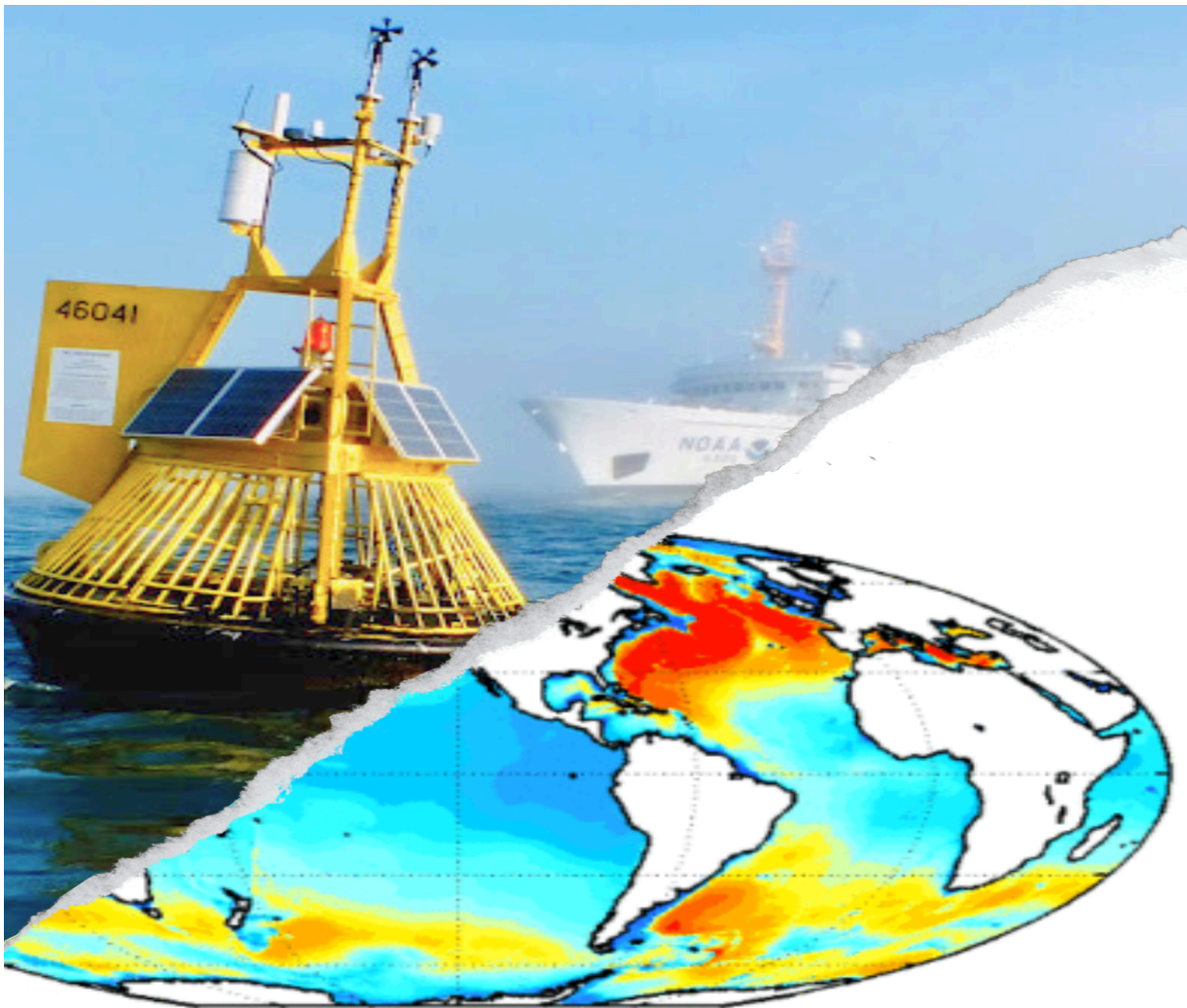


# Connecting Observations to Models: Biogeochemical Observing and Modeling Workshop

2024 Summary Report and Suggested Steps Forward



## **NOAA Technical Memorandum OAR-OAP-6**

U.S Department of Commerce | National Oceanic and Atmospheric Administration | Oceanic  
and Atmospheric Research

Connecting Observations to Models: Biogeochemical Observing and Modeling Workshop  
2024 Summary Report and Suggested Steps Forward

Convened by NOAA Ocean Acidification Program, NOAA Global Ocean Monitoring and Observing Program, NASA Ocean Biology and Biogeochemistry Program and the Ocean Carbon and Biogeochemistry Program February 22, 2024 in conjunction with the Ocean Sciences Meeting in New Orleans LA.

Report Editors: Erica Ombres, Heather Benway, Kelsey Bisson, Alyse Larkin, Liz Perotti, Liza Wright-Fairbanks

<https://doi.org/10.25923/wpdj-ja69>

U.S. Department of Commerce  
Gina Raimondo, Secretary

National Oceanic and Atmospheric Administration (NOAA)  
Dr. Rick Spinrad, Under Secretary of Commerce for Oceans and Atmosphere & NOAA  
Administrator

Office of Oceanic and Atmospheric Research (OAR)  
Dr. Steve Thur, Assistant Administrator for OAR

## Acknowledgements

This workshop and report were a joint effort led by NOAA Ocean Acidification Program, NOAA Global Ocean Monitoring and Observing Program, NASA Ocean Biology and Biogeochemistry Program and the Woods Hole Oceanographic Institute Ocean Carbon and Biogeochemistry Program. We would like to thank all of those who participated in the workshop. Without your thoughtful and engaged participation this workshop and report would not have been possible. We would also like to thank NOAA's Global Ocean Monitoring and Observing Program and the Ocean Carbon Biogeochemistry Program for their generous financial support that allowed this workshop to take place. We would also like to thank the Ocean Science Programming committee for allowing space for this event. And most importantly we would like to recognize the report contributors who volunteered their time to help write and review the various sections of the report.

All report contributors are listed below in alphabetical order by last name:

Heather Benway, Woods Hole Oceanographic Institute Ocean Carbon and Biogeochemistry Program

Kelsey Bisson, NASA Ocean Biology and Biogeochemistry Program

Joey Crosswell, Commonwealth Scientific and Industrial Research Organisation

Sandupal Dutta, John Hopkins University

Cynthia Garcia, NOAA Global Ocean Monitoring and Observing Program

Anand Gnanadesikan, John Hopkins University

Kalina Grabb, Woods Hole Oceanographic Institute

Amanda Fay, Columbia University

Rui Jin, John Hopkins University

Kyla Kelly, NOAA Global Ocean Monitoring and Observing Program

Hayley Kwasniewski, University of Colorado Boulder

Alexa Labossiere, Virginia Institute of Marine Science

Alyse Larkin, NOAA Global Ocean Monitoring and Observing Program

Jonathon Lauderdale, Massachusetts Institute of Technology

Jenna Lee, Princeton University

Yajuan Lin, Texas A&M Corpus Christi

Jacqueline S. Long, Submarine Scientific

Erica Ombres, NOAA Ocean Acidification Program

Liz Perotti, NOAA Ocean Acidification Program

Anna Rufus, University of Oxford

Cristina Schultz, Northeastern University

Nick Ward, Pacific Northwest National Laboratory

Liza Wright-Fairbanks, NOAA Ocean Acidification Program

Yifan Zhu, University of Connecticut

- Cover Image credit: (Top) NOAA research ship and buoy from a West Coast Ocean Acidification mission. Credit: NOAA PMEL. (Bottom) Model visualization of inferred Dissolved Inorganic Carbon from inferred by GLODAPv2 taken from [Stock et al. 2020](#).

# Contents

<b>Acknowledgements</b> .....	<b>2</b>
<b>Contents</b> .....	<b>3</b>
<b>Executive Summary</b> .....	<b>4</b>
<b>Overview</b> .....	<b>6</b>
<b>Common challenges and findings</b> .....	<b>8</b>
<b>Topic Summaries</b> .....	<b>11</b>
Biological Carbon Pump.....	11
Episodic and Extreme Events.....	15
Machine Learning.....	18
Marine Carbon Dioxide Removal.....	21
Ocean Carbon Budget.....	24
Ocean Acidification.....	28
Polar Systems.....	32
Trophic Interactions.....	35
<b>References</b> .....	<b>38</b>

# Executive Summary

Authors: Alyse Larkin, Liz Perotti and Liza Wright- Fairbanks

Reviewers: Heather Benway, Kelsey Bisson and Erica Ombres

As the Earth experiences increasingly severe impacts of global climate change, it is critical to integrate optimized ocean observing networks with biogeochemical models for understanding, policy, mitigation, and adaptation. However, ocean observers and modelers form distinct scientific communities with separate training, methodologies, and vocabularies. To reduce communication barriers and address cutting-edge scientific questions, NOAA, NASA, and the Ocean Carbon & Biogeochemistry (OCB) Project Office co-convened the “Biogeochemical Observing and Modeling Workshop: Connecting Observations to Models” at the 2024 Ocean Sciences Meeting. The workshop aimed to provide a space for ocean modelers and observers to make connections, address observing and modeling needs, and identify synergies and areas for research co-development. More than 100 participants voted on the 14 key topics for discussion, which focused on ocean carbon processes, extreme events, trophic interactions, polar systems, and machine learning. Participants provided feedback on critical gaps in (1) observation networks, (2) data management, (3) observational versus model resolutions, and (4) avenues for fostering collaboration. This report presents the synthesis and recommendations of the workshop.

During the 2024 OSM workshop, modelers and observers worked together to address needs in the two fields, identifying synergies and areas for research co-development along the way. Critical needs emerged for observing systems, modeling, data management and enhancing collaboration.

Observing system needs included increased sampling resolution over time and space, specifically year-round and sub-surface observing of chemical and biological metrics. Critical modeling needs focused around the expansion of Model Intercomparison Projects (MIPs) to improve model performance.

Coordinated data management practices are key as BGC observing and modeling efforts expand. Standardized open-source data storage, metadata, and submission processes will greatly benefit the field. Importantly, data should follow Findable, Accessible, Interoperable, and Reusable (FAIR) data practices, which will ensure interoperability between researchers and disciplines. Coordination across platforms, disciplines, and national lines is critical to dispel duplication of efforts and encourage targeted system enhancements.

Communication and collaboration within and across disciplines stood out as the key to enhancing collective efforts across BGC modeling and observing communities. Iterative and creative scientific processes can be encouraged through targeted collaborative activities and networking events tied to international conferences. Resources for building and fostering multidisciplinary teams early in the scientific process are necessary; without financial support, teams are unable to co-design projects to the best of their ability. Working together, BGC modelers and observers will be better equipped to address emerging needs in the ocean science sphere.

Looking to the future, sustained investment in observing infrastructure that transcends disciplines and strategically combines temporal and spatial coverage of the ocean is essential to address the challenges that lie before us. Filling observing gaps will require continued progress on development and deployment of sensors and platforms that can access even the most difficult regions. Observing System Simulation Experiments (OSSEs) and data assimilation projects present opportunities for fruitful collaboration that will benefit the BGC research community as a whole. Working together to continue enhancing BGC modeling and observing will ensure the community is prepared to address emerging scientific challenges, such as marine carbon dioxide removal and closing the ocean carbon budget. Finally, investment will need to go beyond the science to provide outlets that convene observer and modeler communities for networking, training, and building a common lexicon and understanding.

# Overview

Authors: Erica Ombres and Liza Wright-Fairbanks

Reviewers: Heather Benway and Alyse Larkin

Ocean biogeochemical observing networks and models are continually being developed and enhanced in support of research and monitoring, decision making, operational forecasting, and other marine ecosystem stakeholder applications. Anthropogenic climate change impacts on marine ecosystem function are wide ranging and constantly evolving, underscoring the need to foster a sustained dialog to build and strengthen collaborations between biogeochemical observing and modeling communities. With this aim in mind, NOAA's Ocean Acidification and Global Ocean Monitoring & Observing Programs, NASA's Ocean Biology & Biogeochemistry Program, and the Ocean Carbon & Biogeochemistry Project Office co-convened a mini workshop, *Biogeochemical Observing and Modeling Workshop: Connecting Observations to Models*, during the February 2024 Ocean Sciences Meeting (New Orleans, Louisiana).

To ensure focused and purposeful interactions, the organizers polled prospective participants across their respective networks in advance on potential topics of interest. Over 100 responses were collected from biogeochemical observers and modelers ranging from students to advanced career stages. Common interests included expanding observations, data management, coupling chemical and biological measurements, addressing contrasting resolutions in data sets, using uncrewed systems to fill gaps, marine carbon dioxide removal, sustained funding opportunities, support for data products, community engagement and inclusivity, and channels for engagement between observers and modelers. Workshop organizers used these responses to identify topical discussion areas and design a common set of guiding questions to frame discussions.

Over 100 people participated in the workshop, which provided an interactive space for biogeochemical modelers and observers to communicate with each other and with funding agencies about challenges and opportunities in this space. To kick off the workshop, participants voted on discussion topics based on a selection of topics derived from the results of the pre-workshop interest survey. Nine topics were assigned to discussion tables. The chosen topics were:

1. Ocean Carbon Budget
2. Episodic and Extreme Events
3. Machine Learning
4. Biological Pump
5. Ocean Acidification
6. Trophic Interactions
7. Polar Systems
8. Marine Carbon Dioxide Removal
9. Deoxygenation\*

\*While this topic was discussed during the workshop, it is not represented in this report due to various factors.

Participants rotated tables to engage in two 30-minute topic discussions. A moderator guided the discussion at each table and the group captured responses captured either on a physical brainstorming page or in an online notes document. The four questions that framed the discussions were as follows:

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?

Participants identified observing and modeling needs that are unique to each topic. There were also several common high-level challenges and opportunities discussed spanning multiple topics. The discussions, outlined below, provide a blueprint for improved collaboration and more integrated approaches to research, observing system design, and model development.

# Common challenges and findings

Authors: Heather Benway, Kyla Kelly and Erica Ombres

Reviewers: Alyse Larkin, Liz Perotti and Liza Wright- Fairbanks

## **Observational needs and challenges**

A universal need of the ocean biogeochemical observing community is increased sampling resolution to fill sampling gaps and reduce 3D spatial and temporal biases. For instance, wintertime sampling remains a significant challenge due to ice coverage and adverse sea conditions. Several regions (e.g., polar, tropical Pacific, Indian Ocean, etc.) and depths below the surface layer of the ocean are relatively undersampled. Across biogeochemistry disciplines, specific variables and processes are necessary to measure but remain undersampled. For example, measurement, monitoring, research, and verification (MMRV) of marine Carbon Dioxide Removal (mCDR) projects require information about baseline ocean biogeochemistry tailored to community needs. In addition to constraining contributions from higher trophic level processes, the biological pump observing community requires measurements of physicochemical particle properties, including sinking velocity, porosity, and chemical composition for more accurate calculations of particulate organic carbon flux. Ocean biological parameters are globally undersampled relative to physics and chemistry and are especially lacking in subsurface and benthic systems. Biological rate measurements (e.g., grazing, productivity, viral lysis, and respiration), which tend to be more sought-after in models, 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 vs. incubation-based approaches. Co-collection of biological, chemical, and physical data via the augmentation of existing and development of new observing systems is recommended to provide a more holistic understanding of ocean processes.

Filling observing gaps will require continued progress on development and deployment of sensors and platforms that can access even the most difficult regions. Sustained investment in observing infrastructure that transcends disciplines and strategically combines temporal and spatial (latitude, longitude, depth) coverage of the ocean is essential to address the challenges that lie before us. This infrastructure will likely include a combination of repeat hydrography lines, time series, Long-Term Ecological Research stations (LTERs), sentinel sites for extreme events, autonomous platforms (e.g., floats, gliders, moorings), platforms of opportunity (e.g., commercial fishing and cargo ships), airborne and satellite-based measurements, among others. Observation System Simulation Experiments (OSSEs) may be a useful tool to coordinate and optimize observing system design, reallocating resources from over- to undersampled regions. 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.

## **Modeling needs and challenges**

Gridded biogeochemical data products (e.g., GLocal Ocean Data Analysis Project, or GLODAP and Surface Ocean CO<sub>2</sub> Atlas, or SOCAT) are important tools for supporting ocean research,

ocean and climate monitoring, and model evaluation and development. These products will require continued advancement of Machine Learning (ML) and statistical analysis tools to address spatial data gaps.

Cloud-based computing environments (e.g., [Pangeo](#)) provide an open-source framework that streamlines access to standardized data and model outputs, software, and data analysis tools. This not only centralizes and democratizes access, but it facilitates collaboration and model intercomparison. Model Intercomparison Projects (MIPs) have become effective community exercises for assessing model performance and improving process understanding and system sensitivity.

Rather than accessing datasets after the completion of a project, modelers need the opportunity to engage with observationalists earlier in the planning stages of a project or process study to develop a common understanding of data collection challenges and opportunities (e.g., biological and biogeochemical stocks vs. rate measurements). Modelers bring extensive data assimilation and analysis tools to inform data collection (e.g., OSSEs), which can help observationalists design more effective sampling strategies. Data assimilation, which combines model outputs and observations to improve system understanding, provides another opportunity for fruitful collaboration and capacity building between modelers and observationalists, particularly around addressing the shared challenges of data aggregation across multiple sources.

### **Data management needs and challenges**

We must continue to strive towards more Findable, Accessible, Interoperable, Reusable (FAIR) ocean biogeochemical data systems. Standardized reporting of observed data and metadata would greatly enhance Interoperability and Reusability and will require development of community-vetted reporting guidelines. The use of controlled vocabularies that are machine readable and adoption of standardized units would 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 data set is of a sufficient caliber for their models (e.g., climate vs. weather).

With numerous data repositories, each with a unique format and vocabulary, finding and aggregating data remains challenging for modelers. Continued advancement of semantic approaches that enable the user to query across databases, as well as tools like Environmental Research Division Data Access Program (ERDDAP) that enable data extraction in different formats for different applications is strongly recommended to maximize return on investment in data streams and repositories.

### **Enhancing collaboration**

Explicit financial support for enhanced collaboration, including targeted community activities (e.g., workshops, hackathons, etc.), shared resources to reduce communication barriers between observationalists and modelers, and perhaps even requirements for modeling and observing communities to engage with data scientists and managers will encourage transdisciplinary product development. Proposed solutions to address communication barriers

included glossaries, language workshops, and “matchmaking” tools and activities to enhance sustained community dialog, and dedicated personnel to help with data interpretation/use. Funding entities should encourage projects with co-development designs that integrate observations and models. OSSEs are one example of this type of project where the observers and modelers work together iteratively. This collaboration would be further facilitated by increasing the accessibility of modeling data for observer use, enabling observers to design model-informed field campaigns. Project kickoff meetings and other community building activities should be leveraged in order to facilitate more direct interactions between data scientists and managers, observationalists, and modelers.

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 for cross-training and application of models, observations, and data science approaches would go a long way towards developing more versatile researchers.

# Topic Summaries

## Biological Carbon Pump

Authors: Jonathan Lauderdale, Anna Rufas, Yajuan Lin

Reviewers: Anand Gnanadesikan, Kyla Kelly and Alyse Larkin

The biological carbon pump (BCP) is a key process for ocean carbon sequestration via the transfer and remineralization of particulate organic carbon (POC) to the deep ocean, yet it remains poorly constrained. To enhance the skill of BCP modeling, the community at the workshop recommended increasing the observations of marine particle physicochemical properties (for example, particle stoichiometry), improving quantification of uncertainty in POC flux, collecting comprehensive biological data, and better understanding of deep ocean sequestration timescales. Other aspects of the BCP, such as carbon export associated with vertical migrations on diel to seasonal timescales remain unquantified. The report also emphasizes the importance of establishing standardized observation protocols and ensuring data accessibility to promote effective data synthesis and cross-disciplinary collaboration.

**To enhance our mechanistic understanding and modeling of the BCP, it is imperative to focus on spatial, temporal, and parameter-specific gap filling; particle measurements; uncertainty quantification; and support for long-term monitoring.**

There is a significant lack of observations in the ocean's mesopelagic zone (extending from around 100 m to 1000 m depth) concerning the fate of carbon and its vertical attenuation, which are crucial aspects of deep ocean biological carbon sequestration. Additionally, there is a strong need for high-frequency observation data on nutrient budgets and plankton community composition to resolve fine-scale patterns and diel/migratory dynamics. Key nutrient data, such as iron (Fe) and ammonium (NH<sub>4</sub><sup>+</sup>), are often scarce because their concentrations require highly specialized techniques and frequently fall below the detection limit. Moreover, understanding zooplankton and micronekton community composition has been challenging due to limitations offered by sampling with direct *in situ* methods such as net tows (e.g., gelatinous and fragile individuals break, faster individuals will escape, and different mesh sizes have to be used to collect different size classes).

To fill gaps in existing data, a gridded climatology of POC flux would be useful. In the meantime, we should prioritize data rescue efforts to recover and digitize historical data sets, which are important for assessing long-term trends and enhancing model accuracy.

Physicochemical particle properties, such as radius, sinking velocity, porosity, and chemical composition, are critical variables for accurately calculating POC flux. Marine particles are the key vectors of the BCP and characterizing them properly is essential to inform the next generation of models trying to mechanistically resolve the particle characteristics and compositions that exert bottom-up control on the transfer efficiency of POC to the deep ocean. Stoichiometry of the particle's constituents (i.e., the ratio of C:N:P:Fe...), and their variability during remineralization, play an important but poorly constrained role that directly affects the sequestration of carbon in the deep ocean. Sediment traps are the only observational

technology that provides direct measurements of POC flux, enabling the collection of sinking marine particles for subsequent chemical and microscopic analysis in the laboratory.

Biological community structure, function, and interactions represent a critical gap in the observing and modeling spheres. Specific needs include data across multiple trophic levels (from bacteria and viruses to phytoplankton, zooplankton, and micronekton as well as the upper trophic levels), top-down controls like grazing rates and viral lysis, and studies of vertical migrations, and ecological interactions between functional groups (at finer taxonomic resolution).

Thorough uncertainty quantification in POC flux measurements would contribute critical knowledge to the field. It is imperative to document POC flux data's various sources of uncertainty, such as natural variability (associated with location, depth, and season), operational biases in sampling, inter-platform biases, sampling effort, and parameterization of equations for deriving quantities from observations. It is also important to achieve consensus among international research projects on common metrics for reporting uncertainty. The current variety of uncertainty metrics in the POC flux literature includes standard deviation, standard error, confidence intervals, percentile intervals, and interquartile ranges, amongst others.

Allocating more funding for maintaining and establishing new time-series programs in the ocean would enable the collection of "direct" long-term POC flux data at key depths, particularly at export (100 m) and sequestration (1000 m) depths, indispensable for evaluating the efficiency of the BCP in transferring POC to the deep ocean (>1000 m). Ideally, comprehensive measurements should encompass the entire process, from surface production (new and recycled) and reprocessing, to carbon export and remineralization.

**Increasing discoverability, synthesis, and model development through data management practices requires standard protocols, support for data interpretation, and the creation of a centralized data repository of BCP-relevant measurements.**

Establishing standardized protocols for data acquisition (e.g., core variables, sampling effort, sampling depths, timing of the sampling) and statistical processing (error quantification and propagation), is crucial to ensure comparability between datasets across projects. The pioneering data protocols of the EXPORTS program to acquire POC flux data ([https://oceanexports.org/docs\\_science\\_plan.html](https://oceanexports.org/docs_science_plan.html)) can serve as a model for upcoming international research projects focused on the BCP.

Dedicated personnel from research programs can assist in interpreting datasets (e.g., outlier removal, caveats of different sampling methods, and their sensitivities), promoting the use of already available observational datasets and their correct use by less experienced users, such as modelers.

Creating a centralized data repository would make a great impact on the field. Currently, there exist multiple separate data repositories and interfaces for accessing POC flux data (e.g., BCO-DMO, BODC, SeaBASS, PANGAEA), each with varying levels of data access, reporting units, and reporting measures of uncertainty. This calls for the establishment of a centralized repository, or aggregator of metadata, for all particle flux data, with common data reporting

guidelines and associated metadata to prevent issues like double-counting and improve data discoverability. A cloud-based data platform is a promising solution for the research community to deposit, manage, link, and share data efficiently.

**Resolving contrasting resolutions between data and models, requires data and model compatibility, integration of diverse data, and quantitative evaluations given the variable temporal scales of the BCP.**

Observations and models of the BCP operate at different spatial and temporal scales, with local observations often used to adjust large-scale models to investigate, for example, climate impacts. Factors such as deployment depths, sampling locations, sampling effort, timing of the sampling, and the measurement integration times of the various POC flux collection methods that exist (spanning from days to months) impact how well data represent the long-term mean (climatological) value of POC flux. A comprehensive, process-based understanding of the observations is vital for making informed choices about which datasets to include for parameter calibration and model validation.

So far, there have not been concerted efforts to compare and integrate the diverse multi-platform POC flux data (moorings, shipboard deployments, autonomous vehicles, BGC-Argo profiling floats, satellite-based estimates) globally and over time, potentially necessitating models for spatiotemporal interpolation onto regular grids and statistical downscaling.

Quantitative comparisons between observations and models are essential to evaluate their mismatch. This includes several approaches like (i) model generation of synthetic data at time-series sites that match the temporal resolution and extent of the observations (this helps identify whether models reproduce the right results due to overfitting or due to the right representation of BCP mechanisms); (ii) evaluating if models can replicate BCP responses to transient events, such as synoptic storms or El Niño/La Niña cycles (this helps identify missing processes or feedbacks required to improve the model's representation of variability, rather than just aligning with climatological/long-term averages); (iii) using statistical approaches such as a Relative Operating Characteristic (ROC) analysis to evaluate a model's predictive accuracy for specific events (this method classifies model-observation comparisons as hits, misses, false alarms, or correct rejections, with the area under the ROC curve indicating model's skill).

**Collaborative efforts and co-development, particularly of moderately sized process studies, will encourage growth between observationalists and modelers.**

Encouraging collaboration between observationalists and modelers from the outset of designing research programs, rather than leaving the design solely to observationalists and involving modelers in the final stages to "improve climate model projections". This ensures that the data collected aligns closely with the needs and capabilities of planned modeling efforts, and vice versa.

Diverse group collaboration through workshops and hackathons harness so-called "collective intelligence". These settings require participants to work together to find solutions in a fast-paced manner. In particular, hackathons shift the day-to-day routine, provide a creative safe

space in which to ask “curious” questions, brainstorm ideas, challenge strongly held assumptions, and experiment freely, allow decisions to be made quickly, and empower teams with the tools and varied backgrounds with which to experiment and attempt to provide quantified answers.

Moderately sized process studies present an ideal opportunity for model-observation co-design over varied timescales, with tractable observational and numerical requirements, and a direct pipeline towards integrating observational insights into parameterization of phenomena, leading to potential model improvements. Oceanic process studies may be bespoke if a particular set of variables are sought (e.g., the EXPORTS campaign), or leverage long-term time-series collecting consistent sets of core measurements, such as the Hawaii Ocean Time-series (HOT), the Bermuda Atlantic Time-series Study (BATS), and the Porcupine Abyssal Plain Sustained Observatory (PAP-SO). Laboratory and shipboard incubation-based process studies can similarly co-design to discover, or constrain, biological rates and feedbacks.

## Episodic and Extreme Events

Authors: Heather Benway, Joey Crosswell and Cristina Schultz

Reviewers: Kalina Grabb, Alexa Labossiere, Jenna Lee, Rui Jin and Nick Ward

There are numerous challenges associated with obtaining observations of extreme events (e.g. fires or severe storms), including dangers posed to researchers, potential damage to equipment, difficulties predicting extreme events, lack of timely preparation for field campaigns, and uncertainties about the spatial and temporal extent of event impacts. Therefore, proper framing of extreme events as potential key players in biogeochemical cycles is needed to prioritize high-risk, high-reward research endeavors and maintain research infrastructure and financial resources that could be deployed on short notice.

### **New technology is key to filling spatiotemporal data gaps for episodic and extreme event prediction and understanding.**

To effectively capture and assess the impacts of extreme perturbations in dynamic and complex environments with unknown extents, it will be essential to conduct time-resolved in situ measurements in and around areas that frequently experience such extreme events. To help define baseline conditions and also capture event-scale perturbations, emphasis should be placed on developing and deploying robust new technologies, including autonomous sampling platforms (e.g., gliders, saildrones, floats that can operate and track emerging features in shallow coastal regions, etc.), continuous sampling and other low-cost, high-access technology that can be established at scale (e.g., biogeochemical sensors and temperature loggers on fishing vessels), and leveraging existing continuous or high-frequency time series programs. Geostationary satellite missions such as the Geosynchronous Littoral Imaging and Monitoring Radiometer (GLIMR) will provide concentrated biological and biogeochemical monitoring in the Gulf of Mexico and southeastern US, which are heavily impacted by tropical cyclones.

### **Extreme event sentinel sites would provide opportunities for comprehensive analysis of impacts**

Developing a network of sentinel sites that encompass a dynamic range of extreme event (large storms, tropical cyclones, wildfires) impacts would provide a common set of standardized, time-resolved observations to enable collaborative and comparative interdisciplinary research to improve baseline and event-scale process understanding, including timescales of hydrologic forcing and delivery of material from land to ocean; responses of different organisms and elemental cycles to these pulses; identification of early warning signs for these events; and improved understanding of recovery rates and thresholds for regime shifts.

New strategies and partnerships to coordinate among and augment existing observatories (e.g., Long-Term Ecological Research (LTER), National Ecological Observatory Network (NEON), National Estuarine Research Reserve System (NERRS), Ocean Observatories Initiative (OOI), etc.) would be foundational steps towards meeting the dynamic needs of event-based sampling. Recommended paths include establishment of monitoring networks and short-term, rapid-response funding mechanisms that can support sampling campaigns on short notice.

**Data standards and community building are needed for the extreme event community of practice to facilitate comparative analysis.**

Findable, Accessible, Interoperable, and Reusable (FAIR) data practices include publication of complete datasets (rather than just statistics), reporting of uncertainties, and standardized data and metadata reporting guidelines to improve discoverability and interoperability within and across repositories and also help inform the use of such data. For example, adding metadata field(s) and/or flags indicating that a dataset is linked to sampling of an extreme event or manipulation experiment mimicking extreme events would not only facilitate larger-scale synthesis and/or modeling studies focused on extreme events, but it would also ensure that these data were not used to characterize baseline conditions. Adding this granularity to metadata will also require the community to agree on a common definition of “extreme” (e.g., perhaps some agreed upon percentage departure from established local baseline?). Dedicated time and resources will be required to support community consensus on the establishment of both a standardized set of core measurements and data and metadata reporting standards.

**Extreme event model development should be supported through integration with observations.**

Studying extreme events requires close interactions between observationalists and modelers, which should be fostered through community activities (workshops, hackweeks, field campaign design, etc.). The disconnect between modelers and observationalists stems in part from limited understanding of the different methods and vocabularies used by the two communities. Therefore, establishing common vocabulary, improving model and methodology documentation, and promoting mutual education would be highly beneficial. Some of the paths to achieve this integration include funding calls that encourage or even require projects to integrate observations and modeling, workshops aimed at cross-training and defining common terms, and communication outlets to foster sustained dialog and collaboration.

To ensure more effective outcomes, the collaboration between modelers and observationalists must begin at the early stages of a project, not after the project has ended. For example, modelers should be engaged in the planning of observing networks, field campaigns, and process studies to better understand data collection and interpretation challenges. Conversely, observationalists should partner with modelers in data synthesis and comparative analysis activities to better understand the computational and statistical methods involved. There are several types of activities that are ripe for these interactions. Synthesis and comparative analysis of event-scale datasets would be highly beneficial for model development and validation. Model intercomparison exercises are needed to determine sensitivity of key processes to different parameters and also identify missing processes in specific models and whether they are resolution-dependent. Intercomparison exercises would also allow us to assess the relative utility of property or stock measurements (nutrients, carbon, oxygen, etc.) versus flux or rate measurements in different regions. Stock measurements can be acquired from any platform or observing network, whereas fluxes and rate measurements are more complex, thus requiring greater investment of resources and time.

The drivers/forcings of biogeochemical processes during extreme events are, by definition, outside of the 'normal' ranges that have generally been better observed and parameterized. Thus, there is a need for high-resolution observations to constrain the length scales over which key processes vary, both in time and space under extreme conditions. This is particularly important for high-order and/or non-monotonic relationships. Defining the length scales of variability for key biogeochemical processes will establish benchmarks for the ideal convergence of observational and modeling resolutions. In practice, spatiotemporal resolutions will continue to be limited by available resources, but a better understanding of length scales will inform sensitivity analyses, cost-benefit decisions, and directions for new, more efficient approaches such as autonomous sampling and AI/ML-based parameterizations.

In the face of funding limitations for observations, there are also parallel recommendations that would improve the utility of models in the meantime. Regional models provide higher spatial resolution to better represent event-scale dynamics operating in coastal regions. Dynamical and statistical downscaling of global outputs could also improve models in a relatively short time frame and increase their use for decision making in the near future.

**Funding mechanisms to support international collaboration will positively impact research development around extreme events.**

There is a critical need for funding mechanisms that support collaborative research that transcends geopolitical boundaries, since extreme events are often linked to larger climate-ocean phenomena with impacts that span nations and ecological provinces. For example, one phase of the El Niño Southern Oscillation can simultaneously lead to increased cyclone activity and floods in North America and increased droughts and fires in Australia. The climate feedbacks and risks of these extreme events cannot be fully understood without well-coordinated modeling and observation activities at an international scale. There has been major progress toward this type of international collaboration, particularly in the fields of satellite observations, global ocean and atmospheric observation networks, community modeling activities (e.g., [FLAME](#)), and international community- and capacity-building initiatives like the UN Ocean Decade. Continued funding and community building mechanisms to support global collaboration will not only be more cost-effective, but will be critical to the development of a collaborative and coordinated extreme events research and monitoring network.

# Machine Learning

Authors: Sandupal Dutta, Anand Gnanadesikan and Rui Jin

Reviewers: Amanda Fay, Hayley Kwasniewski and Liz Perotti

Models that are used to predict ocean biogeochemical cycling encode a host of relationships between environmental variables such as temperatures and mixed layer depth, chemical fields such as nutrients and carbon, and biological fields such as phytoplankton and zooplankton biomass. A key question is whether these mathematical relationships realistically combine to produce the emergent behavior of the ocean biogeochemical system to allow predictions to be made in areas without observations. Because both the individual relationships and their combinations can be highly nonlinear, machine learning (ML) methods have the potential to serve as a methodology to capture them.

## **Spatiotemporal biogeochemical and observing coverage needs improvement to inform machine learning.**

Preliminary work has shown that ML methods can be used to improve satellite estimates of biogeochemical cycling (Ioannou et al., 2011), extrapolate in-situ observations of zooplankton (Moriarty and O'Brien, 2013), pCO<sub>2</sub> (Chen et al. 2019), and metals (e.g. Roshan, DeVries and Wu, 2020), merge transport models and tracers to capture rates of biogeochemical cycling (John et al., 2020), and to find the emergent relationships between biological variables and controlling environmental drivers (Rivero-Calle et al., 2015; Holder and Gnanadesikan, 2023). However, even these successes point to a number of required improvements in current observational efforts.

Chemical observations used for all of these applications are sparse in space and time, with much of the current effort for variables like pCFCs or metals focussed on a small number of repeat transects. While these measurements are critical, efforts to miniaturize sensors for a wide variety of tracers, enabling deployment on floats and gliders, could pay major dividends in understanding biogeochemically relevant shifts in ocean circulation. For example, while tracers like iron and ammonia are critically important predictors of phytoplankton biomass in observations and ESMs (Holder and Gnanadesikan, 2023), we do not have a picture of their spatiotemporal variability comparable to what we have for phosphate and nitrate.

In terms of biological observations, a leading theme amongst workshop participants was the need for better resolution of the biomass of both phytoplankton and zooplankton functional groups. For example, cyanobacteria, diatoms and coccolithophorids are known to have quite different impacts on carbon fluxes, but there remain significant differences between pigment-based and backscatter-based retrievals of their spatiotemporal distributions (Mouw et al., 2017). Similar issues exist for estimating trends in zooplankton biomass (Bezerra et al., 2023). A second example is that surface observations and remotely sensed ocean color measurements may not be representative of the whole water column. While we have large-scale measurements from acoustic doppler current profilers (Bianchi & Mislan, 2016) and backscatter profiles from profiling floats (Koestner et al., 2024), these techniques group multiple functional groups into a single measurement. A third opportunity exists in terms of understanding sub-monthly variability of biomass, which could better constrain raw growth and

loss rates, which tend to come into balance on longer time and larger spatial scales (Behrenfeld, 2010). And finally, while global datasets from programs like the Coupled Model Intercomparison Project and GEOTRACES are available to the research community, coastal datasets are often far less discoverable.

### **Data standardization, quality control, and open access will enable machine learning training on large datasets.**

One of the promises of machine learning is that it can find and use nonlinear relationships between biogeochemical variables by training on and synthesizing large datasets. Comparing such relationships may help resolve some issues introduced by the different temporal and spatial resolutions of model and observational data. However, there are a number of practical barriers to achieving this synthesis. One is the standardization and quality control of data so that measurements are comparable. For example, phytoplankton biomass is often tracked in models in terms of nitrogen, but estimated observationally in terms of chlorophyll. Which organisms are included within a functional group in observations is often not clear from available metadata. For example, the large and small phytoplankton are often designated at different thresholds or the cutoff is unclear for particular datasets. Continuous plankton recorder measurements are often reported in terms of presence/absence or counts instead of biomass. Raw data emerging from programs like GEOTRACES often shows clear biases between cruises and across methods. FlowCAM observations may depend critically on aspects of the operation of the instrument not reported in the literature (Owen et al. 2022). And while 'omics data can suggest which processes are important to model in a given region, converting them to estimates of biomass or rates remains challenging. Absent standardization and quality control and appropriate metadata, advanced ML methods run the risk of "garbage in-garbage out" with the additional problem that outlier detection is not as straightforward as it is with classical linear regression.

Obtaining model data for use in ML methods is relatively easy when it comes to global climate models participating in various global model intercomparison projects. However, observationalists are often uncertain how to use such information, as it cannot capture the particular conditions seen during a given experiment and is often at too coarse a resolution (both in space and time) to be useful for regional or coastal experiments. Making more output available from models forced by observations on both global and regional scales would be helpful. Standardization is also needed in terms of model outputs of phytoplankton community composition (PCC) both in terms of the constituent sub-classes in the PCC and the methodology followed for the classification. This will enable inter-comparison of results across different models using various statistical tools. Rapid advancements in the fields of Explainable and Interpretable AI give us new techniques of model interpretation that can be used for such analyses

Opportunities exist to make ML tools available to the community so that observationalists can compare relationships seen in models or derived from global datasets with those seen in individual cruises. Workshops that would bring the community together both to increase familiarity with these tools, their requirements and limitations, and to use them on both models and observations could be extremely useful producing insightful and robust comparisons between observations and model outputs.

# Marine Carbon Dioxide Removal

Authors: Alyse Larkin, Jacqueline S. Long and Cristina Schultz

Reviewers: Heather Benway, Joey Crosswell, Rui Jin, Nick Ward and Liza Wright-Fairbanks

Anthropogenic emissions of carbon dioxide (CO<sub>2</sub>) to the atmosphere have been the most significant driver of climate change over the past century. According to the IPCC 6th Assessment Report (AR6), strategies that remove carbon dioxide from the atmosphere are necessary to limit global warming to 1.5-2°C. In the marine environment, these strategies include ocean alkalinity enhancement, electrochemical and photochemical approaches to directly remove CO<sub>2</sub> from seawater (direct ocean capture); techniques to enhance the growth of primary producers through ocean fertilization, artificial upwelling/downwelling; macroalgal cultivation; and efforts to restore and protect natural carbon sinks. While early mCDR pilot studies and modeling efforts are already underway, there remains uncertainty about additionality, durability, and environmental impacts. Well-integrated modeling and observation efforts are vital to rigorous assessment of mCDR approaches.

## **mCDR efforts require strategic observing system deployments, co-developed models, and BGC sensor refinement.**

To enhance model development applicable to mCDR projects, a significant expansion of observing capacity is essential. This expansion should focus on deploying more sensors in diverse and strategic locations, including coastal areas and sediment pore waters. Observations need to capture metabolic rates, silica cycles, and microstructure measurements of turbulence to better understand local dynamics. The use of autonomous surface vehicles (ASVs), autonomous underwater vehicles (AUVs), water column profilers (e.g., wire walkers), and moorings will be instrumental in establishing strategically located observing platforms within an mCDR intervention site. These platforms will facilitate higher-resolution measurements in space, depth, and time, which are critical for refining models.

Furthermore, there is a need for a two-way interaction between modeling and observing strategies to optimize site selection and sensor placement for data collection (e.g., Observing System Simulation Experiments, OSSEs). The models must be able to accommodate higher-resolution biogeochemical observations, such as those provided by Biogeochemical Argo floats and other autonomous vehicles. They must also be able to simulate the mesoscale dynamics of micro- and macronutrient transport and their environmental impacts, which are crucial for accurate modeling of mCDR interventions involving biomass.

Ongoing refinement of sensors that can help quantify the carbonate system (e.g., pH, total alkalinity, pCO<sub>2</sub> and DIC) yields promise for a denser and more expansive network of observations that are essential for model validation. Growth in low-cost sensor production combined with ever-expanding autonomous platform options and vessels of opportunity (e.g., commercial fishing vessels) offer opportunities for cost-effective collection of observations with the spatiotemporal resolution that can support mCDR work, in which project developers are largely operating in a startup environment with limited funding.

**mCDR research can be accelerated through transparent data processes and novel data assembly centers.**

Regardless of funding source, transparency and public availability of data, methods, and software emerging from mCDR research, field trials, and model development is essential for the responsible advancement of mCDR as a viable climate mitigation strategy. Data management of mCDR experimental information should follow best practices that support FAIR (Findable, Accessible, Interoperable, Reusable) and CARE (Collective benefit, Authority to control, Responsibility, and Ethics) principles as established by the broader ocean science community. Given the wide range of stakeholders and prospective data users, as well as the applied nature of mCDR research, the management of these datasets presents unique challenges. For example, mCDR practitioners should focus on creating cloud-accessible gridded data and products with comprehensive data and metadata documentation. The development of minimum data and metadata reporting standards would facilitate data publication and uptake by models. The establishment of an international open portal to pre-register experiments would ensure that practitioners are aware of these reporting standards prior to their experiments and make their data more discoverable. Such a portal could also facilitate valuable dialog and collaboration between observationalists and modelers in the early stages of the project.

Two potential avenues for mCDR data management include the creation of new databases and products or the integration of these data into existing repositories. One advantage of novel data assembly centers and databases for mCDR is their potential to be tailored to meet the diverse needs of broad stakeholders in this emerging field. For example, data products that provide centralized resources to compile related experiments would help accelerate the field. Integration of novel mCDR databases into the IOC Ocean Data and Information System "Catalogue of Sources" would assist with international data synthesis. However, challenges associated with building novel data resources include difficulties with linking datasets to existing data synthesis products (e.g., SOCAT, GLODAP), issues of data provenance and sovereignty, and funding limitations. An alternative approach would be to integrate mCDR data into existing databases and repositories, which would necessitate the creation of common vocabularies and semantic tools to facilitate discoverability and aggregation of these data across repositories. AI-based approaches such as "OceanGPT" could assist with the process of integrating mCDR information into existing data services by providing improved search engine capabilities (i.e., discoverability), data synthesis, and end-user quality control.

**Communication between mCDR observationalists and modelers must be fostered through common vocabularies, discussion forums, and funding opportunities.**

Model development has largely relied on using varied sources of data collected for different purposes because funding opportunities to co-develop models and observational datasets are limited. Due to the lack of synchronicity, modeling and observational communities have also developed different scientific languages, with terms and definitions that are not always clear to each other. Because mCDR strategies rely on intentionally modulating different ocean variables, properly understanding the scales at which these disturbances act is of particular interest to all the scientific community working in this space. Therefore, establishing a common vocabulary and improving communication between modelers and observationalists throughout the planning

and implementation of research projects is a necessary first step to bridge some of the gaps in process understanding and scalability of mCDR interventions. Actions that could build integrated, interdisciplinary research include increasing funding opportunities focused on co-developing datasets and models and establishing well documented protocols that can be reviewed by both communities.

A discussion forum in workshops and conference sessions could help to identify mechanisms that need to be better represented in models. One such example that arose during this workshop is benthic processes, which are generally oversimplified in ocean models, thus limiting our ability to quantify the efficacy and potential deleterious effects of mCDR interventions that rely on burial. Benthic observations tend to be sparse, are largely concentrated in coastal areas that experience high spatiotemporal variability, and are acquired using a range of methods and technologies with limitations that are not always known to modelers. Given the centrality of the benthos to so many proposed mCDR approaches, a sustained dialog between benthic observationalists and modelers will be critical to informing the representation of benthic biogeochemical and ecological processes that impact mCDR efficacy and durability.

While improved communication between different scientific communities will lead to more comprehensive datasets that can be used to inform and validate models at different spatial scales, basic proof of concept experiments (such as actively burying organic matter in different environmental conditions) and high-intensity sampling campaigns in model-guided locations will be crucial to mechanistically represent mCDR strategies in models. Importantly, *in situ* mCDR experiments and perturbations may have long-ranging spatiotemporal impacts, which also must be monitored and reported in a transparent manner. Marine CDR experimental research will involve substantial investment of federal and private resources, interdisciplinary teams, and rapid timelines (data analysis, reporting, publication, etc.), which will require streamlined funding and evaluation mechanisms. For example, research funding must keep pace with venture capital investment, and data archiving methods and peer reviewing must be more efficient to ensure that information is made available quickly.

### **Early communication will prepare scientists for the execution of mCDR field trials.**

Enhancing communication between observers and modelers is essential in the current nascent stages of mCDR field trials. This connection facilitates the effective preparation and execution of these trials, ensuring that both observational insights and modeling forecasts are aligned and mutually informative. Multiple community platforms have already been established to foster these interactions. Webinars and workshops including discussions between modelers and observationalists have been held. To strengthen these relationships and have lasting impact, research that integrates observations and models should be prioritized by funding agencies, regulatory bodies, marketplace registries, and suppliers.

# Ocean Carbon Budget

Authors: Amanda Fay, Erica Ombres and Liza Wright-Fairbanks

Reviewers: Sandupal Dutta, Alyse Larkin, Jonathan Lauderdale and Anna Rufus

The ocean is one of the largest reservoirs of carbon on our planet, exceeded only by geological reservoirs. This makes the ocean carbon budget a key piece of the Earth's carbon cycle. Despite its importance to global climate dynamics and environmental policies, the ocean carbon budget is not thoroughly constrained. Equipping the marine biogeochemical observing system to produce useful data for carbon cycle models is critical for fully constraining the ocean carbon budget.

## **Targeted approaches to improving spatiotemporal and biological observing coverage will inform the innovation needs for developing carbon models.**

Temporal coverage was identified as one of the highest importance improvements for modelers. Higher temporal resolution observing, up to hourly measurements, would alleviate errors associated with fine-scale changes in the system. Winter has historically been under-sampled for biogeochemical parameters, and ensuring seasonal coverage in targeted areas would improve model fidelity.

Spatial coverage needs include subsurface and coastal measurements. The subsurface ocean is critical to storing carbon and mitigating climate change. Models of the subsurface ocean (below the surface layer; epipelagic to abyssopelagic) are often initialized with gridded data products. This type of forcing necessitates a synthesis of observing system data, but the current observing system does not capture measurements at the resolution required for such a product. Additional observing assets in the subsurface, combined with machine learning techniques, would aid the development of subsurface carbon products. Coastal zones are critical areas for protected marine species, human interactions with the environment, and terrestrial connections to the ocean carbon budget. Increasing observing capabilities in these dynamic areas will ensure accuracy in models attempting to close the ocean carbon budget.

Connectivity is critical in terms of the value of the ocean carbon budget in the broader Earth system given that the ocean is connected to the atmospheric and terrestrial carbon systems. Those linkages need to be addressed by both the observing and modeling communities. Additionally, integrating field ocean and satellite observations will help unlock opportunities for broad-scale surveys of ocean carbon from space.

Biological variables that are often under-observed were identified as a key gap in the existing observing system. For instance, viruses and the microbial loop directly influence the flow of carbon via mortality in the ocean. Simultaneous rate measurements of bacterial and phytoplankton communities are key to teasing apart the drivers of marine carbon cycling. Additionally, zooplankton food web dynamics and diel vertical migration contribute significantly to these processes.

Targeted approaches to designing carbon observing systems will play a tremendous role in helping to fully understand the ocean carbon budget. While it is important to increase observing capabilities through the addition of sensors and parameters, those increases will not be

impactful without ensuring they target areas key to understanding the various processes that control the ocean carbon cycle. Tailoring specific sensors to different environments can account for sources of error like regional variability, observing depth, maintenance access, and biofouling. Identifying key parameters and suitable sensors is the first step to improving the observing system. Observing system simulation experiments (OSSEs) can help determine the ideal carbon observing system (sensor- and network-wise) in an area.

Innovation is key to ensuring the carbon observing system gets the coverage it needs to inform models. Continued development of carbon system sensors and platforms designed with easy integration of those sensors in mind will keep the field moving forward. Connections between scientists, policymakers, and industry can contribute to positive developments in carbon observing and modeling. Effective communication between these groups, along with communication of the science to decision-makers, will ensure that observing and modeling efforts are impactful to society.

### **Collaboratively designing online platforms to support streamlined, standardized data search and submission will improve carbon observing system and model development.**

Streamlined data search and submission can help improve accessibility of the data. Searchable dashboards with the option to filter data by parameter, rather than by cruise or region, would greatly increase accessibility. Acknowledging that a whole system overhaul is hard, steps can be made to improve this process for many groups.

The design of online platforms for data access is an evolving topic in observing communities. In one example, the Argo float community, there are multiple data repositories for subsets of float data. On one hand, this creates a bottleneck for making data discoverable and digestible. On the other hand, it allows users to choose which host sites they find most accessible or think will have longevity of access for their purposes. An alternative option is to host standardized entrance points for accessing all available observations from specific platforms (e.g. Argo). However, broad synthesis efforts may encounter data sovereignty issues when attempting to combine datasets from multiple groups or nations.

Metadata standardization is crucial to ensuring compatibility across datasets. Ideally, data repositories should provide step-by-step instructions for submission of complete and accurate metadata. Units should be standardized to the extent possible to increase data usability. Data users often utilize observations that are easy to access, and including accurate metadata will ensure those observations are used correctly. Metadata reporting could be improved through standardization of uncertainty quantification and reporting. The metadata should, at a minimum, include a discussion of the factors causing uncertainty in each data set (e.g. system complexity, equipment limits) and the degree to which the data represent the system.

Collaboration between data managers and scientists will decrease bottlenecks and limitations. With open communication and incentivized cooperation, it would be easier to ensure that observations and submissions are standardized so that the community can use the data as well as report findings that will continue to prove the need for future research.

Machine learning and AI will help unveil currently hidden data correlations, but more observations are needed in order to gain additional, statistically significant insight from such methods. Observations must continue to be made consistently and with regularity so machine learning methods may be verified.

**Resolving contrasting resolutions between observations and models requires quantitative comparison studies and uncertainty analyses of ocean carbon uptake, transport, and storage.**

With recent computational advances, models are able to be run at increasingly fine resolutions. To ensure model accuracy, it is necessary to compare the output from those models to available observations. As model resolution improves, finer-grid cells require higher resolution in-situ data for cross comparisons. This may require sustained observations, observing system optimization experiments, and identification of areas with the greatest model uncertainty for targeted observing.

On the other hand, sometimes the observing system captures ocean processes that are beyond the model's present capabilities. Identification of those processes and the types of observations that inform them can help modelers determine the most effective improvements for their models. Additionally, it is possible that model output is accurate despite having inaccuracies in the model code (e.g. getting the right answer for the wrong reasons). Collecting data to validate the base equations that determine model output will help ensure accuracy.

For differing resolutions of modeled vs. in situ conditions, current best practices are to report an average of the observations within a model gridcell and time step. However, thought should be given to whether each of the included observations are of similar quality before taking a straight mean of the ensemble. Without such consideration, valuable information from high-quality observations could be lost or obscured.

**Ocean carbon budget knowledge sharing can be facilitated through synthesis products, online platforms, and in-person events.**

Having one go-to website or platform to host all relevant tools and data products along with contact information for the content creators would help reduce duplications of effort. Instead of redeveloping a data repository/archive that already exists, the research community could instead focus on improving or adding to existing data search tools. Currently, websites are focused on specific needs; for example, the Surface Ocean CO<sub>2</sub> Atlas ([SOCAT](#)) database hosts surface ocean pCO<sub>2</sub> data, and the Ocean Carbon and Acidification Data System ([OCADS](#)) database hosts ocean acidification data. Models are often hosted on project-specific websites and not commonly available from one central platform.

A common concern is ensuring that existing databases are able to talk to or query one another. This type of machine-to-machine connectivity could be assisted by AI and machine learning methods. Artificial intelligence is an emerging resource for the ocean carbon community and while technology allows for advancement in machine learning and data extrapolation, there is no substitute for real observations of the world's oceans. Observations must continue to be made

consistently and with regularity because without that the machine learning methods are unverifiable.

Another way to enhance these connections or relationships is to support workshops at the beginning of research programs that provide base level information for utilizing observing data. For example, BGC Argo workshops are held to walk users through data types, data format, data access, and various open access tools that can be used for data processing.

Time, effort, and funding are required to facilitate training and knowledge exchange between observers and modelers. Hosted discussion opportunities could help to mature the relationships between observationalists and modelers. Grant programs should take into consideration the time it takes to establish these relationships and provide sufficient time and resources in their award packages.

Within the BGC observing and modeling communities, each researcher has their own priorities and goals. Currently, there is not a system for easy communication of those priorities between models and observationalists. Strengthening communication and collaboration between observers and modelers is key to move the field forward. Observations are often collected opportunistically without a systematic approach that would prioritize collection in regions and times of the year that are most needed for models. Modelers may not have specific needs until a model is built and run, but funding and project momentum can be lost between the model run and any follow-up observation needs. Community conversations and open-access resources are a minimum for moving this field toward achieving its end goals.

# Ocean Acidification

Authors: Alexa Labossiere, Yifan Zhu,

Reviewers: Anand Gnanadesikan, Liz Perotti, and Liza Wright-Fairbanks

Ocean acidification (OA) refers to the ongoing change in seawater chemistry across Earth's oceans, primarily driven by the absorption of about a quarter of anthropogenic carbon dioxide (CO<sub>2</sub>) emissions (Friedlingstein et al., 2023). This process decreases ocean pH levels and carbonate ion concentrations, impacting the formation of calcium carbonate-based structures of marine organisms such as corals, shellfish, and certain planktonic species, which might have cascading effects on marine food webs and ecosystem functioning.

## **Ocean acidification observing systems should be targeted to critical and historically undersampled ecosystems.**

Understanding the historical evolution of ocean acidification across time and space is essential for assessing its severity and projecting its impact on marine ecosystems. However, limitations in observational data present challenges for accurate model hindcasts, so data coverage needs to be enhanced in time and space. There are historical data limitations due to a scarcity of high-quality dissolved inorganic carbon (DIC) and total alkalinity (TA) data before 2005, which hinders accurate hindcasts necessary for historical comparisons. Limited accessible carbon system measurements further impede validation of hindcast models. Additionally, there are spatial heterogeneity challenges as coastal zones exhibit greater variability than open ocean environments. That means that high resolution observational data are needed to accurately capture these variations in regional ocean models.

Particularly critical impacts of ocean acidification are likely in the subsurface (or bottom depths in coastal systems), where water rich in CO<sub>2</sub> is close to being undersaturated with respect to aragonite due to multiple oceanographic and biogeochemical processes. Current observation approaches primarily focus on surface waters, and so there is a need for increased data collection from deeper depths to understand OA related processes. Expanding the range of measured carbon parameters, like organic alkalinity, is also necessary for a comprehensive understanding of the marine carbon cycle. Additional OA-related data, specifically calcification rates, are not commonly collected, but are important in understanding the consequences of OA on marine biota. More calcification rate measurements and studies on the feedback between OA and calcification are needed to help incorporate OA impacts to biota into ocean models.

Ensuring data quality and implementing data quality control (QA/QC) measures in observational datasets is crucial as models rely on these data for parameterization and validation. Verifying the quality of data obtained from various databases presents significant challenges, potentially impacting the reliability of model outputs. Defining the acceptable data quality standards and providing information on measurement uncertainties is essential for assessing the reliability of "climate" and "weather" quality data (e.g., Tilbrook et al., 2019). There have been issues of data quality identified with measurements based on sensors. Sensors are susceptible to drifting, particularly for real-time pH, *p*CO<sub>2</sub>, DO, and nitrate measurements in the Ocean Observatories Initiative (OOI), and thus often suffer from issues related to data quality and lack regular updates

of QA/QC'd data. Therefore, data curation via thorough QA/QC procedures are essential to ensure data integrity and credibility.

**Assessments of existing ocean acidification and carbon databases will help inform gaps and best practices for future data management efforts.**

Enhancing discoverability for stakeholders, particularly model developers, is essential. Numerous databases and portals are available, organized from national (e.g., [NCEI-National Centers for Environmental Information](#), [BCO-DMO- Biological & Chemical Oceanography Data Management Office](#), [SeaBASS- SeaWiFS Bio-optical Archive and Storage System](#), [IOOS National Data Portal](#)) to regional level (e.g., [NANOOS-Northwest Association of Networked Ocean Observing Systems](#), [MARACOOS- Mid-Atlantic Regional Association Coastal Observing System](#), [Chesapeake Bay Program DataHub](#), [San Francisco Estuary Institute Regional Data Center](#), [CalCOFI- California Cooperative Oceanic Fisheries Investigations](#)), as well as program based (e.g., [OOI](#), [Argo](#), [GEOTRACES](#), [GO-SHIP-Global Ocean Ship-based Hydrographic Investigations Program](#), [LTER- Long Term Ecological Research](#)). Despite this, many scientists are still unaware of their existence, leading to underutilization, and may encounter challenges in comprehending the differences among databases. For example, NCEI aggregates data from various sources, while other databases, like OOI, maintains its own data portal, further complicating accessibility. Regional databases provide localized support for modelers but comparing them with larger-scale global databases like the [World Ocean Database \(WOD\)](#) and [Global Ocean Data Analysis Program \(GLODAP\)](#) presents challenges such that users are often uncertain if there is overlap among these databases. Therefore, it's essential to assess whether global scale datasets already include regional datasets. In addition, all of these data repositories and portals differ in metadata and data quality requirements.

There are existing databases and data portals, such as the [Ocean Carbon Acidification Data System \(OCADS\)](#), [Global Ocean Acidification Observing Network \(GOA-ON\)](#) data portal, and [The Surface Ocean CO<sub>2</sub> Atlas \(SOCAT\)](#) data portal, which act as specialized repositories for OA data, but require increased publicity and user engagement to optimize utility. We would recommend creating a database catalog to assist modelers in navigating and accessing these resources. Moreover, official tutorials and tutorial videos should be made readily available on these databases' websites to enhance accessibility. User-friendliness is important and databases like OCADS, which offer indexing by variable type, are praised for their ease of use, facilitating improved data discovery and application. Furthermore, databases could aim to develop visualization tools to enhance user experience, similar to the MODIS satellite database. Additionally, some large, publicly accessible databases face challenges related to data quality and irregular updates of QA/QC'd data, so greater standardization and transparency of data quality control between databases would be helpful with maintaining consistent data standards. There is a growing trend towards mandatory data sharing in many scientific journal policies. Further enforcement and expansion of these policies across more agencies and institutions is necessary to ensure open access to data. Open data initiatives are vital and existing programs, like the European Copernicus program, are a precedent for open data in models, serving as an example for other regions and disciplines.

## **Existing observational data can validate ocean acidification models, but limitations persist.**

Coupled interdisciplinary model systems provide a powerful tool to construct continuous oceanic fields in space-time that cannot be achieved through observations alone. Model simulations provide a four-dimensional framework for the analysis of coupled physical-biological-chemical processes that is not accessible by any other means. However, it is absolutely crucial that these models be firmly grounded in data, in order to make these simulations truly relevant to the real ocean. Improved computer capabilities have made higher spatial resolution models more feasible and many models (e.g. down-scaled regional models) exist at high enough resolutions to simulate ocean acidification processes. However, resolution can be a significant problem for observational data as there are tradeoffs between spatial and temporal resolution. It is also difficult to create climatological records from traditional cruise based data, which tends to be collected in limited time periods and locations.

Recent development of integrated ocean observing systems capable of collecting data continuously has improved the temporal resolution of OA data. Profilers and autonomous observing vehicles are able to improve spatial resolution, but may sacrifice temporal resolution. Data quality varies between sensors and climate-quality laboratory analyses, making it difficult to compare between different modes of observing. For example, pH sensors are common, but are rarely climate-quality. Sensors for other carbon related variables (e.g. DIC and TA), are not currently available, so there is a need for continued development of high-quality, cost-effective sensors for all carbon related variables.

Leveraging existing observational data to validate model simulations is crucial for testing model credibility. The conjoining of observations and models not only provides a useful methodology for process studies, but also maximizes the utility of observations and aids in their interpretation. Although expanding the spatial and temporal resolution of OA observations is vital, obtaining climate-quality data is equally important.

## **Cross-discipline communication provides the opportunity for creating universal terminology and identifying underutilized ocean acidification resources.**

There are existing channels to connect observers and modelers, but more conversations and collaborations are still necessary. Workshops to connect observers and modelers in the ocean acidification field have been held, but more workshops would help connect observationalists and modelers and facilitate conversations. A barrier to this communication is lack of common language between the two groups, so it is important that there are opportunities for translating between the disciplines or establishing universal terminology and definitions to help with communication. Language workshops have been held at the University of Bergen to share and help establish these definitions. A workshop titled “Co-creating a shared framework for ocean data management: Finding common ground on terminology” will be held in Fall 2024 at The North Pacific Marine Science Organization ([PICES](#)) annual meeting. [US CLIVAR](#) also hosts a meeting in Fall 2024 to bring scientists from different disciplines together to fill the gap and optimize ocean observing networks. Another major existing channel of communication is through interdisciplinary projects. Collaboration between observationalists and modelers from

the beginning of the research rather than at the end as an afterthought is important in ensuring efficient flow of information and help ask better questions. Funding agencies should prioritize these interdisciplinary projects to encourage these collaborations.

One major gap in these conversations and collaborations is the lack of accessible and available modeling data for observers. Just as observations are vital for model development and validation, model output can be very useful to observers, but is currently underutilized. Model output can be useful in cruise planning by helping with site selection and model-based ocean forecasting systems can even give real-time predictions of ocean conditions. There are some existing model-based visualization systems where live OA related output (e.g., aragonite/calcite saturation state) is viewable, such as [LiveOcean-NANOOS](#), [OCEANSMAP-MARACOOS](#), and [CBEFS](#), but getting access to archived model output can be more difficult. All the model output is not always publicly available although some journals require the model output publication. Observers may struggle to figure out where or who to go to for model output access and there can be logistical concerns including file storage constraints that can prevent access. More frequent publishing of model output (St-Laurent and Friedrichs, 2024), especially in easily-accessible formats would be useful in connecting observers and modelers. This could be in a format of an integrated network of regional model output.

# Polar Systems

Authors: Cynthia Garcia, Hayley Kwasniewski

Reviewers: Yajuan Lin and Cristina Schultz

Polar regions are crucial to Earth's biogeochemical cycles, profoundly affecting global climate systems and marine ecosystems. Their sensitivity to climate change and their crucial role in global processes like carbon and nutrient cycling underscore their importance. Recent advancements in observation technologies, such as autonomous platforms and remote sensing, have mitigated some challenges associated with data collection in these remote and extreme environments. Despite this progress, there remains an urgent need for better integration of observations into models to more accurately capture the complex interactions within these systems. Moreover, the expansion of data collection into underrepresented areas and seasons, particularly during polar winters, is critical. This includes improving data resolution and interoperability to better align observational data with model requirements, thereby enhancing model development and predictive capabilities in both the Arctic and Antarctic regions.

## **Comprehensive data collection, multi-platform observation integration, and model development are needed in polar regions.**

Several key challenges and needs emerged in identifying current gaps in observations for model development in Polar regions. These include better resolution of temporal and spatial scales, enhanced data collection in underrepresented areas and seasons, and better data interoperability and usability. There was consensus on the need for better resolution of different temporal and spatial scales to meet diverse modeling needs in both the northern and southern high latitudes. This is underpinned by both the current state of polar research and the specific requirements of model development. Models often require data with high spatial and temporal resolution to accurately simulate complex processes. However, current observations are frequently limited to broader scales due to logistical and technological constraints. The variability is often lost in coarser datasets, leading to models that may oversimplify the real complexity of the environment. There was also a need to resolve seasonal biases in data collection, particularly during the winter months. The dynamic nature of polar environments, characterized by rapid changes in conditions, also requires observations that capture these fast transitions (e.g., ice melt and formation).

There was also a strong call for more comprehensive data collection in high-latitude regions. The geographical coverage needs expansion, especially in areas like under sea ice where key biogeochemical processes occur. The Southern Ocean was highlighted for its data collection bias towards specific areas like the Weddell Sea and the Drake's Passage. Areas like the coastal regions lack necessary observations like ice-shelf melt rates and other biogeochemical parameters. Additionally, global reanalyses often exhibit a bias toward lower dissolved inorganic carbon (DIC) in shelf and coastal regions, primarily because most of the data is sourced from open ocean areas and fails to account for changes occurring on the shelf. In the Arctic, there are fewer observations on the Eurasian side due to physical processes and geopolitical limitations. Expanding data collection to include more diverse regions and conditions would provide a more accurate representation of these environments in models.

Another major theme was the need for improved interoperability of observational data from various sources to enhance model development. This includes making observation data easier to interpret and use in models and using known and widely used metadata standards. The discussions highlighted the importance of converting observational data into forms that are interoperable and reusable. This also includes providing data that are spatially and temporally resolved and focusing on essential rate parameters like mortality rates, grazing rates, respiration, and primary and secondary production.

To enhance observational practices for model development in polar research, integrating ship-based hydrographic and process surveys (GO-SHIP, LTER), emerging technologies such as autonomous platforms (BGC-Argo floats, Saildrones, and Wave Gliders), and remote sensing is vital for improving data resolution across diverse and harsh conditions. Interdisciplinary approaches that combine physical, chemical, and biological observations, including 'omics' data, will enhance the comprehensiveness of datasets, aiding in the understanding of cross-scale interactions. Furthermore, establishing long-term monitoring stations and advocating for community-wide standards in data collection and processing will ensure the generation of compatible and detailed time series, essential for accurate model simulations and broader scientific analysis.

### **Unified databases with advanced search capabilities will enhance data discoverability and usability in polar research.**

To enhance discoverability, synthesis, and model development through data management practices, workshop participants identified several key areas for improvement, each of which supports a more integrated and effective use of biogeochemical data in polar research. This includes better data discoverability and accessibility, supporting efforts towards standardization and interoperability, enhancing communication and collaboration between observationalists and modelers, investing in training and capacity sharing, and implementing effective data management policies.

One of the primary discussions centered around the need for better data discoverability and accessibility through integrated databases that consolidate data from multiple sources, such as NOAA, NASA, or NSF. Participants suggested creating federated or unified databases to facilitate easier access to a comprehensive array of datasets. This would not only enhance the usability of the data but also ensure that various data types, from historical to real-time datasets, are readily available for synthesis and analysis. Developing these databases with advanced search functionalities (i.e., incorporating AI) data analytics, and user-friendly applications is crucial to supporting the broader research community. There was also a strong consensus on the importance of standardizing data collection methods and formats. Standardization would ensure that data from different times and places could be easily compared and synthesized, addressing interoperability issues that currently hinder effective data integration. This includes adopting common protocols and methodologies, exemplified by initiatives like GEOTRACES, which facilitate inter-calibration and data comparison across international research efforts.

Finally, there was a call for policies that ensure funding for data management is included in research proposals or in Data Management Plans (DMPs). This approach would help maintain

high standards in data archiving and retrieval, ensuring that both new and historical data remain accessible and useful for ongoing and future research initiatives.

**Sustained in-situ observing is necessary in polar regions to alleviate resolution differences between models and observation.**

Some of the previously mentioned solutions would also support resolving resolution differences between data and models. Data assimilation and the development of consistent data storage processes will foster conversations between modelers and observationalists. Further, greater, more holistic on-the-ground seasonal and geographic data collection in the polar systems will remain a top priority. This should include, but is not limited to, sustained repeat-hydrography, mooring with high temporal resolution, optimization of sensor placement, and interdisciplinary process studies. AI has also been identified as a tool with the potential to address contrasting resolutions between data and models. Lastly, models require both stationary and non-stationary data to develop analyses, and modelers should be able to access newer data as it comes. This should be considered when developing observational studies, both in method of acquisition and storage.

**Early career training and education in polar research can improve collaboration between observers and modelers.**

Enhancing communication between data managers, observational scientists, and modelers was also highlighted as essential. The workshop discussions pointed to the need for platforms and tools, workshops, and webinars that facilitate direct interactions and enable modelers to specify their data needs. Such tools and targeted discussions would help align the terminologies and expectations between different communities, thus improving the data's overall utility for modeling purposes.

Investing in resources for training and education, particularly for early-career scientists, also emerged as a significant theme. Workshops and training programs focusing on data management, coding, hackathons (i.e., Ocean Hack Week), and the integration of observational data into modeling frameworks are necessary to equip the next generation of researchers with the skills needed to navigate the complexities of biogeochemical data. Additionally, workshops and conferences that bring observers and modelers together to discuss connections (e.g., interdisciplinary discussions during the LTER annual meetings), share ideas, and move forward new objections would improve data analysis for the long term. Working with networks/affinity groups that focus on observational data and modeling provides platforms with existing cohesion and/or community that may improve coordination and collaboration.

# Trophic Interactions

Authors: Anand Gnanadesikan, Kyla Kelly and Hayley Kwasniewski

Reviewers: Jenna Lee and Liza Wright-Fairbanks

Studying trophic interactions requires a comprehensive understanding of entire marine ecosystems, 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. However, increased communication, improved data management, and emerging technologies can be used to improve analyses.

## **Ecosystem modeling is challenged by the need for biological rate measurements at high spatiotemporal resolution.**

We can learn a lot about the role of zooplankton in biogeochemical models by considering the implications of the fact that on monthly time scales and spatial scales of hundreds of km, the phytoplankton growth rate  $\mu$  and mortality rate  $\lambda$  are roughly in balance (Behrenfeld, 2010). As described in Dunne et al. (2005), if the mortality rate  $\lambda$  has some dependence on the phytoplankton biomass  $P$  (i.e.  $\lambda = F(P) = \mu$ ) we can invert this balance so that biomass is a function of growth rates.

While oversimplified, this idea illustrates some key truths about ecosystem modeling. First, the solutions developed by ecosystem models are emergent, involving the interaction of growth and the functional dependence of mortality on biomass. This is challenging, as some of these rates are very hard to measure at one location, never mind across environmental conditions. Moreover, because by necessity models must group a range of disparate organisms into functional groups, phenomena like “the grazing of phytoplankton by zooplankton” or “averaged zooplankton mortality” are themselves emergent from a host of specific interactions between the species making up each functional group. Second, model solutions are very sensitive to rates and to their formulation. For example, if the zooplankton grazing  $\lambda$  has a different dependence on temperature than phytoplankton growth rate  $\mu$ , biomass will reflect this dependence.

Additional coverage of biological sampling across seasons and in undersampled regions would fill critical knowledge gaps and enhance model development of trophic interactions. This could be achieved by deploying more Imaging FlowCytobots (IFCBs), tow cameras, and other automated sampling technologies in undersampled regions to collect continuous data year round. Imaging technologies identifying zoo- and phytoplankton community composition and size distribution would enable models to better constrain food web transfers. Machine learning algorithm development may also enhance data interoperability.

## **Pre-observation communication between observers, modelers, and all involved parties can improve the observation-database-modeling pipeline for complex and under-observed trophic interactions.**

Trophic levels, which are inherently complicated and connected in ways we do not completely understand, are challenging to model. There is a current gap between what is recorded by observations and what is needed to develop, run, and adjust models. Model parameterization

often requires observations like rate measurements and quantifying and reporting size fractionated groups vs the more general label of copepod or phytoplankton. This disconnect is caused by a lack of communication, inconsistent data reporting standards, and barriers to accessing observational data. Changing data management practices could alleviate some of these issues. Improved communication between observers and modelers, increased data accessibility, and standardized data reporting represent promising solutions to better understanding trophic interactions.

Observing ocean processes is a complicated task requiring significant time to plan and align funding, equipment, vessels, and personnel. On board vessels, trophic interactions represent a potentially more time-consuming process (e.g., locating individuals/populations and remaining in one general place long enough to make worthwhile observations). Sometimes the method of data gathering cannot change (e.g., fishery vessels gather important data for the scientific community, but prioritize fishery research over piggyback projects). However, communication early on and throughout the observation-database-modeling pathway can help address mutual interests when possible. Communicating what kinds of data are useful and knowledge-sharing between parties early in the planning process is critical. This communication should include all parties reasonably involved, i.e., industry partners, observers, database managers, and modelers. Using the fishery example, communication, collaboration, and/or incentivization with industry partners could improve data observation outcomes by coordinating specific sample/data collection times that are relevant to multiple parties. Modelers and database managers could collaborate on ways to house data that allow for easy application to scientific inquiries.

Complicating analysis further, different data streams utilize different formats (e.g., depth in the water column is reported as negative and positive values depending on the source). The community would greatly benefit from the standardization of data reporting that includes consistent usage of variable names and formats. Clear descriptions of data type, available access platforms/files, and which data are in such files would further improve usability. Accessing data online is another barrier to completing modeling experiments. Making databases more discoverable and user-friendly would improve efficiency. Databases should also enact standard protocols for data manipulation, re-uploading, and metadata. For example, data should be static and not removed after publishing. This would require collaboration with database managers. Budgeting for this critical part of data science should be more commonplace, and perhaps even required, in grant applications, ensuring effective ways to share data. Furthermore, artificial intelligence may be a useful tool in aggregating data.

### **Community relationships and sustained funding can help provide an observational baseline to assess biological change through models.**

One potential approach to closing the resolution gap is to focus on matching community relationships, rather than spatiotemporal distributions of organisms. For example, given measurements of primary productivity and distributions of biomass, some of the key rates needed for modeling can be inferred from relationships between trophic levels, such as those described in Section 5.1 (Dunne et al. 2005). Furthermore, modelers need a better observational baseline to compare and assess variability and change. Spatially and temporally

high resolution observations must be sustained and expanded to continue providing key data for models. However, current funding structures (e.g., 3 year grant cycles) do not support sustained observations, nor an adequate time frame for both collecting and analyzing interannual observational data. Alternative grant structures should be considered to support these types of projects. Finally, data should be collected with a resource management perspective (i.e., for higher fishery-relevant trophic levels). It is important to consider stakeholder and end-users of these models so the necessary data can be collected. Therefore, goal-oriented and focused data collection are necessary for obtaining desired models and products.

**Cross-training and targeted workshops will strengthen modeler-observer relationships and co-produced science to improve understanding of trophic interactions.**

Modelers should know where their data comes from and observers should know how their data is used/constrained in models. Cross training may be an effective way to foster better understanding between modelers and observers. Encouraging both groups to attend each other's workshops and meetings, focusing on early career scientists, and hosting workshops specifically designed to bring both groups together, could be effective for improved connection and communication. Additional training opportunities (e.g., modeler participation in research cruises) could foster better understanding between the two groups. Industry representatives should also be included in these conversations.

# References

- Behrenfeld, M. J. (2010). Abandoning Sverdrup's critical depth hypothesis on phytoplankton blooms. *Ecology*, 91(4), 977-989.
- Bezerra, W. C. A., Figueiredo, G. M., & Kozlowsky-Suzuki, B. (2023). Can we meaningfully estimate the impacts of climate on zooplankton biodiversity? A review on uses and limitations of marine time series. *Marine Pollution Bulletin*, 195, 115515.
- Bianchi, D., & Mislán, K. A. S. (2016). Global patterns of diel vertical migration times and velocities from acoustic data. *Limnology and Oceanography*, 61(1), 353-364.
- Chen, S., Hu, C., Barnes, B. B., Wanninkhof, R., Cai, W. J., Barbero, L., & Pierrot, D. (2019). A machine learning approach to estimate surface ocean pCO<sub>2</sub> from satellite measurements. *Remote Sensing of Environment*, 228, 203-226.
- Dunne, J. P., Armstrong, R. A., Gnanadesikan, A., & Sarmiento, J. L. (2005). Empirical and mechanistic models for the particle export ratio. *Global Biogeochemical Cycles*, 19(4).
- Friedlingstein, P., O'Sullivan, M., Jones, M. W., Andrew, R. M., Bakker, D. C. E., Hauck, J., et al. (2023). Global Carbon Budget 2023. *Earth System Science Data*, 15(12), 5301–5369. <https://doi.org/10.5194/essd-15-5301-2023>
- Holder, C., & Gnanadesikan, A. (2023). How well do Earth System Models capture apparent relationships between phytoplankton biomass and environmental variables?. *Global Biogeochemical Cycles*, 37(7), e2023GB007701.
- Ioannou, I., Gilerson, A., Gross, B., Moshary, F., & Ahmed, S. (2011). Neural network approach to retrieve the inherent optical properties of the ocean from observations of MODIS. *Applied Optics*, 50(19), 3168-3186.
- John, S. G., Liang, H., Weber, T., DeVries, T., Primeau, F., Moore, K., ... & Taburet, G. (2020). AWESOME OCIM: A simple, flexible, and powerful tool for modeling elemental cycling in the oceans. *Chemical Geology*, 533, 119403.
- Koestner D., Stramski, D & Reynolds R. A. (2024) Improved multivariable algorithms for estimating oceanic particulate organic carbon concentration from optical backscattering and chlorophyll-a measurements , *Frontiers in Marine Science*,10 <https://www.frontiersin.org/articles/10.3389/fmars.2023.1197953>
- Mouw, C. B., Hardman-Mountford, N. J., Alvain, S., Bracher, A., Brewin, R. J., Bricaud, A., ... & Uitz, J. (2017). A consumer's guide to satellite remote sensing of multiple phytoplankton groups in the global ocean. *Frontiers in Marine Science*, 4, 41.
- Moriarty, R., & O'Brien, T. D. (2013). Distribution of mesozooplankton biomass in the global ocean. *Earth System Science Data*, 5(1), 45-55.
- Owen, B. M., Hallett, C. S., Cosgrove, J. J., Tweedley, J. R., & Moheimani, N. R. (2022). Reporting of methods for automated devices: A systematic review and recommendation for studies using FlowCam for phytoplankton. *Limnology and Oceanography: Methods*, 20(7), 400-427.

Rivero-Calle, S., Gnanadesikan, A., Del Castillo, C. E., Balch, W. M., & Guikema, S. D. (2015). Multidecadal increase in North Atlantic coccolithophores and the potential role of rising CO<sub>2</sub>. *Science*, *350*(6267), 1533-1537.

Roshan, S., DeVries, T., & Wu, J. (2020). Constraining the global ocean Cu cycle with a data-assimilated diagnostic model. *Global biogeochemical cycles*, *34*(11), e2020GB006741.

St-Laurent, P., Friedrichs, M. A. M. (2024). An atlas for physical and biogeochemical conditions in the Chesapeake Bay. SEANOE. <https://doi.org/10.17882/99441>

Tilbrook, B., Jewett, E.B., DeGrandpre, M.D., Hernandez-Ayon, J.M., Feely, R.A., Gledhill, D.K., et al. (2019). An enhanced ocean acidification observing network: from people to technology to data synthesis and information exchange. *Front. Mar. Sci.* *6*, 337. <https://doi.org/10.3389/fmars.2019.00337>