

US National BioGeoSCAPES Workshop Report Virtual Meeting November 10-12, 2021

An US Ocean Carbon & Biogeochemistry (OCB) Report November 2022 AUTHORS Benjamin S. Twining Bigelow Laboratory for Ocean Sciences

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Workshop Summary

DioGeoSCAPES (BGS) is an international program being developed to understand controls on ocean D productivity and metabolism by integrating systems biology ('omics) and biogeochemistry (Figure 1). To ensure global input into the design of the BGS Program, countries interested in participating were tasked with holding an organizing meeting to discuss the country-specific research priorities. A United States BGS planning meeting, sponsored by the Ocean Carbon & Biogeochemistry (OCB) Project Office, was convened virtually November 10-12, 2021. The objectives of the meeting were to communicate the planning underway by international partners, engage the US community to explore possible national contributions to such a program, and build understanding, support, and momentum for US efforts towards BGS. The meeting was well-attended, with 154 participants and many fruitful discussions that are summarized in this document. Key outcomes from the meeting were the identification of additional programs and partners for BGS, a prioritization of measurements requiring intercalibration, and the development of a consensus around key considerations to be addressed in a science plan. Looking forward, the hope is that this workshop will serve as the foundation for future US and international discussions and planning for a BGS program, enabled by NSF funding for an AccelNet project (AccelNet - Implementation: Development of an International Network for the Study of Ocean Metabolism and Nutrient Cycles on a Changing Planet (BioGeoSCAPES)), beginning in 2022.



Figure 1. Schematic of interdisciplinary science model of BioGeoSCAPES, connecting geochemical and biological/'omic and in situ sensor observations with data processing and models to scale from metabolisms to ecosystems (Levine and Leles, 2021).

US National BioGeoSCAPES Workshop Report

Meeting Goals

- 1. Communicate current status of the international BGS planning effort
- 2. Engage US-based scientists from a range of disciplines who can help develop and champion the BGS program
- 3. Identify US science priorities and ways to contribute to a US and international BGS science plan

Originally planned to be an in-person meeting at Woods Hole Oceanographic Institution, the meeting was held virtually due to concerns about COVID-19. Fortunately, this decision allowed for greater participation, including from several invited international colleagues, as well as a lower carbon footprint. The meeting was attended by 154 total participants (See Appendix A for participant list), with consistently around 90-100 simultaneous participants throughout the meeting. Participants represented 68 different universities and research organizations from around the United States from all career stages. In addition, several participants from other countries were invited to share perspectives from their national BGS planning efforts. The virtual meeting used Zoom and Gather.Town platforms video conferencing and virtual poster sessions, respectively, as well as the online collaboration tool Google Jamboard. Below is a summary of daily activities and presentations.

Day 1, November 10, 2021

The meeting started with a series of four brief talks (available on <u>YouTube</u>) to introduce participants to the existing vision and planning history for a BGS Program.

Adrian Marchetti (University of North Carolina at Chapel Hill) began with an explanation and brief history of the BGS program. Efforts to bring the US 'omics and biogeochemical communities together began in 2010 with an OCB-sponsored workshop on the <u>Molecular Biology of Biogeochemistry</u>. This stimulated the <u>GeoMICS cruise</u> in 2012, which tested approaches to collect and synthesize molecular and biogeochemical data. It was clear from that effort that there was more work to do to standardize and streamline data pipelines and 'omics protocols. The benefits of doing this were shown by the GEOTRACES and Tara Oceans Programs. Possible intersections of these global datasets were explored at a 2016 joint OCB-GEOTRACES workshop focused on the internal cycling of trace elements in the ocean. However, spatial heterogeneity and biological dynamics make it difficult to integrate biological and geochemical data post hoc. Thus, with an appreciation for the value of globally-integrated data, as well as an understanding of the need to carefully connect measurements in time and space, the seed for BGS was planted during a 2018 small international interest scoping workshop at the Jonsson National Academies Center in Woods Hole with participants from 10 countries (2018 workshop report).

Alyson Santoro (University of California, Santa Barbara) expanded upon the lessons and limitations of previous global ocean programs (e.g., Global Ocean Sampling Expedition, Tara Oceans, GEOTRACES). While each project produced a globally coherent dataset that has been used by many scientists beyond those that collected the data, there has been a lack of co-located biology and chemistry measurements and limited mesopelagic and bathypelagic sampling. Santoro also explained the steps of developing and organizing the international GEOTRACES Program, which took numerous international meetings and intercalibration efforts over a 10-year period to agree on objectives and sampling schemes. As a member of the GEOTRACES Standards & Intercalibration committee, Santoro highlighted the GEOTRACES governance structure, which enables coordination, while recognizing unique national funding mechanisms, and also oversees production and distribution of an intercalibrated global dataset. Santoro also described the Marine Microbial Eukaryotic Transcriptome Sequencing Project (MMETSP) as an example of coordinated community science where the

whole is greater than the sum of its parts.

Maite Maldonado (University of British Columbia) explained international efforts to coordinate national BGS planning workshops, which have already occurred in Japan, Israel, Canada, China, France, and now the US (this meeting). Maldonado highlighted smaller-scale existing BGS-like projects, including <u>AtlantECO</u>, new cruises by Tara Oceans, and cruises led by Indian and Australian scientists. Three pending proposals to EU (Martha Gledhill lead), US (Mak Saito lead), and Canadian (Maldonado and Erin Bertrand leads) agencies will hopefully support the next organizational steps for a BGS program. Finally, Maldonado introduced 4 questions that each national BGS community has been asked to address: 1) feedback on the BGS mission statement, 2) areas for national contribution, 3) most compelling BGS science questions, and 4) impediments that could be mitigated with training or collaboration. A goal of this workshop was to work towards answers to these questions.

Ben Twining (Bigelow Laboratory for Ocean Sciences) finished the introductory talks by expanding on the motivation and context for a BGS program. There is now broad recognition for the impacts of climate change on the ocean, as well as for the role of the ocean in global human and ecosystem health. Indeed, several goals of the UN Decade of Ocean Science for Sustainable Development could be addressed by an international BGS program. Twining also described challenges to a BGS program that need to be tackled, such as bridging across scales and disciplines, standardizing measurements and protocols, and transcending boundaries between disciplines. An AccelNet Implementation proposal was submitted to US NSF to support development of an international BGS program, and Twining described the numerous communities and networks identified in the proposal. The AccelNet proposal has now been funded, and efforts are underway to coordinate with international partners on leadership and governance structures. Accelnet activities and leadership structures will be implemented via an open and transparent process. A successful BGS project will accomplish several compelling, valuable global outcomes, including: 1) creating a baseline understanding of microbial communities and their metabolic function, as well as new tools for data visualization and integration; 2) developing knowledge of biogeochemical hierarchies and feedbacks in the ocean; and 3) training a new generation of multi-disciplinary scientists who can effectively integrate knowledge of molecular- and global-scale processes.

The introductory talks were followed by questions/discussion, and participants then divided into virtual breakout groups to address three topics targeting inclusive community-building:

- 1. What existing communities should we connect with?
- 2. What are good examples of community-building efforts within and beyond the oceanographic community?
- 3. What are potential barriers to interdisciplinarity and inclusivity in a global effort, and how can we address them?

Summary of Day 1 Breakout Discussions

Each breakout group captured notes using an electronic collaboration document (Google Jamboard), and groups were encouraged in advance to allow all participants to speak and contribute to the board. Meeting organizers then summarized these discussions in plenary the following day. In response to question 1, participants identified a number of existing communities that could be tapped, including the US Marine Biodiversity Observation Network (MBON), NSF-funded centers (C-MORE and C-DEBI), US time-series programs (Hawai'i Ocean Time-series Program, HOT and Bermuda Atlantic Time-series Study, BATS), the Earth Microbiome, genomic repositories (e.g., NCBI, DOE's Integrated Microbial Genomes & Microbiomes, IMG), and the network of Long-Term Ecological Research (LTER) sites. Both MBON and LTER were held up as examples of community-building in response to question 2, as well as GEOTRACES and the data science community, specifically the Software Carpentries data and informatic workshops. Finally, in response to

question 3, participants identified intercalibration activities as important for community building, and workshops and summer schools as important for inclusivity. Workshops were also seen as an important tool for addressing communication barriers, for example, between modelers and observationalists.

Day 1 ended with a poster session (15 poster presenters) hosted virtually on gather.town. See Appendix B for list of poster titles and presenters.

Day 2, November 10, 2021

Day 2 consisted of a second poster session on gather.town (14 poster presenters), followed by three presentations on BGS intercalibration activities. See Appendix B for a list of poster titles and presenters.

Introduction to Intercalibration Efforts

Mak Saito (Woods Hole Oceanographic Institution) first provided an overview of the definitions and importance of intercalibration. Saito discussed how intercalibration using reference materials enables three activities: Application of different analytical methods, involvement of different analysts, and development and incorporation of new methods, all three of which a large international program such as BGS will have. In order to combine measurements across large spatial and temporal scales, use of reference standards and intercalibration efforts from participating laboratories will be critical. A continual intercalibration and standards effort, as well as an internationally interoperable data system, should be the foundation for an international big data BGS Program. Examples were provided from the GEOTRACES Program, including how numerous peer-reviewed publications were produced documenting intercalibration efforts and how these efforts resulted in a significant amount of collaboration and community-building that helped lay the foundation for academic research in the GEOTRACES Program. Finally it was stressed that intercalibration and intercomparison efforts are important work, and that those interested in participating in BGS could engage by organizing or participating in intercalibration efforts. If an intercalibration doesn't yet exist for a potentially useful parameter, organizing an effort would be a useful contribution as well. It was recognized that it will likely take multiple efforts to create community consensus and build trust within each community.

Metaproteomics Intercomparison

Mak Saito then presented results from ongoing Metaproteomic Intercalibration efforts. This is a volunteer effort supported by OCB, which provided funds for sample shipment and a workshop. Saito provided an introduction to metaproteomics as a relatively new and useful data type, and presented the project team, advisory board, and project participants. It was mentioned that the Metaproteomic Intercalibration effort evolved from a prior OCB Best Practices in Ocean Metaproteomic Data Sharing Workshop, the results of which were published and are available at <u>Ocean Best Practices</u>. In addition to improving the quality of the measurements themselves, this intercomparison effort has promoted (and continues to promote) broader community confidence in this relatively new data type, as well as providing an opportunity for community-building within the metaproteomics community. The Metaproteomic Intercalibration effort had wet-lab and informatics components, with the wet-lab component using large-volume samples collected from the BATS station. Fourteen laboratories from the US, Canada and Europe participated in the study. Saito presented the results from the wet-lab intercalibration. Over 37,000 unique peptides were identified in total, with 4,000-10,000 shared peptides identified in pairwise comparisons amongst datasets. This was interpreted as abundant peptides being reproducibly identified in different labs, with more variability in rarer peptides detected due to the stochasticity of mass spectrometry data collection algorithms. Good

agreement in taxonomic attribution of proteins was also observed. It was pointed out that this was an initial intercomparison effort, and that future efforts should conduct intercalibrations with new algorithms (data-independent acquisition) and using absolute quantitation methods. The results are in preparation for a peer-reviewed publication.

Nucleic Acid Intercalibration Update

Paul Berube (MIT) gave a presentation summarizing the activities of the OCB Nucleic Acid Intercalibration Workshop (see report) that occured in January 2020 at University of North Carolina at Chapel Hill. This workshop brought together experts from around the country to solicit ideas and make advancements for coordinated activities on this topic. Intercalibration and development of reference materials will be needed to enable studies combining nucleic acid data from a variety of laboratories around the world that use different sequence library preparation and bioinformatic pipelines. Workshop participants agreed that components of sample collection and processing are likely a major source of variability. The value in collection of large volumes using new sampling technologies like the AUV Clio was highlighted. While biases are known to exist in downstream pipeline components such as sequencing and bioinformatics, participants thought that biases introduced during these earlier steps could be more easily identified and addressed.

Several types of reference standards were discussed as potentially useful: mock communities, collections of cultured non-marine cells to add to samples to help with quantification, and addition of purified nucleic acids for quantification as external or internal standards to account for run-to-run variability. It was envisioned that use of a reference material could be a requirement in BGS efforts, enabling absolute quantitation of gene or transcript abundances. Workshop participants proposed that sources of variability in the upstream pipeline should be examined by a small number of laboratories to develop best practices. Then the larger community could be involved in intercalibration activities to assess precision and accuracy across different labs in the US and other nations (e.g., collaboration with AtlantEco team). Continued community-driven efforts in this area will benefit both BGS and microbiome science.

Summary of Day 2 Breakout Discussions

Following these plenary presentations, small groups were created to discuss the US perspective on key science drivers for the BGS program and the methodological capabilities needed to address them. Results harvested from the meeting participants will be used to provide feedback to the international community (via this report as associated documents and videos), as requested in Maite Maldonado's international presentation. Eleven breakout groups of ~6-10 participants were created randomly, and notes were collected using Google Jamboards. The questions posed to breakout groups were:

- 1. What hypotheses could be addressed by BGS program, towards the goal of coalescing around highlevel motivations?
- 2. What are compelling questions that can't be addressed by a single group and really require a coordinated program?
- 3. What are the key intercalibration needs to help support and realize our science goals?

Summary of Question 1 Discussions

For question number 1, it was clear from the array of responses that the BGS program has the potential to address a number of fundamental and exciting biological and chemical oceanographic questions. The results are summarized in Table 1, collated from jam board notes from the 11 groups and broken down by

themes of Carbon and Elemental Cycling, Climate Change and Environmental Stress, Ecosystem Structure and Biogeochemical Function, Ecological and Biogeochemical Theory / Modeling, and Methodological and Study Design. Similar science questions emerged from multiple discussion groups, demonstrating a strong coherence of ideas among participants. One of the overarching themes of the science questions was related to "who is there and what are they doing?" – connecting biogeography of (micro)organisms and biogeochemical function. Another theme was basic scientific discovery within the mesopelagic and deep ocean that are undersampled with regards to microbial oceanography and biogeochemistry. Building on this, once a global baseline of biogeochemistry and organism distribution is established for the first time, multiple groups expressed interest in studying how these systems will respond to environmental change and how this large suite of observations could be used to develop new theory and predictive modeling capabilities. Finally, there was also interest in continued methodological improvements to help address the above science questions - e.g., further development of estimations of biogeochemical rates using highthroughput global omic datasets and improved rate methods.

It is not unprecedented to have multiple science questions for global programs. The big data capabilities of co-collected global-scale geochemical and 'omics datasets have the potential to address multiple research avenues simultaneously. Indeed there has been a high rate of data reuse of trace metal and isotope (GEOTRACES), and 'omics programs (Tara and others). In the latter GEOTRACES example, each ocean section expedition focused on multiple science questions based on geographic specificity (e.g., studies regarding hydrothermal vent, aeolian dust, oxygen minimum zone, and coastal input processes). With improvements in metadata consistency and intercalibration, this ability to facilitate analysis of multiple research questions on a global scale and over varying timescales is an exciting aspect of BGS.

Summary of Question 2 Discussions

Question 2 focused on the compelling science questions that a large coordinated program could answer. These responses were harvested from Jamboard notes, and summarized in Table 2. While there was some overlap with the responses from Question 1, there was a coherent response among discussion groups that linking processes across scales, as well as guantifying scales of variability, is best achieved through these types of collaborations. Several groups pointed to quantifying global spatiotemporal variability in biogeochemical transformations and understanding the role of organisms in driving this variability. Additional comments were made that a BGS-like program is necessary for linking biogeochemical rates to community structure, understanding who is where, and what environmental factors are determining these communities and their functions. Finally several groups highlighted the power of integrating this type of work through global metabolic models. Example guestions included: What controls the fate or persistence of organic matter in the ocean? How will net primary productivity change in response to climate change? What is the role of (micro)nutrients in structuring microbial communities and their function? What are the relationships between environmental conditions, community composition and function, and biogeochemical rates? In addition, multiple groups expressed interest in entraining scientists with eDNA (environmental DNA) expertise in order to link microbial and biogeochemical observations to higher trophic level processes.

Summary of Question 3 Discussions

The third topic of discussion for breakout groups asked participants to discuss the key intercalibration needs to realize the previously discussed science goals. In general, there was a recurring theme of strong support for intercalibration efforts from the "simpler" biogeochemical analytes to the complex 'omics analyses. There was a recognition that intercalibration was foundational to the BGS efforts, enabling comparisons of data internationally and temporally, as well as potentially helping to forge the gap between 'omics observations and estimations of biogeochemical rates. There was also discussion in many groups about the challenges posed by 'omics intercalibrations, with various sub-omic fields (nucleic acids, proteins, metabolites) having unique challenges, such as choosing what to calibrate and how to obtain standards in metabolomics.

Multiple groups expressed interest in development of protocol cookbooks as a means to standardize sampling and analysis methods. There was discussion of lessons learned from GEOTRACES, in particular in the absence of *a priori* knowing the "true" composition of a field sample, developing "consensus results" as the community provided results. The use of defined laboratory mock community standards of mixed organisms was discussed as another alternative for development of standards. Although not included in the discussion question, many groups inevitably were led to the informatics, data management and repository challenges that will be faced by BGS, demonstrating how data aspects will be a particularly important and challenging aspect of BGS.

Finally, there were questions raised about how to support intercalibration efforts, especially in cases where the analytical pipelines can be costly. Lessons could be learned from prior GEOTRACES efforts that used organization grants to support both large sample collection for production of standards and focused intercalibration efforts led by small self-organized teams around specific analytes. Those GEOTRACES efforts were self-organized, bottom-up in leadership (within a larger GEOTRACES-led intercalibration effort), and highly democratized, with open calls to include all analysts interested in participating. The model for funding these intercalibration activities varied, from small teams having NSF OCE support (e.g., particles group, mercury group, etc), to open international calls for participation in intercalibration measurements without financial support for analyses (e.g., bioactive trace metals group) but including workshop travel support.

A poll was conducted during the meeting asking what parameters were in most need of intercalibration (Figure 2). Meeting participants responded that biogeochemical rates (35%), metabolomics/organic geochemistry (25%), transcriptomics (16%), genomics (14%), proteomics (2%), modeling (2%), and other (6%). No participant felt that trace metals and macronutrients were in need of intercalibration, likely due to GEOTRACES intercalibration efforts. In a poll on what should be emphasized first within BGS (Figure 2), participants ranked intercalibration first, fieldwork second, and data management third, demonstrating a community consensus on the foundational importance of intercalibration and data management activities in developing a BGS program.

Scientific Presentations - Part I

The day finished with four short talks providing examples of BGS-type scientific studies. Speakers were chosen to demonstrate a range of studies connecting different 'omics approaches and biogeochemistry, while also representing a range of career stages, geography, and demographics.

Scott Gifford (University of North Carolina, Chapel Hill) described a study of the roles of *Synechococcus* in nitrogen and iron cycling at Station P during the EXport Processes in the Ocean from Remote Sensing (EXPORTS) field campaign using quantitative genomics. Scott highlighted several potential lessons for BGS: 1. It is critical to have 'omics, metabolic, and chemical data measured simultaneously; and 2. Quantitative 'omics data enable moving beyond community surveys and composition to link with chemical and biological standing stocks and rate measurements.

Bethanie Edwards (University of California, Berkeley) discussed ways to integrate lipidomics with biogeochemical measurements to study the plankton chemical signaling, diurnal and bloom dynamics, and the biological and microbial carbon pump. She pointed out that 'omics, rate measurements and geochemical characterizations are all needed to understand processes in marine systems.

Julie Granger (University of Connecticut) presented the use of flow cytometry cell sorting to study population-specific nitrogen utilization. This approach can be combined with population-specific metagenomics/metatranscriptomics and group-specific element analyses and uptake rates. Coupled

together, these provide a means of linking community composition to gene expression and biogeochemical function. This level of understanding is needed in order to predict the response of ocean communities to climate change.

Scott McCain (MIT/Dalhousie University) spoke of efforts to use cellular modeling and metaproteomics to estimate biogeochemical rates from 'omics measurements of genes and proteins. Scott highlighted the frequent disconnect between gene expression and cellular processes, underpinning the need to better understand relationships and controls on cell biology in the ocean. He suggested that expanded knowledge of rates and nutrient quotas might help us explain phytoplankton bloom progression and improve predictions of biogeochemical models.

There were additional questions and discussion from the day's talks, followed by additional opportunities to discuss posters. The poster sessions were well attended and provided a valuable opportunity for participants to share ideas and network.

Day 3, November 12, 2021

The third day of the workshop provided more opportunities to explore potential types of BGS science approaches and to discuss where effort needs to be focused.

Scientific Presentations - Part II

Four speakers provided additional examples of the compelling science questions that are being addressed with combined 'omics and chemical measurements.

Daniele Iudicone (Stazione Zoologica Anton Dorhn Napoli) described the multinational AtlantECO project, which involves the merging of 'omics and biogeochemical measurements, as well as combining 'omics measurements across institutions.

Lihini Aluwihare (Scripps Institution of Oceanography) discussed ways to advance understanding of dissolved organic carbon biogeochemistry through BGS, including studies of exo-metabolites and dissolved organic matter lability across ocean basins. Metabolite datasets are massive, and only a small portion (~11%) of the molecular fingerprints can be identified. Process studies enable carbon fluxes between ecosystem components in spatially-constrained systems to be measured, in concert with NA-omics and indicators of microbial ecosystem composition, physiology and interactions. Thus, 'omics approaches are key tools to help in the interpretation of metabolite datasets.

Sarah Hu (WHOI) explained ways to understand microbial trophic interactions between microbial eukaryotes in deep-sea hydrothermal vents. Gene metabarcoding (for taxonomic identity) and metatranscriptomics (metabolic potential) can be combined with empirical grazing measurements to study carbon connectivity in deep-sea benthic food webs to the water column. A combination of tools also provides understanding of heterotrophic metabolic complexity.

John Casey (MIT) presented simulations of microbial metabolism and physiology in an effort to develop prognostic models of marine ecosystems (both probabilistic and mechanistic). Casey presented work on genome-scale models that apply thermodynamic and stoichiometric constraints with genome information on metabolic networks. An example from the Atlantic Meridional Transect that provides physical and biogeochemical measurements with *Prochlorococcus* ecotype abundance to make inferences about

population dynamism, demonstrating the power of combining 'omics and biogeochemical measurements for developing more realistic and complex ecological models.

Day 3 Breakout Discussions

Participants broke into discussion groups by potential BGS program element.

Field measurements (Survey Cruises and Transects) Break-Out Group

This large group (~15) had a dynamic discussion focused on numerous topics regarding field work, including both process and survey expeditions. From a programmatic perspective, there was discussion of a desire to actively foster inclusion of new and early PIs, as well as including those from smaller institutions. Logistical components were also discussed, including the influence of biology on sampling timing constraints while doing transects/sections, the challenges of acquiring enough material, the need for bulk water samplers, size-fractionated filtering, and robotic samplers. Scientifically, the benefits of conducting full depth basin-scale sections to elucidate connections between biogeography, biogeochemistry, particularly in the deep and the potential for including seafloor habitats was discussed. Synergies and lessons from other programs were also discussed.

Modeling Breakout Group

This group had an engaging discussion about ways in which a BGS program could facilitate the integration of modelers, experimentalists, and observationalists. The group recommened increasing communication between these disciplines and breaking down discipline-specific language barriers as a top priority. There was agreement within the group that such integration would be necessary for a successful BGS program and that modelers should be integrated into BGS projects and sampling design from the onset. A problem-focused modeling-observations incubator program such as a summer school was suggested as a way to facilitate networking across disciplines networking. Past examples of successful cross-disciplinary collaborations were mentioned, including the Amazon River Plume project.

Leveraging Lab Experiments and Cultures Group

This breakout group was made up of 27 participants, reflecting both the excitement for including an experimental component in a future program, but also the uncertainty as to the nature and scope of those efforts. Indeed, scope was a significant topic of discussion within this group and a general, if obvious, consensus was that the overall BGS science questions will determine the role of lab experiments in the program. An example idea that emerged was using cultures to get better kinetic and quota data to better inform models, providing a link between observations/measured rates and models. Participants highlighted that culture experiments under different conditions could be used to establish reference databases for gene expression and metabolite production, which are then used to better interpret field data. The group also discussed the fact that genes and proteins of unknown function still represent major barriers to interpretation of 'omics data, and that lab experiments could be the key to overcoming this. New sampling as part of BGS could be used to generate the raw material (i.e. cultures) for novel experimental efforts by archiving cells at sea for cultivation efforts. Finally, experiments were seen as a key way to extend BGS observations *forward*, in the context of climate change, and to engage scientists for whom participation in field-based studies may present a barrier to participation.

Rates Breakout Group

This group (5 participants) discussed the need for better intercalibration of biogeochemical rates generally, and specifically as part of a BGS program. Rates are the link between chemical parameters and many of the biological 'omics and community descriptors and are thus necessary to build and validate models. The group envisioned a list of core rate measurements that might be addressed: primary production/carbon fixation, including dark carbon fixation; bacterial production; respiration; nitrogen assimilation and turnover of ammonium and nitrate; phosphorus uptake and turnover; and iron (and potentially other micronutrients) uptake rates and turnover. The group discussed the experiences from trace gas intercalibration exercises, as well as the possible value of engaging expertise at US National Institute for Standards & Technology (NIST). The group also discussed the value of a dedicated rate intercalibration cruise (following the model of the US GEOTRACES SAFe cruise) vs. shore-based mesocosms where groups and methods can intercompare. A number of specific components of many biological rate measurements that deserve specific consideration were highlighted: killed controls, filter material and pore-size, timepoint spacing, and appropriate blanks. There was agreement that this topic, while perhaps less exciting as optimizing more novel techniques, is equally important to an effective BGS program.

View from NSF

Biological Oceanography Program Director Mike Sieracki and Chemical Oceanography Program Director Liz Canuel shared their perspectives from the US National Science Foundation. They discussed how community programs gain support from NSF and highlighted how it is important to demonstrate broad community interest, engagement, and enthusiasm, as well as 'readiness', where readiness could include if the methods and technologies sufficiently developed. They also pointed to the need to demonstrate that there are theoretical frameworks to organize and consolidate experimental findings. A BioGeoSCAPES program would result from the community advocating the need for such a program, rather than from a top-down decision to implement a program through the community. Funding would likely come from the core budgets rather than from dedicated new funding. They encouraged BioGeoSCAPES organizers to consider how to leverage investments that NSF has already made in ocean biogeochemistry (e.g., Ocean Observatories Initiative (OOI), Center for Chemical Currencies of a Microbial Planet (C-CoMP), Global Ocean Biogeochemistry Array (GO-BGC), and Southern Ocean Carbon and Climate Observations and Modeling project (SOCCOM)). They mentioned the challenges of the time and space scales that would need to be addressed through BioGeoSCAPES, including challenges in scaling up from the cellular and molecular measurements to the process level, in meshing the time/space scales of sampling with high resolution models, and determining how modelers could incorporate 'omics data.

Summary of Post-Workshop Survey Results

Feedback was obtained from a post-workshop survey, to which 44 participants responded. The respondents had a broad range of expertise, including organic geochemistry, microbial ecology, trace metal chemistry, biogeochemistry and modeling. Overall, there was a lot of positive feedback on the meeting. Here are two examples of feedback on the overall workshop content and organization: "It worked surprisingly well for such a big audience on zoom." and "Given the challenges of a virtual workshop and the limited time available for discussion, I thought the content and activities were well planned. It would have been nice to meet in person and take part in some more informal activities to discuss the state of the field and broader implications of BioGeoSCAPES, but otherwise, I think we were able to address the central questions posed at the first national meeting for the US." Several participants commented on the process, for example two participants said: "I thought it was great, I really enjoyed the format which I think did a good job of giving everyone an equal voice." and "I was impressed at the inclusive tone set by all organizers". There were specific concerns raised, three examples include: "The discussions throughout the workshop were awesome, but it was difficult to focus on coming up with concrete 'big questions' in the breakout rooms.", "There is little discussion of data management and QC, while these should be a core component when

talking about inter-calibration.", and "I was expecting to see more geochemistry/biogeochemistry. The 'Bio' part of BioGeoSCAPES seemed to dominate and the audience/speakers seemed 'Bio' centric." This feedback will be used to try to improve future BioGeoSCAPES Workshops.

Participants were asked to quantitatively estimate the relative contribution of activities to the US BioGeoSCAPES effort and capabilities. The results (Figure 3) showed a balance between field process studies (20-60%), field transect/sectional studies (20-80%), laboratory studies (20-30%), and modeling (20-30%), showing a balance between field transect/sectional studies and field process studies, and a slightly smaller contribution of laboratory and modeling studies.

Regarding the current mission statement, 24 of 44 of the participants recommended simplifying the mission statement, especially removing or rewording the phrase "hierarchical seascape" due to it being too unclear and jargony. Finally, there was strong interest among respondents in future participation, including participating in future workshops and intercalibration efforts.

Outlook and Program Vision

The ocean is experiencing rapid change. Climate change has brought more frequent and intense marine heatwaves, expanding regions of deoxygenation, and shifting ecosystems. The need to understand and predict the impacts of climate change on ocean productivity and biogeochemistry are greater than ever before. Pressure and interest in manipulating large-scale ocean processes to increase carbon dioxide removal is growing, despite a lack of understanding about the efficacy and side-effects of such efforts.

BioGeoSCAPES is envisioned as a program for bringing together an interdisciplinary international community to develop an improved understanding of ocean metabolism using a set of standardized protocols. 'Omics are no longer 'boutique' analyses - there is now a set of basic 'omics measurements that is fundamental to our understanding of what life is present in the ocean, and how that life is interacting with the chemical environment. Moreover, it is critical to integrate insights gained from 'omic analyses with other approaches (e.g., rate measurements, nutrient and trace metal concentrations, etc). BGS will provide a platform for these studies that will both facilitate this type of interdisciplinary work and create a common set of protocols that allow for globally consistent studies and synthesis efforts.

We envision that BGS efforts will include both process studies and large-scale transects to map out these critical properties. Moreover, BGS will provide a space for synthesizing knowledge across the many subdisciplines studying biogeochemistry and for integrating many different approaches from laboratory culture studies, to *in situ* incubations, to process cruises, to global mapping, to modeling. This effort cannot be accomplished by any individual lab or research group or nation. A coordinated, intercalibrated, international program of paired molecular biology and biogeochemical measurements is needed to advance understanding of ocean metabolism to address challenges that the ocean and humans face from climate change.

One approach for achieving a coordinated international program has been referred to as the 'franchise model', which could allow interested participants to self-organize BGS activities and projects focused on specific processes, regions, sections, or time periods. Intercalibrated measurements from such studies would be incorporated into a shared, intercomparable and interoperable global dataset. This approach may be well-suited to both scientific research questions that study complex biological-chemical problems that vary in space and time and the broad US interdisciplinary research capabilities. The franchise model would allow for nimble and cost-effective approaches to addressing BGS research priorities, in comparison with the US GEOTRACES model that relies on large coordinated section cruises every 2-3 years that command large amounts of resources and result in oversubscribed demands on ship berthing and wire time. Such a franchise model could follow the example of GEOTRACES process studies and compliant sections.

Next steps

Development of the BioGeoSCAPES program

As mentioned above, members of the international BioGeoSCAPES community have been applying to funding sources for further development of the program. In the summer of 2022, funding was obtained from US NSF under the Accel-Net (Accelerated Networks) Program to organize meetings and promote educational exchanges. Notably, this program is intended to foster international collaboration and hence, is ideally suited to the development of BGS. Specifically, the grant will support international workshops on science plan development, intercalibration, data management, and integration of modeling. The Accel-Net grant will also support education and training opportunities such as BGS summer schools, participating in and curriculum development for the Ghana School for Coastal Ocean Science, and coordination of international exchanges between laboratories for early career scientists. The Accel-Net Program does not fund scientific research directly, but instead is intended to support community building activities to develop the network-of-networks needed to broaden international collaboration. Many of the activities described as needed in the US and other national meetings can be focused on in the workshops that will be supported by this project, in close collaboration with international partners. Further information will be provided on the Accel-Net BGS effort as it spins up in the coming year. As part of the BGS Accel-Net, leadership teams will be created as needed to ensure execution of proposed international workshops and educational activities. Based on this meeting and recent Ocean Sciences Meeting sessions, there is broad interest in the science of BGS, particularly among early career scientists, and based on this US National Meeting, the US community clearly shows strong support and capabilities for the ongoing development of this international program.

Intercalibration and Data Management Efforts

Essential to the launch of BGS is the ability for datasets to be intercomparable via successful intercalibration efforts, and to be interoperable, allowing data to be synthesized across many international efforts. Because of the complexity of 'omics data, both of these efforts are likely to be particularly challenging. The meeting highlighted recent US-based intercalibration efforts, and also included participation by ocean data managers (e.g., Biological and Chemical Oceanography Data Management Office, BCO-DMO). Inter-calibration and data management capabilities represent foundational pillars of an emerging BGS effort and will thus required immediate and sustained attention and progress over the next 5 years. The newly funded AccelNet project will coordinate two large hybrid workshops, as well as more frequent open virtual presentations/discussion, help to build international collaborations and accelerate progress in this area. While some communities have already self-organized additional grassroots intercalibration efforts are needed and strongly encouraged.

Responses to Questions from International BGS Body

Four questions were posed by Maite Maldonado during her presentation describing international activities (also see summary above). Summaries of responses to these questions follow each question, harvested from group discussions.

1. Suggested changes to the BGS mission statement?

A poll was conducted on the first question, and 40% of respondents felt the mission statement could benefit from some tweaking (see Figure of poll results below). Specifically, the "hierarchical seascape perspective" clause was difficult to understand in a brief mission statement. Other topics were not explicitly addressed, but many of their themes were present throughout the discussions, such as the

capabilities and current needs, and types of studies and how they would relate to science questions (e.g., process, sections, and culture studies).

- 2. How would your nation best contribute to BGS efforts?
- As demonstrated by the large meeting turnout, the US is fortunate to have a large and motivated scientific community interested in BGS. Additionally, the US has a history of supporting interdisciplinary research, both at the funding level and through bottom-up self-organization of interdisciplinary teams spanning biological, chemical, and physical oceanography domains. In addition, the US has a history of international collaboration, most recently within the GEOTRACES Program. The US is well positioned to help the international community launch BGS if we are able to maintain a positive and inclusive sense of community. To this end, continued efforts towards democratization of programmatic development efforts are encouraged to maximize inclusivity, (e.g., self-organized intercalibration efforts, and organization and participation of BGS sessions at meetings). Furthermore, the concept of a "franchise model" of funding, in which self-organized groups can pursue BGS projects that comply with sampling, intercalibration and data management guidelines is one that is broadly appealing to the US community to maximize engagement and science advancement. All of these efforts would be enhanced through international collaboration and coordination.
- **3.** What science questions are most important to your nation with BGS on a 10-yr timeframe? This question was addressed in the breakout groups on Day 2 where participants were divided into 11 groups. Scientific guestions discussed are summarized above and listed in Tables 1 and 2.
- 4. Are there any impediments that the international community could seek to mitigate via training or collaboration?

While this question was not explicitly discussed, the breakout groups on Day 2 focused on the challenges and needs in intercalibration and data analysis and management. There are extensive needs in these areas, and the success of an international BGS program relies on international intercalibration and data management efforts. Brainstorming results from breakout group discussions are summarized in the Day 2 question summary and in Table 3.

References

Levine, N.M, Leles, S.G. 2021. Marine plankton metabolisms revealed. *Nature Microbiology*. 6. 147-148. doi: 10.1038/s41564-020-00856-x.

Table 1. Responses to the discussion question "What hypotheses could be addressed by the BioGeoSCAPES program, towards the goal of coalescing around high-level motivations?" Results collated from 11 breakout groups.

Carbon and Element Cycling

- What controls the fate or persistence of organic matter in the ocean?
- What controls the transformations and vertical fluxes of organic carbon in the ocean?
- Which organisms dominate new and export production?
- What are the remineralization length scales of different nutrients: Is iron more highly recycled at the surface than nitrogen or phosphorus?
- Ecological stoichiometry: What are the carbon, nitrogen, phosphorus and trace element quotas of every even marginally environmentally relevant bug we have in culture?
- What is the exo- and endometabolome of every SAR11, Thaumarchaea, SUP05, etc. we have in culture (this would require massive coordinated effort, similar to MMETSP)
- What is the role of microbes in moderating the flux of material to and from the benthos?
- Is there a unique biomarker to link to the biological pump?
- On the intersection between metabolomics and biogeochemistry, to what extent do ecosystems and microbial diversity interact, and are the interactions bidirectional?
- How does unbalanced deep ocean carbon demand compare to export flux from above?

Climate Change and Environmental Stress

- What are the physiological responses to environmental change?
- How is ocean net primary productivity changing in response to climate change? How will it change in the next century?
- What are the distributions of nutrient stress and viral/grazing pressure as detected/diagnosed by 'omics?
- How is the organic carbon inventory changing in the ocean? What are the roles of microbes, viruses, and their predators in moderating carbon transformations?

Ecosystem and Biogeochemical Structure and Function

- What overarching spatial and temporal patterns in microbial taxa and metabolic function exist across the ocean?
- What are the controls on ocean microbial biogeography and diversity?
- How does the microbial distribution influence biogeochemical function? Sub-themes highlighted focused on the role of light, redox state, nutrients, micro-zones in these distinctions, and identifying overarching patterns that scale from 'microbes' to 'seascapes'.
- "Who's there and what are they doing?" needs to be asked in multiple places at multiple times in order to determine what environmental parameters control activity. Not only who is there but how much different organisms contribute to different processes.
- What is the role of (micro)nutrients in structuring microbial communities and their function? How does metals bioavailability (chemical speciation) affect biodiversity?

- Can relationships between environmental conditions, community structure and function, and biogeochemical rates be elucidated?
- What is the extent of anoxic processes in the oxic water column? Connection of anoxic/suboxic processes to the nitrogen cycle biogeochemical reactions?
- What are the drivers of autotrophy and heterotrophy?
- What are the controls on phytoplankton loss rates?
- Can bulk biogeochemical rates be reconstructed from biological components?
- What is the importance of mixotrophy to ocean ecosystems and biogeochemical cycles?
- Crossing strong gradients (spatial and temporal) are often ideal places to identify important signals (mechanisms)
- How are the deep mesopelagic and bathypelagic microbial communities impacted by export from the surface ocean?
- Can use these high resolution measurements to determine important scales of variability?
- How can we use metabolomics or other 'omics to diagnose nutrient stress, viral and grazing pressure?
- Loss rates for phytoplankton are important in setting scalings between environmental conditions and fluxes. Looking at viruses and zooplankton biomass and how they scale with phytoplankton could be really helpful in constraining such models.
- On ocean sections, where there are physical intersections between biomes, what processes are occurring? How do biota adapt to physical and chemical transitions?
- Can microbial and biogeochemical observations be connected to predictions of higher trophic levels dynamics, including zooplankton and larger metazoa (including fisheries)?

Ecological and Biogeochemical Theory / Modeling

- Studies targeting the paradox of the plankton, applying multi-omics approaches.
- Can 'omics data be applied to inform and improve bottom-up modeling simulations and predictive capabilities?
- Can the central dogma of Biology be studied in the environment across ecosystem diversity (e.g., RNA/Protein, growth rate)?
- What determines whether there is competition of coordination for scarce resources in the ocean environment?
- Where do we find different metabolisms in the oceans and how do we model these dynamics?
- How robust are marine microbial communities? What types of perturbations are needed to push a community beyond an irreversible tipping point?
- Can ecological concepts and theory for macrofauna be applied to marine microbial interactions?
- Collaboration with other discplines such as physical oceanography will provide a greater context to BGS
- What controls the fate or persistence of organic matter in the ocean: biology or chemistry? Does biological community composition control when/where dissolved organic matter is consumed or is chemical recalcitrance more important?

- At the global scale, how much does gene presence correlate with gene usage specifically for things like nitrogen cycling?
- What are the models missing? Are they able to capture future changes if they don't accurately represent present-day diversity and biochemistry occurring?
- Rates are an emergent property of the organisms rather than their transcription; can we obtain higher predictive capabilities using community composition?

Methodological and Study Design

- Can we make the leap from 16S/18S to cell count?
- How does it all fit together: genetics, transcriptomics, proteomics, etc. to link biodiversity to biogeochemical activity?
- What is the relationship between gene expression and rate activity? Which genes are more important than others? (e.g. sentinel genes? organisms?) Could BGS tell us what to monitor for ocean change?
- Need to conduct sampling at larger scales (both time and space) in metabolomics and lipidomics
- How do we connect process-level measurements to big picture processes like carbon flux?
- Need for simultaneous rate measurements along with standing chemical stocks
- Rates are an emergent property of the organisms rather than their transcription, so can we have higher predictive capabilities using community composition data?
- Leverage long-term ocean observing efforts that are making complementary standard measurements like net primary production, export, etc.

Table 2. Examples of Science Questions addressable by the BioGeoSCAPES community. Responses to the discussion question: "What are compelling questions that can't be addressed by a single group and really require a coordinated program?" Results collated from 11 breakout groups.

- Studying the diversity and function of the ocean
- Development and application of global biogeochemical and metabolic models to explore how changes in the ocean result in shifts in metabolic fluxes and metabolisms
- Global spatiotemporal variability of biogeochemical transformations and the organisms that drive them
- Establishing a baseline measurement of global biogeography (taxonomy first) to allow other investigators to build on this foundation
- Quantifying all of the biomass and carbon present to provide as complete a story as possible.
- Who is where, and what environmental factors are determining these communities and their function?
- How do phytoplankton mediate the biogeochemistry of their environment, and how do we scale up observations of small-scale interactions to understand global-scale impact?
- 4D distributions across ocean depth and seasonal changes will necessarily require many groups working together. This also requires sampling over different time scales
- Specific approaches of bottom up vs. top down, how can these be used to inform each other? how are the processes interacting?
- How are the deep mesopelagic and bathypelagic microbial communities impacted by export from the surface ocean?
- Linking rates and community structure
- Assessing scales of biological and chemical variability
- Global models resolve on 100s km and months/weeks. How to marry that with 'omics that yield snapshots that change on much shorter space and time scales?
- How to relate lessons from 'omics to large-scale biogeochemical models? Challenges of temporal and spatial scale mismatches.
- What are the most important compounds and how do we figure it out? Can a specific set of core compounds be focused on? Importance of broad 'omics surveys to overlap with separate studies/time series that focus on processes/fluxes. Including connections to controlled laboratory studies.
- A BGS program needs to include both bottom-up and top-down controls biology on nutrient cycles
- Connections to higher trophic levels and rest of food webs
- Paired (i.e. chemical and 'omics) datasets could be interesting to look at both horizontal and vertical scales.
- Standardization of data collection and formatting improves 'democratization' of data sharing
- 1000-5000m depths are still relatively unexplored for microbiology and biogeochemistry
- Is this program contributing to carbon sequestration or resilience or food production? (functions microbial and biological communities). If so, how to do this
- Flexibility when defining the thresholds of what can be categorized as primary signals, which

depend on ecosystem type, volume, mechanisms occurring and seasonal events.

- eDNA could bridge the gap to larger trophic levels. Would it provide the ability to translate up food web? What kind of samples should be taken and expertise entrained?
- We need to build connections between intercalibrated measurements to understand what they are telling us
- Samples stored and reanalyzed at international level. Nations will share beyond their analytical capacity.
- Scale of experimental effort opens up new opportunities/questions
- There is important information from cultured organisms that inform rates and mechanisms. Incorporating and connecting these to environmental measurements is important.
- Elucidating the close interaction between organisms that we're just starting to discover. Facilitated by metabolites combined with other 'omics.
- Biogeochemical implications of 'omic measurements
- Characterization of organic carbon forms
- Franchise model (giving freedom to science groups to attack different questions using intercomparable/combinable measurements) seems like a good way to figure out the best type of studies
- Integrating across the biological carbon pump and microbial carbon pump requires collaboration between experts on each level of the microbial food web (viral ecology, bacteria and archaea, phytoplankton, zooplankton, fungi).
- How to maintain key structural attributes of an ecosystem (e.g., abundance and biomass) while characterizing the composition and metabolic activity in the ecosystem in the context of varying environmental conditions. How resistant is the system to outside forces? How quickly does it recover? What contributes to resilience?
- Links between community structure and biological rates training datasets for statistical models require datasets that that span space and time beyond what individual investigators can do
- Need a whole-community data collection 'pause' to help with data interpretation
- What is being measured and how does that connect to biogeochemical modeling?

Table 3. Compilation of breakout group responses to the discussion question 3: "What are the key intercalibration needs to help support and realize our science goals?" Results are broken down into themes of 'intercalibration and methods', 'sampling and sample processing', and 'data management and repositories'. Results collated from 11 breakout groups.

Intercalibration and Methods

Discussion on intercalibration itself:

- Intercalibration needs to come first! Need a standard method of sample collection and processing
- Make intercalibration efforts do-able and not onerous for different teams to participate in
- Prioritization of measurements for intercalibration/standards: What are the core methods for high priority for intercalibration?
- Intercalibration is necessary to relate rates.
- Intercalibration of 'omics is a waste of time. Not worth the money. Side note: this comment relates to "standard" 'omics, e.g., 16S, metaG. New techniques such as metabolomics, proteomics, etc. probably still need it!
- Don't forget about "simple" measurements: virus/bacteria/protist counts, carbon fixation, bacterial production, particulate and dissolved organic carbon
- Intercalibration across methods per se: if we know a process is occurring, do our rate methods track it? Do proteomics track it? Do transcriptomics track it?
- What is the best way to intercalibrate for complex analytes?
- How much 'omics intercalibration is necessary?
- Can modeling needs inform intercalibration needs?
- What are the minimum number of replicates needed for reliable 'omics measurements?
- Calibration is needed but also trying to keep the unique specialties of each of the groups
- Intercalibration of whole earth microbiome
- Make 'omics data more quantitative and intercomparable
- Foster connections to human microbiome community, National Institute of Standards and Technology (NIST); identify synergies.
- Utilize GEOTRACES approach of consensus values.
- Access to infrastructure for intercalibration (e.g. each lab needs to have the same equipment, etc.)
- Consistency in methods (e.g., different primers across labs)
- Where are funds going to come from for intercalibration? Some of the workflows are expensive.
- How to balance specialization of labs to answer specific questions versus tradeoffs between streamlining processes but not losing the depth of study within groups?
- Interdisciplinary efforts across studies with different scopes: from small scale to global on individual projects
- Lab standardization via multi lab testing of same samples for intercalibration

- How do we do intercalibration for metabolomics?
- Dissolved metabolomics intercalibration of sorts ongoing
- What are the important molecules? How are those molecules determined?
- How do we annotate lipidomes and metabolomes?
- Which extraction or other methods are 'correct' and selected for intercalibration?
- Develop a cookbook with detailed protocols
- What to do about future comparisons?

Analytes brought up for intercalibration

- Nucleic Acids
- Chemical 'omics
 - ♦ Metabolomics (DOM community is doing one now, but distinct from metabolomics)
 - ♦ Lipids
 - ♦ Proteomics
- Rates
 - ♦ N-fixation rates
 - Primary production rates
 - ♦ Enzyme rates (alkaline phosphatase)
- Flow cytometry
- Flowcam/imaging cytometry
- eDNA
- Microscopy

Standards and Reference Standards

- Develop mock communities for standards
- How do we give feedback to analyses that vary significantly from consensus values?
- Lipidomics and metabolomics can buy standards for many compounds, but not all.
- Obtain lessons from ongoing efforts to standardize image-based measurements?

Sample collection and processing

- Standardize sample collection but don't worry about the rest. This is one way that the International Ocean Discovery Program (IODP) democratizes deep sea science
- Develop sample archive in case methods change in 10 years
- Develop cookbook(s) with detailed protocols
- In discrete samples in a dynamic environment, is there a lag between changes in environments? An organism response to something that has a shorter residence time than response time, what does that mean?
- · What matters in sampling: filter type, flow rates

• Challenge: different groups have different extraction methods. How to select which is 'correct' to pursue for intercalibration? Should we just prioritize the output, not the steps to get there?

Bioinformatics Standardization, Data Processing, and Data Portals / Repositories

- Develop and improve availability of shared (nucleic acid) databases
- Centralized repository for intercomparable data
- Open access analysis pipelines
 - ◊ Standardized bioinformatic pipelines
 - ♦ Should they be standardized?
 - ♦ How to deal with multiple but not necessarily overlapping pipelines
 - Making analysis pipelines publicly available to ensure inter-comparibility of results (scripts through GitHib, software versions and parameter settings, etc.)
- How close are we to some 'omics data being commonplace and standardized enough to lend itself to becoming open access? Metagenomics?
- Scaling smaller scale studies to a global context within these repositories
- Challenge: make 'omics data more quantitative and intercomparable
- · Open data requires good intercalibration of methods

Figure 2: In-Meeting Poll Results (continue over next several pages)

How will you/your group contribute to preparing to BioGeoSCAPES?

ecological-interpretation



How should the US community prioritize its contributions in preparing to BioGeoSCAPES?



US National BioGeoSCAPES Workshop Report

How many more years of international planning and coordination do you think it will take to launch BioGeoSCAPES?



What are the biggest bottleneck(s) in advancing BioGeoSCAPES? e.g. capacity building, collaboration (nations, disciplines), intercal...



US National BioGeoSCAPES Workshop Report

What is the most pressing intercalibration and/or intercomparison need?



I think the preliminary BioGeoSCAPES Mission Statement:



What is your field of study?



Figure 3: Post workshop survey results about the relative contribution of activities to US BioGeoSCAPES effort and capabilities.





Bioinformatics and other data synthesis activities stemming from field operatoins

An intense study of one "model" water column location where all possible analyses (16S, 18S, metagenomics, metatranscriptomics, metaproteomics, untargeted and targeted metabolomics, metabolic and biogeochemical modeling, flow cytometry enumeration, rate measurements, stable isotope probing) are carried out.

Intercalibration activities
Time-series
QC and data management

Appendix A. Meeting Agenda and Schedule from OCB meeting website

OCB Scoping Workshop: Laying the foundation for a potential future BioGeoSCAPES program

Scoping Workshop Objectives

Understanding ocean metabolism on a changing planet is a complex and challenging problem that requires coordination across many different fields. We find ourselves finally at a point in time where international momentum has built and we are methodologically and intellectually poised to take on the challenge of an integrated microbial biogeochemistry program. Critically, we see the international community moving forward with a BioGeoSCAPES initiative and feel it is imperative that the US maintain a co-leadership role. This workshop represents an opportunity for interested US scientists to contribute to the development of key scientific guestions that a coordinated microbial biogeochemistry program could address and articulate how those would bridge disciplines (e.g., questions that are fundamentally biological, chemical, or both). Participants will discuss currently available technical capabilities, as well as obstacles to be addressed in order to address the proposed studies. Project scope will be discussed, with efforts made to develop consensus on how to focus the BioGeoSCAPES program within the broader fields of biological and chemical oceanography. Ongoing 'omics intercomparison and intercalibration efforts (ocean metaproteomics, ocean nucleic acids) will lay critical foundation for BioGeoSCAPES, and participants will provide updates on their status and discuss further efforts that will be needed for those domains. Furthermore, additional analytes that may be of scientific value may be identified as needing intercalibration efforts in order to create globally intercomparable values needed for a large-scale program. For a preliminary schedule, we propose to begin with an introduction by the conveners, followed by several plenary talks to set the stage for the discussions, and then having a combination of large and small group discussions on various topics such as:

- scientific questions of interest (with breakout groups by geographic region and depth)
- analytes of interest and availability of intercalibration standards for ensuring accuracy in largescale sampling programs
- integration of sampling modes and their integration with scientific objectives (e.g., temporal and spatial)
- available and emerging sampling platforms
- challenges of data management and archival, synthesis, and modeling
- scope of the BioGeoSCAPES initiative (i.e. balance of field vs. lab measurements, section vs. process studies
- mechanisms to facilitate international coordination
- potential funding sources and feasibility with the US system

Anticipated Outcomes

An important aspect of the workshop will be using the discussion to develop a list of action items to enable the US program to further the progression towards a global-scale microbial oceanography capability required for a BioGeoSCAPES program. Primary outcomes will include:

- Community-building of a diverse group of national scientists with expertise in microbial biogeochemistry
- Workshop report summarizing workshop findings and future action items
- Read the proposal first two pages include history of this effort

Daily Schedule All times in ET, from 13:00-16:30 each day

Day 1: Wednesday, November 10, 2021

13:00	Welcome, OCB Code of Conduct, and meeting logistics	Naomi Levine
13:10	BioGeoSCAPES: A brief history	Adrian Marchetti
	Lessons from other international programs	Alyson Santoro
	BioGeoSCAPES community building in other countries	Maite Maldonado
	Motivation for BioGeoSCAPES and goals for this meeting	Ben Twining
	Q&A	
	Watch this recording	
	Breakout discussions	
14:15	• What existing communities and networks should we connect with (that are not shown in this diagram)?	
	 List examples of good community building efforts within (and beyond) the oceanographic community we can learn from 	
	• What are potential barriers to interdisciplinarity and inclusivity in a global effort like this and how can we address them?	
15:00	Summary and homework for Day 2	
15:00- 16:30	Poster session on gather.town	

Day 2: Thursday, November 11, 2021

13:00	Welcome: Summarize day 1 breakouts, review plan for the day	Alyson Santoro Adrian Marchetti
13:15	Poster session on gather.town	
14:00	 Updates from intercalibration activities Overview of BGS intercalibration Update on proteomics intercalibration Update on NA 'omics intercalibration Watch recording - Part 1 	Mak Saito Paul Berube
14:30	 Breakout Discussions What hypotheses could be addressed by BGS program, towards goal of coalescing around high-level motivations? What are compelling questions that can't be addressed by a single group and really require a coordinated program? What are the key intercalibration needs to help support and realize our science goals? 	

15:00	Break	
15:10	Talks: Examples of potential BioGeoSCAPES science questions	Scott Gifford Bethanie Edwards Julie Granger Scott McCain
16:10	Summary and feedback via Mentimeter and homework for day 3 Watch the recording - Part 2	

Day 3: Friday, November 12, 2021

13:00	Welcome and summarize day 2 breakouts	Ben Twining Naomi Levine
13:15	Talks: Examples of potential BioGeoSCAPES science questions Watch recording part 1	Daniele Iudicone Lihini Aluwihare Sarah Hu John Casey
14:15	 Breakout discussions Describe successful models of interdisciplinary BioGeoSCAPES science. Brainstorm ways to effectively integrate across disciplines. Brainstorm novel applications of tools to address global questions. 	
15:00	Break	
15:05	Discussion: what are the overarching similarities that make these studies and other studies good examples for BioGeoSCAPES? What are the scientific synergies that could be cultivated to maxi- mize science return?	
15:30	View from NSF	Mike Sieracki
15:50	Meeting wrap-up and discussion of next steps Watch recording part 2	

Appendix B: Meeting Participants

154 registered participants

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Appendix C: Poster presentations

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Sajjad	Akam	Distinct Membrane Lipid Compositions of Anaerobic Methane Oxidizing Archaea - Insights from Peru Margin
Sarah	Andrew	Proteorhodopsin localization and gene expression in a Southern Ocean diatom
Angie	Boysen	Particulate metabolites of the North Pacific reflect microbial community composition and activity
Natalie	Cohen	Metabolic profiles and ecological roles of diverse protists across a coastal-offshore biogeochemical gradient in the North Atlantic Ocean
Jacob	Cram	Network analysis reveals statistical associations between cyanophage host genes and cyanobacterial ecotypes across ocean basins
Clara	Fuchsman	Identifying biogeochemical linkages between bacteria and other trophic levels (protists, viruses, zooplankton) using phylogenetic read placement of metagenomic depth profiles from Oxygen Deficient Zones
Jaci	Saunders	Untargeted proteomics reveals marine microbial community functional shifts across biogeochemical provinces
Benjamin	Van Mooy	Global-scale ocean lipidomic survey reveals new insights on plankton physiology and biogeochemical provinces
Katherine	Barbeau	'Omics approaches to characterizing Fe and C coupling in heterotrophic marine bacteria
Rene	Boiteau	Illuminating the ocean's 'black box' metallome

Irina	Koester	Untargeted metabolomics of organic matter across oxygen gradients in the eastern tropical north pacific ocean
Robert	Lampe	Drivers of diatom abundances and diversity in a coastal upwelling biome
Jesse	McNichol	Progress & prospects for using universal primers for biogeography and modelling
Erin	McParland	Seasonal and diel variability of a depth-resolved exometabolome at the Bermuda Atlantic Time-series Study
Susanne	Menden- Deuer	Phenotypic trait diversity in plankton promotes species co-existence and microbial diversity
Andrew	Allen	Transitions in nutrient supply drive variation in pelagic ocean microbiome biodiversity and distribution in a coastal upwelling ecosystem
Jeff	Bowman	Predicting net community production from microbial community structure in the coastal ocean and beyond
Anitra	Ingalls	Stable isotope probing metabolomics reveals the complex role of glycine betaine in marine microbial communities
Seth	John	Awesome OCIMs such as the AWESOME OCIM are awesome for modeling metalsare they equally awesome for BioGeoSCAPES?
Kaijun	Lu	Evaluating initial peptide hydrolysis rates in seawaters using a tetrapeptide analog: ala-val-phe-ala
Laura	Sofen	Metal contents of small autotrophic flagellates from contrasting open- ocean ecosystems
Xin	Sun	Microbial Niche Differentiation Explains Nitrite Oxidation in Marine Oxygen Minimum Zones
Ying	Zhang	Bacterioplankton Dynamics and Nutrient Cycling Function in Narragansett Bay, RI
Nick	Hawco	Precise, low level iron uptake rates with MC-ICPMS: a trial run at Station ALOHA
Kaycie	Lanpher	Measuring energy charge and flux in marine microbial communities using the adenylate system
Robert	Letscher	Potential BioGeoSCAPES contributions from the Letscher lab: [DON], [DOP], [TEP-C], global biogeochemical-ecosystem modeling
Lauren	Manck	Iron Limitation in the Heterotrophic Bacterial Community of the California Current System
Kimberly	Popendorf	Microbial phosphorus cycling through group-specific uptake rates, enzyme activity, and biochemical allocation
Joshua	Sacks	Dissolved Metabolomics Enables Direct Observations of DOM Cycles

Appendix D: Workshop participant photos

100 participants shown







US National BioGeoSCAPES Workshop Report



https://www.us-ocb.org/ocb-scoping-workshop-laying-thefoundation-for-a-potential-future-biogeoscapes-program/

https://www.biogeoscapes.org/



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