Prospectus to US CLIVAR for new Working Group on Ocean Uncertainty Quantification

1. **Motivation**

Earth science has entered the realm of big data in recent decades. Observing systems now provide the research community with real-time or near-real-time global observations having increased spatial and temporal resolution. Historical and near-real-time observational data streams are analyzed by the research community, ingested by assimilating operational models to produce forecasts on daily to decadal timescales, and used to provide state estimates and reanalysis products. Since all observations are inherently estimates, and therefore have some degree of uncertainty (instrumental, model, and statistical), we must know how well we trust these observations in order to interpret them in the most meaningful way. The scientific community faces specific challenges in uncertainty quantification approaches for in situ, satellite, and model data. For instance, in-situ observations are prone to both instrument and sampling errors. Satellite observations need validation through comparison with in-situ observations, which have different temporal and spatial scales. Data assimilating models have their own physical intrinsic uncertainties, which add to the propagating uncertainties from the quality and amount of data feeding into them. Unfortunately, the continual increase in the amount of available observational and model data only exacerbates on-going issues and limitations associated with the quantification of uncertainties. Although most ocean scientists would agree that quantifying uncertainty is important, this does not mean that we always do it well. An illustration that we may find ourselves at odds between known requirements for scientific practices and programmatic recommendations is the fact that documents such as the Framework for Ocean Observing (that emerged from OceanObs'09) or the GOOS Global Ocean Observing System 2030 Strategy do not contain any reference to "uncertainty" or "error" (or their variants).

For Earth sciences in general, and in particular for ocean sciences, uncertainty quantification (UQ) suffers from a number of perhaps surprising issues: (i) the terminology and vocabulary are often not consistent: for instance, terms such as *accuracy*, *precision*, and *resolution* are often wrongly used interchangeably despite long-established terminology from metrology science (Lequin, 2004); (ii) the knowledge of standard and advanced statistical techniques is sometimes lacking, so that the nature of uncertainty itself (e.g. randomness, serial correlation, etc.) is misunderstood or not calculated accurately (e.g., Parker, 2016, Resplandy et al. 2018); (iii) even when known, statistical techniques can be improperly used (e.g., Nicholls, 2001); (iv) many observational or model datasets lack uncertainty estimates, so that the impact of the data quality cannot be assessed; (v) when reporting uncertainties, ocean observers are faced with different best practices that depend on the observing system, the measurement platform, and the end-user.

In an effort to remedy the issues highlighted above, we propose a US CLIVAR working group (WG) whose aim will be to develop strategies, and identify best practices, for improving the understanding, derivation, communication, and utilization of the uncertainties of ocean in-situ,

remote, and modeled products related to physical variables. In practice, this WG will form a focused forum to discuss how UQ and its associated concepts can be incorporated into scientific research in general, including but not limited to: training of current and future scientists, observing system design, process study conceptualization, data acquisition and processing, modeling and data assimilation. Notably, a point of focus will be to assess how both observationalists and modelers should describe uncertainty in their products in order to facilitate the exchange of data between their two communities. In order to reach achievable goals, the WG will be limited to oceanic physical variables among Essential Climate Variables (ECVs). However, through our reporting activities with US CLIVAR we hope to engage with and learn from current community efforts related to UQ of biogeochemical variables.

There already exists a momentum among oceanographic communities for activities supporting improved quantification and communication of uncertainties. Our proposed WG will capitalize on the outcomes and action items from previous activities on UQ, and serve as a means to provide continuing coordination, progress, and concrete outcomes for this topic. Past or current activities that we will build on include:

- The 2019 US CLIVAR Summit, which included a POS Panel breakout session on UQ. Discussions highlighted the need to promote the writing of a white paper to define a common language for UQ in earth sciences. This is one of the objectives of this WG.
- A breakout session on UQ was held at the OceanObs'19 Conference in Honolulu, HI in 2019. Four speakers emphasized strategies and challenges in UQ for in-situ and satellite observations and data assimilation. The session generated fruitful community discussion, and three priority recommendations emerged which map onto the proposed WG objectives:

    1. *We should train ocean observers and modelers in statistical terminology and techniques for the purpose of uncertainty quantification.*
    2. *Building on existing efforts, we should produce a series of peer-reviewed and open-access documents that define and recommend strategies and best practices for uncertainty quantification in ocean observing.*
    3. *Research programs should require and fund routine uncertainty estimates on ocean observations and derived products and should fund dedicated efforts to develop freely available resources (software and databases) for uncertainty quantification.*

- The Pilot Mission Exploitation Platform (Pi-MEP) for sea surface salinity (SSS), supported by NASA and the European Space Agency (ESA), is an example of a multi-platform, multi-agency integrated project that specifically address the UQ issues associated with remote sensing of ocean variables. The WG will focus on the lessons learned from this effort.
- The International Quality Controlled Ocean Database, or IQuOD, is an international effort supported by CLIVAR, IODE, and SCOR to produce a consistent database of ocean subsurface temperature with systematic quantified uncertainties. This project could be used as reference for the activities of the proposed WG.

2. **Objectives, Tasks, Timeline**

(a) Objectives

The proposed WG will work toward three consecutive objectives:

Objective 1: *Develop a community-driven web platform for UQ knowledge and strategies.* This objective will be achieved by building a robust, fit-for-purpose, dedicated website using a static open-source architecture that integrates with GitHub (for interactive computational environment, i.e. a notebook, development and sharing), Medium (for blog posting), and twitter (for publicizing activities). This website will act as a portal of collected literature, guides, and various resources. It will contain several prominent sections such as a blog post section that will be populated by the WG members on specific aspects of UQ related to their own activities; a literature review section that will bring in references of peer-reviewed articles, open documents, manuals, and books from within and beyond the oceanography and climate literature; and a lecture section that will feature topical lectures that will be assembled by the WG members. Following the completion of the WG, the website will continue to be available to the public for reference.

Objective 2: *Produce peer-reviewed open-access articles on UQ for observational and model ocean data.*

The members of the WG will write two peer-reviewed open-access articles that define and recommend strategies and best practices for uncertainty quantification in ocean observing. Gaps in the literature will be identified as targets for future efforts (for both the WG members and broader community), including discussion at the workshop/summer school organized by the WG (next objective). The first paper will be published in EOS or BAMS to introduce the WG web portal and activities. The second paper will lay out general recommendations for UQ for ECVs, taking particular effort to highlight commonalities between ECVs as well as differences. This review/synthesis paper will address specific applications of the recommended methods to various physical ocean variables, including at the surface (e.g., SST, SSS, fluxes) and at depth (e.g., temperature, salinity, currents).

Objective 3: *Organize a summer school and/or workshop on UQ.*

We will organize a summer school, or a workshop, or a hybrid of the two, on UQ. The exact nature of this event will be determined by the WG. This event will be an opportunity to bring together expertise from the in-situ, satellite, and modeling communities to foster intra- and inter-community dialogue, build consensus on understanding, identify gaps and recommend actions to address them, and develop pedagogical materials. All material emanating from this meeting, including lectures and training materials, will be made available through the WG website.

(b) Tasks and timeline

Year 1: (2020-2021)

- Compilation and curation of relevant literature.
- Development of UQ website and production of material for the site (blog posts, lectures, literature review).
- Engagement with other UQ groups (oceanbestpractices.org, IQuOD, PiMEP, etc.) and other US CLIVAR WGs such as the Data Sciences WG.
- Bimonthly teleconference to advance tasks and monitor progress.

Year 2: (2021-2022)

- Continuation of material production for WG website.
- Drafting and publication of an article to announce the UQ web portal in AGU EOS or BAMS. Drafting and publication in US CLIVAR Variations.
- Town Hall to introduce the web portal and garner community feedback at AGU/Ocean Sciences Meeting (year 2022).
- Plan UQ workshop and/or summer school.
- Bimonthly teleconference to advance tasks and monitor progress.

Year 3: (2022-2023)

- Bimonthly teleconference to advance tasks and monitor progress.
- Continuation of material production for WG website.
- UQ workshop and/or summer school.
- Publication of an article about strategies and best practices for uncertainty quantification in ocean observing.

3. **Publications and Outreach**

Community outreach and engagement will be a major activity of the WG via the material on the website. A town hall meeting/session will be conducted at an AGU Fall Meeting or the Ocean Sciences Meeting. An email list, open to anyone interested, will be created and updates will be sent after each bimonthly WG teleconference. Two publications are planned: one early in the second year to announce the launch of the WG website and publicize its content, and another one at the end of the 3-year activities of the WG focused on best practices for UQ.

4. **Reporting Plan**

The activities of this proposed WG are highly relevant to the goals of US CLIVAR, and particularly to the UQ priority identified by the POS Panel. WG activities will be communicated to the POS Panel through members serving on the Panel (Elipot, Subramanian, Frolov). We will also communicate with, and seek feedback from, the other US CLIVAR Panels, and will report annually at the US CLIVAR Summit or individual panel meetings. We will communicate regularly with the newly-funded US CLIVAR Data Science WG to stay informed on their activities that are

relevant to our own objectives on UQ (for instance, how cloud computing and code-sharing platforms can be used to expand the availability of UQ tools). We will also encourage the Data Science WG to use new UQ tools that will be developed as part of our WG's efforts.

5. **Leadership and suggested membership**

The leadership of the WG will be comprised of Shane Elipot, Kyla Drushka, and Aneesh Subramanian, all of whom were co-organizers of the UQ breakout session at OceanObs19. Kyla Drushka is a previous POS panel member; Shane Elipot and Aneesh Subramanian are currently the two co-chairs of this panel. The suggested memberships for this WG aims at spanning multiple expertise and career levels, notably bringing in statisticians. In order to develop a mutually consistent set of activities, we include the three components of ocean observing for climate (in situ, remote sensing, and modeling/data assimilation). The symbols * and denotes an individual within 5 and 10 years of their PhD, respectively.

Co-chairs:

1. Shane Elipot (U. of Miami)	Observations, POS panel co-chair
2. Kyla Drushka (U. of Washington)	In-situ & satellite observations
3. Aneesh Subramanian (U. Colorado)	DA & modeling, POS panel co-chair

Core Group Members:

4. Chelle Gentemann (Earth & Space Res.)	Satellite SST, cloud computing
5. Patrick Heimbach (U. of Texas-Austin)	DA & modeling
6. Mark Bushnell (US IOOS)	In-situ observations
7. David Moroni (NASA JPL)	Remote sensing, engineering
8. Carol Anne Clayson (WHOI)	Air-sea fluxes; US CLIVAR SSC member
9. Amy Braverman (NASA JPL)	Statistics; Data Science WG
10. Donata Giglio* (U. Colorado)	Argo, scatterometery, EarthCube
11. Mikael Kuusela* (Carnegie Mellon U.)	Statistics; UQ; spatio-temporal statistics
12. Sergey Frolov (NOAA ESRL)	DA & modeling; POS panel

Contributing Members:

13. Alek Petty ★ (NASA Goddard)	Polar ocean and sea ice research
14. Wendy S. Parker (Durham U., UK)	Philosophy of Science, UQ
15. Roberto Sabia (European Space Agency)	Remote sensing, satellite salinity
16. Adam Sykulski ★ (U. Lancaster, UK)	Stochastic modeling, data science

6. **Resource Requirements**

- Funding for the creation of a dedicated website for resources and tools.
- Bi-monthly teleconference support.
- Page charges for two publications (e.g., EOS and Frontiers).
- Organizational support for a 50-participant 3-day workshop/training in 2022, location to be determined.

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