



DEPARTMENT OF COMMERCE RESEARCH PERFORMANCE PROGRESS REPORT (RPPR)

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AWARD INFORMATION	
1. Federal Agency: Department of Commerce / NOAA	2. Federal Award Number: NA21OAR4310251
3. Project Title: Biogeochemical Argo Calibration Algorithms	
4. Award Period of Performance Start Date: 09/01/2021	5. Award Period of Performance End Date: 08/31/2024
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REPORTING INFORMATION	
Signature of Submitting Official: Brendan Rae Carter	
16. Submission Date and Time Stamp: 06/30/2023	17. Reporting Period End Date: 05/31/2023
18. Reporting Frequency: <input checked="" type="radio"/> Annual <input type="radio"/> Semi-Annual <input type="radio"/> Quarterly	19. Report Type: <input checked="" type="radio"/> Not Final <input type="radio"/> Final
RECIPIENT ORGANIZATION	
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ACCOMPLISHMENTS

24. What were the major goals and objectives of this project?

We proposed to create the following products:

1. Empirical seawater property estimation routines: This effort will be aimed at developing and validating empirical seawater property estimation routines with a focus on properties that are not part of the marine carbonate system, improving the quantity and quality of information that can be obtained from observation efforts like GO-BGC.
2. A homogenized seawater pH data and metadata product: Research efforts have recognized the difficulty of creating internally consistent pH data products due to the variety of measurement strategies used for pH and the varying completeness of metadata. This effort will collate cruise metadata, propose recommended adjustments for cruise pH, and release a companion product with these adjustments applied.
3. An estimation algorithm-based data Quality Control assistance tool: Disagreements between measured and estimated values can help call attention to anomalous measurements that warrant further attention, whether because the measurements are problematic or because they are unexpected and interesting. We will create a tool that will make these comparisons fast and easy, and that will put the results in the context of expectations from statistics. Using this tool when ingesting data into data products will improve the quality of the products and the efficiency of data quality control efforts.

25. What was accomplished under these goals?

1. Postdoc Larissa Dias began her tenure at UW working on this grant
2. Jonathan Sharp's GOBAL-O2 manuscript (detailed in the previous report) was submitted and has been through several rounds of peer review.
3. The pH metadata data product has been updated for GLODAPv2.2022 and is now incorporated into a paper describing the Ocean Carbonate System Intercomparison Forum working group activities. This paper includes several community statements and has been through 8 rounds of coauthor review while phrasing on specific statements was debated, has been through PMEL internal review, and is now being subjected to NIST internal review. It should be submitted for peer review within the month.
4. ESPER has been retrained to include depth as an additional predictor. While this inclusion has not been found to meaningfully improve the fidelity of the predictions from the algorithms, the inclusion of depth as a predictor diminishes the size of the prediction discontinuity when transitioning between LIR-pH and ESPER-LIR-pH (i.e., updating to the newest algorithm doesn't change things as much when you include depth, which is helpful for the people managing the float data products). This is a requested feature for future updates by the float data quality control community and, upon verifying this behavior over the previous year, the option to include depth as a predictor will be incorporated into ESPER updates going forward.
5. Larissa has been trained in the code used to generate updates to ESPER. We are currently awaiting the release of GLODAPv2.2023 to commence algorithm retraining in earnest, but she has had success with retraining ESPER on her machine. Our hope is also to incorporate the "TRACE" anthropogenic carbon estimation strategy which should be a marked improvement over the calculations currently used in ESPER without meaningfully increasing the computational burden of the estimate. The TRACE and GLODAPv2 efforts are both separately funded, though it is our hope to use funding on "this" project to bring Larissa into both efforts in a limited capacity. Her involvement should help make sure she is versed in these related efforts and broaden the "postdoc training" impact of this grant. These efforts will collectively represent less than 10% of her time, however.
6. Larissa has been training in Python programming and simultaneously writing scripts that will translate the ESPER routines from Matlab to Python. This could, we hope, result in an additional publication detailing the slight differences in the Python and Matlab algorithm estimates (differences that result from interpolation differences between the coding languages), and greatly increase the impact of the algorithms by extending the algorithms to the growing Python community. The translation is being done in a way to ensure that the translation of future updates can be accomplished programmatically rather than through manual coding.
7. Larissa is attending meetings including the OAP community meeting, the OCB meeting, and the (upcoming) GOMO community meeting. She has so far obtained two external grants for the travel for these meetings and, as a result, has not overburdened the travel budget on this grant. This is excellent professional development for Larissa and these activities have provided networking with her peers working on related GOMO-funded projects. We are also looking at OSM2024 to present research from this project.
8. Larissa has begun planning work on the effort to incorporate float pH into the ESPER training data products. It is our current plan to generate versions of ESPER both with an without float pH used as training data. The float pH data are nearly essential for capturing surface ocean seasonality, but there are some applications (e.g., float calibration) for which it is not desirable to incorporate the (much more uncertain) float pH measurement.

Attach a separate document if more space is needed for #6-10, or #24-50.

ACCOMPLISHMENTS (cont'd)

26. What opportunities for training and professional development has the project provided?

As noted above, this grant has supported Postdoc Larissa Dias while she is learning a programming language, engaging in research, networking with peers, presenting at conferences, and attending subject matter workshops. Larissa has also become involved in a weekly journal club organized by fellow lab postdocs.

Jonathan Sharp had a highly successful postdoc, funded in part by this grant, and has been hired on to a "research scientist" position. We are in the process of helping him secure PI status and he is rapidly developing a research portfolio that is closely adjacent to the work that is conducted under this grant (though not overlapping, except when explicitly funded by this grant). We anticipate that Jon will continue to be a leader in biogeochemical algorithm development.

27. How were the results disseminated to communities of interest?

The products have been presented at formal and informal presentations from Larissa Dias and PI Carter. PI Carter has presented on aspects of this project four times this calendar year. The first papers associated with this grant are currently making their way through peer review and more are nearing submission. We also work closely with the float data management teams at NOAA and correspond with those at MBARI to ensure that the products that we are creating are useful for their needs.

ACCOMPLISHMENTS (cont'd)

28. What do you plan to do during the next reporting period to accomplish the goals and objectives?

1. Complete the translation routines for Python. Submit a short technical paper detailing this product variant for publication.
2. Retrain ESPER to incorporate GLODAPv2.2023 and (if it is ready in time) TRACE anthropogenic carbon estimation. Publish a paper detailing these updates and providing an assessment and validation for the new methods and documentation for the changes and the rationales behind making the changes.
3. Retrain this updated ESPER with float data in the surface ocean to better resolve surface ocean seasonality. As time permits we will also incorporate additional oxygen data and generate the algorithm estimates for Dissolved Organic Carbon. Depending upon timing, the documentation of this float/seasonal ESPER variant might be in a separate paper from the products listed in (2) or in the same paper.
4. Begin work on the ocean chemistry "Quality Control Assistance Tool" QCAT. QCAT will be most useful for the community if it benefits from the seasonality representation by the products in (3), so this will be the last work in the queue for the coming reporting period.

PRODUCTS

29. Publications, conference papers, and presentations

The GOBAI-O2 paper led by J. Sharp is partially funded by this work and is in revisions.

OCSIF recommendations paper is nearing submission (and contains the pH metadata data product funded by this effort).

All other papers are to be led by postdoc Larissa Dias and are in prep.

PRODUCTS (cont'd)

30. Technologies or techniques

The GOBAI-O2 uses a novel combination of predictors with an increasingly common machine learning strategy to great effect, but this is more of an iteration on existing approaches.

We are currently using neural networks and locally interpolated multiple linear regressions as estimation tools. Larissa Dias is taking a machine learning workshop with the goal of assessing whether it makes sense to also incorporate Random Forest Regression or Extreme Gradient Boost estimation (or alternatives). Often these methods perform best, but come at a meaningful cost in the form of slower computation and higher-memory-footprint algorithms.

We are testing the use of generative AI to make the translation of Matlab code to Python more efficient.

31. Inventions, patent applications, and/or licenses

Nothing to Report

PRODUCTS (cont'd)

32. Other products

Nothing to Report

PARTICIPANTS & OTHER COLLABORATING ORGANIZATIONS

33. What individuals have worked on this project?

Brendan Carter (PI)
Andrea Fassbender (PI)
Richard Feely (PI) - primarily involved with postdoc selection
Jonathan Sharp (Postdoc)
Larissa Dias (Postdoc)

PARTICIPANTS & OTHER COLLABORATING ORGANIZATIONS (cont'd)

34. Has there been a change in the active other support of the PD/PI(s) or senior/key personnel since the last reporting period?

(Unrelated) Projects have been funded that allow PI Carter and Jonathan Sharp to continue to work at 100% time across multiple projects for the entire duration of this grant while still working for the proposed amount of time on this grant.

35. What other organizations have been involved as partners?

No other partners are funded, but this research touches upon several communities working on marine biogeochemistry.

PARTICIPANTS & OTHER COLLABORATING ORGANIZATIONS (cont'd)

36. Have other collaborators or contacts been involved?

These efforts have an extensive network of collaborators within the BGC Argo, Data Management and Synthesis, and Ocean Carbonate System analysis and interconversion communities.

IMPACT

37. What was the impact on the development of the principal discipline(s) of the project?

GOBAI-O2 stands to resolve a debate between modelers and observationalists over the magnitude of the rate of global ocean deoxygenation. The findings suggest that the deoxygenation rate found by modelers has been underestimated just as the rates found, previously, by observationalists were greatly overestimated due to the sparsity of the data and the mapping approaches employed.

The seasonal-pH algorithms have the potential to be incorporated into global interior ocean carbon estimation strategies. These estimates could potentially allow near-real time quantification of the full 4 dimensional distribution of carbon in the ocean. Significant work remains (including the work funded by this proposal) to make this possibility a reality however, and additional feasibility testing is required to quantify the likely uncertainty on the estimates produced by such an approach.

The predictive algorithm updates stand to ensure this strategy remains the best available approach for interior ocean float sensor calibration.

The QCAT tool could improve data quality control for marine biogeochemistry generally and form the basis for the creation of internally-consistent data products out of datasets that lack deep measurements (e.g., coastal data synthesis).

IMPACT (cont'd)

38. What was the impact on other disciplines?

Nothing to Report

39. What was the impact on the development of human resources?

Postdoctoral and PI supports has allowed the scientists to remain working with the field and continue their growth as scientists.

IMPACT (cont'd)

40. What was the impact on teaching and educational experiences?

Pls Carter and Fassbender have provided mentoring for postdocs Sharp and Dias. Sharp has also guest lectured at an oceanography class and, in summer of 2022, Sharp mentored an undergraduate intern (Reese Barrett) who has subsequently decided to begin a graduate program in chemical oceanography with the Carter Lab at the University of Washington (she will be working on separately funded work, but will continue to be exposed to this research and she worked on related research during her internship).

41. What was the impact on physical, institutional, and information resources that form infrastructure?

Nothing to Report

IMPACT (cont'd)

42. What was the impact on technology transfer?

Nothing to Report

43. What was the impact on society beyond science and technology?

Nothing to Report

IMPACT (cont'd)

44. What percentage of the award's budget was spent in foreign country(ies)?

0 , null

CHANGES/PROBLEMS

45. Changes in approach and reasons for change

Earlier versions of ESPER were written exclusively in Matlab, and the translation of ESPER from Matlab to Python is a non-trivial task that was not originally planned for this research. Four things changed our thinking and led us to believe it made sense to do the translation first:

1. The Python community continues to grow in oceanography
2. Before being accepted at a journal, the ESPER manuscript was rejected from another journal (despite being very favorably reviewed by the editor and others) because it was only available in a costly programming language.
3. Larissa and Carter agreed that improving her coding ability in Python is an important professional development goal for Larissa.
4. Larissa finished experimenting with the ESPER update code before the GLODAPv2.2023 or TRACE components were ready.

CHANGES/PROBLEMS (cont'd)

46. Actual or anticipated problems or delays and actions or plans to resolve them

The main delay has been the slow process of hiring and onboarding Larissa (she began at the start of 2023 and worked remotely until 06/2023). It is looking likely that an extension of 1 year would be helpful to complete the funded work (but the deadline is still too far away to be sure whether that will be necessary).

47. Changes that had a significant impact on expenditures

Nothing to Report

CHANGES/PROBLEMS (cont'd)

48. Significant changes in use or care of human subjects, vertebrate animals, biohazards, and/or select agents

Nothing to Report

49. Change of primary performance site location from that originally proposed

Larissa needed to work remotely from Texas for the first months of this year due to familial obligations. She has recently relocated to Washington/Seattle.

PROJECT OUTCOMES

50. What were the outcomes of the award?

Development of a novel oxygen product and set of estimation algorithms that incorporate profiling float observations as training data.

DEMOGRAPHIC INFORMATION FOR SIGNIFICANT CONTRIBUTORS (VOLUNTARY)

Gender:

- Male
- Female
- Do not wish to provide

Ethnicity:

- Hispanic or Latina/o Not
- Hispanic or Latina/o Do not
- wish to provide

Race:

- American Indian or Alaska Native Asian
- Black or African American
- Native Hawaiian or other Pacific Islander
- White
- Do not wish to provide

Disability Status:

- Yes
 - Deaf or serious difficulty hearing
 - Blind or serious difficulty seeing even when wearing glasses
 - Serious difficulty walking or climbing stairs
 - Other serious disability related to a physical, mental, or emotional condition
- No
- Do not wish to provide

Attach a separate document if more space is needed for #6-10, or #24-50.