

# TOOLS IN HARMONY

## INTEGRATING OBSERVATIONS AND MODELS FOR IMPROVED UNDERSTANDING OF A CHANGING OCEAN

By Erica H. Ombres, Heather Benway, Kelsey Bisson, Alyse A. Larkin, Elizabeth A. Perotti, Elizabeth Wright-Fairbanks, Joey Crosswell, Sandupal Dutta, Cynthia Garcia, Anand Gnanadesikan, Kalina Grabb, Amanda Fay, Rui Jin, Kyla Kelly, Hayley Kwasniewski, Alexa K. Labossiere, Jonathan Lauderdale, Jenna Lee, Yajuan Lin, Jacqueline S. Long, Anna Rufas, Cristina Schultz, Nicholas D. Ward, and Yifan Zhu

### INTRODUCTION

Increasingly complex and severe impacts of global change require collaboratively developed tools that simultaneously address multiple applications/uses. It is critical to come together as a research community to co-develop ocean biogeochemical observing networks and models that support research and monitoring, decision-making, operational forecasting, and other stakeholder applications. Despite serving as two major research tools in ocean science, ocean observing and modeling tend to act as distinct scientific communities composed of researchers with different skill sets, training, preferred methodologies, and vocabularies. This division often results in missed opportunities for synthesis, challenges in data integration, and inefficient use of resources. Bridging these divides is essential for addressing urgent challenges in ocean sciences.

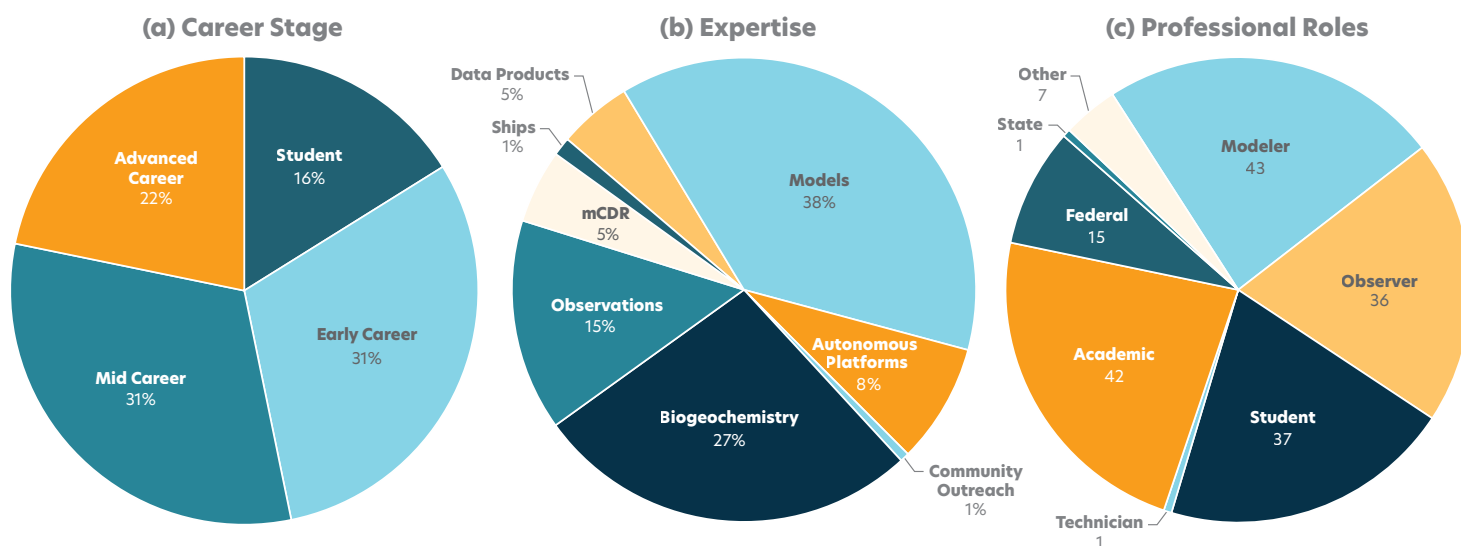
To reduce communication barriers and facilitate discussion on scientific questions of mutual interest, NOAA's Ocean Acidification Program and Global Ocean Monitoring and Observing Program, NASA's Ocean Biology & Biogeochemistry Program, and the US Ocean Carbon and Biogeochemistry Project Office co-convened a workshop—Biogeochemical Observing and Modeling Workshop: Connecting Observations to Models—during the February 2024 Ocean Sciences Meeting (New Orleans, Louisiana, USA). This workshop provided a space for scientists trained in different disciplines of ocean modeling and observing to make connections, assess observing and modeling needs and capabilities within focused areas of interest, and identify synergies and collaborative opportunities. Here, we share high-level recommendations and opportunities for enhanced collaboration that emerged from the workshop to inform and activate the broader oceanographic community. A more detailed synthesis of the workshop discussions is available in the full workshop report (Ombres et al., 2024).

### WORKSHOP DYNAMICS: FOSTERING A DIALOG

To ensure focused and purposeful interactions, workshop organizers polled prospective participants prior to the workshop across their respective ocean biogeochemical (BGC) networks on potential topics of interest. One hundred twenty-four (124) responses representing a range of career stages, expertise, and professional roles were collected ([Figure 1](#)). Workshop organizers used these responses to identify topical discussion areas and design a common set of guiding questions to frame small group discussions. Common interests included ([Figure 2](#)):

- Ensuring adequate observational coverage for the questions and scales of interest
- Addressing data management challenges
- Collecting chemical and biological measurements simultaneously
- Addressing contrasting resolutions in datasets
- Deploying autonomous observing technology to fill spatial and temporal gaps
- Evaluating marine carbon dioxide removal (mCDR) methods
- Investing in long-term research efforts
- Supporting development of data products
- Ensuring community engagement and inclusivity
- Increasing opportunities for integration of observations and models

Over 100 people participated in the workshop, which was designed to provide an interactive space for ocean scientists to communicate with each other and with funding agencies about challenges and opportunities in this field. To kick off the workshop, participants voted on the topics they were most interested in discussing. The selected topics included: ocean carbon budget, episodic and extreme events (EEEs), machine learning (ML), biological carbon pump (BCP), ocean acidification, trophic interactions, polar systems, and mCDR.



**FIGURE 1.** Demographics of the respondents to a pre-workshop survey, including (a) career stage and (b) expertise. Respondents also suggested major discussion points that interest the biogeochemical observing and modeling communities. Responses were used to shape the topical discussion areas presented to workshop attendees. Respondents represented a wide variety of career stages and expertise focus areas. Students are enrolled in an undergraduate or graduate degree program, early career was defined as <7 years from completion of terminal degree, and mid- and advanced career were self-selected. (c) Workshop attendee professional roles. mCDR = marine carbon dioxide removal

Participants chose two of the topics identified and participated in two 30-minute discussion periods on these topics. Throughout the discussions, participants identified observing and modeling needs, data management challenges, and opportunities for collaboration for each discussion topic (Table 1).

Four questions framed the discussions:

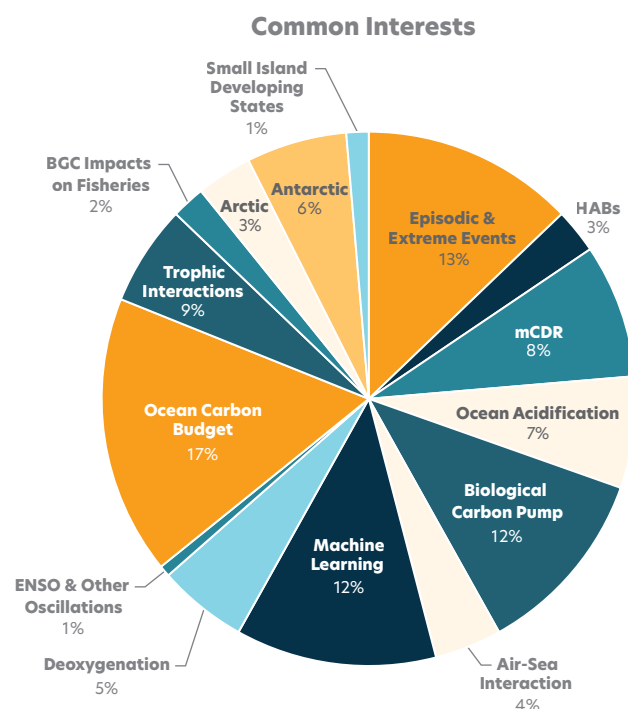
1. What expansion beyond current observations is needed for model development?
2. How can we increase discoverability, synthesis, and model development through data management practices?
3. How do we resolve the contrasting resolutions between data and models for increased understanding?
4. What channels exist for connections between observers and modelers? How can we foster more conversation?

## KEY FINDINGS AND RECOMMENDATIONS FOR ADDRESSING CONTEMPORARY OCEAN RESEARCH CHALLENGES

Several overarching challenges and opportunities emerged from the topical discussions, providing a blueprint for improved collaboration and more integrated approaches to research, observing system design, and model development. These opportunities and suggestions for future actions are highlighted below.

### DESIGNING INTEGRATED OCEAN OBSERVING SYSTEMS

Today's ocean research and monitoring activities face a fundamental challenge: the need for seamless integration of observing systems and models to promote understanding and prediction of ocean processes. While observational gaps limit model development, model limitations also affect our ability to optimize



**FIGURE 2.** Workshop attendee topical discussion area interests.

observing strategies. This interdependency requires rethinking how we design and implement both tools to address contemporary challenges in ocean research.

Critical gaps persist in our observing capabilities that affect both monitoring and modeling efforts. The ocean BGC observing community particularly needs increased sampling resolution to reduce three-dimensional spatial and temporal biases. For instance, wintertime sampling remains a significant challenge in high-latitude

regions due to sea ice coverage and adverse sea conditions (Heimdal et al., 2024). Several regions (e.g., polar, tropical Pacific, Indian Ocean) and depths below the surface layer of the ocean are relatively undersampled (Abrahamsen, 2014; Levin et al., 2019; Smith et al., 2019). Across biogeochemistry disciplines, specific variables and processes are necessary to measure but remain undersampled.

Measurement, monitoring, reporting, and verification of mCDR projects require information about baseline ocean biogeochemistry (Fay et al., 2024; Ho et al., 2023). The biological pump observing community requires the constraint of high trophic level processes in addition to measurements of physicochemical particle properties, including sinking velocity, porosity, and chemical composition,

**TABLE 1.** Abridged summary of priorities for addressing needs and challenges related to biogeochemical observations, models, data management, and collaboration for each discussion topic.

OBSERVATIONS	MODELS	DATA MANAGEMENT	COLLABORATION
<b>Biological Carbon Pump (BCP)</b> The BCP is a key process in the ocean carbon cycle involving transfer and remineralization of organic carbon to depth. Biologically mediated biogeochemical (BGC) transformations occurring against a backdrop of complex physical dynamics make the BCP a uniquely challenging process to measure and model.			
<ul style="list-style-type: none"> <li>• Prioritize deep (mesopelagic and deeper) measurements and time series</li> <li>• Observing gaps: physicochemical particle properties, key nutrients like iron and ammonium, community structure and function, trophic interactions, vertical migration, biological rates (grazing, viral lysis)</li> <li>• Uncertainty quantification</li> <li>• Gridded climatology of particulate organic carbon (POC) flux</li> <li>• Data rescue and digitization</li> </ul>	<ul style="list-style-type: none"> <li>• Integrate diverse multi-platform datasets over space and time</li> <li>• Perform quantitative evaluation of observation and model mismatch</li> </ul>	<ul style="list-style-type: none"> <li>• Standardized guidelines for data collection, metadata reporting, and data processing (data aggregation and error propagation)</li> <li>• Centralized repository or aggregator of metadata for BCP-relevant measurements</li> </ul>	<ul style="list-style-type: none"> <li>• Conduct moderately sized BCP process studies that integrate sampling and modeling activities from the outset</li> <li>• Hackathons and community activities that build capacity and facilitate idea and knowledge exchange</li> </ul>
<b>Episodic and Extreme Events (EEEs)</b> EEEs such as storms and wildfires may generate large BGC fluxes over short periods of time, thus serving as major players in BGC cycles and marine ecosystem health. However, EEEs pose safety and logistical challenges, and observations and models require high spatiotemporal resolution to understand their impacts.			
<ul style="list-style-type: none"> <li>• Develop and deploy robust (able to withstand EEEs) platforms and technologies to fill spatial and temporal gaps (including satellite remote sensing, e.g., geostationary missions like NASA GLIMR)</li> <li>• Leverage existing observatories (e.g., OOI, LTERs) to conduct event-based sampling</li> <li>• Establish sentinel sites where a dynamic range of EEE impacts occur (storms, cyclones, wildfires) for sustained data collection</li> </ul>	<ul style="list-style-type: none"> <li>• Regional models and/or dynamical or statistical downscaling of global outputs to constrain event-scale dynamics</li> <li>• Organize early collaboration to ensure sampling resolution is adequate for models</li> </ul>	<ul style="list-style-type: none"> <li>• Adopt common definition of “extreme” (% departure from baseline)</li> <li>• Create metadata fields and/or flags for EEEs</li> </ul>	<ul style="list-style-type: none"> <li>• Funding mechanisms and community activities (model intercomparison, data synthesis, comparative analysis) that <i>require</i> integration of observations and models for knowledge sharing and capacity building</li> <li>• Mechanisms to support collaborative international EEE research</li> </ul>
<b>Machine Learning (ML)</b> Models used to predict ocean BGC cycling encode a host of relationships between environmental variables. A key question is whether these mathematical relationships realistically combine to produce the emergent behavior of ocean BGC systems to allow predictions to be made in areas with sparse observations.			
<ul style="list-style-type: none"> <li>• Increase spatiotemporal resolution of BGC (especially nutrients like iron, ammonium) and biology (plankton biomass) observations to improve ML algorithms</li> </ul>	<ul style="list-style-type: none"> <li>• Increase availability of model outputs for ML reanalysis</li> <li>• Standardization of model outputs of phytoplankton community composition</li> </ul>	<ul style="list-style-type: none"> <li>• Improve data standardization, quality control, and open access to facilitate synthesis and ML training on large datasets</li> </ul>	<ul style="list-style-type: none"> <li>• Make ML tools available to the community</li> <li>• Workshops for ML training</li> </ul>
<b>Marine Carbon Dioxide Removal (mCDR)</b> Anthropogenic CO <sub>2</sub> emissions have been the leading driver of climate change over the past century. To limit warming and associated climate and ecosystem impacts, multi-sector efforts are underway to explore human intervention strategies to remove CO <sub>2</sub> from the atmosphere and sequester it long-term in the ocean (NASEM, 2022). Well-integrated modeling and observing efforts are vital to rigorous assessment of these approaches.			
<ul style="list-style-type: none"> <li>• Strategic BGC observing system deployments (water column and benthos) for mCDR projects to assess efficacy and impacts</li> <li>• Work with industry to produce and refine BGC sensors and autonomous platforms (e.g., AUVs, ASVs, moorings) that specifically focus on relevant carbonate chemistry parameters</li> </ul>	<ul style="list-style-type: none"> <li>• Optimize sampling strategies using OSSEs</li> <li>• Improve representation of particulate inorganic carbon distributions within models</li> <li>• Prioritize development of models that simulate regional and mesoscale dynamics</li> </ul>	<ul style="list-style-type: none"> <li>• Transparency and public availability of data, methods, and software emerging from mCDR research</li> <li>• Adopt common vocabularies and data/metadata reporting standards</li> <li>• Create mCDR data flags to note datasets that contain results from experiments that modify natural ocean conditions, and/or novel data assembly centers for mCDR projects</li> </ul>	<ul style="list-style-type: none"> <li>• Integration of observations and models starting in early stages of mCDR projects to build common vocabularies and understanding</li> <li>• Research funding must keep pace with venture capital investment to ensure rigorous scientific evaluation of emerging technologies</li> <li>• Efficient data archiving and peer review to make information available more quickly</li> </ul>

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TABLE 1. Continued...

OBSERVATIONS	MODELS	DATA MANAGEMENT	COLLABORATION
<b>Ocean Acidification (OA)</b> The absorption of ~25% of total anthropogenic CO <sub>2</sub> emissions (Friedlingstein et al., 2023) has shifted ocean chemistry toward reduced pH and carbonate ion concentration, with adverse consequences for marine life at all trophic levels, particularly calcifiers. Constraining OA trends on local/regional to global scales and developing predictive capacity to inform decision-making requires cutting-edge technology for climate-quality measurements and advanced models.			
<ul style="list-style-type: none"> <li>Observing gaps: Historical DIC and TA data to validate hindcasts, subsurface observations where big OA impacts occur, organic alkalinity, calcification rates</li> <li>Develop high-quality, cost-effective CO<sub>2</sub> system sensors, especially DIC and TA</li> <li>More careful QA/QC (w/climate- and weather-quality guidance) of OA-relevant BGC sensor data</li> <li>Targeted sampling of critical and historically under-sampled ecosystems (e.g., polar regions)</li> </ul>	<ul style="list-style-type: none"> <li>Leverage existing observational data to validate four-dimensional OA model simulations</li> <li>Make model outputs and model-based visualization systems more accessible</li> </ul>	<ul style="list-style-type: none"> <li>Assess data overlap and connectivity (interoperability) across existing specialized ocean carbon repositories from regional to global scale</li> <li>Develop centralized catalog of OA-relevant data resources to facilitate discovery and uptake by stakeholders</li> </ul>	<ul style="list-style-type: none"> <li>Promote cross-disciplinary communications to create universal OA terminology and identify underutilized OA resources</li> </ul>
<b>Ocean Carbon Budget</b> The ocean is the largest reservoir of mobile carbon on our planet, containing 45 times more carbon than the atmosphere and 15 times more than land plants and soils (Friedlingstein et al., 2023). Despite its importance to global climate dynamics and environmental policies, the ocean carbon budget is not thoroughly constrained. Equipping the marine BGC observing system to produce useful data for carbon cycle models is critical for quantifying the role of the ocean in the global carbon cycle.			
<ul style="list-style-type: none"> <li>More subsurface and coastal observations, increased temporal resolution (hourly when possible), use of autonomous assets to reduce seasonal bias</li> <li>Integrate in situ and satellite-based ocean carbon measurements</li> <li>Increase biological sampling to better understand contributions of zooplankton, viruses, microbes, etc., to ocean carbon cycling</li> <li>Continued development of carbon system sensors and platforms designed with easy integration of those sensors</li> </ul>	<ul style="list-style-type: none"> <li>Use models to inform temporal and spatial sampling resolution requirements in different regions (i.e., OSSEs)</li> <li>Conduct quantitative model-data comparison studies and uncertainty analyses of ocean carbon uptake, transport, and storage</li> </ul>	<ul style="list-style-type: none"> <li>Need tools to streamline access and search for synthesis and modeling in data from platforms like Argo (e.g., searchable dashboards that filter data by parameter, standardized entrance points for accessing all available observations)</li> <li>Standardized metadata reporting, especially data uncertainty source and quantification</li> <li>Collaboration between data managers and scientists to design FAIR data systems</li> </ul>	<ul style="list-style-type: none"> <li>Centralized library of relevant tools, data products, and content creators to promote collaboration</li> <li>Workshops to support uptake and processing of observations, e.g., BGC-Argo</li> <li>Ongoing investment in training, knowledge exchange, and funding opportunities for data-model integration</li> </ul>
<b>Polar Systems</b> Polar regions are crucial to Earth's BGC cycles, profoundly affecting climate and marine ecosystems. Recent advancements in observing platforms and technologies have mitigated some of the challenges associated with data collection in these remote and often extreme environments. Despite this progress, there is an urgent need for more model-data integration to explore complex interactions and feedbacks in these ecosystems.			
<ul style="list-style-type: none"> <li>Geographic: more coastal/shelf and under-ice observations, expanded coverage in the Southern Ocean (beyond the Weddell Sea and Drake Passage) and the Arctic (Eurasian data)</li> <li>Temporal: reduce seasonal bias, high-resolution/continuous coverage across transitions like seasonal ice melt, more time series programs</li> <li>Integration of in situ, autonomous, and remote observations</li> </ul>	<ul style="list-style-type: none"> <li>Increased resolution of polar observations in space and time through logistical and technical innovation (platforms, sensors, vehicles, etc.) that overcome environmental challenges</li> <li>Develop/improve AI methods to address contrasting data vs. model resolution</li> </ul>	<ul style="list-style-type: none"> <li>Develop unified databases with advanced search capabilities to enhance data discoverability and usability</li> <li>Standardize data collection and data/metadata reporting guidelines to improve interoperability</li> <li>Standardize inclusion of funding in projects for implementing FAIR data practices that ensure accessibility of both new and historical data sets</li> </ul>	<ul style="list-style-type: none"> <li>Capacity building activities (e.g., hackathons) on data uptake, assimilation, synthesis, data-model integration</li> <li>Opportunities for sustained dialog among data managers, observers, and modelers (e.g., community workshops, project meetings, webinars)</li> </ul>
<b>Trophic Interactions</b> Studying trophic interactions requires a holistic understanding of marine food webs, from physics to plankton to marine mammals. Marine trophic interactions span several temporal and spatial scales, making them a complex system to observe and model.			
<ul style="list-style-type: none"> <li>Biological rate measurements</li> <li>Improved biological baselines through sustained time series programs to detect patterns of variability and change</li> <li>Imaging data to measure community composition and size distribution to better constrain trophic transfer</li> <li>Resource management and stakeholder needs should guide sampling</li> </ul>	<ul style="list-style-type: none"> <li>Support goal-oriented pre-observation communication among all involved stakeholders to improve model pipeline for complex and under-observed trophic interactions</li> </ul>	<ul style="list-style-type: none"> <li>Overall need for discoverable data in common formats for uptake and aggregation, including:</li> <li>Standardized reporting of variable names and formats</li> <li>Clear descriptions of data type, included variables, and access point(s)</li> <li>Adoption of standard protocols for data manipulation, re-uploading, and metadata</li> </ul>	<ul style="list-style-type: none"> <li>Cross-training activities to build mutual awareness of data collection and modeling challenges</li> </ul>

for more accurate calculations of particulate organic carbon flux. Ocean biological parameters are globally undersampled relative to physics and chemistry and are especially lacking for subsurface and benthic systems. Biological rate measurements (e.g., grazing, productivity, viral lysis, and respiration) important for model accuracy are relatively sparse due to the time and resources required to obtain them. Rate measurements are further limited by a lack of standardized approaches and poorly constrained discrepancies between in situ and incubation-based approaches. Co-collection of biological, chemical, and physical data via the augmentation of existing and the development of new observing systems is recommended to provide a more holistic understanding of ocean processes.

Filling observing gaps will require continued progress in development and deployment of sensors and platforms that can access more extreme depths and environments. Sustained investment in observing infrastructure that transcends disciplines and strategically combines temporal and spatial (latitude, longitude, depth) coverage of the ocean is essential in order to address the challenges that lie before us. This infrastructure will likely include a combination of repeat hydrography lines (e.g., RAPID array, Extended Ellett Line), shipboard time-series programs (e.g., Bermuda Atlantic Time-series Study, Hawaii Ocean Time-series, Porcupine Abyssal Plain Sustained Observatory, the Global Ocean Ship-based Hydrographic Investigations Program), Long-Term Ecological Research stations, long-term monitoring stations (e.g., Ocean Observatories Initiative and NOAA Ocean Acidification Observing Network moorings), sentinel sites for extreme events, autonomous platforms (e.g., floats like BGC Argo, gliders, autonomous surface vehicles), platforms of opportunity (e.g., commercial fishing and cargo ships), and airborne and satellite-based measurements, among others. Observation System Simulation Experiments (OSSEs) may be useful for coordinating and optimizing observing system design in order to inform reallocation of resources as scientific grand challenges and priorities change. Improved coordination and integration of coastal observing assets is especially critical for monitoring and addressing ongoing threats to human communities and the marine ecosystem services on which they rely.

Gridded observational BGC data products (e.g., Global Ocean Data Analysis Project [GLODAP], Surface Ocean CO<sub>2</sub> Atlas [SOCAT], World Ocean Atlas [WOA]) are important tools for supporting ocean research and climate monitoring as well as model evaluation and development. These products will require continued advancement of artificial intelligence (AI), machine learning (ML), and statistical analysis tools to address sampling gaps and to improve spatial resolution. Additionally, measurements that appear to be very important in the current generation of models (ammonium and iron) are not currently available as gridded variables.

Cloud-based computing environments (e.g., [Pangeo](#)) provide open-source frameworks that streamline access to standardized data and model outputs, software, and data analysis tools. They centralize and democratize access and also facilitate collaboration and model intercomparison. For example, Model Intercomparison

Projects (MIPs) have become effective community exercises for assessing model performance and system sensitivity to anthropogenic changes. However, more sophisticated approaches are needed to evaluate why the models differ from observations and from each other, and further to guide improvements in how fundamental processes are represented. Shared computing environments allow users to work collaboratively with models produced by MIPs whose sizes might be prohibitive for personal computers.

Co-development design should be implemented in future projects/endeavors. Rather than accessing datasets after the completion of a project, all involved end users must have the opportunity to engage early in the planning stages of a project or process study to develop a common understanding of data collection priorities, challenges, and opportunities. Models and data assimilation and analysis tools can inform data collection (e.g., OSSEs), which can help optimize sampling strategies. Similarly, model-data integration activities such as data assimilation, which combines model outputs and observations to improve process understanding, provide a unique collaboration and capacity building opportunity to raise awareness of the challenges associated with finding and aggregating data from multiple sources. Therefore, model reanalysis products with essential ocean BGC variables (Task Team for the Integrated Framework for Sustained Ocean Observing, 2012) should also be prioritized, at least at a regional level.

## HARMONIZING OCEAN DATA MANAGEMENT AND SYSTEMS

The success of integrated ocean research depends critically on the ability to harmonize our approach to ocean data management and data serving systems. Development of systems and processes that are findable, accessible, interoperable, and reusable (FAIR) is central to this effort. This requires comprehensive approaches to data collection, documentation, and sharing. Standardized reporting of observed data and metadata greatly enhances interoperability and reusability and will require the development and adoption of community-vetted reporting guidelines. The use of controlled vocabularies that are machine-readable (i.e., the Marine Metadata Interoperability [MMI] Ontology Registry and Repository) and the adoption of standardized units streamline data aggregation and ingestion into models. Additionally, requiring quantitative reporting of quality control and uncertainty measures as part of metadata would allow scientists to judge whether or not the quality of a dataset is suitable for their applications.

With numerous data repositories that utilize different data and metadata practices and formats, finding and aggregating data are challenging. Continued advancement of semantic approaches like Resource Description Framework (RDF) that enable a data user to query across databases, as well as tools like ERDDAP that provide a consistent application programming interface, or API that enables data extraction in different formats for a range of applications, is strongly recommended to maximize return on investment in data streams and repositories. Transparent provenance



information and versioning for datasets should also be provided to enable appropriate data reuse.

Lastly, engaging with international initiatives like the Global Ocean Observing System (GOOS) and Ocean Data and Information System (ODIS) helps align data management practices across the international ocean science community. Development of community-driven data management guidelines and best practices through inclusive working groups and workshops, and establishment of governance structures to maintain standards and address emerging needs, will ensure broad buy-in and sustainability.

## ENHANCING COLLABORATION

Explicit financial support for enhanced collaboration, including community activities (e.g., workshops, hackathons), and sharing of resources to reduce communication barriers between stakeholders are needed. Proposed solutions to address communication barriers include glossaries, language workshops, and “matchmaking” tools and activities to enhance sustained community dialog, along with dedicated personnel to help with data interpretation/use. Funding entities should encourage projects with co-development designs that integrate observations, models, and data science throughout the projects.

The oceanography community must move away from the idea that scientists are either modelers or observers. Modeling and observations are both tools that support knowledge generation. Providing more opportunities at all career stages and developing career structures that incentivize cross-training and application of models, observations, and data science approaches will go a long way towards developing more versatile researchers.

Looking to the future, it is essential to sustain investment in observing infrastructure that transcends disciplines and strategically combines temporal and spatial coverage of the ocean. Filling observing gaps will require continued progress in development and deployment of sensors and platforms that can access even the most remote and challenging (in space and time) ocean environments. Techniques like OSSEs and data assimilation tools and approaches provide opportunities for fruitful collaboration that will benefit the BGC research community as a whole. The community can prepare to address emerging scientific challenges, such as mCDR and closing the ocean carbon budget, by working together to continually improve ocean BGC modeling and observations. Finally, continued investment in community-building will provide opportunities for networking, training, and building a common lexicon and shared understanding.

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## AUTHORS

**Erica H. Ombres** ([erica.h.ombres@noaa.gov](mailto:erica.h.ombres@noaa.gov)), Ocean Acidification Program, National Oceanic and Atmospheric Administration (NOAA), Washington, DC, USA. **Heather Benway**, Ocean Carbon and Biogeochemistry Program, Woods Hole Oceanographic Institution (WHOI), Woods Hole, MA, USA. **Kelsey Bisson**, Ocean Biology and Biogeochemistry Program, National Aeronautics and Space Administration, Washington, DC, USA. **Alyse A. Larkin**, University Corporation for Atmospheric Research (UCAR), Global Ocean Monitoring and Observing, NOAA, Silver Spring, MD, USA. **Elizabeth A. Perotti**, Ocean Acidification Program, NOAA, Silver Spring, MD, USA. **Elizabeth Wright-Fairbanks**, University Corporation for Atmospheric Research (UCAR), Ocean Acidification Program, NOAA, Silver Spring, MD, USA. **Joey Crosswell**, Environment, Commonwealth Scientific and Industrial Research Organisation, Brisbane, Australia. **Sandupal Dutta**, Earth and Planetary Sciences, Johns Hopkins University, Baltimore, MD, USA. **Cynthia Garcia**, Global Ocean Monitoring and Observing Program, NOAA, Silver Spring, MD, USA. **Anand Gnanadesikan**, Earth and Planetary Sciences, Johns Hopkins University, Baltimore, MD, USA. **Kalina Grabb**, Marine Policy Center, WHOI, Woods Hole, MA, USA. **Amanda Fay**, Lamont-Doherty Earth Observatory of Columbia University, Palisades, NY, USA. **Rui Jin**, University of Washington, Seattle, WA, USA. **Kyla Kelly**, Global Ocean Monitoring and Observing, NOAA; University of Southern California Sea Grant, Los Angeles, CA, USA. **Hayley Kwasniewski**, Environmental Studies, University of Colorado Boulder, CO, USA. **Alexa K. Labossiere**, Virginia Institute of Marine Science, William and Mary, Gloucester Point, VA, USA. **Jonathan Lauderdale**, Massachusetts Institute of Technology, Cambridge, MA, USA. **Jenna Lee**, Princeton University, Princeton, NJ, USA. **Yajuan Lin**, Life Sciences, Texas A&M University – Corpus Christi, TX, USA. **Jacqueline S. Long**, Submarine Scientific, Santa Cruz, CA, USA. **Anna Rufas**, University of Oxford, UK. **Cristina Schultz**, Civil and Environmental Engineering, Northeastern University, Boston, MA, USA. **Nicholas D. Ward**, Pacific Northwest National Laboratory, Sequim, WA, USA. **Yifan Zhu**, Marine Science, University of Connecticut, Groton, CT, USA.

## ARTICLE CITATION

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