Reports to SCOR (2020)

1. Name of group

Working Group 148: International Quality controlled Ocean Database (IQuOD)

2. Activities since previous report to SCOR (e.g., virtual or in-person meetings, email discussions, special sessions). Limit 1000 words

IQuOD in-person meetings:

- The 6th IQuOD workshop took place at Ifremer, Brest, France during 29-31 October 2019. The workshop focused on developing a "roadmap" for the v1.0 data release. The workshop report is available here http://www.iquod.org/documents.html

IQuOD Intersessional meetings (virtual):

- 28 February, 2020. The next planned release of the IQuOD product was reviewed, task team goals for the release were reviewed.
- 31 March, 2020. Focus on Expert QC and Intelligent Metadata task teams. Website was reviewed.
- 20 April, 2020. Discussion about future funding for the IQuOD Project.
- 28 April, 2020. Uncertainties themed discussion.

3. Documents published since previous report to SCOR (e.g., peer-reviewed journal articles, reports, Web pages) and should be limited to publications that resulted directly from WG activities and which acknowledge SCOR support

Updates to the webpages: www.iquod.org.
New Google Scholar publication list:

https://scholar.google.com/citations?hl=en&user=qYD_0r8AAAAJ&view_op=list_works&authuser=1

Journal Articles:

Casteleo, G., 2020. A Framework to Quality Control Oceanographic Data. https://doi.org/10.21105/joss.02063

Matthew Palmer, Paul Durack, Maria Chidichimo, John Church, Sophie Cravatte, et al.. Adequacy of the Ocean Observation System for Quantifying Regional Heat and Freshwater Storage and

Change. *Frontiers in Marine Science*, Frontiers Media, 2019, 6, pp.416. ⟨10.3389/fmars.2019.00416⟩. ⟨hal-02286221⟩

Ponte, Rui M.; Carson, Mark; Cirano, Mauro; Domingues, Catia M.; Ezer, Tal; and Zhang, Xuebin, "Towards Comprehensive Observing and Modeling Systems for Monitoring and Predicting Regional to Coastal Sea Level" (2019). *CCPO Publications*. 309. https://digitalcommons.odu.edu/ccpo_pubs/309

Meyssignac B, Boyer T, Zhao Z, Hakuba MZ, Landerer FW, Stammer D, Köhl A, Kato S, L'Ecuyer T, Ablain M, Abraham JP, Blazquez A, Cazenave A, Church JA, Cowley R, Cheng L, Domingues CM, Giglio D, Gouretski V, Ishii M, Johnson GC, Killick RE, Legler D, Llovel W, Lyman J, Palmer MD, Piotrowicz S, Purkey SG, Roemmich D, Roca R, Savita A, von Schuckmann K, Speich S, Stephens G, Wang G, Wijffels SE and Zilberman N (2019) Measuring Global Ocean Heat Content to Estimate the Earth Energy Imbalance. Front. Mar. Sci. 6:432. doi: 10.3389/fmars.2019.00432

Engagement with user communities:

Goni Gustavo J., Sprintall Janet, Bringas Francis, Cheng Lijing, Cirano Mauro, Dong Shenfu, Domingues Ricardo, Goes Marlos, Lopez Hosmay, Morrow Rosemary, Rivero Ulises, Rossby Thomas, Todd Robert E., Trinanes Joaquin, Zilberman Nathalie, Baringer Molly, Boyer Tim, Cowley Rebecca, Domingues Catia M., Hutchinson Katherine, Kramp Martin, Mata Mauricio M., Reseghetti Franco, Sun Charles, Bhaskar TVS Udaya, Volkov Denis, 2019: More Than 50 Years of Successful Continuous Temperature Section Measurements by the Global Expendable Bathythermograph Network, Its Integrability, Societal Benefits, and Future. Front. Mar. Sci. 6:452. doi:10.3389/fmars.2019.00452

Storto Andrea, Alvera-Azcárate Aida, Balmaseda Magdalena A., Barth Alexander, Chevallier Matthieu, Counillon Francois, Domingues Catia M., Drevillon Marie, Drillet Yann, Forget Gaël, Garric Gilles, Haines Keith, Hernandez Fabrice, Iovino Doroteaciro, Jackson Laura C., Lellouche Jean-Michel, Masina Simona, Mayer Michael, Oke Peter R., Penny Stephen G., Peterson K. Andrew, Yang Chunxue, Zuo Hao, 2019: Ocean Reanalyses: Recent Advances and Unsolved Challenges. Front. Mar. Sci. 6:418. doi: 10.3389/fmars.2019.00418

4. Progress toward achieving the group's terms of reference. List each term of reference separately and describe progress on each one. Limit 1000 words

1. To develop, implement and document algorithms for assignment of "intelligent" metadata – i.e. an informed guess as to likely values for missing information – for temperature profiles where crucial metadata is missing.

- Work is being led by Stephen Haddad at the Met Office to implement a Machine Learning ensemble approach. This is being funded through an internal secondment. All the code is

open source (Python) and freely available at https://github.com/Fracappo87/XBTs_classification

2. To evaluate and document the most effective combination of automated quality control (AutoQC) procedures for temperature profile observations. International collaboration will be required for the design and coordination of benchmarking experiments using high quality reference datasets.

- The manuscript "Benchmarking of automatic quality control checks for ocean temperature profiles and recommendations for optimum sets" by Good, Mills et al. is currently in preparation for Frontiers in Marine Science. We expect to submit the paper in the next month or two (June or July 2020).

3. To establish and implement a set of optimal automated quality control procedures, by reaching international community consensus and using the knowledge gained in the benchmarking tests from ToR-2 (above); to produce and publish a reference guide for best practices in automated quality control of ocean temperature profiles; and to develop and freely distribute an open-source quality control software toolkit to promote wide and rapid adoption of best practices by the oceanographic community.

- The optimal set of automated QC checks are documented in Good, Mills et al (in prep). All code is freely available at https://github.com/IQuOD/AutoQC

4. To examine and document the feasibility of machine learning and other novel computational methods for enhanced quality control, to potentially minimize labor costs associated with human expert quality control procedures.

- Work is ongoing and testing of an expert QC interface with a machine learning engine is underway. The machine learning toolbox is described in Castelao (2020) "A Framework to Quality Control Oceanographic Data" in Journal of Open Source Software

- Guilherme Casteleo provided a demonstration of the expert QC interface at the Ocean Sciences Meeting 2019 which was well received.

5. To develop, implement and document internationally agreed best practice methods for assignment of uncertainty estimates to each temperature observation.

- A manuscript for journal publication of the uncertainty values applied to the v0.1 IQuOD release is currently underway. Publication expected by end of 2020.
- Improving the uncertainties for future IQuOD releases is an ongoing task and we aim to publish details of enhancements and improvements with each release.

6. To freely disseminate (interim) versions of the IQuOD global temperature profile database (and added value-products) as it evolves over the next 3 years, in user-friendly file formats.

- The main task for this year has been working towards a first full-release of the IQuOD v1.0 dataset. This will be the first product to include an internationally-coordinated optimised

automated QC flags. The main purpose of the IQuOD workshop in Brest during Oct/Nov 2019 was agreeing on a "roadmap" to deliver this data product. While we had a target for October 2020 for completion, this now is subject to delay associated with COVID-19 lockdown in IQuOD member countries.

7. To share knowledge and transfer skills in instrumentation, regional oceanography, quality control procedures and data stewardship with international scientists in both developed and developing nations.

- The IQuOD 6th workshop and intersessional meetings are the primary means by which this ToR has been addressed in the last 12 months.

- The last workshop had attendees from over 10 countries from many areas of expertise including data collection and management, quality control experts, and end users from the modelling community.

5. WG activities planned for the coming year. Limit 500 words

- Publication of the IQuOD v1.0 product
- Publication of Auto QC paper associated with the v1.0 product
- Publication of Uncertainties paper associated with the v0.1 product
- Seeking endorsement from UN Decade of Ocean Science for Sustainable Development
- Seeking funding for FTE to continue the IQuOD project work (potentially NERC UK)
- Completion and delivery of Machine Learning-based intelligent metadata for XBT observations, including probabilistic information to inform Monte Carlo studies for future XBT bias corrections.
- Duplicate checking routines built and shared via github
- Measuring progress by testing the IQuOD releases by end-users.
- Hosting of the IQuOD products on the NCEI World Ocean Database platform will continue as the platform moves into a cloud-based storage environment.

6. Is the group having difficulties expected in achieving terms of reference or meeting original time schedule? If so, why, and what is being done to address the difficulties Limit 200 words

IQuOD currently has no long-term funding for its participants and relies on engagement and in-kind funding from the participants' home institutions. We continue to achieve what we can under limited funding conditions. Additionally, Covid-19 has impacted on everyone's ability to contribute to the project.
We will continue to actively source funding for IQuOD into the future and have regular online contact within the group.

7. Any special comments or requests to SCOR. Limit 100 words.

Many thanks to the SCOR committee for their support over the last 3 years. IQuOD would like to continue as a SCOR WG if possible, and we request a one-year extension to our 3-year term to allow us to finalize one of our planned activities for the upcoming year.

If appropriate, we may request a letter of support for funding proposals in the future. We also request thoughts on how we can maintain a relationship with SCOR and related relevant SCOR WGs for mutual benefit.

Additional information can be submitted and will be included in the background book for the SCOR meeting at the discretion of the SCOR Executive Committee Reporter for the WG and the SCOR Secretariat.