting, export depths and scales of remineralization (Cram et al., 2018; Guidi et al., 2015), is crucial to our understanding of contemporary and future oceans. Additionally, PCC can enhance the parameterization of end-to-end ecosystem models designed to simulate biogeochemical, ecological, fishery, management, and socio-economic processes within marine ecosystems (Turner et al., 2021; Caracappa et al., 2022). There is also much debate as to the future of the ocean's role in absorbing anthropogenic carbon, as well as the role that biology, specifically different phytoplankton types (e.g., coccolithophores), will play in different climate scenarios. Earth System Models (ESMs) are used to explore, understand, and forecast the role of oceans

in the global carbon budget, including the role of oceans in future climate scenarios (IPCC,⁴ CMIP,⁵ etc). For most ESMs, understanding the role that biology will have in future carbon sequestration relies on our understanding of oceanic PCC, in part due to the relationship between phytoplankton size and sinking rate (i.e., Guidi et al., 2015; Henson et al., 2022).

Whether categorized by taxa, function, or size, the particular mix of phytoplankton detectable by a given in situ sampling is discernably variable across regions, seasons, and conditions (Margalef, 1958); underscoring a strong need for studying what we collectively call PCC through ocean remote sensing. During the past 25 years, numerous studies have shown that space-based instruments can reach beyond estimates of total phytoplankton biomass and quantify certain aspects of PCC (e.g., Bracher et al., 2017; IOCCG, 2014). Such insights on PCC have mostly relied on *Chl a* or multi-band phytoplankton absorption spectra (see Mouw et al., 2017 and references within), information that inherently creates large uncertainties from the inverse problem standpoint, i. e., solving for various components of PCC from a limited number of observations (Defoin-Platel and Chami, 2007; Sydor et al., 2004).

As the needs of aquatic research surpassed the capabilities of current ocean color satellites, the community responded with various instrument concepts, materialized in specific calls by the National Research Council Earth Sciences Decadal Survey (National Research Council 2007) and National Aeronautics and Space Administration (NASA, NASA, 2010) among others (McClain et al., 2022; Muller-Karger et al., 2018a, 2018b). The need to resolve PCCs into ecological and biogeochemical relevant taxonomic components is one of the main underlying motivations for NASA's Plankton, Aerosol, Cloud, ocean Ecology (PACE) mission (Werdell et al., 2019). The PACE mission, to be launched no earlier than January 2024, will respond to community needs for a highly calibrated, ocean-focused hyperspectral radiometer combined with multi-angle polarimeters that satisfy multiple scientific needs, including better resolution of phytoplankton diversity (McClain et al., 2022; Werdell et al., 2019).

PACE is the first global ocean and atmosphere hyperspectral mission (Fig. 1). PACE will collect ocean color imagery over a period of one-to-two days from a sun-synchronous polar orbit at 676.5 km (inclination of 98°), with an ascending equatorial crossing time at 1 pm. The spacecraft will host three instruments: a hyperspectral imaging radiometer named OCI (for Ocean Color Instrument, developed by NASA Goddard Space Flight Center (GSFC)) and two polarimeters, named SPEXone (for Spectro-polarimeter for Planetary Exploration, developed by collaborators at Space Research Organization of the Netherlands, Hasekamp et al., 2019) and HARP2 (for Hyper Angular Research Polarimeter, developed by the Earth and Space Institute of the University of Maryland Baltimore County, Martins et al., 2002).

The OCI has hyperspectral capabilities that continuously span from the ultraviolet to near-infrared, with nominal spectral steps of 2.5 nm and average bandwidths of ~5 nm across a spectral range of 340–890 nm. The spectral steps decrease to 1.25 nm (with the same ~5 nm bandwidths) in the spectral regions of chlorophyll *a* fluorescence and oxygen A and B band absorption, resulting in roughly 230 total wavelengths of information (Table 1). Additional bands in the near- and shortwave-infrared support heritage atmospheric products and will also bring improvements to atmospheric correction in optically complex

³ ShellGIS, an application developed to predict growth of numerous aquaculture species using remote sensing inputs, <http://www.shellgis.com/examples/TFWMidMaine.html>. ShellGIS team is part of the PACE early adopter program.

⁴ IPCC stands for Intergovernmental Panel on Climate Change, <https://www.ipcc.ch/>

⁵ CMIP stands for World Climate Research Programme Coupled Model Intercomparison Project, <https://www.wcrp-climate.org/wgcm-cmip>

waters over large freshwater and coastal estuaries (Frouin et al., 2019; Ibrahim et al., 2018). The spatial resolution of OCI imagery will be $\sim 1 \text{ km}^2$ at nadir with a swath width of 2663 km (supporting global coverage once every two days, given geometry constraints applied to atmospheric correction). In practice, pixels sizes at the center of the swath will be $\sim 1.1 \text{ km}^2$ given OCI's 20-deg tilt. Due to the specific optical design, time-delayed integration, lunar, spectral calibrations, and tilt mechanism OCI will produce high-quality data over a very high dynamic range of radiances from highly absorbing waters to ecosystems rich in inorganics.

The role of the two PACE polarimeters, SPEXone and HARP2 (Table 1), is primarily to improve our understanding of cloud and atmospheric aerosol properties (Chowdhary et al., 2019; Remer et al., 2019; Sayer et al., 2022). Improved characterization of the atmospheric properties will enhance the retrieval of ocean surface reflectances, and there is hope that information about the microphysical properties of particles from polarimeters may also prove useful for phytoplankton studies (Jamet et al., 2019). SPEXone is a hyperspectral polarimeter (385–770 nm, 5 nm steps), measuring light at 5 viewing angles, collecting information in narrow 100 km swath at 2.5 km^2 . HARP2 is a multispectral (nominal 441, 549, 665, 866 nm), hyper-angular instrument, with a wide swath that matches OCI and a ground sampling distance of 3 km^2 .

By identifying the needs, challenges, and future of estimating PCC from space using hyperspectral instruments, this paper contributes to a decades-long community effort to improve remotely-sensed phytoplankton datasets (e.g., Bracher et al., 2017; Bracher et al., 2022; De Moraes Rudorff and Kampel, 2012; IOCCG, 2014; Mouw et al., 2017; Nair et al., 2008). This paper, thanks to the large community of future users of PACE data, is a review of where we, as a scientific community, are, and where other we, a larger community of scientific and non-scientific users of PACE data, could go in the future. After evaluating user community needs (Section 2) and identifying several applications

Table 1

Instrument specifications for OCI, HARP2 and SPEXone (modified from Table 2 from Werdell et al. (2019)).

	OCI	HARP2	SPEXone
UV-NIR range (bandwidth)	Continuous from 340 to 890 nm* in 2.5-nm steps (5)	441 (16), 549 (10), 665 (11), and 866 (40) nm (nominal)	Continuous from 385 to 770 nm in 2-4 nm steps
SWIR channels (bandwidth)	940 (45), 1038 (75), 1250 (30), 1378 (15), 1615 (75), 2130 (50) and 2260 (75) nm	None	None
Polarized bands	None	All	Continuous from 385 to 770 nm in 15-45 nm steps
Number of viewing angles	One, with fore-aft instrument tilt of $\pm 20^\circ$ to avoid sun glint	10 for 440, 550 and 870 nm and 60 for 670 nm (spaced over 114°)	5 (-57° , -20° , 0° , 20° , 57°)
Swath width	$\pm 56.6^\circ$ (2663 km at 20° tilt)	$\pm 47^\circ$ (1556 km at nadir)	$\pm 4^\circ$ (100 km at nadir)
Global coverage	1–2+ days	2 days	~ 30 days
Ground pixel	1 km at nadir	3 km	2.5 km
Institution	GSFC	UMBC	SRON/Airbus

that will benefit from improved PCC estimates (Section 3), we outline current approaches to identifying PCC using in situ data, a critical step in developing PCC retrieval algorithms (Section 4). We then describe the existing approaches that PACE will build on to derive PCC from space (Section 5). Finally, we conclude the paper by identifying some of the existing challenges and gaps, address what PCC will mean in the era of PACE, and discuss how PACE will allow the community to advance understanding of the role that phytoplankton diversity plays on earth and how it is likely to change in the future. A description of all the



Fig. 1. Artist's rendition of NASA's Plankton, Aerosol, Cloud, ocean Ecosystem satellite flying over cloud-covered Earth's Ocean. The Ocean Color Instrument is visible on the front of the platform, while two polarimeters (located on the bottom side of the platform) are not visible from this view. Credit: NASA Scientific Visualization Studio.

abbreviations found in this paper can be found in Table 2.

2. Community needs

There is a consensus across the ocean color user community that better resolution of phytoplankton diversity from space will improve our knowledge and understanding of marine ecosystems (e.g., Kavanaugh et al., 2021), ocean health (e.g., Smith and Bernard, 2020), shifts in communities across freshwaters (Rasconi et al., 2015; Verbeek et al., 2018), and the ocean's effects on the global climate (IPCC, 2019).

Table 2

Acronyms and symbols used in the text.

CDOM	Colored Dissolved Organic Matter
CDR	Carbon Dioxide Removal
CHEMTAX	CHEMical TAXonomy
CHIME3	Copernicus Hyperspectral Imaging Mission for the Environment
<i>Chl a</i>	Chlorophyll a
CMIP	Climate Research Programme Coupled Model Intercomparison Project
CoP	Community of Practice
DNA	Deoxyribonucleic Acid
EOSDIS	NASA's Earth Observing System Data and Information System
EOV	Essential Ocean Variable
ESM	Earth System Models
FAIR	Findable, Accessible, Interoperable and Reusable
FCM	Flow cytometry
GIOP	Generalized IOP algorithm
GLIMR	Geosynchronous Littoral Imaging and Monitoring Radiometer
GSFC	Goddard Space Flight Center
HABs	Harmful Algal Blooms
HARP2	Hyper Angular Research Polarimeter
HICO	Hyperspectral Imager for the Coastal Ocean
HNLC	High Nutrient Low Chlorophyll
HPLC	High performance liquid chromatography
IFCB	Imaging FlowCytobot
IOCCG	International Ocean-Color Coordinating Group
IPCC	Intergovernmental Panel on Climate Change
GCOM-C	Global Change Observation Mission – Climate satellite
JAXA	Japan Aerospace Exploration Agency
LEO	Low Earth Orbit
MAAs	Mycosporine-like Amino Acids
MERIS	Medium Resolution Imaging Spectrometer
MODIS	Moderate Resolution Imaging Spectroradiometer
NASA	National Aeronautics and Space Administration
NASA	NASA bio-Optical Marine Algorithm Dataset
NOMAD	
NIR	Near-Infrared
OB.DAAC	NASA's Ocean Biology Distributed Active Archive Center
OCI	Ocean Color Instrument
PACE	NASA's Plankton, Aerosol, Cloud, ocean Ecology
PAR	Photosynthetically Active Radiation
PCC	Phytoplankton Community Composition
PhytoDOAS	Extension of the Differential Optical Absorption Spectroscopy (DOAS, a method for detection of atmospheric trace gases), developed for remote identification of oceanic phytoplankton groups
POLDER	Polarization and Directionality of the Earth's Reflectance
PSC	Phytoplankton Size Class
$R_{rs}(\lambda)$	Remote Sensing Reflectance
SBG	Surface Biology and Geology mission
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
SeaBASS	SeaWiFS Bio-optical Archive and Storage System
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
SMD	Science Mission Directorate
SPEXone	Spectro-polarimeter for Planetary Exploration
SPM	Suspended Particulate Matter
SRON	Netherlands Institute for Space Research
SST	Sea Surface Temperature
SWIR	Short-wave Infrared
TOA	Top-of-atmosphere
UMBC	University of Maryland, Baltimore County
UV	Ultraviolet
UVP	Underwater Vision Profiler
VIIRS	Visible Infrared Imaging Radiometer Suite

However, the required resolution (taxonomic or otherwise) of phytoplankton diversity varies widely within the user community.

A request for input was directed to the PACE Community of Practice⁶ (CoP) to identify PCC taxonomic resolution needs. The PACE CoP is a diverse group of users composed of modelers and observational researchers, academic and government scientists, local to international decision-makers, and industry professionals within various sectors, including air quality and atmospheric, terrestrial, and marine/ocean applications (Fig. 2).

Responses indicate that data consumers most need resolution down to a few traditionally recognized “taxonomic groups” (e.g., diatoms, dinoflagellates), followed by plankton pigments, and then groups defined by functionality (Fig. 3). A large portion of questionnaire respondents would be satisfied with “whatever taxonomic grouping is available” beyond *Chl a* alone. Approximately 25% of the users prioritized species-level resolution, with 10% of users relying on PACE to resolve specific species (such as the HAB forming dinoflagellate *Alexandrium*). While this short questionnaire provides preliminary insights into the needs of the PACE user community, it does not provide information on how these needs relate to each subcommunity.

The above-mentioned needs are likely driven by the spatiotemporal constraints of each respondent's focus, ranging from local to global spatial scales, and from daily, monthly, interannual, and decadal scales. In a similar way, user-specific capabilities to access and manipulate the data may also drive the differences in needs across the PACE CoP.

3. Applications

A deeper look into the type of applications that use data on phytoplankton diversity (and would benefit from remote sensing data on PCC) highlights the complexities that come with defining PCC and the associated temporal, spatial, and phytoplankton diversity resolution. Hereafter, we present some examples of applications that range from local to global and the level of phytoplankton diversity resolution associated with them.

Monitoring of local and regional water quality, including forecasting HABs, is a critical societal application that requires “local” knowledge and data (e.g., Lekki et al., 2019; Smith and Bernard, 2020). Algal blooms occur in coastal and freshwater systems worldwide and include a variety of potentially harmful species that can impact wildlife, pet, livestock, and human health (Lundholm et al., 2009; Michalak, 2016). To address the need for products capable of detecting, quantifying, characterizing, classifying, and being used in forecasting applications will require finely tuned algorithms for specific HAB (or any other) algal type (Schaeffer et al., 2015; IOCCG, 2021), resulting in products at an appropriate temporal and spatial resolution to capture the transient nature of these events. PACE, similarly to the majority of heritage ocean color missions, will have adequate temporal resolution, and some limitations with regard to the spatial resolution required to detect developing HABs in water bodies smaller than PACE resolving capabilities. Therefore, synergies and cross-product generation with other missions with smaller spatial resolution (< 1 km) but less optimal temporal resolution (e.g., NASA's upcoming Surface Biology and Geology (SBG⁷), the European Space Agency's Copernicus Hyperspectral Imaging Mission for the Environment (CHIME⁸), could be combined to alleviate this weakness. Lastly, low latency (i.e., the time between data collection and availability) is also critical for timely public-safety decisions in response to HABs, which requires near-real time processing of the PCC data product.

⁶ https://pace.oceansciences.org/app_community.htm

⁷ SBG stands for Surface Biology and Geology - <https://sbg.jpl.nasa.gov/>

⁸ CHIME stands for the Copernicus Hyperspectral Imaging Mission for the Environment - https://www.esa.int/Applications/Observing_the_Earth/Copernicus/Going_hyperspectral_for_CHIME

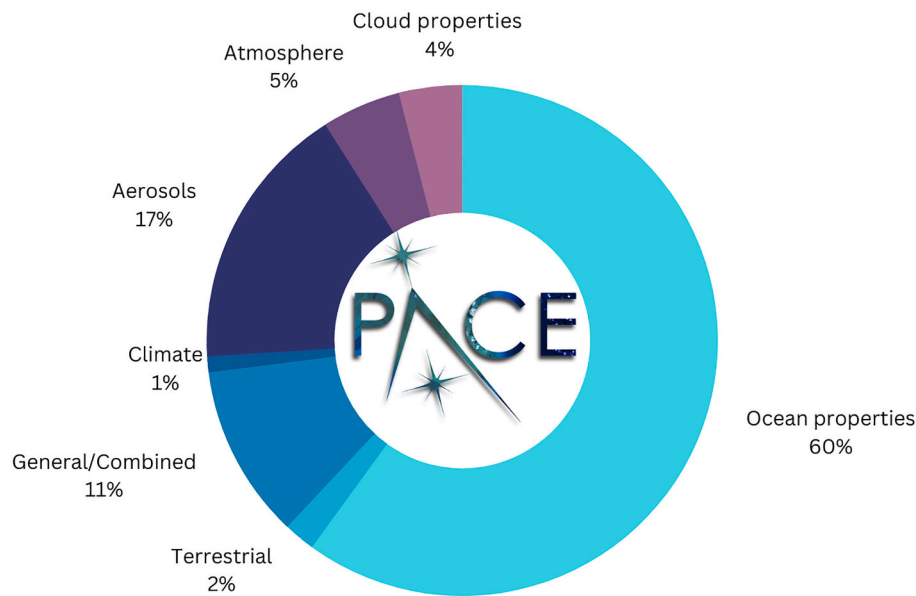


Fig. 2. Self-identified research focus areas grouped into thematic areas, as dictated by PACE Community of Practice members (as of October 2023, 402 members). As Community of Practice grows, their distribution across the thematic areas might change.

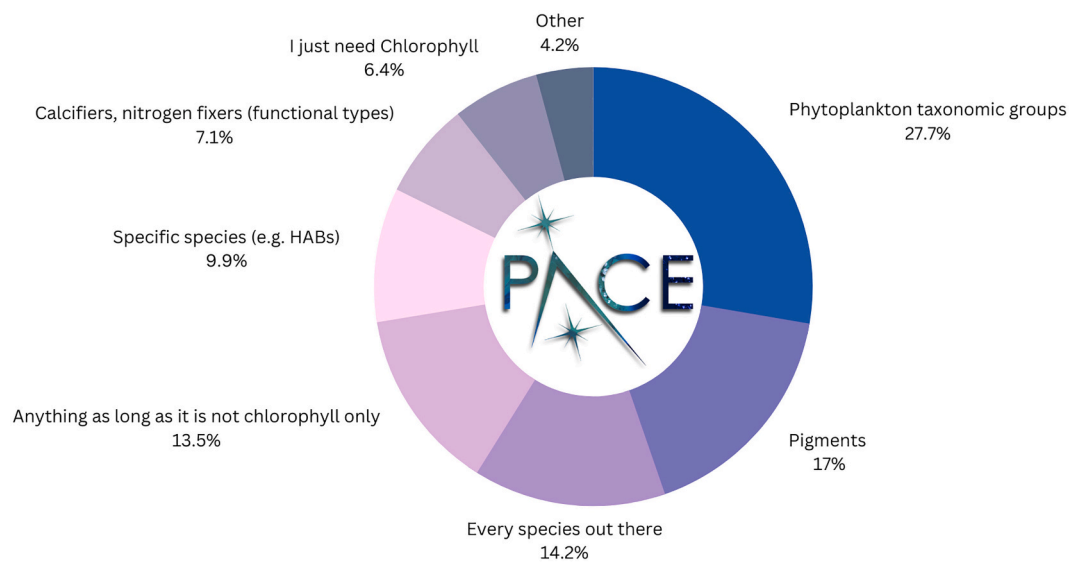


Fig. 3. Needs of the PACE Community of Practice, based on the responses collected from a questionnaire with multiple choice predetermined answers with opportunity to write in an answer (those are grouped and depicted in figure as ‘other’).

The fisheries industry has also increasingly integrated phytoplankton data into management activities for the purpose of: (1) fish stock assessment, (2) harvesting by identifying suitable fishing zones, and (3) fisheries management (Forget et al., 2009). The appropriate PCC definition for fisheries applications could range from single species (e.g., HABs) to more functional or taxonomic information to support fish stock assessment and management to promote best fishing practices.⁹

At the global scale, satellite-derived PCC products can also be used to improve climate applications and research (Fig. 4). Using existing satellite observations of total phytoplankton biomass, natural climate

variability, such as El Niño, has been shown to directly affect phytoplankton composition, with changes trickling up the food web to the higher trophic levels (e.g., due to the change in nutrient dynamics, Fisher et al., 2015; Franz et al., 2021; McCabe et al., 2016; McKibben et al., 2017; Racault et al., 2017; Rousseaux and Gregg, 2012). In a similar way, PCC products can help indicate effects of the anthropogenic driven changes in aquatic ecosystems. This has been demonstrated using long term in situ datasets (e.g., Rivero-Calle et al., 2015) and models (Anderson et al., 2021; Cael et al., 2022; Dutkiewicz et al., 2013). While prior analysis suggested natural variability compounded climate trends in current chlorophyll ocean color records (Henson et al., 2010), recent research is suggesting that ocean color itself (i.e., remote sensing reflectances) is demonstrating significant, global climate trends in 20 yearlong records (Cael et al., 2023a). PCC records from remote sensing may assist with understanding observed trends and interpreting those trends in reference to the whole ecosystem structure and role that

⁹ pezCA, an application developed by the Federación Costarricense de Pesca (FECOP) in Costa Rica, that combines policy and real time satellite based products to identify potentially favorable fishing areas, <https://pezca.org/>. pezCA team is part of the PACE early adopter program.

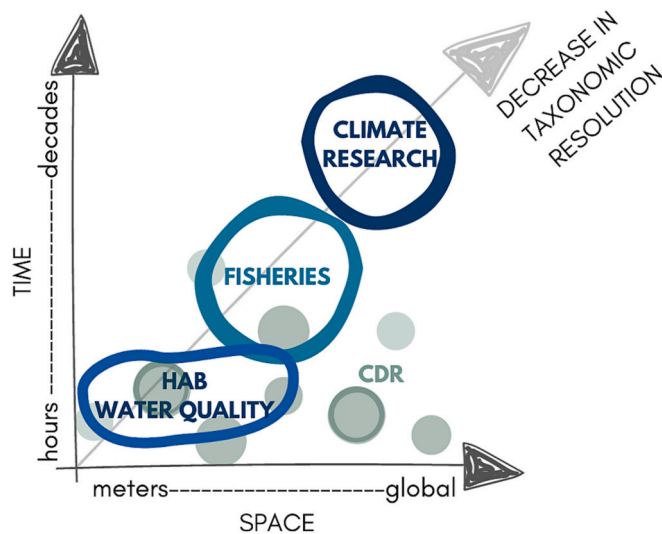


Fig. 4. PACE will provide data to answer scientific questions about phytoplankton community composition (PCC) at local to global scales. The user community, already actively engaged in developing frameworks and pipelines that use PACE data or support mission objectives, comes from different sectors, whose scientific objectives are sometimes distinct and sometimes overlapping. This illustration provides example research interests at different scales and from different sectors. CDR stands for Carbon Dioxide Removal.

oceanic ecosystem plays in the global carbon cycle. On more local scales, in polar regions, a rapidly shifting landscape (due to the unprecedented ice loss) is modifying the ecosystems, and composition and seasonality of phytoplankton (Eayrs et al., 2021; Meier et al., 2021; Nardelli et al., 2022). Understanding of such close coupling of PCC, sea ice, polar food webs, and carbon flux (Flexas et al., 2022; Neeley et al., 2018; Schofield et al., 2018) will benefit greatly from continuous monitoring of PCCs from space.

Numerical models, including simple inverse and food web models as well as more complex ESMs, provide an opportunity to integrate satellite PCC data as well as in situ data in a global context (Dinauer et al., 2022; IOCCG, 2020; Siegel et al., 2023). However, data assimilation is often limited by the availability of data with appropriate units and levels of detail, such as PCC categories, and quantified uncertainties. As detailed by Le Quéré et al. (2010), not only is phytoplankton biomass (usually resolved into functional, taxonomical, and/or size groups) important for modeling applications, but so are parameters such as growth rates and export rates. Moreover, sufficient continuity of measurement (including the various seasons, see also Dutkiewicz et al. (2020)) at the global scale is required to study the feedbacks between climate and ocean biogeochemistry. Assimilation of data on PCC to improve those models will decrease uncertainty in the role of the ocean in the global carbon budget (Ciavatta et al., 2018; Skákala et al., 2018) and decrease the societal and monetary impact of such uncertainties e.g., Bontempi et al. submitted. Importantly, reported uncertainties are crucial for improving models through parametrization or data assimilation, or informing ocean color science. These uncertainties will also enable better understanding of regional, temporal bias, and instrument-based bias, especially in merged products originating from multiple instruments (Dutkiewicz et al., 2020; Gregg et al., 2017).

Lastly, society will have to continue to respond to the growing challenges associated with climate change. It is becoming increasingly evident that controlling future Earth warming to well below +2.0 °C (preferably within +1.5 °C), as is the aim of the McCabe et al., 2016 Paris Agreement, will require deployment of large-scale technologies to reduce carbon dioxide emissions (Fuss et al., 2014; IPCC, 2021). Several ocean-based Carbon Dioxide Removal (CDR) methods have been proposed to curb on-going global warming (GESAMP, 2019; National

Academies of Sciences, 2022¹⁰). Some of the CDR approaches that rely on the ocean, such as ocean iron fertilization or seaweed cultivation, can dramatically alter upper ocean ecosystems and phytoplankton communities (National Academies of Sciences, 2022). An important part of the monitoring, reporting, and verification process of CDR will be understanding the impact of these technologies on the ocean, including the assessment of effects on PCC, net primary production, and carbon export. Remote sensing observations, such as those from PACE, will also be key to quantifying the success of ocean CDR strategies, monitoring their effects on ocean ecosystems (e.g., potential taxonomic shifts in PCC leading to harmful algal blooms), and providing data needed for ESMs to improve our understanding of the role these perturbations have on ocean ecosystems and the global carbon cycle.

4. In situ methods

Many methods exist to quantify phytoplankton composition for mixed natural communities. While no individual method captures the vast diversity of marine phytoplankton across multiple dimensions (taxonomy, size, morphology, genetics, metabolism, etc.), many of these methods provide specific information that is useful to describe PCC across observations and support future PCC models. Some methods (HPLC derived pigments) have been used extensively to develop and validate satellite remote sensing approaches for PCC. Other methods (imaging-in-flow cytometry, DNA metabarcoding) offer globally distributed datasets with high taxonomic resolution that have great potential for future PACE PCC applications. Here, we review the general approaches for many common methods of phytoplankton observation and summarize their notable strengths and weaknesses, particularly with respect to remote sensing approaches (Table 3).

4.1. Cell counting approaches

4.1.1. Light microscopy

Microscopy-based phytoplankton enumeration and biovolume calculation are a common approach for development and validation of ocean color PCC algorithms, especially for HAB detection (Pan et al., 2011; Soto et al., 2015; Wolny et al., 2020). In combination with cell volume to carbon models (e.g., Menden-Deuer and Lessard, 2000; Worden et al., 2004), this method offers a crude route to phytoplankton carbon biomass. Standard compound and inverted microscopes are commonly used for the visualization of phytoplankton communities from water samples, offering taxonomic classification for nano- to micro- size ranges (>3–5 μm) in live or preserved samples (Karlson et al., 2010). The light microscopy methods used vary with size and concentration of phytoplankton within samples and on the accuracy and taxonomic resolution needed when determining PCC. A small volume of sample (1 ml or less) is only suitable for counting nano- and micro-phytoplankton (>2 μm) samples with a high concentration of cells (e.g., >10⁵ or 10⁶ cells L⁻¹, Godhe et al., 2007; LeGresley and McDermott, 2010; McAlice, 1971). However, when cells are in low concentrations or samples represent a more diverse community structure, a greater sample volume (<25 mL) is needed to adequately capture both small-sized and numerous cells, as well as large-sized and rare cells (Elder and Elbrächter, 2010; Haas and Marshall, 1989).

There are notable limitations to microscopic approaches. Due to the small volume of material examined for some samples, certain taxa may be over- or under-represented. Settling chamber approaches that allow for larger sampling volume and better optical resolution, resulting in a larger phytoplankton size range, are time-demanding (hours/days) in comparison to the small volume approach (minutes, Elder and Elbrächter, 2010). Uncertainties in these methods can be highly

¹⁰ <https://www.nationalacademies.org/our-work/a-researchstrategy-for-ocean-carbon-dioxide-removal-and-sequestration>

Table 3

Comparison of different methods, capabilities, and their connection to expected PACE products (from perspective of algorithm development and validation).

Method	Volume sampled (approx.)	Size range detected (approx.)	Taxonomic resolution	What is actually measured?	PACE-relevant examples
Light microscopy	1–200 mL	10–200 µm (nominal)	To species level	Cell concentrations and/or biovolume (can estimate cellular carbon)	Brewin et al. (2011a); Soto et al. (2015); Wolny et al. (2020)
HPLC pigments	1–10 L	>0.3 µm (nominal); 0.7 µm for non-combusted GF/F)	Group level	Pigment concentrations	Bracher et al. (2015); Chase et al. (2017); Kramer et al. (2022); Sun et al. (2023); Uitz et al. (2015)
Flow cytometry	0.1–2 mL	0.2–50 µm (instrument and volume dependent)	<i>Prochlorococcus</i> , <i>Synechococcus</i> , pico- and nano-eukaryotes	Cell concentrations and optical properties (can estimate cellular carbon)	Lange et al. (2020), Kramer et al. (2020)
Imaging-in-flow cytometry	2–5 mL	6–150 µm (nominal)	To species level	Cell concentrations + biovolumes (can estimate cellular carbon)	Chase et al. (2022)
DNA metabarcoding	0.5–10 L	>0.2 µm (filter dependent, nominal)	To species level	Relative sequence abundances and/or barcode gene concentrations	Catlett et al. (2021)

variable, depending on the optical material (LeGresley and McDermott, 2010), fixatives (modifying cells sizes and internal structure), enumeration method, sample volume, and assumptions used to determine biovolume and resulting carbon content (Vuorio et al., 2007; Willén, 1976). However, regardless of the approach used, the greatest limiting factors (and additional sources of uncertainty) are analyst skill level, their experience, and time required for sample analysis (see Clayton et al., 2022 and references within).

4.1.2. Flow cytometry

Flow cytometry (FCM) can enumerate particles and plankton from the size of viruses to cells >50 µm, depending on the instrument used and its configuration, and the whole size spectrum can be captured when combined with complementary methods (microscopy, imaging in-flow cytometry, e.g., Chase et al., 2020; Haëntjens et al., 2022). Recent evolution in FCM technology can also provide continuous or near-continuous monitoring of phytoplankton community dynamics and structure, and the support for other ecological studies (e.g., Hunter-Cevera et al., 2021; Swalwell et al., 2011). FCM delivers cells single-file in sheath fluid past an excitation laser(s) and a set of optical detectors, allowing investigators to identify specific groups of plankton based on their fluorescence (given selected excitation wavelengths) and directional scattering properties. Additionally, some flow cytometry instruments have capability to sort different cell types (based on their fluorescence and scattering properties) into separate streams, allowing for more detailed analysis (e.g., phytoplankton group specific carbon content, Graff et al., 2012; Casey et al., 2013). Samples can be run “live” or preserved (Lepesteur et al., 1993). Published relationships can then be used to convert cell size (in µm) to cell biovolume (e.g., Calvo-Díaz and Morán, 2006) and carbon (e.g., Menden-Deuer and Lessard, 2000; Worden et al., 2004). Fluorescence emission from the excitation of pigments can be used to distinguish specific phytoplankton populations for some groups, such as the pico-sized cyanobacteria *Synechococcus*, which produces an orange fluorescence signal when the phycoerythrin in the cell is excited by a blue laser, distinguishing them from other small cells (Olson et al., 1988). Fluorescent dyes may also be used to enumerate different groups of cells without specific marker pigments (Rose et al., 2004).

Uncertainty in PCC data from FCM can come from both the sample collection and data analysis. Previous studies focusing on microscopy have demonstrated that fixatives can impact the autofluorescence signal or cause cell loss and cell shrinkage by phytoplankton cells if samples are stored for long periods of time, e.g., >1 month (Marie et al., 2014; Sato et al., 2006; Vaulot et al., 1989). The instrument calibration method determines the model used to derive cell size from fluorescence or scattering, usually relying on standardized set of spherical beads with or

without specific fluorophores. Uncertainties also arise during data analysis when discrete populations of cells are separated (sometimes subjectively by operator) based on fluorescence and scattering parameters. Prefiltering usually removes issues due to the clogging by larger, chain organisms and can define the upper size range for a given analysis. Nevertheless, FCM is an effective approach that can provide enumeration of pico and nano-sized cells, which usually dominate the biomass in open ocean phytoplankton communities, novel datasets that support development of PCC algorithms (e.g., Lange et al., 2020; Kramer et al., 2020; Thyssen et al., 2015).

4.1.3. Imaging-in-flow cytometry

Imaging-in-flow instruments have revolutionized collection and analysis of aquatic samples for the qualification and quantification of PCC. These approaches combine flow cytometric enumeration with the digital photography of particles that can be used for taxonomic identification. A number of different imaging-in-flow instruments, such as the Imaging Flow Cytobot (IFCB; Olson and Sosik, 2007), Underwater Vision Profiler (UVP, Picheral et al., 2010), and FlowCAM (Sieracki et al., 1998), have been developed over the last two decades and capture different regions of the size spectrum (Lombard et al., 2019). Unlike standard microscopy, these instruments allow for automated, rapid collection of plankton and particle images over high spatial and temporal resolution that can be classified and enumerated (sometimes iteratively) after collection using image recognition by machine learning.

An imaging in-flow system typically contains an objective, an excitation laser, and fluorescence detectors to detect *Chl a* fluorescence and light scatter. A water sample is drawn through a flow cell and past the optical package, where particles that are excited by the laser get magnified by the objective (like a microscope) and imaged by a color or monochrome camera. The images are interpreted based on morphological characteristics and/or size dimensions that may be used by a machine learning classifier or manually attributed to specific types of particles, plankton, or phytoplankton. As with every method, there are challenges that must be considered. Imaging-in-flow systems typically measure the larger range of phytoplankton (e.g., > ~6 µm for the IFCB). The large number of images that are collected creates challenges regarding the time needed to complete automated and manual classification, and in the interpretation and sharing of results (Durden et al., 2017; Kerr et al., 2020). Advances in machine learning techniques and other automated approaches (Orenstein et al., 2022; Sosik et al., 2020), in particular deep learning such as convolutional neural networks, will increase the accuracy of automated classifications and reduce the analysis time, thereby increasing throughput of PCC data. The scientific and environmental monitoring communities using these methods are

coming together to overcome these challenges not only for image post-processing, but also dataset creation and taxonomic training augmentation (Clayton et al., 2022; Neeley et al., 2021). Overall, imaging-inflow methods present great potential for describing PCC in situ, particularly for PACE applications, given the relative ease of sampling and high taxonomic resolution.

4.2. Indirect approaches

4.2.1. HPLC phytoplankton pigments

High performance liquid chromatography (HPLC) allows for the direct quantification of a number of different phytoplankton pigments. HPLC pigments are currently one of the most widespread approaches for characterizing PCC in ocean color studies: samples have been collected throughout the global ocean, at time series observatories and along transect cruises, across depths and over seasons (e.g., Kramer and Siegel, 2019; Uitz et al., 2006). HPLC methods for quantification of pigment concentrations have also been highly standardized, with successive quality control efforts to ensure consistency between measurements (Hooker et al., 2012; van Heukelem and Hooker, 2011).

Pigment-based taxonomy is fairly low resolution and depends heavily on the HPLC pigment library used to determine PCC (e.g., Catlett and Siegel, 2018). Existing methods to characterize PCC from HPLC pigments typically rely on biomarker pigments to separate phytoplankton groups based on broad taxonomic association (i.e., diatoms with fucoxanthin, dinoflagellates with peridinin) or size classes. Any pigment-based PCC method has to make necessary assumptions, as most pigments are shared between phytoplankton groups and are not unambiguous biomarkers (Jeffrey et al., 2011 and references therein). PCC methods using HPLC pigments are further complicated by environmental and physiological variations occurring on a range of temporal scales that impact pigment production and intracellular concentration (e.g., Catlett et al., 2023; Dierssen et al., 2015; Henriksen et al., 2002; Neeley et al., 2022; Zapata et al., 2004). Given these variations in pigment concentration and composition, statistical methods that make assumptions about constant relationships between taxa abundances and pigment ratios as well as neglecting co-linearity among pigments must be used cautiously for evaluating PCC (e.g., CHEMTAX; Mackey et al., 1996). Evaluation of such variability, by combining HPLC and another independent metric of pigment packaging, could facilitate development of better models that can be used for remote sensing.

Phytoplankton pigment light absorption directly impacts the shape and magnitude of remote sensing reflectance spectra; thus, HPLC pigments are an effective measurement for development and validation of ocean color algorithms (e.g., Chase et al., 2017; Kramer et al., 2022; Torrecilla et al., 2011; Uitz et al., 2015). Studies that compare HPLC pigments with other, higher-resolution taxonomic approaches have variable success, depending on the ecosystem and the taxonomic resolution of the comparison (Chase et al., 2022; Havskum et al., 2004; Lin et al., 2019; Pan et al., 2011). More comparisons between HPLC pigments and other methods using larger datasets will allow for better constraint of pigment-based PCC, and thus more accurate ocean color algorithms using PACE data.

4.2.2. DNA metabarcoding

Numerous molecular approaches are available to quantify phytoplankton diversity, population dynamics, and PCC (Johnson and Martiny, 2015). DNA meta-barcoding is now one of the most widely used methods to provide a holistic view of PCC including diverse members of the phytoplankton community. DNA meta-barcoding refers to targeted amplicon sequencing of highly conserved, hypervariable “barcode” genes. These data are usually compositional (i.e., estimate proportions rather than concentrations or counts), which complicates analysis and interpretation of PCC (Aitchison, 1982; Gloor et al., 2017). However in last decade some exciting approaches, such as the work by Lin et al. (2019) where they used the internal standards to get quantitative

estimation of DNA abundance, have been developed to remove this constraint (also see Satinsky et al., 2013 and Pierella Karlusich et al., 2022).

The taxonomic resolution of DNA meta-barcoding varies from division- to species-level depending on a number of factors including the analysis workflow or the specific Amplicon Sequence Variants (ASV). Uncertainty in relative sequence abundances is introduced by both wet lab and bioinformatic procedures and is difficult to quantify (Catlett et al., 2020; Yeh et al., 2021). In general, nucleic acid sequencing data are generated through a series of complex biochemical reactions that make it difficult to evaluate and constrain analytical uncertainty. Consistent use of positive and negative controls to ensure reproducibility in sequence analysis has only recently become common practice (Bradley et al., 2016; Parada et al., 2016) but is still omitted by many investigators. Positive controls should be replicates of environmental samples or mock communities, e.g., known combinations of phytoplankton taxa grown in culture (Catlett et al., 2020), while negative controls should contain no genetic material. Interpretation of relative (or absolute) sequence abundances is not straightforward in practice, as the number of barcode gene copies per cell or unit biomass can vary across taxa depending on the chosen barcode gene (Gong and Marchetti, 2019; Zhu et al., 2005). Despite these caveats, several recent studies have demonstrated that DNA meta-barcoding workflows can provide accurate and precise estimates of the relative sequence abundances of most phytoplankton (Catlett et al., 2020; Yeh et al., 2021). Some barcode genes also provide relative sequence abundances that scale roughly with cell size, biovolume or biomass proportions (de Vargas et al., 2015; Godhe et al., 2008; Zhu et al., 2019).

DNA meta-barcoding data have not been employed in direct validation of satellite algorithms to the best of our knowledge, but these studies suggest high potential for their use in efforts to validate the next generation of PCC algorithms developed for PACE (Catlett et al., 2023). Despite some methodological challenges, the ability to sample a nearly comprehensive range of size classes, the detailed resolution of phytoplankton taxonomic and functional diversity, and the growing appreciation for the quantitative potential of well-validated nucleic acid sequencing workflows make these methods primed for in situ PCC quantification.

4.2.3. Phytoplankton optics

Phytoplankton, either due to their size, or morphological (external or internal) characteristics have a taxa-specific contribution to the scattering of the light in the water column (Organelli et al., 2018; Poulin et al., 2018; Stramski et al., 2001; Stramski and Kiefer, 1991; Whitmire et al., 2010), and that signal is present in the $R_{rs}(\lambda)$ as well. Ocean color measurements can provide rudimentary estimates of the slope of the particulate backscattering or particulate attenuation spectra through the inversion of $R_{rs}(\lambda)$ (e.g., Roesler and Boss, 2003; Loisel et al., 2018). Particulate backscattering itself, which is readily retrievable from in situ or satellite derived $R_{rs}(\lambda)$ (e.g., Werdell et al., 2013) can be used to infer phytoplankton size composition (Kostadinov et al., 2022). Backscattering can be affected by internal and external morphological characteristics that impact the shape of the slope (see Organelli et al., 2018), whereas particulate attenuation is mostly dependent on particle size. Increased values of attenuation spectral slope are associated with particle populations that have higher proportions of smaller size particles, same as for backscattering slopes (e.g., Boss et al., 2001). This approach is highly applicable to the open ocean where changes in particle population are driven by PCC change and could offer an additional dimension in information when distinguishing the phytoplankton with different mineral components (such as silica and calcium carbonate).

Absorption of the phytoplankton is to the first extent driven by the pigments present in the cell. Chlorophylls, and other (sometimes taxaspecific) cellular pigments (see section 4.2 and references therein) determine the shape of the absorption spectra (Mobley, 2022 and references within). Synergically, pigment packaging and the structure of

protein-pigment complexes will have a significant effect on the phytoplankton absorption spectra. Shape, peak, and width of the specific absorption features can be used as a tool to detect different taxa from in situ measurements of absorption (e.g., Chase et al., 2013; Ciotti et al., 2002; Hoepffner and Sathyendranath, 1991; Hoepffner and Sathyendranath, 1993). While some of these features (e.g., Chlorophyll peaks) are visible in $R_{rs}(\lambda)$ and therefore easy to relate to pigment concentrations, ocean reflectance inversion models (e.g., GIOP – Werdell et al., 2013) are often used to derive phytoplankton absorption from the $R_{rs}(\lambda)$, that is ultimately used to infer PCC distribution.

4.2.4. Other approaches

Here we offered an abridged overview of most used techniques to quantify PCC in situ. However, many other techniques, and modification to the listed ones exist, and can be used for quantification of PCC for the needs of the remote sensing community. For example, size fractionated filtration (with cutoffs at nano and micro size range) can be used to establish the contribution of the specific size spectra to specific pigment concentration (chlorophyll of any other one; e.g., Brewin et al., 2014; Ward, 2015). Fluorescence (natural or through use of fluorochromes) can be used in microscopy to improve taxonomic resolution. Multi-spectral fluorometry can be used to resolve larger taxonomic groups with specific pigments (e.g., Chekalyuk and Hafez, 2013). Most recently, holography has inserted itself as a viable, new technique to quantify and decipher PCC (Walcutt et al., 2020).

Each of methods reviewed in this chapter give a unique view of the phytoplankton community composition, and sometimes incomplete one (due to the inherent technical limitations of the individual approach). Incorporating several approaches offers a more accurate view of PCC (Nair et al., 2008). However, it is important to note that artificial

“breaks” in taxonomic spectra due to the limitations of the individual techniques, are still a challenge, and recomposing such information is not a straightforward process (e.g., Haëntjens et al., 2022).

5. Phytoplankton composition from space

5.1. Heritage multispectral PCC remote sensing algorithms

Heritage approaches for deriving phytoplankton composition from ocean color typically exploit relationships generated from pairing in situ phytoplankton data with either in situ $R_{rs}(\lambda)$ or top-of-atmosphere (TOA) satellite radiometry. Until recently, satellite and in situ radiometry measurements were mostly collected at multispectral resolution. Therefore, the methods developed to derive PCC relied on the multi-spectral information ($R_{rs}(\lambda)$) and could be applied to SeaWiFS, MODIS, and multispectral ocean color missions operated by other space agencies (Alvain et al., 2005; Alvain et al., 2008; Ben Mustapha et al., 2014; Sathyendranath et al., 2004; Werdell et al., 2014; Westberry et al., 2005). In general, their applicability and success (and associated uncertainties) depend heavily on the in situ training datasets, and the formulated methodology. Recent reviews have demonstrated that existing ocean color PCC approaches agree on a global scale, but disagree considerably on regional scales (e.g., Bracher et al., 2017; IOCCG, 2014; Kostadinov et al., 2017; Mouw et al., 2017). These results are, in a way, not surprising, as models used are forced to perform over large-scale patterns that vary over several orders of magnitude in targeted parameters, as well as, in the case of coastal waters, high heterogeneity on small spatial scales. These reviews also identified numerous gaps in ocean color-based PCC (including mismatches between in situ, satellite and model data, the lack of uncertainty estimates

Table 4

Compilation of published algorithms to assess phytoplankton community composition. Algorithms are considered global if they are designed for/applied to more than one major ocean.

Application	PCC product(s)	Algorithm validation data	Remote sensing approaches	Hyperspectral (or polarization?) in situ approaches
Global	Taxonomic group(s)	Direct cell observation (cultures and/or field microscopy)	Subramaniam et al. (2001); Westberry et al. (2005) Subramaniam and Carpenter (1994) Alvain et al. (2005); Alvain et al. (2008); Ben Mustapha et al. (2014); Bracher et al. (2009); Hirata et al. (2011); Losa et al. (2017); Moore et al. (2012); Palacz et al. (2013); Sadeghi et al. (2012); Soppa et al. (2014); Xi et al. (2020)	Torreccilla et al. (2011)
		Pigment concentrations	Brown and Yoder (1994) Brewin et al. (2010); Brewin et al. (2015); Devred et al. (2006); Devred et al. (2011); Fujiwara et al. (2011); Hirata et al. (2008); Hirata et al. (2011); Kostadinov et al. (2010); Li et al. (2013); Moore and Brown (2020); Mouw and Yoder (2010); Roy et al. (2013, spectral a_ph also used in development); Sun et al. (2023); Uitz et al. (2006)	
		Spectral signatures	Kostadinov et al. (2009); Kostadinov et al. (2022) Bricaud et al. (2012)	
	Size classes, size index, or PSD	Mie modeling, Coated Spheres model Spectral signatures	O’Shea et al. (2021); Wang et al. (2018)	Bracher et al. (2015); Chase et al. (2013); (Chase et al., 2017); Kramer et al. (2022); Taylor et al. (2013); Uitz et al. (2015)
	Accessory pigments	Direct cell observation (microscopy of cultures and/or field data or imaging-in-flow cytometry)	Chase et al. (2022); Raitos et al. (2008) Réve-Lamarque et al. (2017)	Kirkpatrick et al. (2000); Lubac et al. (2008); Millie et al. (1997); Xi et al. (2017); Xi et al. (2015)
Regional /Local	Taxonomic group(s)	Pigment concentrations	Di Cicco et al. (2017); Kramer et al. (2018); Palacios et al. (2015); Sathyendranath et al. (2004); Werdell et al. (2014)	Catlett and Siegel (2018); Isada et al. (2015); Shaju et al. (2015)
		Spectral signatures	Gittings et al. (2019)	Craig et al. (2006); Wynne et al. (2008)
	Size classes, size index, or PSD	Pigment concentrations	Ciotti and Bricaud (2006)	
		Spectral signatures		
Accessory pigments	Pigment concentrations	Bracher et al. (2015); Pan et al. (2010); Sun et al. (2022)	Aguirre-Gómez et al. (2001); Hoepffner and Sathyendranath (1991); Hoepffner and Sathyendranath (1993); Liu et al. (2019); Lohrenz et al. (2003); Wang et al. (2016); Ye et al. (2019)	

for the satellite data, and the spectral limitation of existing sensors) that advanced ocean color missions such as PACE will be able to address. Looking towards PACE ocean color and polarimetry data, we can draw from the knowledge gained from these previously developed methods, which address global-scale data products as well as more regional taxon or phytoplankton group specific products.

The breadth of methods for detecting PCC from space includes approaches that rely on total biomass (e.g., Hirata et al., 2011), or other proxies for abundance, rather than spectral shape or features, as well as methods that rely on single or multiple ocean color products; $R_{rs}(\lambda)$, carrying information from both scattering and absorption components (e.g., Morel and Prieur, 1977; Xi et al., 2021); phytoplankton absorption (Brewin et al., 2011b; Bricaud et al., 2007 and similar, derived from $R_{rs}(\lambda)$ via semi analytical models such as Werdell et al., 2013); or backscattering (Kostadinov et al., 2009). Different mathematical and statistical approaches (e.g., Gaussian decomposition, principal component analysis, derivatives, machine learning etc.) have been used to extract the information on PCCs from the abovementioned datasets. A more comprehensive list of algorithms is presented in Table 4. The types of PCC retrievals that result from previously developed methods are highly variable. Certain algorithms focus on the retrieval of single taxa, while others retrieve multiple taxa or fractional contributions of multiple taxa. These retrievals are generally reported as probability of detection, as the dominating portion of biomass (usually *Chl a*), as the proportion of the total *Chl a* concentration, or in concentration units such as abundance (e.g., cells) per volume. In contrast, phytoplankton size classes (PSCs) are used to define the heterogeneity in size distribution of phytoplankton communities; mainly reporting three size classes: the pico-, nano-, and microphytoplankton (<2 μm , 2–20, and > 20 μm , respectively after Sieburth et al., 1978). Very often, picoplankton size fraction is used to separate pro- from eukaryotes, but effectiveness of these limits must be reconsidered and revisited in depth after PACE and the in situ validation sites start providing more information. Some approaches rely on the backscattering to retrieve PSCs, and in combination with modeling, retrieve the particulate and phytoplankton size distribution, expressed as % of total biomass or total phytoplankton carbon (Kostadinov, 2016; Kostadinov et al., 2022). Other methods estimate the contributions of each of these three classes to total *Chl a*, through assigning HPLC-determined accessory pigments to taxonomic groups, and the groups to size classes (as per Vidussi et al., 2001, Uitz et al., 2006). Numerous revisions and evaluations of the “Diagnostic Pigment Analysis” approach to estimating PSCs from accessory pigment concentrations have been published and provide a body of literature for reference regarding the development and validation of PSC algorithms from space. Ultimately, these accessory pigments themselves can be used to estimate PCC (Table 3).

Identification of phytoplankton composition down to the species level is possible in some cases for certain taxa with unique optical properties. One example is the cosmopolitan coccolithophore species *Emiliania huxleyi*, which when present at high concentrations (blooms) in the surface layer, can profoundly impact the optical properties of the upper ocean (Balch et al., 1991; Balch, 2018). This detection is not based on the absorption properties of the phytoplankton, but rather on its intense scattering properties (Neukermans et al., 2018), which lead to “milky white” seas observable even in broadband satellite sensors like AVHRR (Loveday and Smyth, 2018). Similarly, algorithms have been developed to detect the blooms of dinoflagellate *Karenia brevis* due to its consistently lower backscattering properties compared to other types of blooms found in the same region (Craig et al., 2006; Cannizzaro et al., 2008; Soto et al., 2015). The addition of vacuoles or intracellular spaces that create high scattering also has a substantial effect on $R_{rs}(\lambda)$ even at relatively low biomass and has led to approaches for discerning cyanobacteria (Matthews et al., 2012; Matthews and Bernard, 2013; Schaeffer et al., 2015). Combination of increased scattering due to the intercellular gas vesicles and pigment specific signal in $R_{rs}(\lambda)$ was the base of early algorithms used to detect cyanobacteria *Trichodesmium* from space

(Subramaniam et al., 2001; Subramaniam and Carpenter, 1994). More recent approaches rely on the dense surface accumulations (sea slicks, Hu et al., 2010; McKinna et al., 2011), or rely on *Trichodesmium* specific bio-optical properties (Dupouy et al., 2011; Westberry et al., 2005; see review in McKinna, 2015).

5.2. Anticipated benefits of the PACE instruments

5.2.1. Hyperspectral Ocean color

Hyperspectral $R_{rs}(\lambda)$ from PACE will provide, by definition, additional information content over existing multispectral data and their associated algorithms. Several studies have addressed optimal spectral resolutions and/or band placement for radiometric measurements, starting with work from Lee et al. (2007). Wolanin et al. (2016) demonstrated that band placement requirements depend on both the method as well as the target phytoplankton groups to be retrieved, and they suggest that hyperspectral (vs. any lower spectral resolution) observations are ideal. Torrecilla et al. (2011) used field data of concurrent phytoplankton absorption and remote-sensing reflectance measurements and demonstrated the advantage of high-spectral resolution data over multi-spectra data for discriminating phytoplankton pigment assemblages in the open ocean, including the benefits of spectral derivative analysis. Vandermeulen et al. (2017) used a database of in situ hyperspectral reflectance measurements from a wide range of water types to demonstrate that a spectral interval of 5 nm is optimal to separate differently light absorbing phytoplankton groups while also accounting for measurement uncertainties. Further, Kramer et al. (2022) found a similar result where the performance of statistical models for predicting phytoplankton pigment concentrations was greatly reduced above a spectral interval of 5 nm. Hence, PACE radiometry can be used to separate the contribution or fine scale spectral features of phytoplankton and large-scale spectral features of the other oceanic constituents (>100 nm, e.g., CDOM, backscattering) as recently demonstrated by Kramer et al. (2022).

Hyperspectral phytoplankton absorption and $R_{rs}(\lambda)$ spectra are more effective than multispectral data during derivative, Gaussian, and clustering analyses for pigment assemblage discrimination and size-based, phytoplankton community composition assessment (Chase et al., 2017; Kramer et al., 2022; Lange et al., 2020; Roelke et al., 1999; Torrecilla et al., 2011; Uitz et al., 2015). This finding reflects the relative similarity of spectral absorption of different phytoplankton pigments and groups (e.g. Garver et al., 1994; Mao et al., 2010), which necessitates the use of optical information at a high spectral resolution to discern subtle differences in spectral absorption and reflectance that are the result of differently absorbing phytoplankton pigments. By focusing on changes on small spectral scales some of these approaches minimize the source of noise in absolute signals (usually associated with atmospheric correction approaches – see Ibrahim et al., 2018).

Existing algorithms that take advantage of hyperspectral $R_{rs}(\lambda)$, have demonstrated their capability on data collected by previously flown hyperspectral instruments; either by quantifying *Chl a* or phytoplankton absorption to differentiate targeted taxonomic groups. Studies based on the Hyperspectral Imager for the Coastal Ocean (HICO) (Lucke et al., 2011) have successfully demonstrated the use of hyperspectral $R_{rs}(\lambda)$ to observe a phytoplankton bloom in Monterey Bay, CA (Ryan et al., 2014), to differentiate a red tide ciliate bloom (*Mesodinium rubrum*) in Long Island Sound, NY at high spectral and spatial resolution using unique yellow fluorescence features (Dierssen et al., 2015), and to map PCC in coastal China using machine/transfer learning approach (Zhu et al., 2019). Recent publications have also shown high-quality retrievals of *Chl a*, phycocyanin, and phytoplankton light absorption spectra from HICO imagery over freshwater and coastal ecosystems (Gitelson et al., 2011; O’Shea et al., 2021; Pahlevan et al., 2021), and discrimination of cyanobacteria monospecific blooms in large (Wynne et al., 2008) and small lakes (Kudela et al., 2015). In the open ocean, the PhytoDOAS method, which makes use of hyperspectral $R_{rs}(\lambda)$, has been applied to

SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric Chartography) to discern blooms of cyanobacteria, coccolithophores, and diatoms (Bracher et al., 2009; Sadeghi et al., 2012).

The OCI on PACE will be able to measure ultraviolet (UV) wavelengths at the same high spectral resolution as the visible portion of the spectrum. Information from the UV part of the ocean color signal will bring additional means to constrain the phytoplankton community structure; directly and indirectly (e.g., through a better characterization of other oceanic constituents such as CDOM). Numerous phytoplankton species produce specific Mycosporine-like amino acids (MAAs) of individual spectral characteristics (Llewellyn and Ains, 2010), with additional UV absorbing compounds (Jeffrey et al., 1999) that could impact the remote sensing reflectance and be traced back to either species composition or community-specific response to environmental conditions (e.g., polar regions, Ha et al., 2018). Using in situ measured $R_{rs}(\lambda)$ Kahru and Mitchell (1998) demonstrated that the presence of a HAB species, *Lingulodinium polyedra* could be distinguished from diatom-dominated populations by the light absorption of MAAs, compounds produced by dinoflagellates to protect organelles from harmful UV rays. This approach was recently validated using a UV band from JAXA's GCOM-C satellite to track the spatial and temporal distribution of this specific HAB (Kahru et al., 2021). However, if this approach will be used in the future for quantification of the targeted species, variability of cell concentrations of MAA and its response to environmental factors must be further evaluated.

5.2.2. Polarimetry

PACE will carry two polarimeters, HARP2 and SPEXone, that will measure polarization of light in addition to the intensity. Light polarization, dependent on wavelength and highly sensitive to scattering angle, carries valuable microphysical insights about particles. PACE polarimeters are targeting primarily properties of atmospheric particles. As such, these measurements will indirectly advance the retrieval of PCC from hyperspectral OCI information by improving atmospheric correction through better characterization of aerosols (e.g., Harmel and Chami, 2011). Regarding the measurement of oceanic properties, these instruments are limited by their mode of operation; collecting information on coarser spatial resolution (3–4 km vs 1 km for OCI) and measuring approaches that maximize the number of scattering angles. However, a similar instrument, ESA's POLDER (Polarization and Directionality of the Earth's Reflectances), has been previously used in combination with modeling to offer information about characteristics of oceanic bulk particle composition (Loisel et al., 2008).

Related approaches could be used to derive additional information about marine particles from PACE's polarimetric data, encompassing their morphology (e.g., Chowdhary et al., 2012), composition (e.g., Chami and McKee, 2007; Quinby-Hunt et al., 1989), and attenuation coefficients (e.g., Ibrahim et al., 2016), some of which are impossible to achieve through traditional ocean color radiometry measurements. Such information could be used in better retrievals of PCC and constrain uncertainties associated with phytoplankton products (see Harmel, 2016; Jamet et al. (2019); Neukermans and Fournier (2018) and references within). However, it is important to note that despite the long history of research of polarization in the ocean (dating back to 1950s) there is still a basic need to first better understand the Muller matrix (i.e., inherent polarization properties) of different marine particles/phytoplankton as a prerequisite to potential meaningful interpretation and use of polarization properties of natural light fields, such as polarized water-leaving light derived from PACE's polarimeters.

5.3. Other approaches to deriving PCC from space

In addition to the development of PCC algorithms that solely rely on optical properties of phytoplankton, the scientific community has developed various approaches that use non-optical proxies including model outputs or results from analysis of lower-level data (e.g., variables

derived from multiple measurements¹¹) to derive PCC. These data are referred to as Level-4 data products and include satellite-based models, machine learning approaches that could incorporate ancillary data, and Earth System Models (ESMs). Such approaches have the advantage of being able to integrate in situ, model, and/or satellite data to gain insights that would not be achievable with the use of phytoplankton optical properties alone and can provide information on variables that might not currently have designated algorithms (e.g., Anderson et al., 2009; Brewin et al., 2015; Brewin et al., 2015; Moore and Brown, 2020; Sun et al., 2023; Ward, 2015).

Several satellite-based models have emerged over the years that result in phytoplankton taxonomic composition as well as phytoplankton size information (e.g., Xi et al., 2021). Hirata et al. (2011), for example, used satellite *Chl a* to derive the fraction of both phytoplankton composition and size fraction. California Harmful Algae Risk Mapping (C-HARM) is routinely (since 2014) using a combination of multispectral $R_{rs}(\lambda)$, remote sensed *Chl a*, sea surface temperature and Regional Ocean Modeling System framework to forecast distribution of *Pseudo-nitzschia* spp. and associated toxins (Anderson et al., 2019). By combining hyperspectral in situ $R_{rs}(\lambda)$ and sea surface temperature in a principal component analysis framework, Lange et al. (2020) derived cell counts for several smaller phytoplankton groups across the Atlantic, demonstrating improved performance for such a combined approach over a multispectral one (Fig. 5).

Machine learning approaches to estimate phytoplankton composition have also been developed in the last decades. Raitos et al. (2008) developed an artificial neural network that incorporates ecological and geographical information (e.g., longitude, latitude, season) with ocean color products (e.g., *Chl a*, normalized water-leaving radiance, PAR), bio-optical characteristics, and remotely sensed physical parameters (e.g., SST, wind stress). Using this approach, they were able to discriminate four major phytoplankton functional types based on probability of occurrence (diatoms, dinoflagellates, coccolithophores, and silicoflagellates) with an accuracy of >70%. Palacz et al. (2013) used another approach that relies on an artificial neural network to simulate the global distribution of PCC with a focus on diatoms and coccolithophores in the high nutrient low chlorophyll (HNLC) regions. A recent approach by Chase et al. (2022) utilizes *Chl a* in combination with environmental variables (sea surface temperature and salinity) to retrieve diatom carbon biomass in the North Atlantic. This approach is a clear demonstration of improvement in PCC retrieval due to the inclusion of environmental variables as well as imaging in-flow cytometry data to define PCC during algorithm development (Fig. 6). These approaches become even more relevant in coastal and freshwater systems where phytoplankton light absorption features in $R_{rs}(\lambda)$ are masked by strong light absorption and backscattering by other optically relevant constituents, hence, auxiliary environmental and physical information could further constrain the solution space enabling high-quality PCC retrievals.

Finally, ESMs integrate in situ and satellite data through parameterization, forcing, and/or assimilation. ESMs can provide global coverage (no gaps due to high solar zenith angle, clouds, polar night, etc.) and can provide information on components of the ocean biogeochemical cycle that cannot currently be derived from satellite data alone (IOCCG, 2020). These models do encompass the diversity of phytoplankton as either functionality (e.g., diatoms, cyanobacteria, diazotrophs, etc.; Bopp et al., 2005; Gregg and Casey, 2007) or size classes (e.g., Ward et al., 2012; Ward and Follows, 2016). ESMs make assumptions that are aligned with our current understanding of phytoplankton dynamics (i.e., nutrient uptake, growth rate, sinking rate etc.). Some models also assimilate satellite ocean color products (e.g., Gregg and Casey, 2007; Jones et al., 2016; Shulman et al., 2013) in models including PCC as functional groups (e.g., Ciavatta et al., 2018; Skákala

¹¹ earthdata.nasa.gov

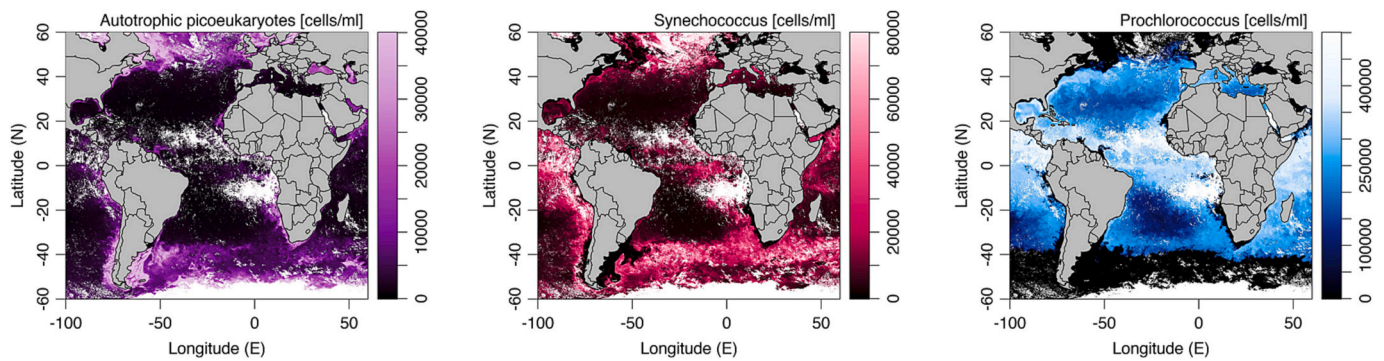


Fig. 5. Spatial distribution of the autotrophic picoeukaryotes, *Synechococcus*, and *Prochlorococcus*, stated as concentration of cells per volume, derived from MODIS Aqua (modified after Lange et al., 2020). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

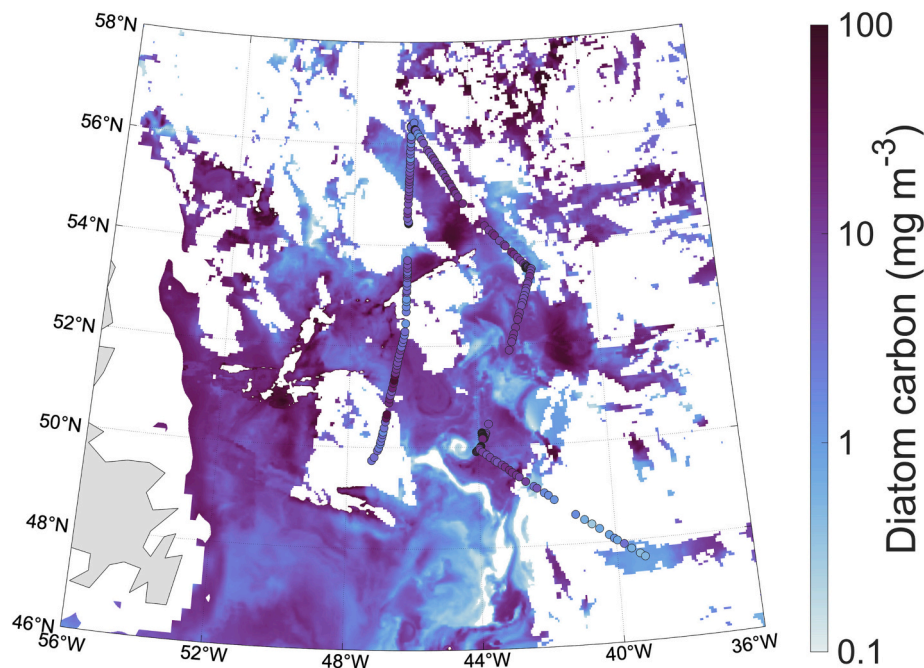


Fig. 6. Diatom Carbon concentration derived from three component neural network model, following Chase et al., 2022.

et al., 2018) or size classes (e.g., Xiao and Friedrichs, 2014).

5.4. Challenges of deriving PCC from space

In the previous sections, we highlighted approaches that are currently used to detect the dominant phytoplankton groups in the world aquatic ecosystem from ocean color imagery. In vast areas of open ocean, living and not living particles that don't contain photosystems (i.e., detritus, heterotrophic bacteria) are more abundant than phytoplankton. While all these particulate (and dissolved) components of the open oceanic systems contribute to the ocean color, the strong light absorption by phytoplankton pigments dominates the contribution to the ocean color signature, which has been identified as a promising signal in terms of identifying groups of phytoplankton (Alvain et al., 2008; Devred et al., 2006). As algal particle concentrations increase, the scattering properties can also have important implications for retrieving different types of algal blooms and surface scums (Hu, 2022). As demonstrated by Garver et al. (1994) both pigment assemblages and pigment packaging effects (self-shading effect in large cells) contribute to the observed similarities in absorption spectra among phytoplankton, making it challenging to differentiate between different species solely based on their spectral characteristics. They found that >99% of the

variance in the particulate absorption spectra was related to the biomass, and <0.5% was related to the presence of auxiliary pigments (Garver et al., 1994). The combined effects of assemblage effective cell diameter and phytoplankton biomass, together with non-algal optical contributors, are not easily interpreted from $R_{rs}(\lambda)$ as these quantities have ambiguous effects on the bulk optics (Evers-King et al., 2014). Recent information content studies have shown that the spectral signatures of absorption by different phytoplankton groups are similar within the uncertainty of the measurement mainly because of the considerable overlap in pigment composition, and thus spectral absorption, between different groups spatially and temporally across aquatic ecosystems (Cael et al., 2020). Also, correlation among reflectances of different wavelengths can decrease information content in hyperspectral data, limiting the capability of derivation of independent parameters (Cael et al., 2023b).

Using the hyperspectral reflectance spectra from UV to NIR (320 to 715 nm) incorporates significantly more information (than traditional multispectral) including backscattering of the phytoplankton and associated particles, as well as fluorescence information, and may yield further taxonomic resolution. New methods to differentiate fractional phytoplankton composition from reflectance detected six different groups globally including diatoms, dinoflagellates, haptophytes, green

algae, prokaryotes, and *Prochlorococcus* (Xi et al., 2020). However, such approaches may not apply to all coastal and inland waters. In the North Sea, Castagna et al. (2021) found that blooms of *Phaeocystis globosa* are synchronous with those of the diatom *Pseudo-nitzschia delicatissima*, both harmful bloom-forming species with similar pigmentation and optical properties.

Remote sensing algorithms and biogeochemical models can be derived and tuned for the regional or local phytoplankton groups down to specific taxa, if they are known to occur in an area and do not have similar optical properties compared to other local taxa (examples listed in section 5.1 and Table 3). For example, in South African waters, five different probabilistic indicators of harmful algal blooms were retrieved relevant to the aquaculture industry including waters with high and low density of dinoflagellates, *Pseudo-nitzschia* dominated waters, as well as waters with mixed assemblages of high and moderate phytoplankton concentrations (Smith and Bernard, 2020). We have only begun to assess the hyperspectral scattering and fluorescence properties that may also aid in differentiating different types and stages of blooms, as well as relationships to seasonal trends and other remotely sensed quantities including polarization parameters, temperature, photosynthetically available radiation, and salinity (see Section 4.2.3). Sometimes inclusion of environmental parameters (such as SST) improves the algorithm capabilities. In those situations PCC model outputs and such environmental variables are no longer independent – something that will have to be taken into consideration when doing long time series analysis (or trying to divulge climate driven trends).

Some studies have developed hyperspectral techniques to differentiate over 20 different species of phytoplankton (e.g., Zhu et al., 2019). While the statistical approaches used in such studies are robust, the lack of validation data across the breadth of space and time hinders the widespread application of such tuned approaches. The chosen approach for treatment of error and uncertainties in these applications determines the difference between retrieving four to five phytoplankton groups rather than >60 (Cael et al., 2020). A recent study using a large HPLC pigment dataset confirmed that only a limited number of phytoplankton groups (~4) may be differentiated globally including cyanobacteria, diatoms/dinoflagellates, haptophytes, and green algae (Kramer and Siegel, 2019). However, they also demonstrated that, on regional scales, pigment association varies, suggesting that regional algorithms could resolve up to 6 taxonomic groups. Data from the Santa Barbara Channel, California revealed that around five phytoplankton pigment communities, which are covarying assemblages of phytoplankton groups, could be differentiated based on their spectral properties (Catlett and Siegel, 2018; Catlett et al., 2021).

Another challenge of deriving PCC from space is that the vertical structure of phytoplankton in the ocean is not always homogenous as many of the models are assuming; phytoplankton layers are often found across the oceanic ecosystems. Depth on which specific phytoplankton is, as well as a thickness and number of layers with different PCCs will heavily influence observed $R_{rs}(\lambda)$ at the surface, as that signal represent optically weighted contribution of all components, with the note that surface community will have the strongest influence on the signal itself. These vertical distributions are not simple to resolve either from the perspective of total biomass (Gordon and McCluney, 1975; Morel and Berthon, 1989; Stramski and Stramska 2005), fluorescence signal (Erickson et al., 2019) size structure (Uitz et al., 2006), or PCC (Lange et al., 2018; Werdell et al., 2014).

Another challenge requiring attention is the mismatch in the products that some of the remote sensing PCC approaches produce and in situ measurements. Above mentioned approaches that output % of biomass (chlorophyll or carbon) to specific size class or group, are hard to validate, as in situ datasets for those parameters are rare, or modeled (carrying a lot of assumptions, therefore errors), or unavailable. In those situations, validation is carried through comparison with in situ measurements that explain PCC in different units (see section 4), leading to additional uncertainties that are often unaccounted for. Furthermore,

there is a spatial and temporal mismatch between in situ and remote sensing data. The current approach, where a 5×5 pixel (nominally) box is centered on a pixel closest to an in situ data point, has shown success at validating indices of total phytoplankton biomass on open ocean scales. A key reason for this is the high dynamic range of *Chl a* concentration (and by proxy, total phytoplankton biomass) in the ocean, which may not be the case for individual phytoplankton taxonomic groups. Issues of sub-pixel variability, however, are not trivial in heterogeneous and dynamic ocean regions, including coastal areas that are likely to have strong tidal influences, river runoff, stratification, sediment resuspension, and other biophysical interactions that create patchy water mass distributions (e.g., Aurin et al., 2013; Ryan et al., 2005). In addition, diel variability in phytoplankton processes causes changes in cell size consistent with patterns of cell growth during the light period and cell division late in the day (Sosik et al., 2003) that is visible in optical properties, including $R_{rs}(\lambda)$ (e.g., Briggs et al., 2018; Claustre et al., 2002; Concha et al., 2019; Gernez et al., 2014; Henderikx Freitas et al., 2020; Poulin et al., 2018; Stramski et al., 1995; Stramski and Reynolds, 1993). In regions with considerable spatiotemporal variability, for example, matching the seasonal climatology can be a useful tool to evaluate and validate different algorithms (Henderikx Freitas and Dierssen, 2019). In situ observations of radiometry (e.g., using drones), or parallel observations of radiometry and PCCs (e.g., field experiments) can facilitate the challenges of spatio-temporal heterogeneity (Gray et al., 2022). Going forward, thoughtful approaches that take in consideration the spatiotemporal variability of PCC, phytoplankton growth stages, and associated bio-optical retrievals should be applied to the validation of these remote sensing products.

6. Phytoplankton from PACE

In this review we presented a three-pronged approach to define PCC from PACE; as information that is needed by the users, definable by in situ methodology, and detectable from satellites (Fig. 7). In the preceding sections we defined current capabilities to resolve phytoplankton taxonomy from in situ and space-based observations. We described the strengths and weaknesses of each approach. We also described the availability of various techniques for phytoplankton enumeration and identification, from pigments to DNA to microscopy to imaging in flow

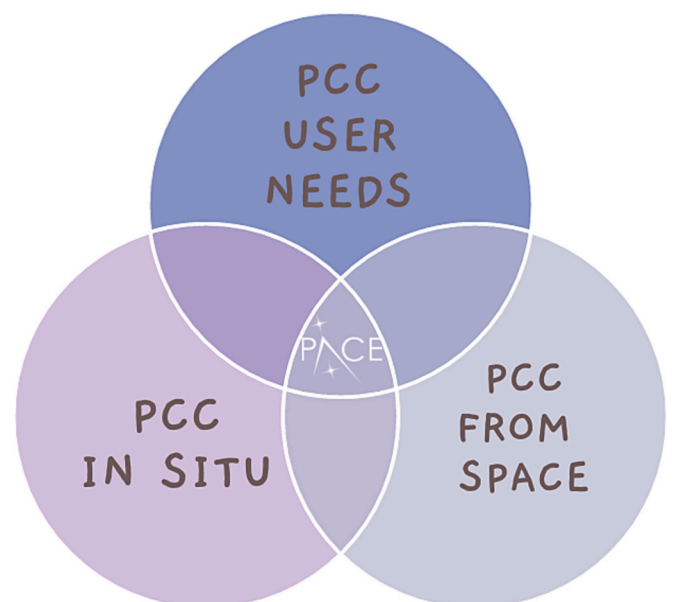


Fig. 7. PCC from PACE is an intersection of user's needs, facilitated and constrained by the spaceborne technology aboard the satellite, and our capability to measure and define the phytoplankton community structure in situ.

approaches. The current suite of satellite PCC algorithms is largely only capable of deriving size classes, with a few that can discriminate unique taxonomic classes. Now the question is: what is possible with PACE? Although we would like to satisfy every user's needs, we must be realistic in our assumptions or expectations, and limitations that are outside of the sphere of technological capabilities of PACE instruments and our methods in situ.

6.1. In situ data requirements

Even with PACE's technological advancements, its potential to characterize the phytoplankton community will still depend on the availability of pigment and taxonomic data—that is, how well PCC is assessed in situ and subsequently used in algorithm development and validation. Previously, most PCC algorithms developed for application to satellite data have relied on phytoplankton accessory pigment concentrations to define the phytoplankton groups of interest. A challenge arises in that the biomass of a given phytoplankton group cannot be directly defined using accessory pigment concentrations, as there are assumptions and approximations made when defining groups via pigment proxy (Jeffrey et al., 2011). Diversifying the types of in situ data used to define PCC (see Section 4) as well as use of multiple types of in situ taxonomic approaches will not only will improve the development of robust PACE PCC algorithms, but it will be critical as we go forward, as each data type has its advantages and limitations (see Catlett et al., 2023). Additionally, the limited number of validation exercises have been ad-hoc, and to ensure the quality and fidelity of the PCCs produced from PACE, validation must be done in a continuous standardized fashion (PACE mission, 2020).

The first steps for validation of PACE algorithms will be using a solid foundation built upon heritage ocean color missions such as SeaWiFS, MODIS, MERIS, and VIIRS. From these missions, we have learned that the development, usability, and reliability of ocean color data depends on the availability of quality field data from (and prior to) launch date through the final days of the mission. Here we define “quality field data” as that which have been collected and processed following vetted

community protocols, and deposited in an open access long-term data repository, especially those following up-to-date international data standards. The need for calibration and validation of optical oceanographic data during the SeaWiFS era set the stage for development of the SeaWiFS Bio-optical Archive and Storage System (SeaBASS), which today is one of the largest data repositories for optical oceanographic data. SeaBASS is part of NASA's Ocean Biology Distributed Active Archive Center (OB.DAAC), operating under NASA's Earth Observing System Data and Information System (EOSDIS). In addition to serving the ocean color community as a long-term data repository and data distribution (via OB.DAAC), SeaBASS is responsible for compiling and curating data used for calibration and validation activities of ocean color satellite missions, including PACE. Most of the radiometric and bio-optical data used for validation is shared via NASA NOMAD (NASA bio-Optical Marine Algorithm Dataset), which is a publicly available, global, high-quality in situ bio-optical data set for use in ocean color algorithm development and satellite data product validation activities.

When it comes to measurements of phytoplankton and community composition, SeaBASS has been primarily limited to phytoplankton pigments and relatively few flow cytometry and imaging datasets. As HPLC based *Chl a* has historically been the preferred validation data type for ocean color *Chl a*, community has developed standard protocols, and has participated in numerous round robin comparisons, that allowed standardization of not only *Chl a*, but the whole HPLC pigment suite across international community (e.g., SeaHARRE round robin series, Hooker et al., 2012). In preparation for PACE and to expand phytoplankton data availability beyond pigments, SeaBASS implemented community protocols outlined in Neeley et al. (2021) for standardizing image data collected using imaging-in-flow instruments, such as the IFCB, UVP and FlowCAM, and associated metadata and other documentation. Standards and best practices for other taxonomic datasets, such as traditional microscopy and flow cytometry are either published or underway (Neeley et al., 2023). Following these community standards, imaging, flow cytometric, and classical microscopy datasets are organized to be interoperable with Ocean Biodiversity Information System and aligned with Darwin Core terminology when possible.

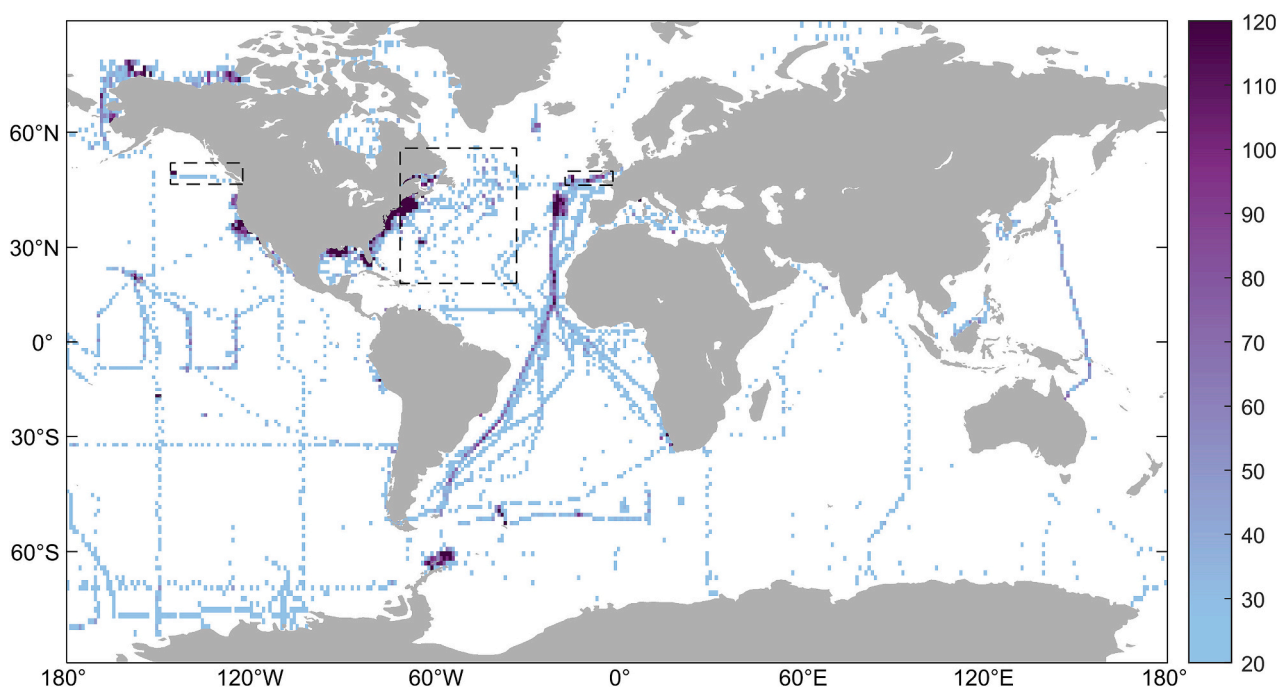


Fig. 8. Geographical distribution of the current inventory of taxonomic data in NASA SeaBASS database (as of October 2023). Color-coded is the density of HPLC data (samples per pixel). Dashed squares indicate the area where NAAMES and EXPORTS campaigns took place, the only campaigns that contributed additional taxonomic (imaging, flow cytometry and genetic) data to SeaBASS.

Incorporating molecular taxonomy datasets would be the next step, as currently, these data are not easily accessible for validation or dataset-building purposes. In parallel, community accepted protocols are being developed for a whole suite of other PACE products, including hyperspectral remote sensing reflectance (Zibordi et al., 2019). As these new datatypes are added to the validation pipeline, they will be included into future versions of NOMAD datasets.

Currently, in situ data on phytoplankton concentration and composition are still heavily biased towards some regions and/or are not directly available (Thompson and Carstensen, 2022). For example, SeaBASS currently contains only 2 large datasets (from NAAMES and EXPORTS cruises) that contain imaging, flow cytometric, and DNA data on top of more abundant HPLC taxonomic information (Fig. 8). To allow for the above-mentioned applications, it is critical that we have data that allow us to calibrate/validate satellite products, as well as to validate ESM outputs (Dierssen et al., 2020). As stated by Thompson and Carstensen, 2022, this network needs to be carefully planned in order to provide the information that we will need to understand and manage climate variability and change. Several recent grassroots initiatives address the geographic biases in SeaBASS (or NOMAD) towards ocean data by sharing a large database of hyperspectral $R_{rs}(\lambda)$ (> 7500+) along with their co-located *Chl a*, CDOM, and SPM across global freshwater and coastal (Lehmann et al., 2023), and coastal and open ocean ecosystems (Casey et al., 2020) but with no accompanying PCC datasets.

Finally, error propagation and attribution of uncertainties to PCC products are paramount. This information will determine whether an algorithm can be applied effectively and/or broadly. While uncertainty has long been a topic of discussion in the ocean color community, only recently have significant strides been made to improve uncertainty estimation and error propagation to the measured or modeled products (IOCCG, 2019; Kostakis et al., 2021; McKinna et al., 2019). With more complex algorithms, such as the ones used for estimation of PCC, uncertainty associated with underlying ocean color observations (Ibrahim et al., 2022; Zhang et al., 2022) accumulates through each step in the algorithm hierarchy (Siegel et al., 2023). Ancillary data present sources of uncertainty, as well as the theoretical assumptions or empirical data used to develop the PCC algorithm (Brewin et al., 2017; Xi et al., 2021). As PACE has a requirement to estimate uncertainty at the level of $R_{rs}(\lambda)$, such cumulative uncertainty should be calculated and reported with the PCC products and used in future validation exercises in combination with contemporary validation metrics (McKinna et al., 2021). Such uncertainty propagation exercises can be helpful when developing future PCC algorithms, to elucidate the interpretation of (e.g., climate driven) trends in PCC observations from space. In addition, having uncertainty as part of the harmful algal blooms (HABs) detection report is crucial for water quality managers, especially when it comes to determining the potential public health risks and implementing appropriate responses. Ultimately – all said above outlines the need for a stronger collaboration with other communities in oceanography – such as phytoplankton ecology – to facilitate and elucidate better ways of defining phytoplankton groups – knowledge that can be used to inform and improve future PCC algorithms.

6.2. Data accessibility and open science

Chl a, as a heritage ocean color product, sets a high bar when it comes to data objectives and potential recognition as an Essential Ocean Variable (EOV, see Muller-Karger et al., 2018a, 2018b). Wilkinson et al. (2016) describe widely-accepted “FAIR” data objectives, listed below with a description of the relevant OB.DAAC practice:

- Findable: total *Chl a* estimates from multiple satellites and sensors are indexed on the Earthdata Search website, including spatial and temporal filters.

- Accessible: single or multiple total *Chl a* datasets may be downloaded on-demand by users or applications that authenticate with a free Earthdata account.
- Interoperable: total *Chl a* datasets are delivered as NetCDF files, which embed metadata in a vocabulary controlled by the Climate and Forecast metadata conventions.
- Reusable: in addition to being in the public domain, total *Chl a* datasets include metadata relevant to the ocean color research (e.g., variable units, sensor calibration parameters, and references to protocols and algorithms) that cover all aspects of the data provenance.

PACE ocean color products, including PCC, will be distributed via OB.DAAC, as soon as the data are available. However, it is important to understand that data will be considered “provisional”, meaning that they will not be validated (or validation is in progress) and quality may not be optimal. Assessment of the PACE data quality, i.e., validation, will be done in several steps, starting with remote sensing reflectance, followed by *Chl a* (and other products in ocean color standard suite), and ultimately PCC (when data is available).

PACE data products for PCC are on the path to achieve each of the FAIR principles; despite being a more complicated variable than total *Chl a* (e.g., PCC is multivariate), there is nothing structurally novel about these products. New components of the vocabulary needed for metadata about phytoplankton composition (Neeley et al., 2021) demonstrate that the ocean color research community is actively engaged in establishing standards for interoperability. The units of PCC variables are well defined, ranging from *Chl a* or carbon density to total or relative abundance. Standard methods will have to be defined so that taxa can be pooled into genera or class (or higher taxonomic levels) depending on the users and goal outcomes. One of the biggest challenges, owing to the types of models that produce Level-4 data products containing PCC variables, will be the complete description of data source and methodology. Variables estimated through semi-analytical algorithms are relatively easy to document, using equations or open-source software and a short list of parameters. It is more difficult to document the provenance of variable estimates that get introduced after a model-fitting procedure, such as in supervised machine learning. In this case, both the fitted, or trained, model itself and any in situ data used while training must both be FAIR (e.g., Schoening et al., 2022). OB.DAAC and SeaBASS are well suited repositories to support the data-intensive model-fitting procedures reliance on in situ data.

The NASA Science Mission Directorate (SMD) objectives for conducting supported missions, including PACE, through open science practices extends beyond open data. The topic of inclusivity, creating new pathways for end users to become involved in science, is also relevant to open science.¹² While the majority of academia and government entities have computational capacity to download and process large datasets, many of those in the broader PACE CoP may have challenges working with a large number of files in scientific data formats containing multiple parameters, like $R_{rs}(\lambda)$, pigments, and light attenuation, and metadata on calibration, validation, and other provenance.

For this reason, the PACE Mission will develop and offer trainings, tutorials, data “recipes”, and other forms of community support to ensure that global users know how to appropriately access and utilize PACE data products (to be available virtually through NASA ARSET, PACE Project, OB.DAAC, and in person in conferences and meetings). Further, the PACE team will continue its work with the PACE CoP to identify further training needs and gaps, and gather feedback post-launch on continued challenges and barriers and the development of new products. The PACE team, for example, is working towards making a new type of merged “Water Quality Product” that will highlight specific products for a wide range of users. Such a merged and simplified

¹² <https://science.nasa.gov/open-science-overview>

data product, drawing from different parameters, will be adaptable and can grow as new algorithms come online. Finally, a PACE Community of Potential will also be convened; versus (and in addition to) the CoP, which is made up of more technical users. The Community of Potential will target individuals or groups (within or outside of PACE CoP) who are unfamiliar with satellite data products and PACE capabilities but may be able to leverage and benefit from PACE data products. Members of the Community of Potential may benefit from additional support on remote sensing at large, and the benefits and applications that PACE specifically could offer. For example, white papers with case studies may be developed so that new users can understand possible applications and uses of PACE data. In addition, certain new international conferences or venues could be identified and targeted where users are less familiar with NASA remote sensing data. Other efforts to engage with new and existing users across the globe – whether for awareness raising, training, or some combination – will be considered as they are identified.

Steps to reduce financial barriers associated with research on PCC include provisioning of cloud-computing services with timely access to PCC data products, that should not only rely on NASA based providers. The Giovanni (Acker and Leptoukh, 2007) and Google Earth Engine (Uğur et al., 2021) systems are in-browser applications coupled to cloud computing facilities that provide low-barrier entries to analysis of earth observation variables. The inclusion of new variables on phytoplankton communities in these or other comparable systems is included in the design objectives for PCC data products. Training on software and online data tools for new users will be integral to the mission.

7. Conclusion

In this paper we have identified the strengths and weaknesses of existing approaches and presented how PACE will address some of the remaining gaps and challenges for quantifying PCC. The knowledge gained from this mission will rely on the existence of appropriate validation products (e.g., quality, coverage, diversity of products available, error and uncertainties requirements), the use of the various approaches currently available (in situ, satellite, and model products) as well as the distribution of data products following FAIR principles including training of the community and developing user friendly data products. Improved characterization of PCC is key to understanding aquatic ecosystems, our ocean's health, and the ocean's effects on global climate. From local applications, such as water quality assessments that are focused on specific phytoplankton taxa, to global applications such as the role that ocean plays in carbon sequestration, the needs for information on phytoplankton composition requires the community to work together to develop the next generation of data products. This is especially critical when it comes to improving our understanding of the impact that climate change has on the ocean and developing effective management strategies for the ocean and other aquatic resources, both today and in the future.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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