4D-BGC: Coordinating the Development of Gridded Four-Dimensional Data Products from Biogeochemical-Argo Observations

Working Group Proposal Submitted to SCOR 2023

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1 Summary/Abstract

Substantial advances in oceanographic observation have been made in recent decades, allowing scientists to address questions relating to ocean physics and biogeochemistry on previously unattainable spatial and temporal scales. Remote sensing technology (1970s-pres.) has enabled highly resolved views of surface ocean properties and the Argo array (2000s-pres.) has generated unprecedented ocean interior temperature and salinity observations. The Biogeochemical (BGC) Argo array has grown over the early 21st century, and its planned expansion will soon generate ocean interior carbon, oxygen, nutrient, and optical data with near-global coverage. Four-dimensional (4D; latitude × longitude × depth × time), gridded, and gap-filled data products of these ocean interior properties are being developed. These products will enhance data accessibility and ease data interpretation, transforming our understanding of ocean biogeochemical processes such as carbon fixation, export and remineralization, ocean acidification, deoxygenation, and nutrient cycling. Regular updates to these 4D-BGC products will allow scientists and decision-makers to monitor changes to important biogeochemical processes in near-real-time. We propose a SCOR working group to facilitate discussion and coordination among different scientific communities around developing, validating, and distributing 4D-BGC products from observational datasets, with a focus on the BGC-Argo array. The emphasis on international and cross-disciplinary collaboration, aimed at addressing global oceanographic challenges, makes this topic highly suitable for a SCOR working group. The ultimate goal of this initiative is to significantly enhance access and utility of BGC observations through 4D-BGC products, and thus refine our understanding of ocean biogeochemistry, improve models and reanalysis products, and inform policy decisions.

2 Scientific Background and Rationale

2.1 Anthropogenic perturbations to the ocean

The ocean is undergoing rapid physical and chemical changes associated with anthropogenic perturbations to the Earth system. About 91% of all anthropogenic heat has been taken up by the ocean (Forster et al., 2021), which has increased ocean surface temperatures by about 0.88 °C since the late 1800s and 0.60 °C since 1980 (Fox-Kemper et al., 2021). Concurrently, the surface ocean has acidified at a rate of 0.017–0.027 pH units per decade and the upper oceans (0–1000 m) have lost about 2% of their oxygen inventory (Canadell et al., 2021).

In the context of this global ocean change, the evolutions of key biological processes like surface primary production and the biological carbon pump are uncertain, largely due to a lack of globally distributed appropriate observations (Boyd, 2015). In particular, seasonal to interannual variability and long-term trends of these critical biogeochemical processes are not well understood. Earth System Models (ESMs) indicate that the biological carbon pump will be altered by physical and chemical ocean changes (Kwiatkowski et al., 2020), and variations in the amount of carbon transported from the ocean surface to depth could have massive implications for future climate (Kwon et al., 2009).

2.2 Argo history

Beginning in 1999, autonomous floats (i.e., Argo floats) measuring temperature, salinity, and pressure and profiling from the surface to 2000 meters every 10 days began being deployed throughout the global ocean (Roemmich et al., 2019). By 2004, the Argo array was global in scale and has been sustained since, allowing for accurate quantification of regional to global heat and salinity budgets in the upper two kilometers of the ocean. The more recent implementation of the Deep-Argo mission (Zilberman, 2017), which deploys floats that profile to 6000 meters, has led to a better understanding of heat uptake by the deep ocean (Johnson et al., 2019).

In addition to the Core and Deep Argo arrays that provide measurements of physical parameters, the Biogeochemical (BGC) Argo program (Biogeochemical-Argo Planning Group , 2016; Claustre et al., 2020) deploys floats equipped with at least one chemical or biological sensor. The extent of the BGC-Argo array is rapidly expanding, with a vision for a sustained array of 1000 BGC-Argo floats distributed globally and measuring six core BGC variables (dissolved oxygen, pH, nitrate, downwelling irradiance, suspended particles, and chlorophyll-a concentration) by the end of this decade (Owens et al., 2022). BGC sensors may also be implemented more widely on Deep-Argo floats in the near future (Roemmich et al., 2019). Core, Deep, and BGC missions are now integrated as OneArgo, which is a sustained action for the UN Ocean Decade.

2.3 Argo-based data products

In their native format, Argo data files provide measured parameters and associated quality flags at a profile-level (Bittig et al., 2019). This differs from the way satellite observations and model outputs are delivered, i.e., in gridded format at defined spatial and temporal resolutions. To bridge this gap, efforts have been made to translate profile-level Argo data into four-dimensional (4D) gridded and gap-filled products of ocean temperature, salinity, and heat content (e.g., Roemmich and Gilson, 2009; Oke et al., 2022; Lyman and Johnson, 2023). These spatiotemporally consistent gridded products of ocean interior physical properties enable the quantification of global to regional and diurnal to interannual variability, as well as anthropogenically forced trends, generating unprecedented insights about ocean heat uptake, steric sea level rise, and patterns of evaporation and precipitation (Johnson and Lumpkin, 2022).

Compared to physical ocean properties, relatively few global-scale, observation-based insights into ocean interior biogeochemical properties and processes have been drawn, largely due to a lack of spatiotemporally consistent 4D-BGC gridded data products. Furthermore, existing estimates often disagree and carry substantial uncertainties. For example, observation-based estimates of historical upper ocean deoxygenation range between 1.35% and 2.70% from 1970 to 2010 (Bindoff et al., 2019) and estimates of the annual net oceanic carbon uptake and ocean interior storage changes differ by a quantity larger than the cumulative annual carbon emissions of the European Union (Friedlingstein et al., 2022).

With the expansion of the BGC-Argo array and the commitment to OneArgo, we are on the precipice of generating paradigm-shifting insights into ocean biogeochemical variability and anthropogenically forced trends, with 4D-BGC products being an important component of this effort. These products will need to be carefully prepared, as BGC-Argo data is much sparser than Core-Argo data. Filling biogeochemical gaps in time and space therefore requires more advanced gap-filling methods, such as machine learning approaches. Proper uncertainty estimates are important to include alongside gap filled products, and can be obtained by comparing gap-filled data to direct observations or by replicating the gap-filling procedure on synthetic data generated from ocean model output, a strategy referred to as an observing system simulation experiment (OSSE).

Some early examples of 4D-BGC products include: bio-optical properties extended from the surface to depth by training machine learning models with BGC-Argo data (Sauzède et al., 2016); dissolved inorganic carbon mapped using ship data and a cluster-regression machine learning approach (Keppler et al., 2023a); and dissolved oxygen mapped using machine learning with Core and BGC-Argo data (Sharp et al., 2022). As efforts like this are pushed forward — generating critical, novel insights into magnitudes and variability of regional and global ocean biogeochemical processes in four dimensions — community coordination in the preparation, validation, evaluation, and dissemination of 4D-BGC products is crucial.

2.4 Surface CO_2 analogues

Analogous to 4D-BGC products, three-dimensional (3D, i.e., latitude × longitude × time) gridded data products of surface partial pressure of CO_2 (pCO_2) have been developed over the early 21st century, primarily based on observations aggregated in the Surface Ocean CO_2 Atlas (SOCAT). These products rely on machine learning regression (e.g., Landschützer et al., 2014) or statistical interpolation (e.g., Rödenbeck et al., 2014) to fill observational gaps, and contribute to estimates of annual ocean carbon uptake in the Global Carbon Budget (Friedlingstein et al., 2022) and regional variability in carbon fluxes as studied in the framework of phase two of the Regional Carbon Cycle Assessment and Processes program (RECCAP2). Approaches to compare methods of creating these 3D products (Gregor et al., 2019), to assess the quality of the observing system (Gloege et al., 2021), and to rely on multiple products when performing global analyses (Friedlingstein et al., 2022) should serve as a roadmap for streamlining efforts to create, validate and update 4D-BGC products.

2.5 Why a SCOR Working Group?

To create and promote the use of high-quality 4D-BGC products and avoid duplicative efforts, effective communication between different scientific communities (BGC modeling, satellite ocean color, ship observations, etc.), involving researchers with diverse areas of expertise located around the globe, is essential (Figure 1). A SCOR working group (WG) can provide the coordination to bring these experts together, facilitating necessary lines of communication within the community. For instance, BGC modelers rely on observation-based fields for model initialization, assimilation, and evaluation, such that effective communication between modelers and product creators is crucial to ensure that requirements in terms of spatiotemporal resolution and accuracy are met. Ultimately, this collaboration will lead to the development of consistent and reliable 4D-BGC products that meet the needs of various scientific communities. Such products will refine our understanding of biogeochemical processes, improve models and reanalysis products, and inform policy decisions.

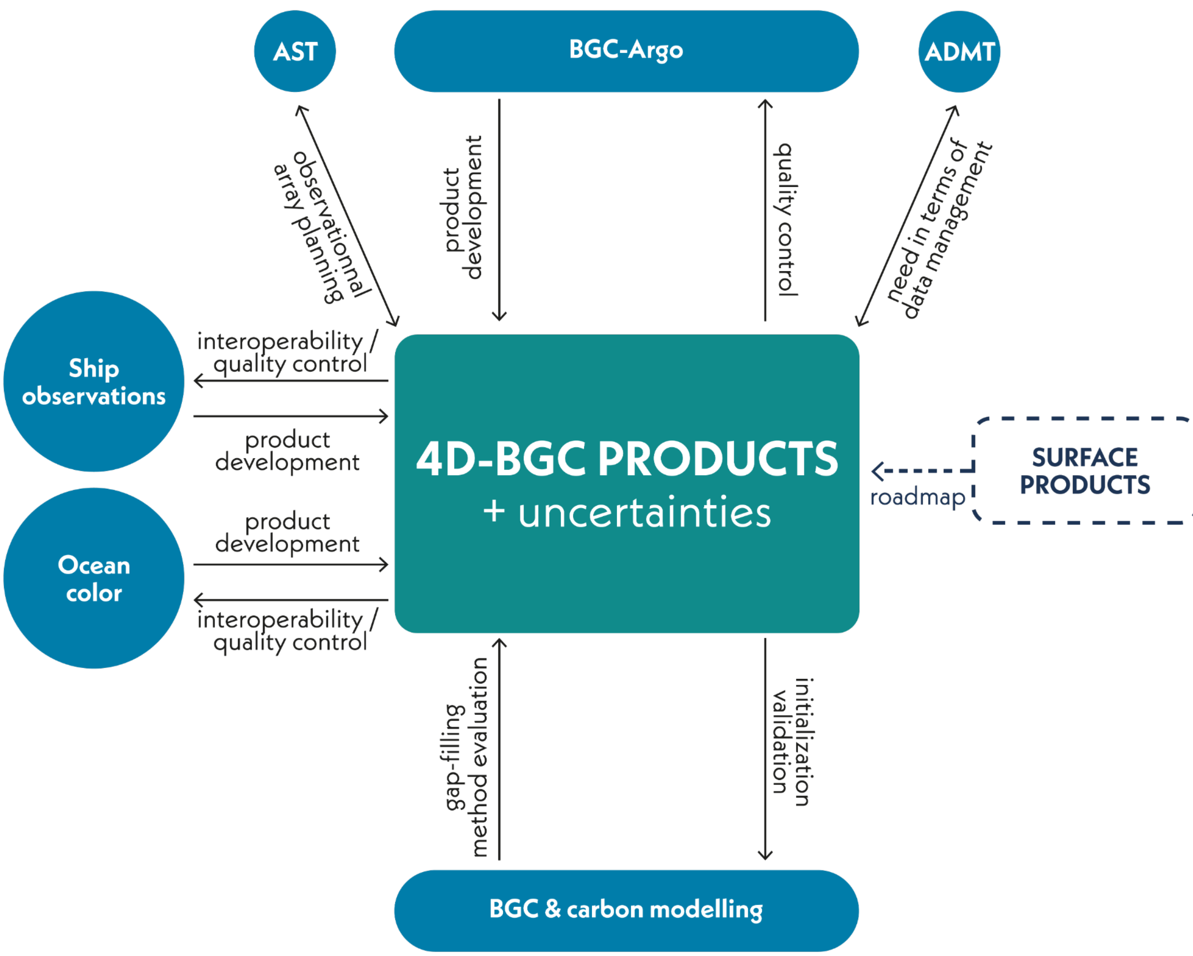

Figure 1. Interaction between communities of interest in 4D-BGC product development. Directional arrows indicate areas in which one community can help another. The BGC-Argo community includes the Argo Steering Team (AST) and Argo Data Management Team (ADMT).

3 Terms of Reference

T1. **Establish connections among 4D-BGC product developers, observational communities and data synthesis efforts, and end-user communities.** This will include planning method intercomparison exercises, developing strategies for merging observational datasets for 4D-BGC product creation, and ensuring that 4D-BGC products are co-developed with stakeholder input.

T2. **Compile an inventory of 4D-BGC products that highlights the original data and methodology used to create each one, provides data access information, and suggests relevant applications.** Through this inventory, promote the broad distribution and use of 4D-BGC products in open-access format for public decision-making and scientific research.

T3. **Synthesize available estimates of global to regional magnitudes, variabilities, and trends of key biogeochemical processes that can be refined by 4D-BGC products, and identify actions that can be taken to achieve those refined quantifications.** Example processes include carbon production and export, subsurface respiration, anthropogenic CO_2 uptake, deoxygenation, ocean acidification, and nitrogen cycling.

T4. **Develop recommendations for methods to create, distribute, and dynamically update 4D-BGC products, as well as strategies to estimate uncertainties from grid-cell to global scales.** These recommendations will promote the creation of consistent and reliable 4D-BGC products with well-quantified uncertainties.

T5. **Build capacity within the oceanographic community, especially among early career researchers and within underrepresented groups, to ensure 4D-BGC product development and usage is sustained and supported.** This will involve training researchers on 4D-BGC product creation, uncertainty estimation, and product-model intercomparison.

4 Working Plan

4.1 Months 1-12

The WG will convene its first in-person meeting (M1) at the 2024 Ocean Sciences Meeting (OSM 2024) in New Orleans, LA, USA. The state-of-the-science on 4D-BGC products will be reviewed and the chairs will present the WG's objectives and working plan.

Members of the WG will share insights from their respective communities as they relate to BGC-Argo data product development (**T1**), with communities distinguished by operational duties (e.g., data managers, data users, product developers, end-users), scientific interests (e.g., marine carbon cycle, bio-optics, ocean color), and contributions to programs and projects (e.g., BGC-Argo, GLODAP). The needs and capabilities of the different stakeholders in the 4D-BGC product development chain will be evaluated. Ocean biogeochemical processes that can be refined by new 4D-BGC products will be identified and reviewed (**T3**).

Members of the WG will be identified at M1 to serve as liaisons with associated committees, projects, and programs. Liaisons will update these partner communities on the WG's activities and gather feedback and input to bring back to the WG (**T1**). Many WG members have direct connections with these communities, which will aid in the identification of members to serve as liaisons (see Section 6). The WG will identify pathways through these partner communities to connect with researchers from developing nations, in particular to entrain new participants in WG activities and to provide trainings to scientists interested in 4D-BGC product development (**T5**). In addition, the WG will plan the establishment of an online repository to provide centralized access to 4D-BGC products (**T2**).

Breakout groups (BG1s) will be formed to focus on different topics, some of which will be addressed in a synthesis paper (SP) on 4D-BGC products. These topics may include the identification and description of 4D-BGC products that have been made available (T2), the synthesis of global estimates of BGC processes and fluxes that can potentially be refined (e.g., carbon production and export, subsurface respiration, anthropogenic CO_2 uptake, deoxygenation, ocean acidification, and nitrogen cycling) (T3), and the development of a plan for organizing the WG's capacity building activities (**T5**). BG1s will initiate conversations at M1, and will conduct virtual meetings over the year (e.g., every two or three months) to review and discuss their assigned topic, brainstorm ideas, and draft language for the SP.

The WG chairs will hold an OSM 2024 session on current and ongoing progress in 4D-BGC product development. One presentation at this session will describe the structure and goals of the WG. Others are expected to provide updates on 4D-BGC products in development from the BGC-Argo array, review related 3D surface biogeochemical products, and describe existing 4D products of ocean physical and BGC properties (**T2**).

4.2 Months 13-24

The WG will convene for its second in-person meeting (M2) during a conference to be determined later. The BG1s will report to the group on their assigned topics. Text prepared by each BG1 will be synthesized into a first draft of the SP on 4D-BGC products (**T3**). Liaisons will report on the interests of affiliated communities as they relate to 4D-BGC product development (**T1**), which will aid in the direction of the WG from this point. Updates on the status of 4D-BGC products will be also provided (**T2**).

At M2, the WG will focus on continuing development of the SP, which will examine the current status and future of 4D-BGC products, their interoperability, and the questions they can address (**T3**). The work towards this SP will involve compiling the 4D-BGC products that have been produced, describing the methods used to create them, and summarizing insights that can be drawn from each one. The WG will continue iterating and refining the SP throughout months 13–24, with the goal of submitting the manuscript by month 22.

An intercomparison exercise among 4D-BGC product development methods will be planned during M2, which will include the identification of gap-filling methods to test, BGC parameters to focus on, and metrics used to compare gridded products (**T1**). This intercomparison exercise may be initiated as a separate project by WG members, but at the very least a recommendation for methodological intercomparisons will be included in the SP.

Breakout groups (BG2s) will be formed at M2 to discuss topics related to the development of a Recommended Practices Guide (RPG) for 4D-BGC product development over the coming year. These topics may include BGC-Argo data access and quality-control (QC) flags, interpolation and gap-filling methods, predictor data products that can assist with gap-filling, evaluation and quantification of uncertainties, and how data products can most efficiently be served and dynamically updated (**T4**).

Committees will be formed at M2, building on the progress of the capacity building BG1, to lead the organization of a webinar series focused on the introduction and promotion of 4D-BGC products and a virtual workshop series on 4D-BGC product development, validation, and utilization (**T5**). The webinar series will communicate and promote the availability of 4D-BGC products to oceanographic researchers who may want to use them to address their research questions. The workshop will train product developers on the tenets of the RPG and elucidate the requirements of 4D-BGC products (e.g., update frequency, spatiotemporal resolution) identified to the WG by interested end-users. A "hack-a-thon" will also be arranged as part of this workshop series to develop code for 4D-BGC product creation, product analysis, and model–product comparisons.

4.3 Months 25-36

The WG will convene for its final in-person meeting (M3) at a conference to be identified later. Conversations at M3 will focus mainly on bringing together ideas and text from the BG2s that met over the previous year into a draft of the RPG (**T3**). The goal will be to publish the RPG by month 36. Updates will be provided on the webinar series and virtual workshop; additional events will be planned for the coming year (**T5**).

The future of sustained 4D-BGC product development coordination efforts will be discussed. The WG may decide to continue meetings on an annual or similar basis, possible future updates to the Recommended Practices guide may be discussed or drafted, strategies for incorporating data from new BGC sensors (e.g., Underwater Vision Profilers, hyperspectral radiometers) may be considered, and the maintenance of the 4D-BGC product repository will be discussed.

4.4 Simple timeline

Month	Events
1	M1; OSM session
2-12	BG1s meet; Liaisons connect with partners
10	4D-BGC repository established
13	M2; SP outlined
14-22	Refine and submit SP
14-24	BG2s meet; Webinars; Training workshops

25	M3; RPG outlined and drafted
26-36	Webinars; Hack-a-thon; Refine and publish RPG

5 Deliverables

D1. **Online repository of gridded BGC-Argo data products (T2):**
A catalog will be developed and integrated with the BGC-Argo website featuring descriptions, statistics, and accessibility information for 4D-BGC products. This will include a process for researchers to submit and update their 4D-BGC products.

D2. **Synthesis paper on 4D-BGC product development (T3):**
This open-access paper will summarize progress in creating 3D and 4D gridded products of physical and biogeochemical ocean properties, review new insights from emerging 4D-BGC products, provide an outlook on this area of research over the next decade, and set goals for critical questions about Earth system processes that 4D-BGC products should address.

D3. **Synthetic datasets for methodological comparisons (T1):**
Model-derived, synthetic datasets (e.g. profiles extracted from ESM output to match Argo float profiles) will be made available to support validation and intercomparison exercises for 4D-BGC product creation methods.

D4. **Recommended practices guide (T4):**
This document will outline recommended practices for the production, validation, evaluation, and distribution of 4D-BGC products from the BGC-Argo array, integrating perspectives from various communities.

D5. **An archive of material (code, presentations, reports) on 4D-BGC products (T5):**
Material developed for virtual webinars and workshops will be retained in an accessible archive. In particular, a programming-based "hack-a-thon" will support the development of open-source code to produce products and compare them with model output.

6 Capacity Building

Our capacity development activities will be guided by the principle that Argo and BGC-Argo data are freely and openly available in near-real-time, with carefully coordinated QC efforts thanks to the Argo Data Management Teams. These features remove financial, geographic, and infrastructure-related barriers that limit capacity development in some other fields of ocean science. Researchers need only an internet connection and the proper training to get involved in the 4D-BGC product development community. Further, 4D-BGC products created from Argo data can be instrumental for economic sectors that rely on the ocean, such as fisheries and ocean-related tourism.

Development and utilization of 4D-BGC products therefore present an opportunity to engage researchers from nations, institutions, and demographic groups that are traditionally underrepresented in ocean science. We will tailor our capacity development activities with this opportunity in mind, prioritizing virtual trainings and communicating the value and significance of 4D-BGC products to audiences who may not typically have access to such information. In addition, we will take advantage of our WG convening in-person at M2 and M3 to plan one or more in-person training events, with at least one being held outside of Europe and North America. We will leverage SCOR's travel grant program to facilitate participation in these trainings, in particular to support scientists from developing nations. We will discuss each of these objectives during M1 and compile a list of committees and organizations that can promote our capacity development activities to researchers in developing nations and underserved institutions.

We will hold a virtual webinar series to disseminate information about available and in-development 4D-BGC products. This series will facilitate the sharing of information among product developers and will help entrain researchers who are interested in entering the product development space. It will also promote the use of available products for novel, value-added studies that may not be pursued by typical Argo data-users. For example, regional studies in the Exclusive Economic Zones of nations that may not have their own observing systems in place could benefit from the unique information offered by 4D-BGC products. We will lean on partner organizations that offer avenues to connect with a wide array of researchers to ensure the webinar series has wide reach.

We will also organize a series of virtual workshops to build capacity in the oceanographic community by (1) encouraging more ocean data scientists to develop and evaluate 4D-BGC products, (2) supporting the development of code to create products and compare them with model output, and (3) incentivizing the design of projects that use 4D-BGC products to answer key scientific questions. One workshop will be focused on machine-learning- and interpolation-based strategies to develop 4D-BGC products and model-simulation-based strategies to estimate their uncertainties. Another "hack-a-thon" workshop will provide attendees the space to develop code for product creation and evaluation and generate ideas for research projects using 4D-BGC products. We will also seek opportunities to integrate presentations and product demonstrations in existing and upcoming capacity building initiatives such as those coordinated by the projects and programs listed in the table below.

To enhance the accessibility and interoperability of 4D-BGC products, one of the WG's deliverables will be the establishment of a well-curated online repository of 4D-BGC products. This deliverable will support capacity development by providing a direct, unambiguous access point for 4D-BGC products. The repository will provide myriad information about the products it contains, and it will be integrated within the existing BGC-Argo website to ensure longevity.

Another deliverable of the WG is a recommended practices guide that will serve as a reference for BGC product development and will complement information disseminated in the workshop series. A section in the recommended practices guide will be focused on ensuring newly produced 4D-

BGC products follow FAIR data principles (Findability, Accessibility, Interoperability, Reuse) and CF (Climate and Forecast) metadata conventions.

Our WG membership is heavily composed of early career researchers (10 of 20 members) and includes participants from six continents. For all WG activities — including the session at OSM 2024, webinar series, and virtual workshop — we will emphasize recruiting early career participants and those from developing nations. We are planning to hold all in-person WG meetings in conjunction with community workshops and conferences to facilitate participant travel to the meetings. We will also target locations outside Europe and North America for M2 and M3.

Finally, we will focus on fostering communication among an international community of interested stakeholder groups, each of which may offer channels to disseminate information about our WG activities and to build capacity among participating scientists to produce and use 4D-BGC products. Examples of these stakeholders, the WG member(s) who may foster connections, and the connections points that can be emphasized to promote sustained 4D-BGC product development from the global array of BGC-Argo floats are provided (alphabetically) below:

Program/ Project	**Member**	**Connection Point to Promote 4D-BGC Products**
Argo Data Management Team (ADMT)	R. Sauzède X. Xing H.C. Bittig	Knowledge of data management and QC procedures is essential for 4D-BGC product development. In turn, reference fields provided by new 4D-BGC products may aid in data QC efforts.
Argo Steering Team (AST)	K. Fennel P. Oke T. Fujiki	Uncertainty fields from 4D-BGC products can inform decisions made by the AST on float deployment locations and mission parameters.
Bluelink	P. Oke	4D-BGC products can add value to Bluelink, which aims to develop global ocean analysis, reanalysis, and forecasting capabilities.
Copernicus Programme	R. Sauzède H. Evers-King	4D-BGC products can be developed using data provided by the Copernicus Marine Service, which can in turn host 4D-BGC products.
Coupled Model Intercomparison Project (CMIP)	N. Mayot	Observational constraints on biogeochemical fluxes provided by 4D-BGC products can inform modeling efforts for CMIP7.
Euro-Argo ERIC	R. Sauzède H.C. Bittig	Improved, cost-benefit-based deployment planning can be conducted based on 4D-BGC product gaps and uncertainties.

FAIR-Ease	R. Sauzède	4D-BGC products can be integrated into the FAIR-EASE European project toward the goal of improving BGC data quality through software standardization and easy cloud development.
Global Carbon Project (GCP)	N. Mayot P. Landschützer	4D-BGC products can address efforts of the GCP to quantify the strength and variability of the ocean carbon sink.
Global Ocean Acidification Observing Network (GOA-ON)	R. Kerr	4D-BGC products can contribute toward GOA-ON's goals to improve our understanding of global ocean acidification and ecosystem responses.
Global Ocean Biogeochemistry Array (GO-BGC)	J. Sharp	GO-BGC will provide significant amounts of data for 4D-BGC product development and can glean important insights from the products.
Global Ocean Data Analysis Project (GLODAP)	S.K. Lauvset H.C. Bittig J.D. Müller	Data synthesized by the GLODAP community can contribute to the development of 4D-BGC products.
Global Ocean Ship-based Hydrographic Investigations Program (GO-SHIP)	S.K. Lauvset	Blending ship data with float data for 4D-BGC product development and using insights from products to inform float deployment locations will require coordination with GO-SHIP.
Integrated Carbon Observing System (ICOS ERIC)	H.C. Bittig P. Landschützer	Observational data and surface carbon fluxes can link with 4D-BGC products for improved estimations on greenhouse gas exchanges.
International Ocean Carbon Coordination Project (IOCCP)	J. Sharp	4D-BGC products serve the IOCCP's goal to promote the integration of ocean carbon and biogeochemistry information into research and assessments to improve our understanding of ocean carbon cycling.
International Ocean Colour Coordinating Group (IOCCG)	H. Evers-King	4D-BGC product development can be informed by the expertise available from the ocean optics community, and are likely to be of high interest to users of satellite ocean color data in research contexts.

OceanOPS	R. Sauzède H.C. Bittig	4D-BGC products can augment visuals provided on the OceanOPS platform and inform data quality indicators that OceanOPS expects to develop.
Regional Carbon Cycle Assessment and Processes phase 2 (RECCAP2)	J.D. Müller	Carbon fluxes inferred from 4D-BGC products can help achieve RECCAP2's goals of improving our understanding of regional sources and sinks of carbon and the processes that control them.
Southern Ocean Carbon and Climate Observations and Modeling (SOCCOM)	L. Keppler	4D-BGC products will be heavily influenced by SOCCOM floats, and can contribute toward SOCCOM's goal of determining the influence of the Southern Ocean on global climate.
Southern Ocean Observing System (SOOS)	R. Kerr	4D-BGC products can contribute to the SOOS mission to deliver essential Southern Ocean observations to stakeholders, particularly in the scope of the Observing System Design and Southern Ocean Fluxes capability working groups.
Surface Ocean CO_2 Atlas (SOCAT)	H.C. Bittig P. Landschützer S.K. Lauvset	Data synthesized by the SOCAT community can contribute to 4D-BGC product development.
Surface Ocean CO_2 Observing Network (SOCONET)	J.D. Müller S.K. Lauvset H.C. Bittig	Researchers who have developed 3D products from surface CO_2 observations as part of the SOCONET mission can collaborate on 4D-BGC products.
Surface Ocean Lower Atmosphere Study (SOLAS)	H. Evers-King	Fluxes of carbon and oxygen between the ocean and atmosphere can be analyzed using 4D-BGC products.
United Nations Ocean Decade	K. Fennel	4D-BGC products will promote progress toward the goals of OneArgo as a UN Ocean Decade Action: to increase Argo's influence on ocean and climate services, predictions, and research.
US Ocean Carbon and Biogeochemistry (OCB)	J. Sharp	OCB priorities related to ocean carbon cycling and biogeochemical fluxes can be addressed by 4D-BGC products.

7 Working Group Composition

7.1 Full Members (EC = early career, fewer than ten years post-PhD and under 40 years of age)

Name	Gender	Place of work	EC	Expertise relevant to proposal
Jonathan Sharp (co-chair)	M	UW CICOES / NOAA PMEL, **USA**	✓	BGC-Argo; Carbonate chemistry; 4D-BGC product development
Raphaëlle Sauzède (co-chair)	F	CNRS / IMEV, **France**	✓	BGC-Argo; In situ optical BGC proxies; Ocean color; Argo data management; 4D-BGC product development
Henry Bittig	M	IOW, **Germany**	✓	Argo data management; GLODAP; ICOS; Method development for mapping and QC; SCOR WG 142
Laique Djeutchouang	M	U. Cape Town, **South Africa**	✓	Sampling scale sensitivity; *p*CO_2 reconstruction from SOCAT, machine learning
Katja Fennel	F	Dalhousie U., **Canada**		Coupled physical-biogeochemical models; Ocean carbon cycle; Ocean observing systems; BGC-Argo
Tetsuichi Fujiki	M	JAMSTEC, **Japan**		Biogeochemistry; Phytoplankton productivity; Autonomous ocean observation platforms
Lydia Keppler	F	UCSD, **USA**	✓	BGC-Argo; 4D-carbon product development based on ship-data; Ocean carbon cycle
Rodrigo Kerr	M	FURG, **Brazil**		Ocean ventilation; Water mass evolution; Ocean acidification, Air-sea CO_2 fluxes; Anthropogenic carbon storage
Jens Daniel Müller	M	ETH Zürich, **Switzerland**	✓	Ocean interior carbon storage and acidification based on ship-data; RECCAP2 coordinator
Andrea Rochner	F	Met Office, **UK**	✓	Ocean carbon cycle; Coupled physical-BGC models; Data assimilation for BGC

Haimanti Biswas	F	CSIR-NIO, India		Marine Biogeochemistry; Climate Change; Phytoplankton; Marine Carbon Cycle

7.2 Associate Members

Name	**Gender**	**Place of work**	**EC**	**Expertise relevant to proposal**
Lucile Duforêt-Gaurier	F	LOG, **France**		Ocean color; Remote-sensing POC bio-optical algorithm to derive POC from optical data
Hayley Evers-King	F	EUMETSAT, **Germany**	✓	Ocean color and ocean optics; Operational user requirements definition and data provision; Capacity building
Peter Landschützer	M	VLIZ, **Belgium**		Ocean carbon cycle; Climate change; 3D surface CO_2 product development
Siv K. Lauvset	F	NORCE, **Norway**		GLODAP; SOCAT; BGC-Argo; 3D BGC product development; Carbonate chemistry
Nicolas Mayot	M	U. East Anglia, **UK**	✓	BGC-Argo; Ocean color; Global ocean biogeochemistry models
Alexandre Mignot	M	Mercator Ocean, **France**		BGC-Argo; Ocean modeling; Data assimilation
Peter Oke	M	CSIRO, **Australia**		Ocean data assimilation; Argo
Katherine Turner	F	U. Arizona / GFDL, **USA**	✓	Ocean carbon cycle; Ensemble optimal interpolation for BGC
Xiaogang Xing	M	SIO MNR, **China**		BGC-Argo; Ocean color; Ocean optics; Marine ecosystem dynamics
Cunjin Xue	M	CAS, **China**		4D-BGC product development; Marine data mining; Machine learning

8 Working Group Contributions

Jonathan Sharp has led the development of a 4D-BGC product of global dissolved oxygen content based on a combination of BGC-Argo and discrete shipboard observations. He has also been involved with efforts to enhance accessibility of BGC-Argo data and has connections with the US OCB and GO-BGC communities.

Raphaëlle Sauzède has led the development of 4D-BGC products of particulate organic carbon and chlorophyll-a concentration based on BGC-Argo observations that are released operationally as part of the European Copernicus Marine Service. In this way she is involved in the Copernicus Thematic Assembly Center Multi-Observation and is also a member of the BGC-Argo Data Management Team.

Henry C. Bittig is involved with various observing systems (e.g., BGC-Argo, ICOS) and data synthesis efforts (e.g., GLODAP). He lead the community paper on BGC-Argo and has established standard routines for sensor calibration and QC (e.g., Argo-O_2; SCOR WG 142; CANYON-B algorithms used for BGC-Argo) as well as for data end user accessibility (Argo "s-profiles").

Laique Djeutchouang has a background in mathematics and statistics, and has led efforts to estimate the sensitivity of surface CO_2 reconstructions to observational density. He has also been involved with characterizations of the ocean carbon sink, in particular as part of the Global Carbon Budget.

Katja Fennel studies the effects of climate change on ocean ecosystems using coupled physical–biogeochemical models. She sits on the Argo Steering Team and BGC-Argo mission team, and has recently led studies to glean large-scale insights on ocean biogeochemistry from BGC-Argo observations.

Tetsuichi Fujiki has conducted time-series observations of the ecosystem and biogeochemistry in the North Pacific using BGC-Argo floats and mooring buoy systems. In particular, he is studying the relationship between phytoplankton dynamics and environmental changes such as warming, acidification, and deoxygenation. He is a member of the BGC-Argo mission team.

Lydia Keppler developed two 4D data products of DIC: a monthly climatology of mapped, global upper ocean DIC and monthly fields of mapped, global upper ocean DIC from January 2004 through January 2019. She has also been involved with and has connections with the SOCCOM, BGC-Argo, US OCB, RECCAP2, GLODAP, and GCP communities.

Rodrigo Kerr supervised the creation of a seasonal 3D high-resolution hydrographic (T, S and dissolved oxygen fields) gridded data set for the northern Antarctic Peninsula, and other compiled products in the Southern and South Atlantic Ocean. He has also been involved with and has connections with SOOS and GOA-ON communities.

Jens Daniel Müller provided a reconstruction of decadal trends in the oceanic storage of anthropogenic carbon and is a core member of GLODAP. He has acted as scientific coordinator of phase two of the project REgional Carbon Cycle Assessment and Processes (RECCAP2) since 2020.

Andrea Rochner is a biogeochemical modeler who worked on assessing coupled physical-biogeochemical models and biogeochemical data assimilation from satellite-, ship-, and BGC-Argo-based observations. Her work focused on the air-sea CO_2 flux. She recently transitioned to a new role in operational forecasting of biogeochemistry on the Northwest European Shelf.

Haimanti Biswas is an observational oceanographer who has worked in open-ocean and estuarine environments, often in the North Indian Ocean. She is interested in the effects of climate change, ocean acidification, and trace metal enrichment on marine phytoplankton; as well as changing organic matter dynamics in the ocean.

9 Relationship to other international programs and SCOR working groups

Some connections between the WG and other international programs are summarized in Section 6, especially as they relate to building collaborations within the oceanographic community to promote the long-term sustainment of 4D-BGC product development efforts. This section will discuss synergies the WG may exploit with international programs and previous SCOR WGs, to help those groups achieve their broad-scale goals.

The WG will interact directly with the **Argo Steering Team** and the **BGC-Argo Mission Team** to direct 4D-BGC product development toward the fulfillment of their objectives, including observing the changing state of the upper ocean, providing products for the initialization of biogeochemical ocean models, and generating insight into ocean carbon uptake and acidification, oxygen and nitrogen cycling, the biological carbon pump, and phytoplankton community composition. Uncertainty fields co-developed with 4D-BGC products, especially gridded fields constructed from OSSEs, will inform observational array planning, helping to fill gaps and identify priority areas for each BGC variable. The WG will also interface with the **Argo and BGC-Argo Data Management Teams** to exchange ideas about how to use float data for 4D-BGC product development and, in turn, how gridded products may inform data QC efforts.

The WG will provide recommendations for international programs that may use 4D-BGC products to address their own scientific objectives. For example, the next generation of climate models developed as a part of the next iteration of the **Coupled Model Intercomparison Project (CMIP7)** would benefit greatly from a new suite of observation-driven 4D-BGC products for model initiation and/or validation. The **Global Carbon Budget (GCB)** evaluates both model- and observation-based estimates of ocean carbon uptake, and has seen a growing divergence between these two estimates in recent years. 4D-BGC products can provide an ocean interior constraint on ocean carbon uptake to compare to estimates evaluated in the GCB.

The WG will connect with experts from the **International Ocean Colour Coordinating Group (IOCCG)** to evaluate how 4D-BGC products, particularly chlorophyll fluorescence, may support the IOCCG's objective to optimize quality of data for calibration and validation.

Researchers pursuing developing data assimilative models, such as the **Biogeochemical Southern Ocean State Estimate (B-SOSE)**, could learn from the development of 4D-BGC products, and vice-versa. Data assimilative models and 4D-BGC products both sit at the nexus of observations and models, and each have their own benefits and limitations. Other groups working on observation-model comparisons, such as the **Marine Ecosystem Analysis and Prediction (MEAP) Task Team of OceanPredict** can derive benefits from the spatiotemporally consistent fields of 4D-BGC products.

The activities that the WG will support are only feasible due to the work of **SCOR WG 142: Quality Control Procedures for Oxygen and Other Biogeochemical Sensors on Floats and Gliders**. This WG pioneered critical advancements in QC for float measurements of BGC parameters, particularly oxygen. The WG will also interface with **SCOR WG 161: Respiration in the Mesopelagic Ocean (ReMO)**. A main application of float-based 4D-BGC products will be to provide estimates of subsurface respiration, which can be compared with results from the ReMO group.

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***11 Appendix** (five key publications for each full member)*

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