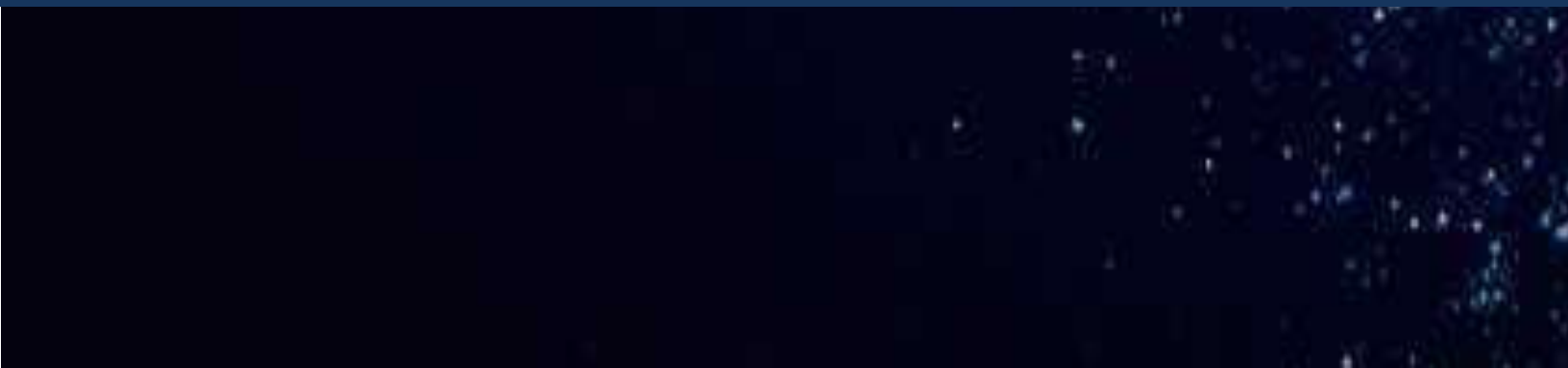
2023 International Quality-Controlled Ocean Database (IQuOD) – 7th IQuOD Annual Workshop

8th IODE SG-IQuOD
4th SCOR WG 148

10-11 July, 2023
Potsdam Institute for Climate Impact Research, Potsdam, Germany



Editors
Rebecca Cowley, CSIRO, Australia; **Alison Macdonald**, WHOI, USA; **Simon Good**, Met Office, UK; **Rachel Killick**, Met Office, UK; **Lijing Cheng**, CAS, China; **Zhetao Tan**, CAS, China; **Guilherme Castelão**, Scripps Institute of Oceanography, USA; **Matthew Palmer**, Met Office Hadley Centre, UK; **Tim Boyer**, NCEI, USA

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- Brigitta Krukenberg, Potsdam Institute for Climate Impact Research, Germany

Organizers

Organizing Committee

- Rebecca Cowley (CSIRO, Australia)
- Simon Good (Met Office, UK)
- Lijing Cheng (Chinese Academy of Sciences, China)
- Guilherme Castelao (Scripps, USA)
- Matthew Palmer (Met Office, UK)
- Catia Domingues (National Oceanography Centre, UK)

Local Organizer

- Brigitta Krukenberg, Potsdam Institute for Climate Impact Research (PIK), Germany

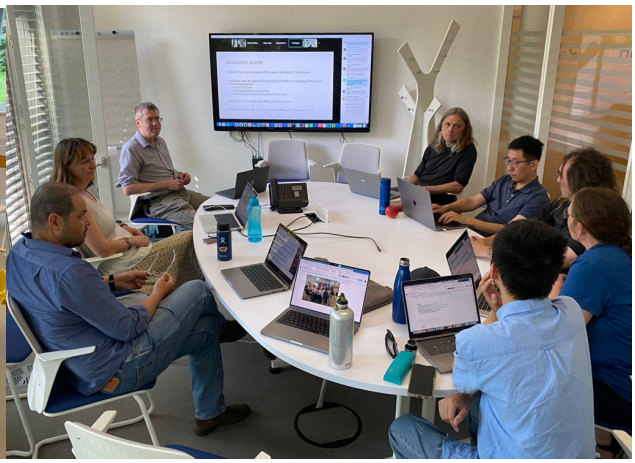
Goals of the workshop

- Ratify new co-Chairs.
- Review work achieved so far.
- Review IQuOD structure.
- Plan for tasks for the coming 12-24 months.

Workshop Documents

All workshop documents and presentations can be found in the Google Drive folder below (access request required).
https://drive.google.com/drive/folders/1--T5Z4QK957g3FI_G9ZIZwVCkVPIZutG?usp=sharing

IODE Portal:
This document is available at the IODE document portal AquaDocs:
https://aquadocs.org/



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1. Welcome – Simon Good

Simon Good welcomed all in attendance (see Appendix A) to the meeting. Introductions were made around the table and online.

1.1. Vote ratifying new co-chairs

The vote to ratify the new co-Chairs was taken. Lijing Cheng and Guilherme Castelao were unanimously voted as new co-Chairs for IQuOD.

1.2. Introductory talk: Progress over the last 3 years and current structure of IQuOD - Simon Good

In the 10 years of IQuoD there have been 5 workshops and multiple publications.
The new IQuOD co-chairs are Gui and Lijing, and Bec will continue to be the coordinator.
A vote was taken to confirm Gui and Lijing as co-chairs to meet our requirements as an IODE project. Their appointment was unanimously approved. We also had a quick run through the agenda.

2. Phase 1: IQuODv0.1 improvements

2.1 IQuOD uncertainty quantification: next steps, Rebecca Cowley

Rebecca reviewed what we have done so far with uncertainty quantification. She outlined some ideas for improving uncertainties that were then discussed by the attendees:
Improvement ideas:

- Engage with others who are working on the same issue and end users
- Review practical publications with uncertainty derivations (see references)
- Define categories for uncertainty calculations, for example:
    - Parameter/variable type
    - Platform type (incorporate cruises?)
    - Regions of high or low variability in-situ data
    - Uncertainty with depth
    - Calibration information
- Work through some small datasets to build uncertainty budgets
- Create some simple excel spreadsheet templates and/or code

Education and outreach:

- Engage with others (who?)

        - Argo DMT
        - QARTOD group
        - BIPM or European Metrology Network (EMN) of EURAMET about Ocean (https://www.euramet.org/climate-and-ocean-observation/sections/ocean)
        - European Metrology Network (EMN) of EURAMET, Ocean part (https://www.euramet.org/climate-and-ocean-observation/sections/ocean)
        - Modellers, OHC estimates – how do the uncertainties improve their outputs?
    - Outreach through OTGA
    - Code/sample calculations available through IQuOD github and website.

Workplan ideas:

- Choose 1 or 2 priority datasets of interest to IQuOD and collaborators
    - Which are good to target? Moorings, XBTs, CTDs etc?
    - Colleagues with datasets ready to go and a requirement to calculate uncertainties
- Work through uncertainty calculations for the datasets
    - What sources of uncertainty should be included?
    - What about undefined biases?
- Create a template of uncertainty calculations for IQuOD to publish and follow
- Identify end users, what is the impact of providing observational uncertainty?
- Publish code and templates
- Journal publication, best practices?

References:

https://www.frontiersin.org/articles/10.3389/fmars.2019.00706/full#supplementary-material
https://www.frontiersin.org/articles/10.3389/fmars.2022.1002153/full
https://os.copernicus.org/articles/7/651/2011/os-7-651-2011.pdf
https://www.frontiersin.org/articles/10.3389/fmars.2019.00578/full
https://opg.optica.org/oe/fulltext.cfm?uri=oe-30-25-45648&id=522186#
https://doi.org/10.1364/OE.470994

Discussion:

The OTGA (OceanTeacher Global Academy): https://classroom.oceanteacher.org/ might be of use in future to engage users in the use of uncertainties and for understanding their complexities

Bias corrections: how do they get included? How do we fold biases into our uncertainties because biases are uni-directional? Lijing says if systematic error is removed by a correction scheme, it can be assumed that what remains are random errors. One can check the spread of the temperatures after applying several bias corrections to define and quantify this uncertainty.

Zhetao has a paper that looks at regional selection: western boundary currents, tropical western Pacific, and ACC (Antarctic Circumpolar Current). We don't want to include natural variability in the uncertainty.
Representativity error: This is application dependent, needs to be calculated by the user. Gael says they use instrumentation uncertainty and representative error. See full notes below.

Would be useful to get 3D maps of representative error. An estimate of representative error could be provided for a specific community. Since, for example, there are often standard ocean model configurations (e.g. NEMO has a 1, ¼ and 1/12 degree tri-polar grid) it may be useful to serve estimates of representative error on these standard grids - in collaboration with the modelling/reanalysis community.

Tim: we still have a lot to do for the instrumental/observational uncertainty. E.g., WOCE data would have a lower uncertainty compared to say, GTS data which one would expect to have higher uncertainty as no QC checks occur for data going into the GTS.

Matt: we should focus on instrument uncertainty. IQuOD should not be responsible for creation of representative error, but we could work with others to help. Could get someone with Matt's group to look at this work.
ACTION: Matt to raise with ME4OH community in due course.

Viktor: Uncertainty in location is also a source that needs to be included. Astronomical navigation period, for example, navigation was done by radio beacon, then GPS/satellite. Could be a crude partitioning to add uncertainty estimates to lat/lon information.

Curation of already published information, much of which has already been done in the first publication. Further curation would mean looking at reports, WOCE/CLIVAR publications etc. to define uncertainties. We should add metadata connecting the tables of uncertainties with the publications that such numbers came from.
We could implement a FAIR code for uncertainties calculations to share with the community.

Gui, Simona: Provide some examples to engage the different users and allow them to make their own use of the code (see for example Chris Atkinson's work on uncertainties in section 4 of the HadIOD user guide: https://www.metoffice.gov.uk/hadobs/hadiod/HadIOD.1.2.0.0_Product_User_Guide_[1.2].pdf. And example code for EN4 in section 5 of the product user guide: https://www.metoffice.gov.uk/hadobs/en4/EN.4.2.2_Product_User_Guide_v1.0.pdf).

Could make a nice publication. The modelling and reanalysis community will need the uncertainties, the mesoscale/sub mesoscale, they need more information. Can't give a unique answer for everyone. Need to select a target user community and solve for them.

Outlier detection would be extremely useful for end users. Can be done without models. Gael could contribute here. Possibility to host a "roadmap" on the IQuOD website to help a variety of users, pointing to maps of spatial variance in temperature, etc.?

Simon: We should be checking and testing instrumental against representativity errors that we are providing. Somehow show that what we are providing is useful.

Christoph: We can calculate an uncertainty budget. The GUM has specific contributions to uncertainties and this is where we should start. Common ground is the uncertainty budget. Start with instrumental uncertainty.
Get rid of outliers as they have an impact on uncertainty calculation. Incorrect outliers should be removed, but good data with natural variability should be maintained, ie, remove bad flagged data.
Alison: removing data already flagged as bad is one thing, but much of the complication in estimating uncertainties arises because it is often difficult to determine whether outliers are real because their determination is scale dependent.

Tim: Instrumental error, and how to move forward. Curate information - already published information and make it available - these are what we are using in IQuOD and publish these values. **Tim will not update the IQuOD values until they have been peer reviewed,** but a user could grab them and use them when they need.

Christoph: Instead of instrument uncertainties we should stick to the term "measurement uncertainties" which encompasses instrument contributions and other uncertainty sources.

Tim: Raises the point of not using geoids, but before the estimate of location had larger errors. And the effect of changing position such as Argo during ascent.
Alison: This location doesn't matter in many cases.
Matt: if a source of uncertainty is not important, we can say so in a paper.

Gael:
IQuOD could aim to provide the tools (estimates & recipes) for data users to assess whether an individual data point should be viewed as an outlier and excluded from the type of analysis they have in mind or not. This is complementary to the goal of providing an error budget, but not independent (e.g. outliers are often flagged if outside of "mean +/- 3 sigma").

Both goals (error budget and outlier detection) need to be viewed as dependent on application. For example, someone working on extreme events will have a different notion of outliers than someone mapping out large scale heat content anomalies. Or someone doing optimal interpolation, and reanalysis work (data assimilation, etc.) might treat instrumental errors of 0.001 degree as negligible compared to representativity error in the upper ocean (e.g. eddy activity not resolved by Argo).

To both goals, I feel it is useful to map out variance fields from data. I did an early version of this in https://journals.ametsoc.org/view/journals/phoc/37/8/jpo3072.1.xml and am suggesting we can update. Now that we have so much more data from Argo, we probably can do this seasonally. And additional emphasis should be put on shallow & coastal regions, which Argo does not cover well.

Mapping variance from data gives a way to test high-res models (Fig 14 of cited paper) e.g. those used in ME4OH (Mapping Evaluation For Ocean Heat). It's also a relevant element of geophysical context for field programs in my mind -- when it's useful to know how variable the observed region is.

What I am envisioning for IQuOD is that it would provide a set of 3D maps (estimated from data distributions) and explain how to use them with respect to error budget and outlier detection. The stamp of approval from the IQuOD community on those maps would enhance the likelihood of different reanalysis groups (optimal interpolation, data assimilation, ...) to converge on a more uniform and coherent approach.

The diversity of use cases seems like it could be effectively addressed/communicated through a set of notebooks published under the IQuOD github & website. These could be written from the perspective of different user categories -- e.g. someone doing high-resolution measurement vs someone doing climate analysis/reanalysis. FAIR is a good framework.

Zhetao: should we include duplicate information in the uncertainty?

People interested in the uncertainty topic for following up:
- Rebecca
- Rachel
- Matt
- Christoph
- Lijing
- Marlos

- Simona
- Viktor
- Tim
- Gael
- Franco

2.2 Metadata and duplicates problem identification and rectification in IQuOD, Zhetao Tan

We began with a presentation by Zhetao on Duplicate Checking.
There has been some work done on duplicate checking that was simple, apart from Gronell & Wijffels and the coding by Edward King. Lack of metadata information is a big challenge.
Zhetao has looked at statistical tools to use 'DNA' to identify duplicates and incorrect/missing metadata. Comparison is done with an intermediate step. Each profile has its unique 'DNA' which is used to reduce the space of comparison and computational cost. WOD data in 1975, 1995, and 2011 and some XBT data (1992-1993) in the Gulf of Mexico are used for the test.
The tests found more than 200 potential duplicates in a single cruise and in total, it found >1,000 duplicated pairs.
Issues found include:
- Partial metadata, i.e. missing some of the metadata.
- The possibility of a different truncation point in data.
- Multiple submissions, sometimes from different organizations.
- Error due to human adjustments on the data.

Looking at the time history of available CTD data, there is a spike in potential duplicates identified in 2011. Many of the identified duplicates were duplicate profiles from tow-yo style CTDs. After identifying true duplicates, that spike disappears, thus the resultant dataset is consistent with the remaining years.

Flags to assign duplicates were proposed. Once confirmed, the decision is left for the expert to confirm that such profiles should be removed.

Discussion:
Duplicate pairs should be identified in a dataset and the procedure should be documented in a written summary to keep track of the duplicated cases.
How to report and fix metadata issues was discussed (see below).

Viktor: Does the algorithm consider triplicates of multiple ones? The answer is yes, they consider that.

If we identify true duplicates, we should remove the duplicate. But keep flag 1 duplicates until any decision is made. The record of which duplicates were identified needs to be kept for future ML purposes. This dataset will be published soon with DOI.

Gui: talked about methods to find duplicates using similar methods in DNA testing. He will pass the information to Zhetao.

Allison: It might matter automatically removing big chunks of duplicates if we later find a better solution. Is it more common to find duplicates in recent data?

Tim: We should not use Machine Learning to remove duplicates. Maybe use it to help find them, but certainly base the final decision on human expert confirmation.

Pathway for reporting:
After identification, we need the confirmation by the expert which takes time. The final step is removal of the duplicates after actual identification. An inefficient process, but what we can do. The WOD needs to be managed by experts around the world. That is the goal for the WOD cloud, but for now, needs to be funneled through Ricardo Locarnini. We will need a second validation before any changes are made.
It may take years to make the cloud product available because of security issues.

Rachel: How do we deal with 'duplicates' where they were both taken for a reason e.g. an XBT and a CTD profile taken at the same time in the same place? We don't want to throw these out as they are valuable for instrument comparisons?
We can nominate experts to review the identified potential duplicates. Can do this by country (eg, Bec can look at Australian data, Alison offered to review US data).
Lijing: Flag issue doesn’t need to go to the WOD; we can provide the flag directly to the country representatives to decide if/what are duplicates.

Identify the metadata problem with flags, the final removal decision is made at the NCEI.
Suggested scheme:

- Flag=0: profile to be retained ;
- Flag=1: need a further check;
- Flag=2: profile to be removed.

Flag 1 profiles need further checks by team members/experts. Flags 0 or 2 should be passed to NCEI for the final decision and removal.

ACTION: Publication to summarize the metadata checking/duplicate checking work. Journal of open sources (JOSS) and ensure that we acknowledge IQuOD and IODE (Link to JOSS: https://joss.theoj.org/). (In progress now)

ACTION: Zhetao to move the code to the IQuOD GitHub (Done)

ACTION: Consider linking GitHub with Zenodo for software publication eg (https://github.com/castelao/inception). Or Software Heritage

Participants who would like to continue to have some input to the duplicate/metadata checking:

- Bec
- Alison
- Lijing
- Zhetao
- Xinyi
- Rachel

2.3 IQuOD bias corrections: next steps, Tim Boyer, Viktor Gouretski

Framing the Challenges:
XBT biases. There is one XBT bias correction being applied to IQuOD (Cheng et al. 2014). User selection is not available for IQuOD, as it is an expert community choice. Do we want to continue to do this? We should formalize its use - with updates every year - Making it official.

There are other biases to consider (e.g. corrections to MBTs and bottles, Viktor is also working on pinniped corrections).

ACTION: Lijing to update the Cheng et al correction (last update was 2017). To update this year.
ACTION: IQuOD 2023 will be released soon, assess if it is possible to add updated bias corrections for XBT.

If the data are part of the Global XBT Network it should already have been QC'd and these flags should be used. Some of the recent XBT data (AOML) may still be the NRT, rather than delayed mode.
ACTION: Tim and Francis/AOML need to check the status of AOML DM XBT data.

Franco says that there are some 0.5 million XBTs in the WOD that might be Plessey probe types. Shoichi Kizu collaborated with Franco for these "archaeological findings". Plessey

made a commercial agreement with Sippican at the end of 1966 and began to build and sell its own version of XBT systems built in the factory in Ilford (Essex): model T4 and T7 probes (there is trace of this in documentation available online), analog recorder strip chart very close to Sippican's MK2A, and launcher. Commonwealth countries and some Northern European countries are the official market for Plessey but there are documents from the Italian parliament from 1980 and 1981 which decide on the purchase of recording systems from Plessey. In some cruise reports from the 80s of English research ships the use of Plessey XBT probes is mentioned and when these profiles are present in WOD they are indicated as XBT of unknown type or unknown brand. The only known performance test of XBT Plessey is the one done in 1990 from Gould on the RRS C.Darwin Cruise 50 (maximum depth value quite different from that calculated with Sippican's FRE). Franco has a Plessey/Sippican T4 with serial number PL 547358, year of manufacture unknown but Plessey discontinued XBT equipment in 1989.
In July 2020 LMS provided this reply.
"Your Questions Regarding XBT's Manufactured and Sold by Plessey Electronics – LMS Comments:
1. Plessey manufactured XBT's starting in the late 1960's, up until the time the Plessey company was dissolved in the late 1980's
2. Plessey purchased thermistors and wire from Sippican for use in their XBT production, for their entire
3. LMS has no information on the customer deliveries of Plessey-manufactured XBT's
4. LMS has no current information relevant to the tables and content of the cited Manual MP0400."

Do we include uncertainty from biases? Lijing says he will just use the three XBT corrections from the paper to provide a spread of corrections.
ACTION: Viktor to recalculate his XBT correction, but would need a deadline.

There are two more XBT corrections out there that need to be assessed and maybe listed as options in the WOD.
ACTION: Can these authors be identified and invited to talk to us?

Capability exists to have a depth dependent uncertainty in IQuOD.

MBT data set - correction scheme was published, but some issues were found (by Rachel) for specific (Canadian) data in homogeneous waters. Viktor began writing corrected corrections - but it would be better to restart the process and create a new calculation - started, but not completed.

Another issue with MBT data comparisons is the reference data is the bottle profiles. They are biased because of depth over-estimation. First need to correct the bottle profiles, then update the MBT profile corrections.
ACTION: MBT updates will not be published, but maybe a correction note/letter? Viktor.
Will need some acceptance by IQuOD that the updates are ok. Tim would like to do some comparisons before giving it the IQuOD stamp of approval.

APB data – there are small systematic thermal biases in upper water column. Suggest we use just the thermal biases identified in the deeper water only. These are from the SRDL recorders only.
For another recorder, there is a depth bias. For the global OHC calculations, they are not significant, but need to be thorough and check all instrument types.Has a regional effect, not a global effect.
Viktor hopes the paper will be published by the end of the year. Probably should wait till published before including in IQuOD.
ACTION: Viktor to send Tim the APB corrections. But, Lijing suggests we wait until next year to include both the MBT and APB corrections together in IQuOD (because further evaluation and confirmation needed).

Bottle corrections are complicated by the possibility of interpolated data. Therefore, they included a table with an envelope of corrections. Lijing checked the impact of the upper and lower limits.
Viktor and Lijing have also looked at biases in Mooring profiles, comparing to Argo globally and found positive biases throughout the water column.
Not published, but needs to be looked at.
ACTION: Investigate the mooring data (Viktor, Lijing).

2.4 IQuOD Intelligent metadata, Matt Palmer

Three papers have been published so far from the MetOffice. The latest one is the most refined. The idea came from IQuOD, but has been taken forward by others which is a nice model.
Next steps:
- Update IQuOD metadata with Haddad et al method
- Come up with a selection of ideas for work and shop around for colleagues to do the work.
- Which other metadata could be subject to similar iMetadata treatment?

A random forest network comes with an uncertainty estimate.

Gui asked about some of the methods & results. We can send questions to Stephen Haddad.
Rachel: The outputs were approximately '60% T4, 40% T6' - or sometimes with more possibilities, the idea is that we could run say 5 versions of EN4, with XBT types assigned based on these probabilities and see what the uncertainty is.

Matt & Gui want to explore the range of outcomes versus a best estimate.

The uncertainties from iMetadata would need to be considered, but might not be independent, so have to be careful when calculating the budgets.

We can show the impact of IQuOD work on OHC by systematically looking at each aspect of QC, uncertainties etc to see the impact.
Funding - look at going for UK university funding for postdocs to look at some of these tests.
ACTION: Matt (and Catia) to explore UK NERC funding options and entrain IQuOD community into proposals as needed.
A combined international funding arrangement such as NERC/NSF was discussed. Matt would support that approach. There are two other international options.
Alison is happy to host a postdoc as well. Would be good to connect with a heat content expert in the US as well.
ACTION: Matt and Alison to investigate NERC/NSF and other international funding options.

Should we adopt the new Haddad et al method? How difficult is it to implement for Tim? All the code to implement the Imetadata assignments is available.
We could treat it as a probabilistic method for now. The immediate thing is to use the best deterministic system, then explore in the future how to be more ambitious.

Tim: how much better would a “best” Haddad method implemented over the current iMetadata coding?
ACTION: Rachel and Matt to look at what the outputs are and refer back to Tim.
From Rachel: A "quick" comparison would be current iMeta OHC compared to the most likely new iMeta OHC - if they look the same then until we have the probabilistic implementation it probably wouldn't be worth the extra effort.

Zhetao - can this method be applied to other Meta data and the answer is yes. We could fill missing metadata such as platform codes, country codes etc. It is potentially also useful for the automatic/expert QC, which could give us another uncertainty sources estimation.

Who wants to be involved in further discussions:
- Tim
- Alison
- Rachel
- Matt
- Gui

3. IQuOD organizational topics - Part 1

3.1 Reframing IQuOD and discussion about the next steps for IQuOD, Gui Casteleao

Ideas for consideration for IQuOD going forward:
- Rotation of steering team and co-chairs.
- Diversity within the steering team.
- A dynamic task team structure built around a single task/publication, then the task team is dissolved.
- The steering team should have a minimum requirement of meeting attendance (could be any meetings), to keep an eye on what is happening. Steering team members are not required to be task team members.

We need to create a roadmap with a big picture for IQuOD. This could be initiated by a group of IQuOD volunteers and then maintained/assessed by the Steering Team.

Funded projects could then come in with work that would fit with IQuOD. They could operate as a task team. We have a group with a lot of experience, mentoring available.

Longer term things might mean that the task team needs to remain in contact. Eg, next steps for uncertainties mean that Bec still leads the task team even if inactive. Same for intelligent metadata. The task teams don't end after an initial paper.

Gui is concerned that we will miss out on legitimacy if we aren't publishing? The back bone of IQuOD is our publications.

Keep the task team structure, label as active/inactive?

The steering team could have a scientific advisory committee. Is this too many layers? Consider inviting Simona or someone from her team to the group to enhance cooperation between the Blue Cloud 2023 project and IQuOD. Simona suggests Christine Coatanoan, Sebastian Meurich, others that might join the steering team.

What do we offer to postdocs/PhD students? Impact, mentoring, learning through discussion, networking. Being on a committee is very helpful to early career people as it gives connections.

The next IQuOD meeting should target a bigger meeting to draw people in and get them involved.
Tim could find out who downloaded IQuOD through WOD select. Help to assess the use of IQuOD.

ACTION: Renew the steering team, then the steering team can make some decisions about any changes we might need. Leave task teams as they are for now.

ACTION: Look at past attendees and others that made presentations and see if we can re-engage with them.

3.2 Terms of reference document review, membership review, steering team review and new members.

Outcomes of task team structure discussion:

- Task teams are following a road map (in general terms).
- Task teams pursue the end goal to suit the work that they want to do. The priorities are defined in discussion with the task team. The task teams should find what is relevant to the project and bring people in to work with.
- Task team leaders are re-labelled as 'Point of Contact'.
    - This can mean a more active role for leads/Points of contact. The leader figures out how goals will be implemented.
    - Task team leads are the point of active communication to the DAC to ensure testing and implementation happens correctly.
- Activities will be more free and flexible.

Task teams:

- **AutoQC**:
    - **ACTION: find POC or combine with ExpertQC to a single QC TT.**
- **ExpertQC**: Gui (POC)
- **Uncertainties**: Bec (POC), Christoph, Marc
- **Intelligent metadata**: Rachel (POC), Matt
- **DAC**: Tim (POC)
- **Data Erratum:** Zhetao (POC) & Ricardo

    - Find others to continue for Zhetao
    - A long-term task team
      ACTION: Change the name of the team. Franco suggests: Metadata error and duplicates.
- **Outreach and education:** Uday (POC)
    - Coordinate with IODE and conduct training programs
    - Outreach to other communities (mapping etc).
- **FAIR Data:** Bill (POC),
    - Data format leader?
    - Fair data team (new name suggestion welcome).

ACTION: Simona & chairs can discuss with Christine Coatanoan and see if she is interested in collaboration for data format design. Christine works with the Blue Cloud project and previously began a formats document for IQuOD.

Data format (possibly "FAIR data") task team people who are interested. Tim has a need for the format team now for the 2023 release:

- Christine
- Bill
- Simona
- Christine
- Gui
- Lijing
- Tim

ACTION: In two months – create a list of what activities are happening now, priorities and a wish list for each task team (achievables, products).

Outreach and Education:
Uday: We need to meet Lucy Scott and team from Ocean Info Hub (OIH). Tim is already working with them with WOD, therefore IQuOD is already involved. The IQuOD website can be linked with OIH by setting up a meeting with Lucy Scott and her team.
The restructuring at IODE has resulted in classifications of projects as (i) Program Component, (ii) Program Activity or (iii) Project. As a result, we need to try to link IQuOD with the other "IODE projects" as much as possible to the 3 already designated IODE programme components ODIS, OBIS and OTGA. In view of this we need to identify suitable components to map IQuOD with.
ACTION: Arrange a meeting with the OIH team and identify components to map IQuOD with.

Steering team:

Simona suggests all the TT leads are members on the steering team. Begin a monthly ST meeting that people may or may not attend.
Alison suggests that leads should not be required to meet if they are not funded.
Steering team members should be in an oversight role.

Lijing proposes that we have a core team to make the plans for IQuOD, then
Keep the Steering Group size of <= 10~12, which is manageable. We agree the "purpose" today and everyone recommends the experts in the following two months with a justification. We will have a meeting in two months to elect the Steering Team members. There should be 5-6 inside the IQuOD, 4-5 outside the IQuOD.

ACTION: Workshop 2024 Funding group activity: Alison, Matt, Gui, Simon, Bec

ACTION: Finalize the TOR document in the next two months. Co-Chairs & ST and Simon.

ACTION: Co-Chairs & everyone to nominate Steering team members and experts in the next two months and send to co-Chairs.

Matt's suggested terms of reference for the Steering Team (starting point for later discussions/inclusion in the IQuOD workplan document):

1. To set the overall strategic direction of IQuOD, including a statement of current priorities / milestones
2. To champion IQuOD and raise awareness of the project among international research networks.
3. To attend IQuOD workshops on an annual basis to review progress of activities and renew priorities when needed.
4. To provide specific advice / expertise to IQuOD activities as needed on an ad hoc basis.

4. Phase 2: IQuOD Auto QC

4.1 AutoQC, Simon Good

Simon suggested we combine the auto QC (AQC) and expert QC (EQC) task teams.
There is still work to be done to join the EQC tool and AQC efforts.
AQC flags are on each measurement. 1 = no test failed. 2=high true positive (flagging most of the bad data at the cost of also flagging some good data). 3=compromise, 4 = low false positive (flagging very little good data, at the cost of missing some bad data). There

is no whole profile flag. No Depth/Press flag. Just Temperature flags on each measurement.
Individual flags could be used to create a whole profile flag if needed.
Tim has included the WOD flag for the Depth, Pressure and other variables.
The IQuOD flag is not compatible with other flag schemes. Should we be providing a whole profile flag?

Some discussion about combining and handling AQC and EQC flags. Can we combine the two?
Yes, it seems so.
We can use the AQC 1-4 flags with GTSPP equivalent flags and have one flag field that is the IQuOD flag.

ACTION: Map the AQC flags to GTSPP flags in a document for users. Or label the flags to match GTSPP approximations or make clear to users which flags to use for other flag schema equivalent.

AQC Code optimization ideas:

- Section out the QC code into Rust and improve speed.
- Can the AQC performance be improved using Argo? Train ROC curve separately on Argo.
- Training dataset: we could develop an Argo dataset instead of relying on only the QuOTA dataset.
- We need to define a representative training dataset for historical data.
    - WOCE global dataset? Scripps folks might be helpful, Bill can talk to them. Zhetao/Viktor had WOCE data already, can share.
    - Alison: What about using a piece of Hydrobase for a training set - a part that we have the accepted/not accepted information? Result of the discussion was to not go with Hydrobase unless we can sort out what we have.
    - GO-SHIP Easy Ocean
    - Can we QC our own dataset and use that?

CoTeDe is being re-written in Rust, that will help with compatibility.

ACTION: Optimize the AQC code to run faster.
ACTION: Incorporate new QC tests.

5. Phase 3: IQuOD Expert QC

5.1 Expert QC

Are there any expert QC data sets we can leverage? Can we define and add some expert QC flags and add them as IQuOD flags? Yes, but let's plan ahead, not rush to get them out with the next release.

- Argo
- XBT
- GLODAP for chemistry, and not looking at T/S the same way that a physical oceanographer would do.
- CCHDO? These data have not been expert QC'd or at least some of them have not.

ACTION: Release IQuOD2023 with autoQC flags only at this stage and build a plan for adding in expert QC flags in future releases.
ACTION: Figure out how to find expert QC'd XBT datasets so we don't see them again through the QC interface. Bec, Tim, Gui. Need to get a list of accession numbers to exclude, including WOCE datasets, to exclude from the expert QC interface.

The current EQC tool needs 3 experts to agree for the flags to be accepted as IQuOD expert QC flags. We don't have the resources to just rely on the current small QC expert group.
Start with the three people now (Bec, Uday and Gui), then we need to expand who becomes and expert and at what level they are considered 'experts'

We require an understanding and agreement between experts for QC cases. Francis suggested an online gathering to discuss special cases and QC decisions.
A monthly study group or similar.
ACTION: Begin a regular EQC gathering to discuss expert QC cases.

There was much discussion about how much of the AQC'd data we should be looking at. The expert QC should be used to create training datasets to then use machine learning to improve the AQC results.
Gui suggests that experts should look at the flags in the middle of the distribution as they are the most uncertain. Gui wants to look at the thresholds and improve them. There was discussion about biasing our results unless we look at all flags.

ACTION: Gui, Simon, Bill to decide what an AQC training dataset will look like and then feed that to the 'experts' for QC and retraining of the ML tool.

In the expert QC tool, there should be an option for the user to choose a region, platform or dataset etc to QC.

Potential contributers to monthly QC gatherings etc:

- Gui
- Simon
- Bill
- Rachel (talks)
- Bec
- Uday
- Others outside IQuOD can be invited.
- Franco
- Simona

Zhetao has done a gradient check that is localized and it is very sensitive to the vertical resolution. The threshold needs to be higher for higher resolution data. Zhetao can be involved in gradient test discussions.

A long term strategy should be prioritising the data that is on the boundaries, but for the training dataset it should be strategically sampled, across regions.

The training dataset can be built from data already expert QCd and will also contain data from older datasets, non-qc'd datasets that we then manually QC.
Future work for manual QC: we can improve the tool and use it through OTGA to teach QC.
Ideally in the QC system you would only be checking flags that fail AQC manually.
Gui is using a ranking system to feed the dataset to the user. To prioritise profiles that are in the extremes of the probability scale.

ACTION: Bec start using Gui's system again - so she can give basic feedback

Gui is running the database and cron jobs from the computer in his home. Should this be moved to the cloud? That would be expensive. The flags collected are in the cloud. The database is not backed up.
ACTION: Gui to consider options for back up of flags collected and moving the system to a supported environment.

We continued discussion about the data flows between EQC and the WOD and then feedback to the AQC training ML tool. Data will come into IQuOD and be held ready for

the next release (2024). The WOD format does not include the information of why the decision was made. IQuOD should keep the reasons with the profile. Tim says we can do that.

ACTION: Consider how flagging reasons can be kept with the IQuOD profile.

Datasets with EQC flags:
- XBT data from Australia (need to retrieve the reason flags). And from NZ.
- Deidre Burn at NOAA has QC'd a lot of data from the Atlantic for OHC estimates, she wanted to use the CoTeDe ML tool. Could use her QC'd data as a training dataset.
- GoShip/CCHDO dataset?
- Med XBTs? QC'd by Franco and Simona
- Moorings datasets etc from IMOS?
- Defence and AIMS Australian CTDs
- Any other datasets we pull in for CARS project.
- MNF data from Australia needs to be sent to WOD.

6. IQuOD organizational topics – Part 2

6.1 Community outreach efforts

Future outreach ideas:
- We can use the engagement with OTGA to teach people how to QC.
- Could look at all sorts of physical oceanography things to support QC.
- Could look at getting financial support for the outreach from the private sector.
- Create a course, which will need a small group to build up a design. The content will take some time to get together.

Uday: The required topics can be shortlisted and then the material can be built over a period of say the coming 6 months and once we are clear that the material is good to go then we will approach OTGA seeking their clearance for the training.

Simona: General QC teaching is good, but we could be more specific by going through all the code available and how to use the QC tools and the IQuOD dataset.
We probably need to start working towards this after the next release.

ACTION: Work towards building content for future teaching efforts over the next 1-2 years.

6.2 How does IQuOD collaborate with other projects?

Lijing listed several ideas:

- Advocate the IQuOD standards and methodologies (e.g. GO2DAT and Blue Cloud 2023 is still in the scoping/developing stage, Lijing/Zhetao will follow these activities and get involved).
- Communicate, discuss, and collaborate with these projects to co-generate best practices for data processing of oceanic data.
- Use local knowledge and expertise (i.e., Blue Cloud 2023 in the Mediterranean Sea) and feed into IQuOD data.
- Reanalysis community: for example, Andrea Storto used IQuOD flags as an ensemble member in his reanalysis data generation. ECCO shows some interest as well. GSOP is a platform that needs to be connected.
- WCRP-GCOS organized a joint project for energy/water/carbon cycles, IQuOD can investigate being endorsed as it is important for T/S data (ocean heat/freshwater).

A suggestion was made to engage more people in these groups, for example, steering team members. Or invite members of these groups to join us.
We should have a town hall at one of the next big meetings.
We should have more to do with Go2Dat, we should incorporate their flags into IQuOD. If the GO2DAT group need temperature and salinity, we could get involved. Lijing and Viktor are interested in having IQuoD move to salinity.

The GEWEX group cannot endorse a particular dataset. The intention is to endorse the products, not the dataset. Lijing says that the uncertainties should come from IQuOD and that is where the endorsement should be.
Marc Le Menn is involved in the MINKE project (https://minke.eu/) which gives cross collaboration there.

6.3 Summarize: Finalize goals and plans for next 12 months - 2 years

Summary of Activities/Papers:

- **IQuOD2023 release and data description/evaluation paper** (Bec leads the paper etc. end of 2023): publish and show the benefits/advantages of IQuOD data. SCOR funding to be used for publication.
- **Duplicate paper** (Zhetao/Xinyi lead, end of 2023): publishing the benchmarking dataset
- **OTGA** (Uday leads, design stage: end of 2023; implementation: before the end of 2024)

- **XBT/MBT/Bottle/APB bias correction: paper and implementation** (Lijing coordinates, Viktor leads the paper, Tim implements; Rachel to test): update CH14/L09/GR10, compare MBT correction schemes; publish Bottle/APB corrections; Implement updated XBT correction to IQuOD2023 (end of 2023); Implement MBT/Bottle/APB in IQuOD2024 version (end of 2024).
- **Uncertainty definition/quantification: next version design** (Bec leads, end of 2023, how to define uncertainty and what can be done?); a paper for the new uncertainty definition/assignment (end of 2024)?
- Improving the code speed/and incorporating new QC tests (Bill, end of 2024):
- Training dataset development, scope out what you need from an expert QC'd dataset to use for the training dataset. (Bill&Gui, version-1 for middle of 2024)
- **Expert QC** (Gui leads; end of 2023).
- **I-meta data** (how to implement, evaluation: Rachel; middle of 2024, report back and SGs decide to implement or not)
- **Organization: Funding seeking** (Gui, Alison, Lijing, Bec, Simon, Matt. all., end of 2023); **Steering teams** (Gui & Lijing leads, 2 months); **Term of references** (Lijing & Gui, 2 months); **Membership** (Bec leads and use google-group)
- **Outreach** (town hall, sessions in next year's EGU/AGU meetings etc. Lijing to check)
- **Pilot activity for Salinity** (Zhetao/Viktor/Lijing/Tim/Simon, end of 2024): Viktor for bias; Zhetao/Simon for QC. (Bec, Tim, Alison to be involved)
- **Check the falsely QC-ed out data in some extreme ocean conditions** (i.e. warm/cold eddies, tropical cyclones etc.), **assess the impacts on OHC estimate, and find a potential way forward** (Lijing/Tim, middle of 2024)

ACTION: Bec will update IODE with the steering team details and put names back on website.

Meetings:

- Bec to put in an abstract for IQuOD for OS. Suggested AGU session to submit to: https://agu.confex.com/agu/fm23/prelim.cgi/Session/192092
- Rachel is always happy to talk about IQuOD if there are conferences she is going to/ can go to.

6.4 Plans for next in-person meeting

How to fund the next workshop:

- Look at CLIVAR funding for workshops and submit a proposal.
- CLIVAR webinar series presentation is an option.
- Could be in conjunction with next ME4OH

- GEWEX open science conference July 7-12 2024 in Sapporo. Earths energy conference and ME4OH meeting/involved.
- OOPC plan to have a workshop next year for energy/water. March to July.
- Could be in conjunction with XBT Science meeting/GTSPP etc at SCRIPPS.

7. Appendix A. Actions summary

Report section	Topic	Action	Who	Due date
2.1	Uncertainties	Matt to discuss the creation of representivity error product with ME4OH community in due course	Matt Palmer	end 2023
2.2	Data Erratum	Publication to summarize the metadata checking/duplicate checking work.	Zhetao, Xinyi	end 2023
2.2	Data Erratum	Zhetao to move the code to the IQuOD GitHub	Zhetao	end 2023
2.2	Data Erratum	Consider linking GitHub with Zenodo for software publication eg (https://github.com/castelao/inception). Or Software Heritage.	Zhetao	end 2023
2.3	Bias corrections	Lijing to update the Cheng et al correction (last update was 2017).	Lijing	end 2023
2.3	Bias corrections	IQuOD 2023 will be released soon, assess if it is possible to add updated bias corrections for XBT.	Lijing, Tim	end 2023
2.3	Bias corrections	Tim and Francis/AOML need to check the status of AOML DM XBT data	Tim, Francis	end 2023
2.3	Bias corrections	Viktor to recalculate his XBT correction	Viktor	end 2023
2.3	Bias corrections	Can the authors of other XBT corrections be identified and invited to talk to us?	Bec	end 2023
2.3	Bias corrections	MBT updates will not be published, but maybe a correction note/letter?	Viktor	end 2023
2.3	Bias corrections	Viktor to send Tim the APB corrections, Viktor to lead publication, Tim implement, Rachel test.	Viktor, Tim, Rachel	end 2024
2.3	Bias corrections	Investigate the mooring data (Viktor, Lijing).	Viktor, Lijing	End 2024
2.4	Imetadata	Matt (and Catia) to explore UK NERC funding options and entrain IQuOD community into proposals as needed.	Matt, Catia	end 2023
2.4	Imetadata	Matt and Alison to investigate NERC/NSF and other international funding options.	Matt, Alison	March 2024
2.4	Imetadata	Rachel and Matt to look at what the outputs are from the Haddad et al imetadata method compared to original method and refer back to Tim.	Matt and Rachel	June, 2024
3.1	IQuOD structure	Look at past attendees and others that made presentations and see if we can re-engage with them.	Bec	end 2023

Report section	Topic	Action	Who	Due date
3.2	IQuOD structure	Find a point of contact for AutoQC TT or combine with ExpertQC to a single QC TT		end 2023
3.2	IQuOD structure	Change the name of the duplicates task team to Data Erratum or similar	Zhetao	end 2023
3.2	IQuOD structure	Simona & chairs can discuss with Christine Coatanoan and see if she is interested in collaboration for data format design.	Simona	end 2023
3.2	IQuOD structure	Create a list of what activities are happening now, priorities and a wish list for each task team (achievables, products).	TT POCs	October, 2023
3.2	IQuOD structure	Arrange a meeting with OIH team and identify component to map IQuOD with.	Uday	early 2024
3.2	IQuOD structure	Workshop 2024 Funding group activity	Alison, Matt, Gui, Simon, Bec	
3.2	IQuOD structure	Finalize the TOR document in the next two months.	Lijing, Gui	October, 2023
3.2	IQuOD structure	Co-Chairs to consider nominations for Steering team members create new ST	Lijing, Gui, Bec	October, 2023
4.1	AutoQC	Map the AQC flags to GTSPP flags in a document for users. Or label the flags to match GTSPP approximations or make clear to users which flags to use for other flag schema equivalent.	Simon, Tim	end 2023
4.1	AutoQC	Optimize the AQC code to run faster.	Bill	end 2024
4.1	AutoQC	Incorporate new QC tests.	Bill	end 2024
5.1	ExpertQC	Release IQuOD2023 with autoQC flags only.	Tim	end 2023
5.1	ExpertQC	Figure out how to find expert QC'd XBT datasets so we don't see them again through the QC interface.	Bec, Tim, Gui	end 2023
5.1	ExpertQC	Begin a regular EQC gathering to discuss expert QC cases.	Francis, Gui	June, 2024
5.1	ExpertQC	Decide what an AQC training dataset will look like and then feed that to the 'experts' for QC and retraining of the ML tool.	Gui, Simon, Bill	June, 2024
5.1	ExpertQC	Bec start using Gui's system again - so she can give basic feedback	Bec, Gui	October, 2023
5.1	ExpertQC	Gui to consider options for back up of flags collected and moving the system to a supported environment.	Gui	end 2023
5.1	ExpertQC	Consider how flagging reasons can be kept with the IQuOD profile.	Tim	June, 2024

Report section	Topic	Action	Who	Due date
5.1	ExpertQC	Work towards building content for future teaching efforts (design stage end 2023; implementation end 2024)	Uday	end 2024
5.1	ExpertQC	Update IODE with the steering team details. And put names back on website.	Bec	end 2023
6.3	IQuOD goals	Submit an abstract to OS2024	Bec	Sep-23
6.3	IQuOD goals	Set a next meeting date/location for in-person meeting	Steering team	end 2023
6.3	IQuOD goals	Publish data paper for IQuOD	Bec coordinate	end 2023
6.3	IQuOD goals	Publish uncertainty paper #2	Bec coordinate	end 2023
6.3	IQuOD goals	Pilot a salinity QC activity	Zhetao, Viktor, Lijing, Tim, Simon	end 2024
6.3	IQuOD goals	Check the falsely QC-ed out data in some extreme ocean conditions (i.e. warm/cold eddies, tropical cyclones etc.), assess the impacts on OHC estimate, and find a potential way forward	Lijing/Tim	Mid 2024

8. Appendix B. Participants

In person attendees	Affiliation
Lijing Cheng	CAS, China
Viktor Gouretski	CAS, China
Zhetao Tan	CAS, China
Rebecca Cowley	CSIRO, Australia
Simon Good	Met Office, UK
Gui Castelao	SIO, USA
Marlos Goes	AOML, USA
Tim Boyer	NCEI, USA
Bill Mills	University of Colorado, USA
Matt Palmer	Met Office, UK
Alison Macdonald	WHOI, USA

Remote attendees	Affiliation
Rachel Killick	Met Office, UK
Uday Bhaskar	INCOIS, India
Ricardo A. Locarnini	NCEI, NOAA, USA
Mohamed CHOUAI	AWI. DE
Simona Simoncelli	INGV (Italy)
Franco Reseghetti	ENEA, Italy
Toru Suzuki	MIRC, Japan
Gael Forget	MIT, USA
Xinyi Song	CAS, China
Christoph Waldmann	University of Bremen, Germany
Francis Bringas	AOML, USA

9. Appendix C. Agenda

Monday 10th July, 2023

Time	Chair	Rapporteur	Topic	Discussion lead
08:00 - 08:30	Arrival and coffee			
08:30 - 08:35	Gui	Alison	Welcome, introductions	Simon
08:35 - 08:40			Vote ratifying new co-chairs	Simon
08:40 - 08:50			Introductory talk: Progress over the last 3 years and current structure of IQuOD. Agenda introduction	Simon, Catia?
Phase 1 - IQuODv0.1 improvements				
08:50 - 09:50	Bec	Alison	IQuOD uncertainty quantification: next steps	Bec Cowley, Christoph Waldmann, Marc Lemenn
09:50 - 10:20	Coffee Break			
10:20 - 11:20	Marlos	Bec	Metadata and data problem identification and rectification in IQuOD. How to streamline duplicate checking, error identification, reporting mechanisms and correction to WOD.	Zhetao and Ricardo
11:20 - 12:50	Lunch break			
12:50 - 13:50	Simon	Alison/Bec	IQuOD bias corrections: next steps.	Viktor/Tim?
13:50 - 14:30			IQuOD Intelligent metadata - which metadata should be subject to IM processes and how it will be implemented?	Matt/Viktor?

Time	Chair	Rapporteur	Topic	Discussion lead
14:30 - 15:00	Tea Break			
15:00 - 16:30	Gui	Bec	Reframing IQuOD and discussion about next steps for IQuOD.	Gui and Lijing
16:30 - 18:00			Map4OceanHeat session	Matt Palmer

Tuesday 11th July 2023

Time	Chair	Rapporteur	Topic	Discussion lead
Phase 2 - Auto QC				
08:30 - 09:15	Lijing	Matt/Bec	AutoQC flagging explanation and discussion on optimal flag presentation and socialization in the community	Tim, Simon, Bill
09:15 - 09:45			AutoQC code optimization, maintenance and community utilization	
09:45 - 10:45			Future AutoQC, further testing and refinement of IQuOD AutoQC tools	
10:45 - 11:15	Coffee Break			
Phase 3 - Expert QC				
11:15 - 11:45	Tim	Simon/Alison	1. Defining expert quality control for IQuOD (how do we use CoTeDe or other tools; how to we certify/recognize an expert to accept their expert decisions; do we coordinate the experts (e.g. similar to Argo cross-DAC qc homogenization).	Gui
11:45 - 12:45	Lunch Break			

Time	Chair	Rapporteur	Topic	Discussion lead
12:45 - 13:30	Zhetao	Bec	2. How do we incorporate expert QC into the IQuOD and what role will machine learning play?	
13:30 - 14:00			3. Discussion of data sets deemed already to be expert qc'ed and how these are incorporated into IQuOD	
IQuOD organization topics				
14:00 - 14:30	Zhetao	Bec	Community outreach efforts (webpage, IODE programs (Ocean Teacher). Who is the IQuOD community? How to promote IQuOD data to users? Papers, students etc? Funding?	Uday, Gui, Chairs?
14:30 - 15:00	Tea Break			
15:00 - 15:30	Gui	Alison/Bec	Community outreach efforts continued	
15:00 - 15:30			How does IQuOD collaborate with other projects? Eg, GLODAP, GO2DAT, Blue Cloud 2023. How do we leverage their efforts in flagging data?	Lijing, Simona
16:00 - 16:30			Terms of reference document review	Simon
16:30 - 17:00			Membership review, steering team review, new members?	
17:00 - 17:30			Summarise: Finalize goals and plans for next 12 months - 2 years Plans for next in-person meeting (Ocean Sciences?). Wrap up	Lijing