



IQuOD

International Quality-Controlled Ocean Database

3rd Annual Workshop Report

4th CLIVAR GSOP IQuOD

2nd IODE SG-IQuOD

1st SCOR WG 148

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Editor

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- Masayoshi Ishii (MRI/JMA, Japan / chair of XBT-Japan)
- Shoichi Kizu (Tohoku University, Japan)
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** XBT-Japan means the Working Group for Recompilation of Historical XBT Database, Japan Group of Experts to Advance IOC Programs.

Workshop objectives

- Update on recent IQuOD activities, particularly SCOR WG 148 and IOC/IODE.
- Delivery status of the 1st IQuOD data/flavour version: progress on the development/implementation of intelligent metadata, (random) uncertainty estimates, exact duplicates flagging, platform for Auto QC benchmarking and setting up public delivery.
- Plans towards benchmarking auto QC procedures using high quality reference datasets.
- Plans towards implementation of further advances for intelligent metadata, uncertainty estimates and duplicates.
- Discussion on potential approaches for expert QC & implementation.
- Discussion on potential approaches for implementation of knowledge transfer and capacity building, particularly in developing countries.
- Establishing synergies between IQuOD & XBT science team.
- Reviewing goals and actions for 2017/18 & planning for the 5th IQuOD workshop.

Table of Contents

1 Session 1	7
1.1 Japanese Data Rescue Activities and Related topics - M. Ishii (MRI/JMA)	7
1.2 The Current IQuOD structure – SCOR WG 148 - Catia Domingues	7
1.3 WOD as Dissemination Tool for IQuOD – Tim Boyer	8
1.4 IQuOD Duplicates - Ann Thresher, Ed King	10
1.5 Update on Assessing the Japanese Navy data - Shoichi Kizu, Tohoku University.	11
1.6 Discussion: GDAC interactions with other task teams and next steps for duplicate checking – Tim Boyer and Ann Thresher	12
2 Session 2	13
2.1 Progress on a new Met Office temperature and salinity dataset with incorporated uncertainties - Rachel Killick	13
2.2 Uncertainty task team: summary of activities - Bec Cowley	14
2.3 Discussion on roadmap for implementation of uncertainty into IQuOD dataset versions - Bec Cowley	15
2.4 Intelligent metadata task team: summary of activities - Matt Palmer, Shoichi Kizu, Toru Suzuki	18
2.5 Discussion on iMetadata	18
3 Session 3	20
3.1 Copernicus Marine Service, the European service for marine in situ data - Thierry Carvel	20
3.2 Coriolis data quality control system - Christine Coatanoan	23
3.3 Further developments of the ICDC automated data quality control scheme with application for ocean climatologies - Viktor Gouretski	23
3.4 CCHDO and IQuOD: synergies - Steve Diggs	24
3.5 Crowd sourcing discussion - Steve, Tim and Alison	25
3.6 Expert QC task team: summary of activities - Ann Thresher	25
4 Session 4	26
4.1 Quality control and duplicates removal for the Marine and Meteorological data from NMDIS/China - LIU Yulong	26
4.2 Introduction to JODC - Takeharu Miyake	27
4.3 Progress of Japanese data rescue - Toru Suzuki	27
4.4 Present Trends in IOC/IODE - Prof. Yutaka Michida	28
4.5 On the use of Climatological Convex Hulls for Detecting Outliers - TVS Uday Bhaskar	29
4.6 Progress on the auto QC benchmarking - Simon Good	29

5 Session 5	31
5.1 GOOS update and IQuOD in the context of Framework for Ocean Observing (FOO) - Toshio Suga	31
5.2 Task team review and Action items	32
5.2.1 GDAC Task Team	32
5.2.2 AutoQC Task Team.....	32
5.2.3 Expert QC and Duplicates task teams	33
5.2.4 New task teams.....	33
5.2.5 Other discussion.....	33
5.2.6 Action items from previous meeting	33
5.3 Finishing tasks and wrap up	36

1 Session 1

Chair: Steve Diggs

Recorder: Alison Macdonald

MONDAY MORNING

M. Ishii gave a formal welcome to all attendees.

1.1 Japanese Data Rescue Activities and Related topics - M. Ishii (MRI/JMA)

A working group called XBT-Japan was organized in 2012 under the Japan group of experts to advance IOC program for recompiling oceanographic database for monitoring Global Warming with high accuracy and providing them to users in various climate-related studies including environmental issues in the Japanese community. It consists of Japanese agencies, institutes, and universities concerned with oceanographic observations. The working group is financially supported by the Ministry of Environment to FY 2017. The Japan group of experts is responsible for the decision-making for the Japanese contribution to the IOC activities. Needless to say, XBT-Japan is ready to collaborate with IQuOD activities.

Three research themes are currently undertaken by the working group: 1) ocean analysis and application to climate studies, 2) recompilation of database and quality evaluation targeting for Japanese observational data, 3) use and improvement of ocean databases. Ishii reported on the progress of several research topics on ocean data rescue, historical analysis of subsurface ocean temperature data, and centennial-scale climate reanalysis.

Questions and discussion

Tim: Are digitized XBT data publically available, and has it been sent to WOD? Not yet, maybe next year.

Catia: Can you include your tests in the benchmarking for auto-qc? Toru will discuss tomorrow – there is a lot of noise in the data. How long is the project? 3 years from last year.

Tom Rossby: will you be able to continue digitizing the remaining data? The problem is cost.

Steve: have you quantified the cost of doing data rescue? Not answered.

Viktor: Do you also have mechanical bathy-thermograph data? Ishii no current work to QC the data, but there are some observations.

Alison: Crowd-sourcing the digitization might be an option for data rescue.

1.2 The Current IQuOD structure – SCOR WG 148 - Catia Domingues

In the first part of the presentation, we reviewed the main objective of the IQuOD project, its expected outcomes, workflow, and current structure (co-chairs, steering committee and task teams/co-leaders). In addition to the 8 main goals of the workshop, we provided:

- Updates on recent IQuOD activities, particularly SCOR WG 148 and IOC/IODE.
- Delivery status of the 1st IQuOD data/flavour version: progress on the development/implementation of intelligent metadata, (random) uncertainty estimates, exact duplicates flagging, platform for Auto QC benchmarking and setting up public delivery.
- Plans towards implementation of further advances for intelligent metadata, uncertainty estimates and duplicates.
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In the second part of the presentation, we provided a summary of the calendar activities since June 2013, with an emphasis on the dissemination activities that occurred in 2016, after the 3rd annual workshop in Hamburg (December 2015). These included an IQuOD session at the Ocean Sciences meeting in the USA and presentations about IQuOD at the OOPC meeting in Europe, CLIVAR Open Science Conference in China (GSOP panel, CONCEPT-HEAT RF, Sea Level session, Town Hall on Sustained Observations, report to SSG). IQuOD's sponsorship by IOC/IODE and ICSU/SCOR were also discussed, particularly the formation of the SCOR-IQuOD working group 148 and its 3-year workplan and main deliverables (with terms of reference at http://www.scor-int.org/SCOR_WGs_WG148.htm).

Questions and discussion

Tom Rossby: There is an historical database to be digitized – is that being done on a national basis? Tom referred to figures in Abraham et al (2013) comparing XBTs with and without metadata. Tim: There is a NODC program that is currently working with ACR to get data digitized with crowdsourcing.

Thierry: Do you have a plan to provide information back to data providers? Catia – it has not been done, but could be – what, Ann depends where the data comes through. Bec – we did say there would be a feedback method we should discuss it.

Mauro Cirano – Brazil is planning to remove it from the Navy– will be one of the first actions of the ministry of oceanography.

1.3 WOD as Dissemination Tool for IQuOD – Tim Boyer

The World Ocean Database (WOD) at the National Centers for Environmental Information (NCEI) is prepared to be the GDAC for IQuOD. The IQuOD data will be served through the WODselect system (<http://www.nodc.noaa.gov/OC5/SELECT/dbsearch/dbsearch.html>). The WODselect system allows for subsetting of the WOD and delivery of the requested data. On the download page for WODselect (test version) there is an IQuOD choice. If a user chooses the IQuOD, they

will receive ocean profile data with IQuOD uncertainties attached to each profile measurement and latitude/longitude, IQuOD intelligent metadata (best estimation of vital but missing metadata), and IQuOD quality flags for each measurement. The WOD with IQuOD capabilities (IQuOD v0.1) is set to be released by the end of December, 2016. There are as of yet no IQuOD quality flags, so WOD and originator (source of data) quality flags will be attached to each measurement. In order to release IQuOD v0.1, both the initial uncertainties and intelligent metadata will need to be set. This information will be in a set of flat files which will be read directly into the WODselect system and applied when the user requests IQuOD data. In this way the uncertainties and intelligent metadata can be modified at set time intervals as information on specific instrumentation and institutional procedures is amassed. The format for IQuOD v0.1 will initially be a modified WOD native ASCII format, a modified WOD comma-separated value (csv) format, and a modified Climate-Forecast (CF) compliant netCDF ragged array format. The newly created IQuOD format team will advise on future IQuOD format design.

Questions and discussion

Gustavo, Steve, Catia: discussed submitting announcing the first product. A publication in EOS or BAMS? We could have another update for OS2018. The IAPSO-IUGG conference in 2017 could be used for the first announcement. Also, our SCOR proposal lists products with a deadline.

ACTION

Viktor: does the format include uncertainty for geographical coordinates? Yes, but not on date. What about bottom depth? That is another order of magnitude.

Thierry: we cannot mix reported data vs. guesses. Yes we need some way to identify what has been changed.

Catia: we have to backward check – Tim – said we wanted the original data, but that is not in there yet. The GTSP has history records in every file. Tim: we don't have history records – at least not yet. We expect to have original data and final data, but not keep the history of changes.

Gustavo: you have raw depth, temp and you provide WOD and IQuOD flags – will you be correcting depths and temperature, in separate file or same file – Tim you could get it either way – you can have either or both.

Gustavo: There should be products derived from the IQUOD data set, for example indicators for ocean currents, MOC/MHT, OHC when we show afterward metrics of success, this is how the new IQUOD data set positively impacted the results.

Tim: The data will be netCDF compliant so should be easily meshed with Argo.

Gustavo: recommended to have the transect number in the IQUOD XBT data set, as scientists also use the repeated ship track data. Tim: This will be included in the data set. It is also possible to create intelligent metadata for launching height. If we know the ship and date we should be able to get bridge height and then get deck height.

1.4 IQuOD Duplicates - Ann Thresher, Ed King

With access to the CSIRO supercomputer, checking millions of profiles for exact duplication has become possible. The first step is to sum the Z, T and S (if present) values for every profile in the WOD database. Sorting by number of values allows you to quickly find those where all of these sums match. These are potentially duplicates.

The more points in the profiles, the higher the probability that the profiles are true duplicates. In practice, if more than 30 points are present, almost all of those identified in this process are true duplicates. 64% of the non-constant T profiles with 27 points are true duplicates. At the other extreme, if you only have 4 points, the probability that you will get false matches is extremely high.

Examining many of these manually reveals some patterns. We see exact duplicates that are 3 years apart, or at positions that are the same within rounding errors, or where one has a decimal position (32.1 degrees) that is matched by a degrees/minutes position expressed as a decimal (31.06 which is really 31°06') or that are in the wrong hemisphere (-62° vs 62°). Some are correctly identified as having the wrong position in WOD. Others remain as duplicate profiles.

The challenge is to decide which one to retain. In some cases this will be simple (decimal vs degrees/minutes positions). In others, more work will need to be done (profiles from cruises apparently 3 years apart).

Further complications come when two profiles carry different metadata or profile data. An OSD profile may have T, S, O, CHLa, NO3,... when the corresponding CTD carries only T and S. In this case we need to merge the profiles retaining the most complete metadata available. We do NOT want to retain both profiles in the IQuOD database.

Preliminary results are encouraging. It seems that it will be possible to check many of these manually.

N points	N dupes	N possible dupes	N const T-dupes	N non-dupes	Total N
4	?	3939 [^]	264,828 ⁺	?	875,125
27	208	93	2902 ⁺	169	3462
30+	3793 [^]		4104 ⁺		7897

+ all T within a profile identical

[^] not looked at individually but all points match

The next step will be to compare profiles of different data types or resolutions. Bathy versions of XBTs undoubtedly still exist in the database. Transmission errors can result in slightly

different positions or time. We therefore intend to compare all profiles within both spatial and temporal boxes. Initially we will use a 2° spatial window and a 3 month temporal window. These can easily be modified to compare different subsets.

Comparing the internal data of profiles with different resolution is tricky and we cannot enforce an exact match. In practice, the closest T in depth from a high vertical resolution profile (XBT or CTD) will be compared to the closest T in depth from a low resolution profile (Bathy or Tesac). If the data is of different precision, the adjustment will be made to compare similar precisions. If more than 90% of the points match, they will be identified as duplicates and checked manually. We hope checking these will give us confidence that our procedure is reliable and we can handle these automatically.

There will be a hierarchy used to decide which of two profiles to keep and in some cases, this decision can be made automatically so these can be efficiently removed from IQuOD.

- Always keep the profile of highest 'quality' i.e.,
 - XBT kept when it matches a BATHY
 - CTD kept when it matches a TESAC
 - If two XBTS or CTDs match, keep the higher resolution profile
- If a CTD matches a bottle cast, however, KEEP BOTH

This is a work in progress and we expect more interesting patterns to appear as we run the duplicate checks.

Questions and discussion

Viktor: Has a small project of North Sea data compilation. The problem is that there are possible duplicates because they are identical in T&S, but they might be different in the other properties.

1.5 Update on Assessing the Japanese Navy data - Shoichi Kizu, Tohoku University.

Kizu-san presented on the work he has been doing assessing historical Japanese Navy data. Generally, the data have poor Metadata – ship position, sampling depths, sampling bottle, thermometers, etc. Unclear data flow of post-war processing – most data was sent to US by 1960 – not sure if these data made it to NODC. JODC started in 1965.

There was an extensive post-war survey by IS by Washington Document Center 1945-46 – collecting documents and interviewing people. The Japanese documents say that copies were made before US collected the data and copying effort and camouflage to avoid requisition by the Allies – i.e. the data sent to the US could be incorrect.

War time data – example taken in 1942 published in 1963 – reported as standard level – captains were told to use specific depths, but it is not obvious how whether they actually

obtained the target depths. Post-war values were reported as both as original depths and interpolated on to standard depths.

1931 – data was reported on standard depths. There is no information about wartime data. Post-war, 1949-1953, #4 Kaiyo is an example of a ship that survived WWII that reported original depth, so it is possible to determine a bias. It suggests that real sampling did not reach the target depths.

The JODC dataset (1921-2010) – shows biases continue into the 1970s.

Bingham et al 1992 – comparing Japan Navy (1938-42) and Transpac 1978-1982 (T-4 XBT) – they found differences. But perhaps this study was affected by these depth biases

Living memory is no longer available.

Correction is not easy and may be impossible, but some uncertainty estimate is possible. Important because it can change view of decadal change rates.

Questions and discussion

Tom Rossby: Perhaps the issue could be modelled. The bias would be greater in the Kuroshio than in the mode waters.

Thierry: Data from the French National Navy throughout 20th century, the measurements are recorded on paper and they have not been digitized. All navies have made these measurements, and they require significant manpower to be digitized and corrected.

Tim: how would you suggest assigning uncertainties? **Ishii:** Uncertain as yet. There are many variables, different ships, types of ships and a mixture of quality. He does not feel ready, but Tim says we need to assign uncertainties to this data also.

Viktor: This is important for heat content calculations based on Nansen casts – can we believe the depths in the logs? It is a question of methodology. Viktor has looked at this for the Soviet ships, and we don't always know how the guesses at depths were made. In the case of the soviet cruises there were manuals that describe these methods. Could some work be done to determine this country-wise?

1.6 Discussion: GDAC interactions with other task teams and next steps for duplicate checking – Tim Boyer and Ann Thresher

Tim and Ann led a discussion on GDAC interactions with other task teams and the next steps for duplicate checking.

Catia: What do we need for the task teams? We need to decide priority for which duplicates are worth checking first.

Tim, Ann: We have to start from one version, freeze it, and anything else has that comes in has to be checked against that. WOD is updated every 3 months – so new profiles can be compared to this. What comes first duplicate checking or auto-qc or are they the same?

Newer data have unique IDs which are embedded in the files (the CRC). Is there a way to get this into the WOD? These are in GTSP. There may still be duplicates because not everyone will put the IDs in. There are now additional metadata in XBT profiles provided by AOML, including contact info. If this info is in GTSP then it can be retrieved (Tim). WOD keeps PI info.

Gustavo: AOML can provide launch heights that would be based on the ship where the XBT deployments were made.

Tim: needs intelligent metadata converted into a form that Tim can use to apply to the WOD.

Catia: Should we be correcting XBTs for biases using the recommendations from the XBT Science team? Catia suggests that IQuOD can provide guidelines for XBT corrections, but not correct the data.

Gustavo: The XBT Science Team have agreed that it is dangerous to confuse users, who are already worried about errors in XBT data.

Catia: she is not convinced that we know what the best one is, because they don't all correct for the same thing.

Gustavo: the group interested in the details of the corrections is very small, most scientists are interested in which data set is the best data set (recommended) to be used. The XBT science team provides recommendations on which correction to use, at it was done during the last XBT Science Team meeting, published in the Cheng et al BAMS manuscript.

Molly: agreed with Gustavo's comments, and could use the correction method as a way to make sensible uncertainty estimates.

Catia: SST groups look at correction ensemble differences.

2 Session 2

Chair: Shoichi Kizu

Recorder: Ann Thresher

MONDAY AFTERNOON

2.1 Progress on a new Met Office temperature and salinity dataset with incorporated uncertainties - Rachel Killick

This presentation gave an overview of the current plan to investigate uncertainties in Ocean Heat Content (OHC) and salinity using an ensemble of datasets. These datasets will be created

using methodology similar to that currently employed by the Met Office subsurface temperature and salinity dataset, EN4.

In addition to using subsurface data these ensembles will take surface data from the Met Office dataset HadIOD (Hadley Centre Integrated Ocean Database). HadIOD currently incorporates surface and subsurface temperature data and subsurface salinity data with the view of including surface salinity data as well in the near future.

In the long term it is hoped that ensemble members can investigate the impact of mapping methods, climatologies, bias correction schemes, QC choices, uncertain metadata and OHC calculation methods. Initially three of these aspects will be focused on: OHC calculation methods, climatologies and XBT correction schemes. As work in IQuOD progresses uncertainties from metadata (or lack of it) can also be drawn in and a current collaboration with IFREMER will aid the addition of a QC choice ensemble.

The ensemble will focus on the years 1950 – 2016 and will have 30 OHC members and currently three salinity analysis members. The salinity measure to be investigated is as yet undecided; it is likely to be anomaly from climatology, but the author is open to suggestions for alternatives or additions to this.

Questions and discussion

Simon: is working with Coriolis and this system to benchmark QC systems. So far, they know results are different but don't yet know why.

Thierry: Do they plan to use long term time series such as Oceansites? Currently trying to do that but not yet.

Lijing: mentioned using Argo climatology but is this Argo only data or is it referring Argo time period? Probably the time period though that includes XBT data which must include correction.

Gustavo: what is the link with IQuOD? Once IQuOD is ready, it could be used as basis for comparison purposes at the very least. UKMet office is integral to the IQuOD development as well as this. Both will converge to one QC system but not yet. This work will assess the quality of different mapping procedures, which will be useful for IQuOD.

2.2 Uncertainty task team: summary of activities - Bec Cowley

A summary of the tasks assigned to the Uncertainty Task Team was given. The definition of uncertainty for IQuOD was presented and still needs some work. It uses the Guide to Uncertainty in Measurement (GUM) as a basis, but is expanded to incorporate things like instrument behaviour, sampling, calibration and metadata uncertainties. Also, uncertainty estimates might include accuracy estimates from manufacturers, published papers, calibration information and expert estimates. The TT has started a table of uncertainties in a format suitable for the WOD, and this was presented for comment. Feedback from the community and experts to assist in population of the table and a paper describing the uncertainty assignments

are still works in progress. A more detailed document about uncertainties might be needed (a 'cookbook'). The current plan is to present uncertainties as a standard deviation.

Remaining questions include: should we be applying uncertainties to date/position information and how? What about uncertainties for data flagged as bad? An uncertainty for data with i-metadata applied?

The formats task group should be separated from the uncertainties task group.

2.3 Discussion on roadmap for implementation of uncertainty into IQuOD dataset versions - Bec Cowley

Catia: how do other groups incorporate or calculate uncertainties? Have we looked at these? Not yet. It is clear that bias will not be included in uncertainty measurements.

The process will be to start with the maximum uncertainty for each group of instruments, then refine this based on the metadata or other information which may increase or decrease the uncertainty for a specific measurement. This will all be in a table but very preliminary at this stage. We will always start with the highest value if you have a range.

Tom: modern instruments should have smaller uncertainty. Yes, that is the plan.

Gustavo: Systems have time-varying uncertainties and then the corrected data will have still another uncertainties.

Lijing: Can we compare XBT with XBT side by side (not just compare with CTDs) to determine uncertainty? This will give us the spread of error/uncertainty for random errors. We can do this regionally as well.

Molly: where did the CTD numbers come from? The table is the worst case value/ What about glider accuracy? These are the issues that would modify the uncertainty assigned to a particular instrument. Modern ctds are better than others. We need information from users to help us track the values for current instruments.

Action: we need the modifiers before Iquod version 0.1 release - we cannot leave large uncertainties that may be deceptive.

Thierry: lab calibration helps and should lead to lower uncertainties, a glider in the water for a long time leads to larger uncertainty. Perhaps we are getting too complicated? Also there may be position/date/time/T/S uncertainties as well. How do we record this? This is where the modifiers come in.

Gustavo: Notes that different glider operators calibrate sensors and carry refurbishment in different ways and this information needs to be known to better complete the table of errors and uncertainties for different observational profile platforms. The underwater glider community is working towards recommending standards for data, QC and sensor calibration

procedures. There will be a US glider meeting at Stennis to discuss this. IQUOD will need presence at that meeting to present the effort on profile data by this group. **Action: Gustavo (who will attend this meeting) will contact David Legler to recommend the participation of Tim Boyer at this underwater glider meeting.**

Steve: (Re: Gliders) Also there was an [EGO meeting](#) in Southampton, one of the subjects they discussed was glider data management. Contact [Yvonne Firing](#) for details.

Tom: So far we are defining the worst-case scenario, but we also need to capture the best case using our modifiers. And is this our responsibility? Or should the providers be the ones tasked with this as in WOCE? So this means we need to gather this information but we don't determine the values. They are fed to us by the experts. What we have now is just a raw starting point.

Alison: We need an example of how these modifiers work. Glider - Yvonne Firing for their start at this problem. Shoichi's work can be an example. Tim explained that the Japanese data didn't have real depth. So worst case is perhaps 10m accuracy in depth. but some ships used better processes and so their uncertainty is better.

Viktor: Note that the uncertainty can go the other way - you might have a worse uncertainty for some instruments that are badly calibrated or badly treated and with known errors that are large. We need to ask people about the data they submit before the memory disappears. This is a work in progress but it requires more time than we have. It's only basic so far. It will improve but take time.

Tim: Will we have something by December that is actually ready for release? Dangerous to put these tables out too early. Even Argo is questioning CTD data and intends to explore the data set to determine quality. Argo requires very high quality data but our reference database has data of mixed quality. Some sources are more reliable and of higher quality than others. In addition to the instrument uncertainty, we also need uncertainties on other data from that cruise. How well calibrated is the data from CTD submissions? OceanSites has done a lot of work like this too, it's hard to assign these uncertainties automatically - they are actually assigned by the PI.

Tim: as you get more information and use more modifiers, this changes the uncertainties applied to a particular dataset. Data source, etc can change your value assigned. Do we need multiple uncertainties? One for the instrument, another for the source or how it's been treated? Or the cruise or the ship... but Tim thinks we need one uncertainty.

Viktor: a lot of data from 1950s and the methods and accuracies used by various organizations are documented and could be used by us to determine uncertainties for that organization or data set. Russian example - manual used for data collection was applied to all Russian collections in that time frame - so estimates of accuracy are easy to determine. But smaller fisheries vessels didn't follow this and so are less accurate. It's not easy to tease this apart.

Tom: we're talking about temperature – but we're also mixing a lot of different instruments... should we organize the table by instrument or system? Would this help us? **Bec:** problem giving this to users – note that this is a database table not meant to be generally distributed. Perhaps history of instruments is way to start but no matter what you do, it's complicated.

Catia: if we have 3 years to do this, what are the priorities? Start from basics and add as quickly as possible to the tables. **Steve:** people like human readable information, but we need a more complicated or multi-dimensional table that can be extended. Is a decision tree a good way to represent this table interactively?

Alison: is this assigned on the fly or once? **Tim** points out it doesn't matter as long as the answer is the same. And these values might change as we gain a better understanding of the data and how it's been treated.

Catia: how do we refine the table right now? We can make a start by using time periods to determine estimates now, particularly for historical data. Modern data can be done more easily now.

Steve: notes we need to contact the experts NOW – their retirement/disappearance makes this urgent that we gather that information as soon as possible, and we can't wait until we have the questions to initiate contact – they can probably help us frame the questions as well. Do we know what the end users want in terms of uncertainty? Modellers have strong opinions... we need to canvass this.

Tom: The uncertainties we are talking about are calibration uncertainties. No – it's more than just that. Perhaps it's a calibration that's not applied... Tom points out that what's most important are biases for climate research. Errors should be random.

Steve: are there others out there struggling with this? And can we leverage their experience? SST groups? This is a different problem. Argo? Gliders? Oceansites? IQuOD needs to request these things from the other groups. Trying to do this ourselves is perhaps not best. **Catia** will go back to GSOP to ask for their input. It is a huge amount of work no matter how we approach it.

So what do we need to do before December? Refine metadata and some of the error estimates? Send table to outsiders and get their opinion of the current state? Need to put it out there!

Tom: we need the context of the evolution of the system.

Molly: if you have bottle data then the CTD data is probably better than if you don't. However, only if the bottle data is actually used (Gustavo).

2.4 Intelligent metadata task team: summary of activities – Matt Palmer, Shoichi Kizu, Toru Suzuki

Progress towards a first version IQuOD intelligent meta-data (iMetaData) algorithm has been made by evolving the approach documented in Cowley et al (2013). While we initially started out trying to replicate Matlab code using Python, it became apparent that a “flow chart” is a more robust way of describing the algorithm and has the advantage of being code independent. Like Cowley et al, the IQuOD iMetaData algorithm uses the profile date, maximum recorded depth and country code to assign the most likely probe type. Some details of the algorithm are still being modeled and will include the use of probes of known type to refine the depth “bins” used for assigning iMetaData probe type.

In the longer term, it would be useful to put the iMetaData into a probabilistic framework – i.e. assign a likelihood to each of the possible probe types (based all available probes at that particular time). The real value in this framework may come from the use of Monte Carlo approaches to provide a more complete assessment of XBT bias correction uncertainty. We will investigate machine learning approaches to assigning probabilities. We should also work with the XBT community to discuss other iMetaData we might want to include, such as XBT launch height, and how this information could be included in future.

2.5 Discussion on iMetadata

Francis: We have known information but are missing xbt-type, how can we actually guess reliably to correct for fall rate? In some cases, if you guess it's a T7, you still don't know what fall rate was attached originally and so you can't correct it! But we can try to quantify the uncertainties by making monte carlo analysis of the data and that feeds into the uncertainty estimate. Having some information is better than having no information.

By restricting the possibilities, you do get a better estimate. Full resolution data is easy to back calculate fall rate equation. Low resolution data is much harder. Even if you know the probe type, that often doesn't give you the fall rate coeffs used. It's a lot of work to work this out with any certainty. Statistical treatments are turning out to be pretty useful.

How will this be implemented? Tim will propose solution to that problem.

XBT science people question: At least half of xbps have no metadata. How are they working out corrections for these? Transect data is well known at AOML and SIO high density/resolution so not an issue with these data. The BAMS manuscript describes what applications (changes in location of currents, MOC, global heat content, etc) need the best QC. The global heat content is currently the indicator that would benefit the most from an improved data set and from the work of IQUOD. At the end, it will be critical to assess the impact of improved data in the computation of the various indicators derived from XBT data.

Lijing: uses this data and guesses metadata. 500-900m is treated differently to shallower probes, as are deeper probes. He doesn't split Sippican from TSK – numbers of the latter are

small so perhaps doesn't affect the outcomes? But they do bias the N Pacific. The process is not complicated so adding this is useful. Corrections don't impact on current location or speed analyses. But when estimating OHC variation on regional or seasonal scales it becomes more important.

Everyone: How will a probabilistic assessment work? Correct in a probabilistic way or correct based on the most probable result? Generate multiple realizations of assignments of intelligent metadata and then apply to different datasets to see effects of the different analyses. How is this information going to be used in determining (or correcting) bias? Matt envisions ensemble product of the ocean past state. Will people know how to use the data? Do we want to just serve our best guess as a basis with perhaps the probabilistic version as an add-on? Perhaps, depends on users and we need to ask them what they want.

Do we apply uncertainty to i-metadata value? So we'll have different versions with different i-metadata? Then let the users explore the effect of these variations. But first we need to provide best guess.

When will this get delivered so we can use this in version 0.1? Tim has already coded this and now we need to define refinements. After discussions, we will finalize processes and then apply it. Matt will change step cutoffs. The people involved need to discuss this this week and then recommend changes to be incorporated.

What about other intelligent metadata? Eg whether data was scientifically calibrated, launch height from ship, etc. Machine learning algorithms with cluster analysis might help. This is thinking about the future and while useful now, we need to finish version 0.1.

Bec: We are using WOD as our portal and they have several formats but they aren't adequate for IQuOD, we need a format based on Argo with original and adjusted values in it and this decision needs to be made soon we need a task team to address this. We don't want to reinvent the wheel so Argo is a good starting point. Christine Coatanoan and Marty Hidas will lead the task team.

Delivery could be a challenge because the current WOD system doesn't handle creation of multi-profile files on the fly. CORA provides multi-dimensional files but with lots of wasted space. Netcdf 4 is the way forward if we need to do ragged arrays, but some tools do not yet read this format.

Catia: Can we help people working on bias corrections by providing intelligent metadata? Operators can help by providing launch height, etc, and we can ask other groups to provide information as well. Italy, India, Brazil, Argentina, Japan and others should be asked to provide Pis, ship ID, etc.

We need – type of XBT, Launch height, (ship ID), recorder type, serial numbers, year of manufacture, etc. JCOMMOPS is updating requirements to include all of this. **Action: Bec will**

supply the list JCOMMOPS are developing. Can we go back to the data from research ships from the early years? And separate cargo ships from research ships?

Some groups are declining in number of deployments so not much data comes in now. Viktor has German contacts who have managed to get data from BSH and we can request it from him. Birgit Klein would be good source of information. Norway has historical data but maybe not releasing it going forward. Tom can help extract more recent data but they may not be ready to share.

We can build list of contacts who can help fill in metadata going forward, and we need to request full resolution data be submitted when possible. Copernicus would be pipeline into BSH and Norwegian data.

Lijing: Chinese researchers wanted to attend IQuOD but didn't have time to organize. They want to work with historical datasets and compile a database of Chinese XBTs. But we can't get the data. Even Lijing can't get it. The data is partially Chinese XBTs and partially TSK probes.

Tim: had someone at BSH who was providing him with historical metadata but the collaboration only lasted 3 years. Need to get that going again.

Catia: points out that many groups are doing auto-qc of various datasets without talking to each other and getting different results.

3 Session 3

Chair: Toru Suzuki
Recorder: Rebecca Cowley
TUESDAY MORNING

3.1 Copernicus Marine Service, the European service for marine in situ data – Thierry Carvel

Copernicus is a European system for monitoring the Earth. COPERNICUS-CMEMS products and services are meant to serve all marine applications: Marine resources, Maritime safety, Coastal and Marine Environment, Seasonal Forecast & Climate.

The service has a multi-platform approach, taking into account sea-level stations, coastal buoys, HF radars, river flows, drifting buoys, sea-mammal or fishes fitted with sensors, vessels, gliders, floats. Copernicus in situ TAC shares the work within 7 regions: Arctic area, Baltic sea, North Sea, Ireland-Biscay-Iberia area, Mediterranean Sea, Black sea and the global ocean.

Within regions, a total of 20 Production Units (PU) perform data collection, formatting, QC and duplicate checks and synchronization between regions. The Production Units work with data providers from EuroGoos Rooses, EU SeaDataNet network of data centres, US NCEI World Ocean

Database, the JCOMM operational networks (Argo and bio-Argo floats, GTSP profiles, OceanSITES moorings, Gosud underway data, DBCP drifting buoys, EGO gliders, CCHDO – GO-SHIP, SOCAT BGC data).

The Marine in situ TAC data are distributed by 7 Distribution Units (DU, one per region), they are listed and described in Copernicus catalogue <http://marine.copernicus.eu/>.

Each Distribution Unit continuously manages an FTP server providing NetCDF CF1.6 data and metadata files.

- The performance of the Dus are tracked by a series of KPIs (Key Performance Indicators): <http://www.ifremer.fr/co/co05010507/KPI/>
- Data downloads are logged and visible on User maps : http://www.ifremer.fr/co/co05010507/user_map.html

The main ongoing activities in 2016

- Setup a dashboard, improve and homogenize KPIs
- Reorganize providers to avoid duplicates in overlapping areas
- Development of Biogeochemical REP products
- Development of Waves products
 - NRT: under development, to be launched April 2017
 - REP: planned for 2018
- Improvement of interfaces
 - Copernicus Modeling centres and scientific users
 - European and International partners -> AtlantOS, IQuOD
 - Big data service: a cloud of observations, 12 columns, 5 billion lines, instant access time
- Communication and training sessions: presentation at EGU General Assembly in Vienna, IQuOD workshop in Tokyo.
- Improve citeability and traceability of data: promote DOI et ORCID for efficient bibliographic surveys and to provide feedback to data providers.

Status of observations available in 2016 on Copernicus in situ global region

Real-time: observations of year 2015

- 1 million de vertical profiles (2 million if the vertical profiles of coastal buoys are included)
- 89 millions of time-series/trajectory observations (TSG, Ferrybox, buoys, moorings, floats)

Historical data, status for the end of 2015

- 16 million vertical profiles, 110 million trajectory points, 45 millions of time-series
- 5 billion of observations from 80 parameters (temperature, salinity, current, oxygen, chlorophyll, nitrates, turbidity, etc...)
- 31 000 platforms

A list of useful links for documentation, data access, service desk

- The global region web page
<http://www.coriolis.eu.org/Data-Products/Data-Delivery/Copernicus-In-Situ-TAC/Organization>
- User's manual, Copernicus implementation of OceanSITES NetCDF V1.3
<http://dx.doi.org/10.13155/40846>
- The quality control manuals
 - http://eurogoos.eu/download/Recommendations-for-RTQC-procedures_V1_2.pdf
 - http://eurogoos.eu/download/RTQC_BGC_recommendations_v2.5.pdf
- The global region REP product : CORA version 4.2
<http://dx.doi.org/10.17882/46219>
- FTP access with your Copernicus account
ftp://MyAccount@vftp1.ifremer.fr/Core/INSITU_GLO_NRT_OBSERVATIONS_013_030

The service desk will answer your questions servicedesk.cmems@mercator-ocean.eu

Questions and discussion

Catia: What is Ferrybox? Data collection on ferries, includes TSG and some BGC parameters. What is the difference between Copernicus and SeaDataNet? SDN is an EU federation between the EU oceanographic datasets. Not designed to handle global data. Copernicus gathers global data, including NCEI.

Tim: Do you plan to or could you serve IQuOD through Copernicus? Possible, but would not like to interfere with NCEI server. Tim says it would be good to have another GDAC to serve the data. Could you serve it through CORA?

Copernicus will provide data to IQuOD (glider, animal etc). It is possible for them to hold the complete IQuOD product for serving. The gliders are talking about a GDAC? They are working on promoting the GDAC for gliders and they are working with other global groups on this. Also working on a GDAC for drifters with MEDS.

Tim wonders if the 2 million vertical profiles in 2015 is correct? Some are not 'true' vertical profiles, the data includes coastal buoys which really should be time-series.

Mauro: Buoy data is QCd in real time, Mauro is analysing this data and Mauro has the full resolution data. GTS only releases the low resolution data, and this is what is pulled in to Copernicus.

Tim: Data around Korea? This is through OceanSITES

Toru: How to you assign a DOI? They have a publisher that assigns a DOI to each version of the product – each snapshot gets its own DOI. Can handle different versions with one DOI, however.

3.2 Coriolis data quality control system – Christine Coatanoan

An overview of the Coriolis quality control system has been presented. First started with the real/near-real time processing for which quality control steps have been described: automatic tests, objective analysis and QC visual software. Objective analysis has been more detailed with a definition of the different alerts provided by the method (standardization alert, spike/offset climatology, red and white alerts defined by comparison of residuals with customized thresholds). An exercise has been performed on some data (CTD & XBT) from the WOD. The results show that 71% do not show anomalies. Less than 5% have significant alerts. Examples of anomalies (from red alerts) have been shown and are clearly identified as anomalies. A suggestion to send anomalies' list as it's done for the Argo dataset has been proposed. A second part of the presentation was dedicated to delayed mode processing at the Coriolis R&D level. A description of the CORA dataset has shown the evolution of the number data integrated in the CORA dataset as well as the distribution per oceanic basins. Another layer of quality control is also performed for CORA with the participation of the CLS tests like altimetry and a focus on coastal profiles, from which feedback has sent to Coriolis when anomalies are detected. A new statistical method based on min max, and developed by J.Gourrion, is also used to perform quality control on the CORA dataset. This approach, that does not require assumptions such as unimodal, symmetric and homogeneously non-Gaussian distribution, proposes minimum and maximum values calculated from a reference historical dataset. The application on the CORA dataset was very efficient at finding biased profiles (accurate in the deep ocean) and has shown lower wrong detection rate.

Questions and discussion

Tim: Are these QC tests included in the IQuOD testing? Yes, but not the minmax test yet. There is some work being done with the MetOffice with the minmax tests. Check with Simon which tests are being implemented in IQuOD.

Tim: Visual QC is done after all the auto tests and the OA testing. In OA testing is only performed on data that does not fail other tests. Ignore the bad data. Christine will send the OA output from the WOD dataset to Tim.

Tom: An easy test would pick up some of the bad data would be a wave frequency test.

3.3 Further developments of the ICDC automated data quality control scheme with application for ocean climatologies – Viktor Gouretski

Viktor showed results from the ICDC Auto QC procedure, a suite of qc checks (global and local). The climatological test requires N=300 obs and is a 2.5 stdev envelope around the median. The distributions are skewed and sometimes are very high in certain areas of the oceans. He has also included freezing temperature test in the temperature range test since the last IQuOD meeting. Profiling floats have fewer failures than the other data types. Failures are usually associated with areas of strong currents/eddies. The same procedure is applied to salinity. He uses the dataset to determine the thresholds, but applies thresholds from different

datasets to each other. The climatology is an update of the WOCE 2013 – Argo climatology of Gourteski and Koltermann, 2004. Also has applied the method to nutrient analysis.

Questions and discussion

Uday: You have new thresholds for the data checks, how are bi-modal checks applied? The single mode is applied using probabilities. Normally there are no bi-modality problems except for a couple of tests. More development can be done to improve the tests.

Thierry: For salinity, 8% of all levels were rejected. This is a big number, but VG is not surprised because it is for the OSD. Argo is more like 2%. A lot of the failures are due to the depth check, which is dependant upon the bathymetry used.

Tim: Stuck value test is difficult to operate as it catches a lot of good data. We should look at Viktor's and Christine's tests to see if the tests have similar useful methods. Viktor's test is applied globally. Looks for constant temperature over a large depth range. Should maybe be tailored for different datasets.

Will Viktor's min/max test catch bi-modal cases? Viktor has not seen this problem of bi-modality in his testing. He uses circles around a location, Jerome uses a different method. Viktor sees skews, not bi-modes.

It is important to look at bi-modal data because qc tests throw out data when these modes exist.

Francis: Are Viktor's methods being applied to IQuOD? All groups are submitting their tests for benchmarking with a goal of assessing all the tests and using the best to put into one set of tests for IQuOD. Francis says we should use the tests available for our own testing. That is the idea, we are sharing and developing the tests.

Bec: Have these updates been transferred to iquod testing? Not yet.

3.4 CCHDO and IQuOD: synergies – Steve Diggs

CCHDO is a data center and data assembly organization, it does not perform QC. CCHDO is moving to being more accessible directly rather than through a web interface. Jim Swift has a clean data project that he is working on which could be of huge benefit to IQuOD. Breck Woens, Brian King and Howard Freeland are all working on Qcing older CTD data and have documented clear QC steps used. GO-SHIP are very interested in the work.

Crowd sourcing works for small, known crowds.

IQuOD should exploit the new Argo reference database for a QC method. We should entrain our emeritus professors to enhance our tasks. Look for small pockets of funding to help.

CCHDO and IQuOD have similar missions and are strongly aligned. Need to review the task teams. Where does CCHDO fit? Steve can help with the uncertainty group with accessing help for feedback.

Questions and discussion

Molly & Catia: Where does the funding come from? NSF, another grant, SeaView. CCHDO make specialised datasets for some of the funding.

Alison: Emeritus group – this is a worry because it is another group of people coming up with their own QC. Does the work Jim & co doing fit? They are looking at a small amount of data that is Argo-based and they are entraining others to look at the BGC data. We need to entrain them in IQuOD. Flagging systems should be aligned between the groups.

Catia: The focus is on historical data for IQuOD, but the Jim et al work is modern data. But we should keep feeding the information back to other groups. Learn lessons from the historical data about what metadata is required for the future.

3.5 Crowd sourcing discussion – Steve, Tim and Alison

Which tasks can we crowd-source? How do we define crowd? Crowd sourcing gives us free help and cheap processing. Which tasks are suited to non-experts? Visual QC: we could have non-experts look at the data, then get the experts to confirm. How do we figure out the workflow?

Tim: www.oldweather.org is a data digitisation project. Each piece is digitised, then compared. Those that don't match go out again. They are reluctant to work with data that doesn't have a story. That is what attracts the crowd. They are open to us being part of the site, but we need a story. They are associated with ACRE who is also getting old records digitised and another group – Reclaim group.

Tom: is there a deliberate effort to contact European countries that have shipping activities going back? This is like the Reclaim project. Norway has a lot of data in file cabinets. **Tom** might be able to encourage them to give it up for sharing with NCEI. **Alison** suggested a contact (Are Olson) who is already involved with Carina.

Can we come up with a web of contacts for data recovery?

Catia suggests offering a prize of a trip to sea on a research voyage to the crowd. This is a good idea. Also we can close the loop and bring the data back into the expert QC. Teachers are a good resource for inspiring students to do these things. Competition for high school classes?

Can we use the crowd-sourcing to give us information on the patterns that people are looking at? Yes, the groups already have methods of getting this out. Already have these inbuilt systems.

Ann: can we look at the data that is good-flagged and assess how many auto QC effectiveness?

Steve: Can we tie our data to the climate discussion, as our story? Maybe the message will be different for different cultures.

Tom: how to explain what is 'bad' data – maybe re-phrase the question and ask people to look for patterns. Grouping data might be more science.

Zooniverse – build your own project in January in Texas. www.zooniverse.org

Summary, what can be crowd sourced:

1. Visual QC is a possibility – need a structure, advertise it – AMS, geological society. Small cost to initiate.
2. Digitisation of old data. Also 'hack-athon' style of digitisation.
3. Duplicate checks?
4. Messages – how can we get our message out? Crowd sourcing can bring out better external messaging. They will learn more about oceanography and getting them more interested in it.

Crowd Source Task Team: Steve, Ann, Alison, Janet, Tim, Tom, Catia, Bill Mills(?)

3.6 Expert QC task team: summary of activities – Ann Thresher

The expert QC task group has not done much yet, while waiting for a few things to happen with crowd-sourcing and machine learning. Need some Auto QC output to assist with an estimate of the size of the problem.

Catia: What is the upper limit of the visual QC. If we assume a number can we make some guesses about how long it will take.

Janet: Is there a timeline? Auto QC should have some data ready next year, crowd-sourcing should have some momentum, then we can make a start.

Alison: There are people in the room that can give information about what are common failures. We should start compiling the list of people who do QC or are experts. Then we have a list to start with.

Action: Everyone to email a contact to Ann.

Tom: we need to put together a package.

Tim: We should all just write down what we have done and what we have found – we can start putting the QC'd data into the WOD and therefore the IQuOD database. This would be a good start for the expert QC task team.

If we can identify the datasets that can be IQuOD datasets, then we can make them part of IQuOD.

Action for expert QC task team: Identify the QC'd datasets. Pass this information on in a nice list. How do we identify if data has been expert QCd?

Argo expert QC team mostly QC salinity, are these people useful for IQuOD? Maybe?

4 Session 4

Chair: Catia Domingues

Recorder: Steve Diggs

TUESDAY AFTERNOON

4.1 Quality control and duplicates removal for the Marine and Meteorological data from NMDIS/China – LIU Yulong

NDIMS Quality Control System and Software was presented and QC of temperature and salinity is performed. They have an Objective Analysis Method for QC. Data Processing is performed by NOOS-China on ocean stations, buoys, shore-based radar, Argo, etc.

Data Products from Fixed Station, Buoy Radar, Cruise obs, etc include: Temperature and Salinity; Currents; waves; Sea Level; sea ice; transparency, etc. They eliminate duplicates. Progress of TS data processing was shown for Argo, XBT and WOD. Future Work includes continuing to upgrade QC and TEST eliminate duplicate data methods

Questions and discussion

Molly: Why do you think that the WOD is not getting all of the Argo Data?

Molly: Are you only putting DM data, or also real-time (**Tim:** both)

Rebecca: Are the duplicate information being given back to Tim/NCEI?

Yulong: yes

Catia: are you willing to benchmark your QC as part of IQuOD?

Yulong: yes

Ann: Big difference between duplicates between data sets, and looking for duplicates in ONE dataset.

Yulong: We are using different methods depending on the dataset. NMDIS are the only ocean data centre in China.

4.2 Introduction to JODC – Takeharu Miyake

The Japan Oceanographic Data Center (JODC) was established in the Hydrographic Department, Maritime Safety Agency in 1965 in accordance with the resolution adopted by the Intergovernmental Oceanographic Commission (IOC) of UNESCO in 1961 as well as the reports of the Council for Marine Scientific Technology in 1963 and 1964. Since its establishment, JODC has been playing the role of an overall marine data bank of Japan through the uniform collection and management of the marine data obtained by various marine research institutes and organizations concerned in Japan and also been providing users with these data. In addition, JODC has been carrying out international services as the National Oceanographic Data Center of Japan under the framework of International Oceanographic Data and Information Exchange (IODE) promoted by IOC.

JODC started the internet data service as J-DOSS in 1995. This type of internet service was the first one among the NODCs. JODC constructed Web-GIS based system for managing the marine geospatial information as CeisNet, for measures with oil spill incident. JODC has a high technology obtained by data processing of oceanographic data in many years, like J-DOSS. Also JODC has experiences gained by offering the geospatial information, like CeisNet. So JODC will try to approach the new system to integrate oceanographic data and human related information. This is called Marine Cadastre. To construct and operate the Marine Cadastre, our experiences and technologies have been utilized until now.

Questions and discussion

Tim: You incorporate data from the Japanese Navy (in JODC database)?

Answer: yes ... (over to Kizu-san)

Shoichi: they are published, therefore yes (qualified his answer)

Toru: not really Japanese Navy

Tim: apologies, wrong name...

4.3 Progress of Japanese data rescue – Toru Suzuki

The Historical XBT Profile Recovery and Rescue Project in Japan.

We collected about 3,300 XBT strip charts from T-6 probe manufactured by Tsurumi-Seiki Co. Ltd. (TSK) in Japan Meteorologica Agency and Japan Coast Guard. In addition, we discovered 700 XBT strip charts which were not stored in JODC database. All profiles were scanned as TIFF file, and traced using Adobe Illustrator and saved as DXF file, and finally converted to temperature data as a function of elapsed time by affine transformation. These data will be compared with

existing standard depth data by visual reading and the differences will be estimated, and also provided to IQuOD in order to be processed by automatic QC and manual/expert QC.

Questions and discussion

Tim: Have you made a comparison of the traces with existing data in WOD? These are the full trace?

Toru: yes

Tim: They would be preferable, you got these off strip charts (Toru:yes), then you match with std level data if the digitization went well?

Tim: You should replace the standard level data with the full resolution trace.

Tom: in the reprocessing of the XBT data, shouldn't you keep the original trace in the archive?

Tim: The original traces are preserved at JODC, but in an active DB, we're only going to keep one copy. The original fall rate the data was digitised from will be kept.

Bec: you have software to digitize

Toru: yes, I use Illustrator

4.4 Present Trends in IOC/IODE – Prof. Yutaka Michida

Prof. Yutaka presented about IOC, established in 1960 under UNESCO to promote international cooperation and coordinate programs. The current structure of IOC was shown, 148 member states. High level objectives include: Healthy Ocean Ecosystems, Early warning, Resiliency to Climate Change, Enhanced Knowledge of Emerging Issues, Emerging Needs in Ocean Issues. IODE was established in 1961 (C. Chandler and Y. Michida : co-chairs 2015-2017), currently there are ~80 member countries.

During the 23rd session of IODE in Brugge (Belgium) , IODE adopted 4 decisions including: restructuring of IODE; revise the strategic plan for IODE; create IOC communication and outreach program. IODE also established Ocean Expert project

Suggestions to IQuOD: Interlinked relationship with other on-going activities closely related to IQuOD (GODAR, WOD, GTSP) be well-established. Progress Reports to IODE Committee on a regular basis for exchange of views.

Questions and discussion

Steve: how often should IQuOD report to IODE?

Yutaka: twice a year

Tom: the ferrybox is a very powerful tool for observations on a regular basis. Is IODE an operating agency, how do we solve problems we have?

Yutaka: IODE is not in a position to coordinate a solution. GOOS also has a ferrybox problem.

Thierry: JCOMM has a data management system for Ferrybox, but GOSUD is a DM repository – a big improvement would be to have more scientists involved – a science team could drive the issues.

Tom: more scientists is all well and good. But Ferrybox is a demanding instrument, Pis don't have time to deal with them. Governments should be involved. Maybe just scientific input, but they shouldn't run the programs.

Yutaka: Agreed. There are two different roles (one for scientists / but there is an operational aspect as well). Scientists can make suggestions – that's their role.

Janet: IODE promotes freedom of data, etc. Do you have any sense of how you're going to enforce/encourage that?

Yutaka: IODE can emphasize importance, but the community should promote this.

4.5 On the use of Climatological Convex Hulls for Detecting Outliers – TVS Uday Bhaskar

A new method of identifying erroneous profile data is discussed. Any parameter like temperature and salinity when plotted against latitude, longitude for a specific depth is plotted shows a particular pattern. This pattern can be used build polygons which can be used to perform QC. An 'n' sided polygon (convex hull) with least area encompassing all the points from climatology is constructed based on the Jarvis March algorithm. The periphery points from the clusters formed while plotting the parameter (e.g.: temperature, salinity) against longitude and latitudes is used for building the polygons. Subsequently, Point-In-Polygon (PIP) principle is used to classify the data as in or out of the polygon. It is observed that all possible outlier associated with the data can be identified using this method.

Questions and discussion

Viktor: I've seen a picture of these polygons, but is the noise simply due to the lack of data? Question: is the method robust enough for the task? Distributions of salinities vs. latitude for different oceans. This was coded up for the Indian Ocean only but can be expanded into other ocean basins.

Bec: Is this going to be coded into the IQuOD project?

Uday: I coded into the Indian Ocean only, I can see the potential for this to be another useful tool.

Ann: Is this coded for salinity – can it be used for temperature.

Uday: Yes, it can be used for temperature and he will look at doing a test.

Gopalakrishna: can we use this for Argo Salinities?

Uday: yes, all salinities.

4.6 Progress on the auto QC benchmarking – Simon Good

The AutoQC project aims to benchmark the automatic quality control checks around the world in order to find an optimum set that can be used to find the set of profiles that we are confident contain only 'good' data, which can be released without further checking, and the set that contains some or all 'bad' data, which will be fed into augmented quality control measures. Our methodology is to code free, open source versions of the quality control checks in Python. The code is stored on GitHub (<https://github.com/IQuOD>) and there is wrapper code that runs the quality control on profiles where the quality of the data is known with a decent degree of confidence and hence can be used to benchmark the performance of the tests. The quality control software is free to use by anyone and this, along with the WOD ASCII data reader that was also developed, should be viewed as IQuOD products.

Since the last workshop a lot of work has gone into adding more quality control checks to the repository. CSIRO and ICDC checks are now included plus 16 checks that have been added through calling the CoTeDe quality control software suite (<https://github.com/castelao/CoTeDe>). In total there are now 50 checks (note that some of

these are variants of the same check, but this allows the relative performance of each to be assessed). Infrastructure improvements have been made; in particular a PostgreSQL database is now used for storing results to avoid memory issues and a Docker image of the AutoQC system is available, which makes it easy to transfer the software between systems. The focus is now turning to running the system on the test datasets that were chosen and finding the optimum set of QC checks, but new QC checks can still be added to the repository and would be very welcome.

Questions and discussion

Viktor: Simon, great job – a big step forward! Which test datasets are at your disposal for these procedures?

Simon: Argo DM data, North Sea Data (from: Gouretski), WOCE dataset, Quota and seal tag.

Viktor: My suggestion is to make use of the highest quality dataset from CCHDO.

Simon: How do we get hold of the data?

Steve: Viktor and Steve are talking already. Tim says that the CCHDO data is already in the WOD, we already have this available in the WOD format so it can be directly downloaded from WOD. This would be a better route. This can be done when Tim gets back to NCEI. It would be useful for the dataset to be delivered in the next month or so.

Ann: WOD has CSIRO XBT data that can be extracted from the WOD for Simon.

Upper 4m removal – might not be a good idea, but up for discussion. Automatic removal of wire breaks is an easy and quick thing to do. The order of the tests run is important in that case.

Simon: At the moment its' set up that each of the tests are completely independent. It's possible to do what you're suggesting, but we'd like to keep each test independent, I think it should be possible to clear-up any of those issues in post-processing.

Ann: it may fail a wire-break test ... you want an expert to look at things **other** than wire-breaks. Some of these tests should be used as pre-screening. Get rid of the obvious problems so they are not getting to the expert qc stage.

Simon: ok, yes – I see what you mean.... We can break down the auto QC tests further.

Janet: Question – like Ann, in a general sense .. will you make recommendations as to whether all of the tests are useful for all things, or something more specific?

Simon: potentially, it depends on how consistent the results are ... Lot's of potential

Bec: we have a vacation student work on IQuOD, how about we point him in your direction to work on this project?

Simon, yes, ok. Have him contact Bill Mills.

Alison: we have lot of people in the room interested in benchmarking ... do you have a deadline for benchmarking?

Simon: hoping to start anytime, really.

Catia: Francis from AOML can add his auto QC tests, in addition there's JODC, Toru as a contact? And Yulong Liu from China, Uday from India? Also, Christine / Thierry from Coriolis?

Thierry: the OA we use is different because it uses a climatology. Might be useful later. Argo tests are already coded in.

Catia: What about the IMOS data center? No, they don't have QC tests.

Marty: we do have a set of test routines for mooring data, not sure

Catia: Y. Michia from IODE ... Could we take advantage and have IODE "market" this and gather interest? OK (Y. Michida)

Gustavo: Now that you have Auto QC procedures, would it make sense to create a set of synthetic temp profiles where we introduce spikes/gradients, etc so we know which one if good

/ bad ... we don't need 100K of them , we can make an assessment about how good each of these are?

Simon: that would be interesting/fantastic

Rachel: Could we use the synthetic data made by Chris Roberts that match ENACT data

Simon: sure ... it would be interesting to see if they're flagging good data. To see if there are false positives. Are these profiles good profiles?

Rachel: they are all good profile, but you could introduce a spike...

Marty: basic questions ... what do you set the thresholds to?

Simon: We are using whatever they were set at originally, we are not choosing. We're not trying to tune it to, would be possible within the framework. We're just trying to work with the tests as they're defined.

Tim: Action item 12: What does IQuOD want out of this? (Creative Commons). If it's served from a US government website, it cannot be copyrighted. Can't license WOD, doesn't seem like a good idea.

Bec: Action item 4: I did send some examples to Bil, Gui and others (XBT), but that's about it.

NEW TOPIC

Ann: (subject – expert QC). It's really 2-3 groups. She suggested to break up the group into

1. Expert QC
2. Auto QC
3. Assessment Group (end of the pipeline)

Alison: crowd-sourcing group is still conceptual

Ann: not talking about the crowd-source group per se, could be people doing the QC or machine learning?

Gustavo: what does Argo do to handle it? It is done by the DACs and is done by float. Checks are performed on salinity.

Viktor: Should the assessment part be done by people who are not here? How are we going to find the right people for the job? The right way to do it is to increase the linkages between the groups.

Tim: let's start marking all the profiles that have been expertly QC'd, put aside all the data that has not be QCd. Make a slow start on the expert QC.

Matt: originally we thought it would take 5 years, but, we really don't know yet.

Gui: Machine learning technique is operational and this can reduce the amount of visual qc that will be needed. Gui to talk with Ann later.

5 Session 5

Chair: Janet Sprintall

Recorder: Rebecca Cowley

WEDNESDAY MORNING

5.1 GOOS update and IQuOD in the context of Framework for Ocean Observing (FOO) – Toshio Suga

We need sustained observations for many applications, a framework was developed at Ocean Obs, '09. Have defined essential ocean variables as part of GOOS as an expansion of the essential climate variables. Incorporates societal issues and

observational group issues. EOVS (Essential Ocean Variables) use a readiness scheme – IQuOD is in the ‘mature’ observations on the readiness scale. GOOS has been revitalised and now has three scientific oversight groups. These three panels work together to articulate the requirements and targets of global ocean observations for climate through GCOS IP 2016. IQuOD fits into the action items from the GCOS IP. IQuOD has been contributing to the FOO.

Questions and discussion

Catia: Is the implementation plan available? Yes, on the web. A final version will be available in a couple of weeks. IQuOD should mention these actions when we need to express the value of IQuOD to the community.

Tom: is Ocean Obs '19 in the works? Yes, probably to be held in Honolulu.

Mauro: What is the link between the regional office and GOOS? The regional alliance is the link (GRA), but there are little resources available and regional groups are relied on to have a forum every few years.

Alison: Interesting that Physics, biology and chemistry as oversight groups are separate, rely on each other. Toshio says yes, there are cross-issues and the new IP describes how these links work between the groups.

5.2 Task team review and Action items

5.2.1 GDAC Task Team

The short term goal is to get out the v0.1. The mechanism is there, ready to go. Tim needs uncertainties and intelligent metadata information. Before December 15 if the first version is to come out at the end of the year.

What about duplicates? Tim does not expect that these will be removed by then.

This will take more time. Aim for next iteration. The formats task team has just formed, so at this stage, we will stay with the WOD ascii format and the netcdf that is available through WOD.

Lower level things include the set up of the WOD select page. Tim needs input on setup. Also, we will need to make the announcement of the first release.

There will be a static copy. **ACTION: Thierry can serve this through CORIOLIS.**

Application of XBT biases: do we apply a correction to IQuOD? Catia would like to see this still as a choice for the user, with information about the use of the data – eg climate studies need a correction. Gustavo says we need to apply a correction as the ‘best’ recommendation. The WOD still posts the selection of corrections. Do we do the same for IQuOD? What do other groups do? Some have one copy of the best, some have different versions available.

Tom and Gustavo say we should not confuse the community. We should keep improving our algorithms and output updates as a community.

Can we add the adjusted fields in? Tim will work on this, but can’t do that in time.

5.2.2 AutoQC Task Team

Thierry: IFREMER can perform OA on the v0.1 and provide feedback to IQuOD.

Should this be part of the QC flags for V0.1? Or is this just feedback at this stage?

Should we be including autoQC flags? WOD flags should be served at the moment. If we flag data with Thierry’s results, we can include that as an IQuOD flag.

Are we ready to put out the v0.1 product? The SCOR proposal states our goals.

5.2.3 Expert QC and Duplicates task teams

We have an action item to get a list of experts together. Duplicate testing needs to continue at CSIRO. Can Yulong and Christine's tests help? Maybe, different process.

5.2.4 New task teams

Crowd Source Task Team: Steve, Ann, Alison, Janet, Tim, Tom, Catia, Bill Mills(?)

Formats Task Team: Marty, Christine,

Funding task team: Steve, Matt, Catia, Alison, Janet, Bec

5.2.5 Other discussion

A machine learning approach to look for false good data has been developed, this can be talked about with Bec, Ann, Catia. Gui has a website that we can start with and he will revive it.

Alison suggests that we take some examples of issues to the experts then ask them for their input so it can be incorporated into the machine learning.

Separating the AQC tests and assessing them is the best way to perform the test.

Important Issues:

Thierry: Do you have a plan to provide information back to data providers?

Catia: it has not been done, but could be.

5.2.6 Action items from previous meeting

Action	Who	Importance	Date	Cost / Effort (FTE)
Make announcement of first IQuOD product. How, Where, When? Eg: BAMS, EOS, Clinglist, GODAE Ocean-view, IAPSO-IUGG, via SCOR/IODE?	Catia and Matt	High	December to March (when ready)	
Request that the XBT Science community provide historical metadata for ships that have deployed XBTs: transect name, launch height, probe type(?), recorder type, serial number, other information that is retrievable. The information can be put into IQuOD as intelligent metadata, or specific metadata if available for particular voyages.	Bec, Gustavo, Janet	Medium	during XBT Science Meeting, Tokyo, Japan	

Action	Who	Importance	Date	Cost / Effort (FTE)
Duplicate-checking code included on Git repository? Chinese duplicate check code too?	Ann, Ed, Yulong, Thierry, Bill, Bec	Medium	early 2017	
Uncertainty table first version finalised and provided to Tim <ul style="list-style-type: none"> Develop CTD and XBT values further (also look at UKMO values, CORA values, others) Seek feedback from IQuOD (table readable). Seek information from modellers Seek information from the Emeritus group 	Uncertainty task team: Bec, Viktor, John G, Rachel, Tim, more volunteers please	High	December	
Request uncertainty information from known groups (eg Glider group, Argo) for modern data streams	Uncertainty task team	Medium	ongoing	
Develop a human-readable uncertainty table/database/web page and promote it, asking for feedback from community.	Uncertainty task team	Medium	High priority – December 2016	
Metadata table finalised and provided to Tim, feedback on TSK information from Shoichi and Toru	Metadata task team	High	December 2016	
Set a date for next meeting and invite Chinese attendees early.	Steering Team?	High	Now	
GDAC to produce IQuOD v0.1.	GDAC task team – Tim	High	December	
Set up of the WOD select page wording for IQuOD	GDAC task team – Tim with Catia and Matt	High	December	
Give the static v0.1 to Thierry for serving at Copernicus. Other places? Assign a DOI.	GDAC task team – Tim, Thierry, Catia	High	December	
Seek feedback from the XBT Science team for choice of correction for XBTs	XBT Science group back to Tim	High	This week	

Action	Who	Importance	Date	Cost / Effort (FTE)
Corrections for MBTs	Viktor	Medium	December	
Choose correction for the MBTs	Viktor to Tim	High	December	
Expert QC'd datasets list to be made and then flagged in the WOD. See section 3.6.	Expert Data QC team – Ann, Steve Diggs, Jim Swift, Tim, others?	Medium	2017	
Hydrobase data needs to be put into WOD if possible.	Tim, Alison, Ruth Curry, Viktor	Low	2017	
Ifremer can perform OA on the v0.1 and provide feedback to IQuOD. Include in v0.1	Thierry, Christine, Auto QC task team	High	December	
Include additional tests from other organisations & known historical sets into auto QC benchmarking tests: eg WOCE, GLODAPv2, others?	Auto QC task team, Uday, Yulong, ICDC, AOML, JODC, GLODAP, Copernicus, BODC (Catia), IODE	Medium	2017	
Find optimum QC set	AutoQC team	high	2017	
What do the flags look like for IQuOD? What can we use/learn from Argo experience? IODE flags?	AutoQC team, Expert QC team, formats team? TT leaders		2017	
Compile a list of experts – IODE list, Emeritus group. See section 3.6.	Ann	medium	2017	
Create Synthetic profiles for helping with AQC tests	Rachel	medium	2017	
Report to GODAE OceanView Science Team Meeting , Kochi, India	Mauro, Matt	high	November	
Interact with international GODAE OceanView Data Assimilation task team to help with expert QC	Mauro to Ann	medium	2017	
Have a discussion about Gui's ideas	Gui, Ann, Catia,	high	December	

Action	Who	Importance	Date	Cost / Effort (FTE)
on reducing the load on expert QC. Machine learning	Bec, Simon, Bill, Alison, etc			
Look at the options for tools (e.g. GUI etc). that are useful for QC for experts	Expert QC group.	Low	2017	
Produce draft document based on Argo formats to determine their suitability for IQuOD	Formats TT	medium	2017	
Develop more capacity building knowledge transfer things	Catia	Medium	2017	
Work towards achieving funding for IQuOD. New TT. Have a webex to start.	Steve, Bec, Alison, Matt, Catia, Janet	High	October, 2016	2 hours
Compare previous minutes together to assess missing items, progress and successes. Write the report up.	Bec	Medium	October, 2016	5 hours
Gustavo will contact David Legler to recommend the participation of Tim Boyer at the underwater glider meeting in Stennis (see section 2.3)	Gustavo	Medium	?	
Supply the XBT metadata list developed by JCOMMOPS	Bec	Low	Next meeting	

5.3 Finishing tasks and wrap up

Need to report twice yearly to SCOR and IODE.

Next meeting to link with IAPSO meeting in August/September in Cape Town/South Africa.

Catia has some small amount of funding for collaboration but needs to be with EU partner.