IQuOD

International Quality-Controlled Ocean Database

3rd Annual Workshop Report

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Editor

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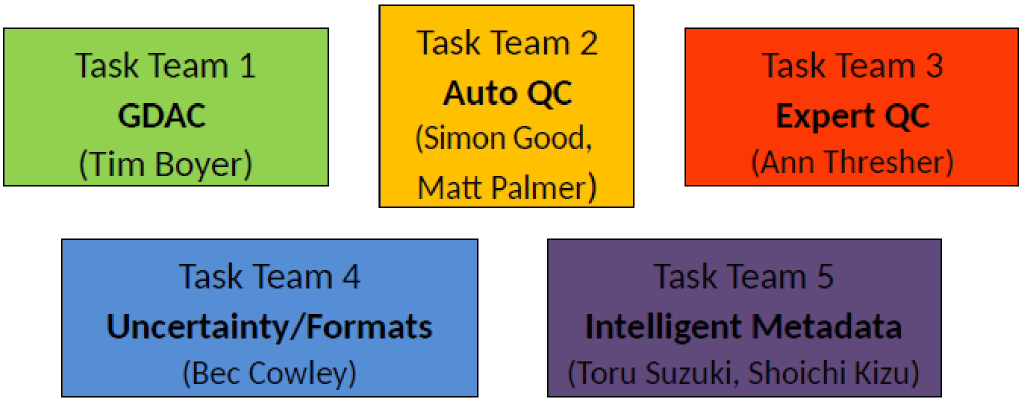
1 Session 1: Overview and Uncertainty/Metadata task teams

Chair: Steve Diggs, Notetaker: Ann Thresher

1.1 Overview of IQuOD activities, Matt Palmer, Catia Domingues

The overarching goal of the IQuOD initiative is to create the most complete, consistent and high quality ocean subsurface temperature database with intelligent metadata and uncertainty estimates for each observation. IQuOD will develop international best practice approaches to data quality control and all data and code will be made freely available to the international research community. The approach will be developed focussing on temperature, but the aim is to provide a template so that the database can be extended into other variables later, such as salinity and oxygen.

IQuOD is organised in to a number of different Task Teams, as shown in the schematic below:



The basic format of the meeting was for each of the groups above to report back on progress and plans – as detailed in the following sections of this report. The focus of the 3rd IQuOD workshop was on the delivery of a first data product. Rather than being a release of a v1.0 IQuOD database, this will instead be an IQuOD "flavour" of WOD – with intelligent metadata and uncertainty information available as an optional data stream.

The outcomes of the group discussions and proposed activities and timeframes to delivering this first data product are reported in section 4.

1.2 IQuOD/GAIC meeting summary

The GAIC (GO-SHIP/Argo/International Ocean Carbon Coordination Project (IOCCP)) conference took place in Galway, Ireland (September 14-18, 2015). Bringing together participants from each of the programs with a focus changes of physical, biogeochemical and biological parameters in the ocean interior. The presentations and discussions spanned a large variety of spatial and temporal scales seeking to respond to the following questions.

- What aspects of the climate system are presently addressed by these programs?
- What aspects should be addressed in the future?
- What are the science synergies among these programs
- What gaps exist in sustained observations?
- What are the roles of emerging technologies

Many of the presentations included research based on multiple platform synthesis. IQuOD should be a part of this conversation and the IQuOD effort could be inform the efforts of the GO-SHIP, Argo and IOCCP communities.

1.3 Uncertainties/formats task team overview. Rebecca Cowley

A meeting of the Uncertainties/Formats task team was held on the 2nd December and Rebecca summarised the discussion, and highlighted some areas for further discussion.

1.3.1 Uncertainties

Goal: Add uncertainties to every temperature, depth/pressure and position data point in IQuOD dataset.

Additional goal: collect salinity uncertainty information if possible.

1. Provide a definition of uncertainty for the IQuOD purposes

    a. Use the GUM (Guide to Uncertainty in Measurement) – will have to derive an uncertainty from published accuracy values, experience, observations (Type B uncertainty)

2. Consider the time available to us to make uncertainty information available for IQuOD. What is realistic and achievable?

What we need to do:

1. Construct the uncertainty table, incorporate information from other groups (John Gould, Bec, Tim, Viktor)

2. Develop a template for feedback from those who collected data – table or document of some sort (John, Bec, Viktor).

3. Expand the experts table (eg Fabien, Loic). Gliders, seal data, etc. (Viktor, Alexander, Bec, Alison, South African – Seb Swart?)

4. Approach experts with a template or basic information and ask for feedback.

5. Produce a journal paper on uncertainties and how they are applied to IQuOD.

1.3.2 Formats.

What we need to do:

1. Define a format for our files (based on Argo, IMOS, GTSPP?). How the data is stored/served could have a big impact on the choice. NCEI can serve data in a format, but can't archive it in individual netcdf files. Will need further discussion with Tim/NCEI. Create the documentation for the format.

2. Decide on QC flag standards – use an existing standard Argo/GTSPP. Two level scheme – what tests were failed in AutoQC. This decision will be dependent upon QC tests and will need more interaction with AutoQC and ManualQC groups.

1.4 Intelligent metadata task team overview and progress. Toru Suzuki

Dr. Toru Suzuki, leader of intelligent metadata task team, presented a draft plan of metadata items and code tables for XBT and its format with quality control flags (http://www.mirc.jha.jp/forum/iquod/metadata/xbt.html). He explained that almost codes were referred by World Ocean Database (WOD) 2013 and WMO common codes using BATHY if available, and indicated that some items which were founded through XBT recover project by the Environment Research and Technology Development Fund of the Ministry of Environment, Japan, have not been coded yet. He also emphasized that quality control flags should be added to all metadata items such as confirmed by data originator/provider, estimated by data center or IQuOD, and unknown. Drs. Suzuki and Matthew Palmer led group meeting and they confirmed that launcher height is necessary information to identify XBT uncertainties so that it should be collected as possible as we can. Dr. Martine Kramp, GO-SHIP coordinator of JCOMMOPS/IOC-UNESCO, talked to identify that information of VOS.

1.5 Historical profile collection – Notes of caution. John Gould

John Gould gave an historical perspective on the errors and uncertainties in the quality of historical profile data.   He focused on the changes in instrumentation for profile collection and for navigation since the start of the 20th century.

In summary he concluded that in the red GPS era navigation was less than perfect and that often water depth was the best indictor of position. Metadata are often unavailable or inadequate and calibration and standards were below those of the present day.

In many cases the purpose of collection (where the operator is solely interested in detecting the position of fronts) may limit the effort expended in ensuring the quality of original data. In a similar way the competence of operators varies from lab to lab (but we know which were the best). This depends on the living memory of people involved in collecting the data. That living memory only goes back to the about the 1970s.

Amongst his conclusions were that priority should be to ensure that **present and future** data are of the best standard so that there is consistency/compatibility of data between observing programmes. This would avoid the situation where, 10 years from now, we have to re-assess today's observations.

1.6 Validating the oldest oceanographic subsurface temperature measurements (1860-1899). Viktor Gouretski

All oldest T-data from the WOD2013 are added by the digitized data from three prominent expeditions during the 1870s: Challenger, Tuscarora and Gazelle cruises.

The uncertainties of the data are estimated based on the data statistics and the available metadata. The validation of the data is done on the cruise by cruise basis.

Multiple WOD cruise identifiers were found to be linked to one and the same cruise and the respective corrections in cruise attribution (country, ship) have been done.

1.7 Progress assessing Japanese wartime surveys. Shoichi Kizu

The simultaneous hydrographic surveys made by Japanese Imperial Navy during WW2 provided plenty of thermal profile data in the western NP at that time. But little is known about their method and quality, so this talk tried to reveal the facts based on available literature and published data tables. The reported sampling depths is like standard-level ones for all profiles, but how they were attained is still unknown. A most plausible story is that they basically used wire-out and angle assuming some wire shape in the water, but it is also inferred that the situation varied from cast to cast.

1.8 IMOS autoQC on mooring and CTD data. Guillaume Galibert

The IMOS Toolbox aims to convert oceanographic time series and profile data files into pre-processed and quality controlled (QC) IMOS compliant NetCDF files. It is written in MATLAB and Java with a graphical user interface and was developed by the Australian National Mooring Network supported through the Integrated Marine Observing System (IMOS).

This toolbox can read data files from a wide range of sensors and platforms including CTDs (Seabird, FSI, RBR), pressure and temperature loggers (Aquatec, RBR), multi-sensor instruments (WET Labs WQM, YSI 6 series) and ADCPs (Teledyne RDI, Nortek). Metadata from a deployment database can also be critically integrated into these data files, following the IMOS NetCDF conventions (https://raw.githubusercontent.com/wiki/aodn/imos-toolbox/documents/IMOS_NetCDF_Conventions_v1.4.pdf). A set of automated and manual QC tests is implemented so that consistent QC'd data will be available through the IMOS portal (https://imos.aodn.org.au/imos123/).

This IMOS toolbox is freely available as a standalone executable and with its source code and documentation on GitHub (https://github.com/aodn/imos-toolbox).

1.9 Production of high quality CTD data. Marcela Charo

Production of high quality CTD data CTD sensors calibration is crucial important for obtaining high-quality data, especially when factory CTD sensor calibrations are not always easy to carry out or when the oceanographic equipment on board (conductor cable, winches, etc.) is not suitably maintained.

Laboratory and field calibrations using water samples and manual quality check are described. Bottle data is complementary information of the water column for analysis of vertical changes, particularly in regions under strong vertical stratification (e.g. thermocline). Also water samples allow a preliminary check of CTD data in real time and detect any malfunction of sensors.

1.10 Implementing uncertainty + I-metadata for IQuOD V1.0. Tim Boyer

Both uncertainties and intelligent metadata will be implemented through criteria lists maintained by the IQuOD group. The uncertainty list will contain a given uncertainty (e.g. 0.3degC) and a set of criteria which, when met, will result in the assignment of the the given uncertainty in the IQuOD dataset. The list will be hierarchical, so for instance an entry with criteria instrument=MBT with an assigned uncertainty of 0.3degC will be superceded if a subsequent entry in the list has instrument=MBT+institute=Scripps+start_year=1953+end_year=1965 with assigned uncertainty 0.15degC where the given criteria are met. In the same vein, intelligent metadata will give a variable and given value (e.g. instrument,TSK T4) and a set of criteria under which the intelligent metadata will be applied (e.g. instrument=XBT type unknown+country=Japan+maximum_depth=550 m). The intelligent metadata list will be hierarchical same as the uncertainty list. The lists will be used to populate the IQuOD dataset and the lists will be stored with each subsequent release of IQuOD data.

2 Session 2. Auto and Expert QC task Teams

Chair: Toru Suzuki, Notetaker: Matt Palmer

2.1 Duplicate task team progress. Ann Thresher, Ed King

Any datasets that result from merging of data from different sources is likely to contain duplicate observations that will need to be identified and removed. This is complicated by occasional errors in metadata for time and space, making a comparison of profiles within a small region incomplete. But comparing every profile within the entire database requires more computing power than we have.

The first step in identifying duplicates was to calculate the sum of the depths, the sum of the temperatures and the total number of points for each profile in the WOD databases for CTD, XBT, OSD and MBTs. Sorting by the number of points, the sum of the depths and the sum of the temperatures, in that order, let us compare the actual profiles for 'matches'. If the difference between the individual depths and temperatures was close to 0, then we presume these are true duplicate copies of a single profile.

2.2 Discussion – duplicate detection results and way forward. Ann Thresher, Ed King

A methodology for identifying duplicate profiles within the WOD netCDF profile database has been developed and trialed. The initial version uses only the profile data points (no metadata) to identify duplicates. Unphysical data values are rejected from each profile and then the sums of each variable (Depth, Temperature and, where present, Salinity) are computed and recorded together with the number of points. These metrics are used as profile signatures to rapidly identify potential duplicates. A second step compares candidate profiles point by point to eliminate non-duplicates. This method, using just depth and temperature, has identified approximately half a million pairs within the 8.5 million WOD profile collection. Having demonstrated this successful proof-of-concept implementation, the method will be refined to better exploit the profile metadata, QC flags and the salinity profiles (where they are available). We plan also to extend the method to find sub-sampled or truncated profiles, and also to utilize spatial and temporal locality to identify potential duplicates. The aim is to provide an accurate list of duplicates to WOD and, where possible, with an indication of which profile is more likely to be genuine.

2.3 Python infrastructure for AutoQC. Bill Mills

A pythonic infrastructure 'AutoQC' for facilitating automatic quality control of subsurface ocean data has been developed for the IQuOD collaboration. AutoQC is developed to be highly modular, supporting additional QC tests with no infrastructural modification, and highly parallel, currently able to evaluate 14 QC checks across 150k profiles from the quota collection in about half an hour on the Amazon Web Services cloud, for a cost of under $2 USD. Future work includes expanding the set of QC checks implemented, constructing an unbiased underlying dataset for developing IQuOD's automatic quality control strategy, and exploring machine learning techniques for optimizing this procedure.

2.4 Examples and implications of the current AutoQC results. Simon Good

The current IQuOD AutoQC system is able to find just under 55% of profiles containing bad data (‘bad profiles’) at a cost of flagging just under 10% of profiles that contain no bad data (‘good profiles’), based on the full QuOTA dataset. We need to find a way to increase the percentage of bad profiles that are being identified. One option would be to (de)tune some of the existing tests to catch more profiles. This was investigated for the EN background check, which is the most effective test at catching bad profiles. It was shown that by tuning one of the parameters used in the test it was possible to catch an extra ~5% of bad profiles at the cost of slightly increasing the rejection of good profiles. Beyond that point the test started to flag large quantities of good profiles. This raises the question – what are the characteristics of the other bad profiles that make them so difficult to find?

There are other combinations of checks that could be of immediate interest to IQuOD. These are ones that flag bad profiles with very low rates of flagging good profiles. For example, results indicate that it is possible to find ~5% of bad profiles without catching any good profiles. It is also possible to find about 30% of the bad profiles with a very low rate of catching good profiles. These are relevant to the manual QC team as, for manual QC, it is important that QC operators are not asked to manually inspect many good profiles. Therefore, although we don't yet have a complete picture of the number of good and bad profiles that will be caught by the system, it would be possible to begin feeding profiles to the manual QC process if this is required.

2.5 Auto QC of CTD data using CoTeDe and Tools for visualizing and validating Auto QC. Gui Castelao

CoTeDe (http://cotede.castelao.net) is an Open Source Python package to quality control (QC) hydrographic data such as temperature and salinity. It was designed to attend individual scientists as well as operational systems with large database, reading the inputs from different formats and types of sensors. To achieve that, CoTeDe is highly customizable, allowing the user to compose the desired set of tests, as well as the specific parameters of each test. Otherwise there are preset QC procedures conforming with GTSPP, EuroGOOS and ARGO recommendations. It is also implemented innovating approaches to QC like the Fuzzy Logic (Timms 2011, Morello 2014) and Anomaly Detection (Castelão 2015). Anomaly detection overcomes the limitations of other machine learning techniques by identifying bad data as anomalous behavior. A multi-dimensional classification criteria allows to distinguish consistent measurements of extreme events from spurious data. On preliminary results the anomaly detection properly identified 4 times more false positives than the traditional approach. More details and examples of use are available in the official documentation.

2.6 2nd level Auto QC GLODAPv2. Alex Kozyr

http://www.imber.info/index.php/News/Newsletters/Issue-n-27-September-2014#toc_3_12.

The Toolbox software looks for stations that are in the same area (the definition of "same area" is a variable and has to be set (normally to 2° of latitude, i.e. ~200 km) but can be changed based on knowledge of horizontal gradients in the area).

The software compares the interpolated profile from each station in cruise A to each interpolated profile from cruise B within the maximum distance for a valid crossover, and a difference profile is calculated for each such pair.

This process is repeated for each station in cruise A and the crossover offset and its standard deviation are calculated as the weighted mean and standard deviation of the difference profiles of each crossover pair (i.e., cruises A and B).

The software performs this process for all cruises in the reference data base and displays the offsets in one figure per cruise pair.

The software performs summary of all biases found for one cruise vs. all cruise in the reference data base

For the GLODAPv2 synthesis work GLODAPv1, CARINA and PACIFICA used as reference database

2.7 Automated QC of temperature profiles implemented at Integrated Climate Data Center and Using global statistics to evaluate quality control – comparison of ICDC and best AutoQC as of December 2015. Viktor Gouretski and Simon Good

The AutoQC procedure developed in ICDC is described in detail, with the examples of the distinct quality check performance. AQC results for the global hydrographic data set (WOD13) are compared for different instrumentation types, demonstrating a quite different percentages of potentially bad observations among these data subsets. The CTD, OSD, and PFL instrument types are characterized by the lower percentage of the flagged observations/profiles compared to the other instrument types.

Comparison between the ICDC AQC and the actual IQuOD AQC

Both AutoQC systems have been applied to the same WOD global temperature profile dataset. The preliminary statistics characterizing the degree of the overlapping between the observations flagged by the two procedures are presented, showing on general a rather low degree of the overlapping. The course for these differences is still to be explained through the in depth comparison of the AutoQC results.

3 Session 3. Expert QC and GDAC Task Teams

Chair: Alison Macdonald. Notetaker: Bec Cowley

3.1 Metadata validation with the IOOS compliance checker. Marty Hidas

The IOOS Compliance Checker is a command-line tool for validating data files against metadata standards. It is an open-source project developed by the US IOOS program (see https://github.com/ioos/compliance-checker), written in Python. Checks for the Climate and Forecasting (CF 1.6) conventions, and the Attribute Convention for Data Discovery (ACDD 1.1) are implemented in the core project. Additional check suites can be added as plug-ins. Currently the checker can read NetCDF files (locally, or remotely via OPeNDAP), and Sensor Observation Services (SOS). It could be adapted to work with other data formats.

At IMOS, the checker is being incorporated into automated data "pipelines", that receive files from data providers, apply processing and compliance checks, make compliant files accessible to the public, and send feedback to the providers about any files that failed the checks. For IQuOD, this tool could potentially be adapted to

* Find gaps or inconsistencies in the input data and metadata;

* Ensure that the output data products meet required standards; or

* Apply a similar framework for automated QC checks.

3.2 Creating a toolbox for validating operational forecast data in MATLAB. Simon Jandt

In the framework of the MyOcean projects and the Copernicus Marine Environmental Service, the Baltic monitoring and forecasting group provides daily a 60h-forecast products for physical and biological parameters. To be able to control the quality of the product, we developed a toolbox to validate these products against observations. The motivation of the development of such a toolbox was to be able to make the validation process easier and furthermore, to be unbound to a certain number of datasets or a certain format of data. So, this toolbox can also be applied for other validation purposes like e.g. quality control of observations.

The structure of the toolbox is structured in modules, one of those contains quality control functions for observations. The implementation of new quality control schemes is an ongoing task. Quality control schemes, adapted from the development in IQuOD, can improve the abilities of the toolbox.

3.3 IQuOD Data Flow. Tim Boyer

The IQuOD data flow is likened to a rivers components:

inflow - raw data (not yet quality controlled by IQuOD manual procedures) will be obtained from the World Ocean Database (WOD) by each manual quality control (qc) group. Quality control flags (and possibly data corrections) will be applied by the groups and the data, now IQuOD data, uploaded back to the WOD. Eventually, as originators adopt IQuOD qc techniques, the originators will provide their data, IQuOD data, directly to the WOD. Auxilary sources, such as Hydrobase qc will also be uploaded. WOD unique cast identifier will be used to keep track of each cast in IQuOD.

outflow - the WODselect system will contain all IQuOD data (a subset of the WOD) and will serve out user requests with IQuOD quality control flags, metadata, and uncertainties. IQuOD data will be distinguished from other WOD data by the addition of the uncertainties (along with identifying metadata specific to IQuOD including intelligent metadata). Full sets of IQuOD data will also be available at NCEI (National Center for Environmental Information, United States). The data will be served in WOD native ASCII, a comma-separated form, and in netCDF. The netCDF form will be a ragged array form to minimize space requirements.

confluence - the netCDF form of IQuOD will be incorporated into a larger NCEI data flow which will include Argo data, the Global Temperature and Salinity Profile Program (GTSPP), ocean currents data, anything with a Climate-Forecast (CF) compliant netCDF form.

3.4 JCOMMOPS monitoring tools: about XBT Metadata format and platform IDs. Martin Kramp

Martin Kramp reported on developments and activities of the **IOC**-WMO Joint Technical Commission for Oceanography and Marine Meteorology (JCOMM) in-situ Observations Programme Support Centre (JCOMMOPS).

He presented in particular the new integrated monitoring and metadata management website/database for the JCOMM Ship Observations Team (SOT, comprising VOS/SOOP/ASAP), Data Buoy Cooperation Panel (DBCP), Global Ocean Ship-based Hydrographic Investigations program (GO-SHIP), OceanSITES and Argo.

One of the main remaining challenges in this regard remains the uniqueness of ship-borne platform IDs, using at present mostly the non-unique ITU radio call sign of the ship. Tasked by the JCOMM Observations Coordination Group (OCG), JCOMMOPS has worked with the International Council for The Exploration of the Sea (ICES) on advanced and unique ship codes assigned by ICES on request to all ships in need of such a code, including those without IMO number. The ICES code now comprises between 4 and 6 characters. JCOMMOPS recommends that all observing networks in need of ships (ship-borne instruments, float and buoy deployments, maintenance, recovery etc.) use these ship codes in the future. Otherwise the cumulated contributions from volunteer ships are very difficult to measure and many synergies cannot be exploited.

Based on the unique ICES code for the ship, JCOMMOPS recommends the implementation of a new ID scheme for ship-borne instruments: At present, SOT BUFR templates allow up to 9 characters for the ID. Even a 6 character ship code (e.g. ABCDEF) would thus allow the addition of another 3 characters to identify the individual and sometimes numerous instrumentation packages (VOS, ASAP, SOOP etc) on a volunteer ship, often installed and maintained by different operators. Sometimes even several stations of the same kind (e.g. 2 weather stations, also using the same GTS header) are on the same ship and can thus make it impossible to identify the origin of the emerging data, if not clearly separated by individual IDs. The PIs of the International Comprehensive Ocean-Atmosphere Data Set (ICOADS) and a VOS working group already reviewed the draft version of the proposed ID scheme and endorse it.

Martin Kramp presented the JCOMM XBT metadata submission format. On a yearly basis, XBT operators should submit combined platform and observation metadata to JCOMMOPS in this format. The new JCOMMOPS system, and the new WMO Observing Systems Capability Analysis and Review Tool (OSCAR), now require however that platform metadata are submitted to JCOMMOPS as soon as a platform exists. The format must thus be divided in two parts, and the migration to BUFR requires in addition the review of the metadata content. Martin Kramp (SOT-SOOP coordinator) and Rebecca Cowley (SOT-SOOP chair) drafted new XBT metadata formats in a side meeting and will discuss this further with a therefore established SOT Task Team (http://jcomm.info/metasoop).

4 Session 4: Towards IQuOD v0.1

Chair: Janet Sprintall. Notetaker: Bec Cowley

4.1 From where we are to delivering IQUOD v1.0 product in early 2016. Led by Matt Palmer

The aim of the first IQuOD data product is to provide 'first cuts' at intelligent metadata and uncertainty information on each individual observation in the database. Rather than being a new database, this will essentially be an IQuOD 'flavour' of WOD where the user has the option of selecting the additional information provided by IQuOD. IQuOD is also delivering a new algorithm/method for removing duplicates (see Thresher/King presentation), although this may be rolled straight into WOD. We are now aiming to deliver this first IQuOD data product in mid-2016, which is a more realistic target than early 2016.

This part of the meeting was organised into two sets of two parallel breakout sessions, organised into the following task teams: (1) Intelligent Metadata; (2) Uncertainty Estimates; (3) Manual QC; (4) Automated QC. There was about 50 mins of discussion dedicated to each topic and then each group reported back for about 15 mins in a plenary discussion session. The focus of groups (1) and (2) was to outline the tasks on a 6-month timescale required to deliver the first IQuOD data product. Groups (3) and (4) considered a 12-18 month time horizon, but had the same goal of highlighting the key tasks/activities with timelines.

The summaries from each group are presented below:

Intelligent Metadata

The discussion started out quite broadly before homing in on what needs to be done to facilitate a first data released in mid-2016. It was felt that (i) XBT type; (ii) Recorder Type; and (iii) Launch Height are all potentially important pieces of information in regards to bias correction algorithms. However, it is not clear whether the importance of (iii) has been demonstrated in the literature yet. Regarding (iii), there may be ways to recover the information on ship deck heights from AOML and/or Scripp's, although this may take a year or more before the information is passed back. The issue of metadata recovery was raised and should form a longer-term aim for the project. It is clear that more sophisticated intelligent metadata algorithms could usefully be developed in the longer term.

Intelligent metadata for other data types was also discussed but it was unclear what sorts of instrumentation would require intelligent metadata and if the effort to derive intelligent metadata for data types other than XBTs would give a notable improvement in the historical temperature database.

For the 6-month timeframe associated with a first IQuOD data release, the following tasks were identified:

- Implement the Cowley et al [2013] algorithm for assigning intelligent metadata

- Evaluate it's performance on XBTs of known type
- Target possible increment improvements on this scheme ahead of IQuOD release
- Incorporate the intelligent metadata into WOD with appropriate flags and links to appropriate references

The resourcing of the above activities is not entirely clear yet, and discussions are underway to clarify this for early in 2016.

Uncertainty Estimates and Formats

The discussion on estimating uncertainties for IQuOD followed on from the meeting held on Wednesday 2nd December, 2015, and centred on what could be achieved in the timeframe given for the first release of IQuOD.

- How far can we take uncertainty estimates? For example, uncertainties could be applied to latitude/longitude, depending on navigation method. Underlying data quality could be assessed according to cruise calibrations or even specific stations on a cruise. This could, in principle be addressed through working with specific cruise reports.
- It was felt that it would be a useful exercise to write up something "on far can we go with uncertainties in profile data" to capture some of these ideas, even if actioning it isn't feasible for the next few years. This discussion could be folded into the publication of the uncertainty assignment method for IQuOD which is a requirement of the first data release (the paper should be submitted at least soon after the data are released).
- Another issue arising is the definition of uncertainty. For example, XBT manufacturers often claim that the instruments are accurate to 0.1C. Taking this to be an estimate of precisions (rather than accuracy, which must include information on bias errors), how does this relate to the statistics of the measurements – is 0.1C the standard deviation? This needs to be clarified to make sure that uncertainties assigned have the same meaning.
- John suggests that we engage with End Users to inform the priorities for geographic locations and time periods.
- John suggested that if we are going to look at cruise reports that we ought to capture the metadata for salinity as well. Gathering information from cruise reports could make a good student project?
- There was discussion of the possible interaction between QC flags and uncertainty estimates – e.g. do some flags imply a greater uncertainty? If we are talking about the random error assignment associated with instrument precision then the two should be largely independent.

Action list for first release of IQuOD:

1. Provide a definition of uncertainty for IQuOD purposes.

2. Provide uncertainties for temperature to the instrument level and available country/institution level. Use the hierarchy table structure presented by Tim Boyer. (John Gould, Bec, Tim, Viktor)
3. The uncertainties should be applied to all available data in the first release to avoid confusion (eg, we will not only apply uncertainties to pre 2000 data).
4. A readable table will be made available on line.

Action list, ongoing items:

1. Develop a template for feedback from those who collected data – table or document. Include salinity uncertainties (John, Bec, Viktor).
2. Add to the existing list of experts (eg Fabien, Loic). Gliders, seal data, etc. (Viktor, Alexander, Bec, Alison, South African – Seb Swart?).
3. Approach experts with the template and ask for feedback
4. Define a format for our files (eg, based on Argo, IMOS, GTSPP). How the data is stored/served could have a big impact on the choice. Get a task team together to start assessing formats with the aim of documenting a netcdf format for IQuOD. Do this in the next few months.
5. Decide on QC flag standards. This decision will be dependent upon QC tests and will need more interaction with AutoQC and ManualQC groups. Get a task team together to start assessing flags. Do this in the next few months.
6. Produce a journal paper on uncertainties, how far we can take the hierarchy of estimation of uncertainty (eg, instrument, manufacturer, country, institute, cruise levels) and how they are applied to IQuOD.

Automated QC

The automated QC work has made good progress in the last year thanks to Simon Good and Bill Mills. Work needs to continue with coding in the tests from each group and the goal is to have the benchmarking tests completed in time for the next workshop and the auto QC tests ready to apply to the second release of IQuOD. The scientifically QCd datasets available were reviewed and making the datasets available is critical for the assessment of the effectiveness of each institutes QC tests.

Bill and Guilherme both expressed interest in developing QC tests that can recognise data faults that are generally not detectable by currently available QC tests. Also in profiles that might be typical of some areas but might be identified as ‘bad’ in the standard QC tests. Usually these sorts of profiles are properly QCd in the manual step. Developing new AutoQC tests for them is highly desirable and could lead to machine learning development.

Benchmarking datasets useful for both Auto and Expert QC:

- QUOTA

- Sea Tag data (Bec needs to provide a version with flags)
- Argo
- North Sea data set (semi-automated, how well do we know the quality?)
- Hydrobase – note that we'd need the raw profiles from WOD in order to infer the QC rejections (Tim and Alison)
- WOCE Hydrography
- CORA – a dataset from Coriolis, which will be presented at AGU Ocean Sciences 2016 in the IQuOD session
- CSIRO XBTs

Actions:

1. A number of datasets were identified as good test candidates for validating AutoQC performance (QuOTA for the 3 or 4 months that were fully manually QCed, seal data, North Sea data, Argo D mode data + others?) CORA was also mentioned but this is in an Argo-like netCDF format so it would make more sense for us to implement a netCDF reader than for Tim to spend time converting the data. Bec to ensure Simon and Bill have the versions given to CSIRO earlier with the QC flags. Conversion to WOD format, including originator flags to be done by Tim. Deadline: May.
2. Bec/Ann to identify the 4 months in Quota that have every profile visually QC'd.
3. We also identified a number of further QC tests to implement; Bill and Simon to assist with CSIRO (Bec) and ICDC (Viktor) tests. Implementation either with Bill's help or do it yourself in this repo: https://github.com/IQuOD/AutoQC.
4. Ann, Bec, and anyone else interested to provide examples of profiles that are flagged in expert/manual QC. Examples to be sent to Bill Mills and Guilherme Castelao.
5. Simon, Bill + all to implement as many QC tests as possible (May).
6. Simon, Bill to use test datasets to determine performance of tests and the best set to use, and check consistency across datasets (June).
7. Simon, Bill to distribute files containing results of applying the best set of tests to interested people (Viktor, Ann, others?) to calculate statistics/check that the results look sensible (in time for the next IQuOD workshop – September?)
8. Simon, Bill + other contributors to draft paper (September onwards).
9. Regarding the AutoQC benchmarking work – the geographic distribution of false positives should be investigated.
10. There may be computational and storage resources available from Amazon – perhaps this should be investigated further?
11. Post the AutoQC "Quick Start" guide to the IQuOD website (Simon/Bec)

Expert QC

Discussions focussed on funding for expert/manual QC and using crowd-sourcing as a method to manually QC many profiles is still very attractive. There is a need to capture the imaginations of the wider public. There is a need to get away from the "doom and gloom" of climate change and reframe the question: "What can you do as a citizen to help?" John Gould has done some work to capture the essence of this messaging, see Appendix 1.

There is a need to identify the manual QC tasks that are essentially independent of the AutoQC work. This would include development of software to aid manual QC. This may also be helpful for efforts in seeking crowd sourcing.

Expert QC and crowd-sourced QC and how they are envisaged to work together was discussed. Ann expressed interest in using the same tool for the public and expert QC, which is very appealing in terms of not having to maintain two interfaces. But this might be challenging given the added complications of public engagement (convenience, aesthetic appeal, intuitive operation etc). Bill showed Alison the infrastructure for crowdsourcing: https://www.zooniverse.org/. These folks know how to engage the public, but it remains to be seen if their platform will satisfy all our needs.

Actions:

1. Ann to describe what the expert QC software interface should look like and discuss with Bill Mills & Guilherme Castelao.
2. Bill to enquire about crowd sourcing activities, e.g. with Zooinverse.
3. Alison to look into crowd source funding for IQuOD. Note that this is different to the crowd sourcing that Bill will investigate.
4. Come up with a list of well QC-ed database, including Hydrobase and the WOCE database.
5. Matt (Catia?) to come up with funding strategy for IQuOD expert QC – e.g. tapping into H2020 proposals or similar.

4.2 Review of action items

Action items from this meeting are summarised in Appendix 3.

The action items from the previous workshop were reviewed by members of the steering team "offline" and the major outstanding actions were briefly discussed among the group at the end of the meeting. These roll-over actions are indicated in Appendix 4.

4.3 Other Communication

4.3.1 2016 Ocean Science Meeting Session

Matt Palmer presented a few details of the IQuOD session at AGU Ocean Sciences 2016. The session title is "Toward a Subsurface Ocean Climate Record and Applications that Improve Understanding of Climate Variability and Change" and appears under the Primary Topic of "Ocean Observing and Data Management". The oral session will take place on Monday 24th February between 14:00 and 16:00. The poster session will also be on Monday 24th February between 16:00 and 18:00.

4.3.2 4th IQuOD Workshop

Kanako Sato announced Japan will host the 4th Workshop and introduced the group that will support the workshop.

XBT-Japan working group has been established for efficient collaboration among MRI-JMA, JMA, JODC, Tohoku University, MIRC, National Research Institute of Fisheries Science, TSK, and JAMSTEC in order to rescue and reconstruct of historical temperature data and evaluate it from the climatological aspect.

Its activities are supported by Ministry of Environment Government of Japan under the Environment Research and Technology Development Fund from 2015 to 2017.

4.3.3 Improving communication/website

This topic was not covered at the workshop and needs to be followed up by the Steering Team (Matt, Bec and Catia).

4.3.4 Regular videoconference meetings

The following schedule for monitoring progress towards the first IQuOD data product was put forward:

- Videoconference end of January 2016 (Task Teams to update Co-Chairs and email plans to steering team)
- Ocean Sciences meeting 21-26 February 2016 [M Palmer to organise meeting with Task Team members present]
- Videoconference end of March 2016 (Task Teams to update Co-Chairs) => Ocean Observations Panel for Climate meeting 6-8 April [M Palmer to seek feedback from OOPC]
- Videoconference end of April 2016 (Task Teams to update Co-Chairs)
- Videoconference end of May 2016 (Task Teams to update Co-Chairs)
- Delivery of first IQuOD product in June 2016
- Announcement at the CLIVAR Open Science meeting, September 2016

4.3.5 CLIVAR scientific/implementation plan

Matt Palmer and Catia Domingues will liaise with Task Team leaders to make progress with the implementation plan. The target date for CLIVAR endorsement is the next IQuOD workshop in September 2016.

4.3.6 Next Steps

All workshop participants to contribute to/review workshop report and actions.

5 XBT side workshop.

5.1 Summary on the achievements since the last XBT workshop. Lijing Cheng

Rebecca Cowley presented for Lijing, who joined us remotely. The presentation summarised the outcomes of the 4th XBT workshop and the work that has been done since. The goals of the workshop were: to reach a consensus on the recommendations made to the scientific community about corrections to historical XBT data; identify barriers to refining/improving corrections; identifying the source of the biases and how they contribute to uncertainty in the historical dataset; how the work on biases can feed into projects like IQuOD. A paper on the workshop led by Lijing, summarising the outcomes and recommendations has been published in BAMS (**Cheng L.,** John Abraham, Gustavo Goni, Timothy Boyer, Susan Wijffels, Rebecca Cowley, Viktor Gouretski, Franco Reseghetti, Shoichi Kizu, Shenfu Dong, Francis Bringas, Marlos Goes, Loïc Houpert, Janet Sprintall, Jiang Zhu, 2015: XBT Science: assessment of instrumental biases and errors, ***Bulletin of the American Meteorological Society***, accepted. doi: http://dx.doi.org/10.1175/BAMS-D-15-00031.1).

Ongoing work since the workshop includes: continue to provide corrected XBT data through the major datacentres; recommendations on essential metadata for future collection of XBT data; continued recovery of side-by-side XBT/CTD data and encouraging more tests yearly; assessing the cause of the time-varying biases in different probe types – including fluid dynamics models (Abraham); the tank fall rate experiments of Bringas and Goni, published in 2015. Future work includes: assessing the link between water temperature and pure temperature bias; evaluating the higher temperature bias in analog recorders (Reseghetti); ongoing communications with manufacturers to reduce uncertainties in thermistors and probe build.

5.2 Inter-comparison of the 10 existing XBT correction schemes. Lijing Cheng

Lijing Cheng presented the updated results on the evaluation of 10 of the existing XBT correction schemes. This is motivated by the scientific question of: How well the existing schemes can correct the XBT bias in the major ocean databases? They used three datasets to examine the performance of 10 of the existing methods. Two of them are Global-scale datasets constructed based on WOD09 and EN3. Another one is Side-by-side dataset. XBT/Reference pairs were constructed so that PFL/OSD/CTD data were used as reference. Then they corrected XBT profiles by different schemes separately and calculated the temperature difference between corrected XBT and CTD. Five metrics were used to define the “goodness” of the correction. The results still indicate the contradiction between Global-scale dataset and Side-by-side dataset, because the best four methods according to Global-scale dataset are not the best in Side-by-Side dataset. Furthermore, they find that quality control is an important source of uncertainty! It is not clear which dataset (WOD09 or EN3) is better.

5.3 Quantification of the effect of water temperature on the fall rate of XBTs. Rebecca Cowley, John Abraham and Lijing Cheng.

The study presented aims to test the impact of water temperature on fall rate by testing the numerical model of Abraham et al, 2012. The thermal gradients method of Cowley et al, 2013 was also employed to compare the effectiveness of the numerical model of correcting the depth error in XBTs. Using the XBT/CTD pair database, the model was used to recalculate the depths of the XBTs in two parts.

Part 1 (289 pairs) involved a forward-stepping algorithm to calculate the velocity at each time step of the probe's fall. A quadratic equation was then fitted to determine the A, B and C coefficients for each probe. Part 2 (2,937 pairs) used the relationship between A and the first surface temperature determined in Part 1 to assign an A value to each XBT dependant on the first temperature. An average B and no C value were used. The model reduced the depth error in the historical XBT data. Compared to the correction of Cowely et al, 2013, the correction was not as uniform, with depths overcorrected at depth and under corrected near the surface. Residual temperature error was similar in the two methods (median of ~0.04°C). The simplified numerical model of fall rate is effective at reducing the depth error, but could be improved by including an offset term and might be combined with other efforts to improve corrections to XBT historical data.

5.4 Gouretski & Reseghetti 2010 correction scheme – an update. Viktor Gourestki

No summary available.

5.5 Evaluation of XBT measurements accuracy in Ligurian and Tyrrhenian Seas. Franco Reseghetti

G.Raiteri[1], F.Reseghetti[1], M.Borghini[2]

[1] ENEA, SSPT-PROTER-BES, 19032 Pozzuolo di Lerici (Italy)

[2] CNR-ISMAR, U.O.S. La Spezia, 19032 Pozzuolo di Lerici (Italy)

The aim of this analysis is to give an estimate of the accuracy of XBT measurements from SOOP program in the Central Mediterranean sea (Ligurian and Tyrrhenian seas). The line Genoa-Palermo (active since September 1999 but with breaks in 2001-2004 and 2007-2009) has about 80 different data taking for a total amount of more than 2300 XBT profiles of different type. The distance between consecutive drops was typically of 10-12 nautical miles for the most part of data taking. The repetition rate varied from monthly to seasonal sampling. Raw XBT data are used (without application of any filter and interpolation to transform to 1-m reduced values or correction to fall rate equation). ARGO profiles from Tyrrhenian and Ligurian Seas are available since August 2004. Profiles with good QC flag have been downloaded from CORIOLIS Data Centre (Brest, France). XBT vs. CTD comparisons were conducted by ENEA and CNR-ISMAR in Tyrrhenian Sea since 2003. CTD profiles were obtained from a Sea-Bird SBE 911 *plus* device.

Pairs of XBT and ARGO (and XBT and CTD) temperature profiles are included in the analysis if the difference between the geographical coordinates is less than 0.1° in latitude, 0.15° in longitude and 7 days in time. The window dimensions are similar to the standard sampling distance (10-12 nm). The main results concerning T4/T6/T7/DB probes are shown below (temperature differences are in °C).

XBT vs. ARGO	0-bottom	0-100m	100m-bottom	XBT vs. CTD	0-bottom	0-100m	100m-bottom
mean	0,11	0,33	0,03	T4-T6	0,07	0,23	0,03
st. dev.	0,44	0,76	0,12		0,27	0,55	0,09
median	0,05	0,08	0,05		0,04	0,09	0,03
mean	0,12	0,23	0,07	T7-TD	0,04	0,1	0,03
st. dev.	0,56	0,98	0,11		0,24	0,52	0,07
median	0,07	0,09	0,07		0,03	0,03	0,03

If only data below 100m depth are considered, XBT profiles from SOOP in the Mediterranean have to be considered slightly warmer than real, with a reasonable value of uncertainty, and in substantial agreement with the results obtained from XBT probes deployed during comparison with CTD.

5.6 XBT Science at Scripps: Recent Highlights. Janet Sprintall

Sprintall presented some recent science highlights from the Scripps Institution of Oceanography (SIO) High Resolution XBT (HR-XBT) network in the Indian and Pacific Oceans. The highlights included using Argo, altimetry and the HR-XBT data to examine variability in East Australian Current western boundary current (Zilberman), examining frontal variability in the Southern Ocean and its impact on air-sea gas exchange (Sprintall) and the use of XBT data in Ocean State Estimation models (Cornuelle). The SIO HR-XBT network relies on international partnerships to help facilitate the implementation of the program. Some transects have now been occupied for 30 years.

Sprintall also led a discussion on the plans for an XBT Science Paper. In general, the response by the workshop participants was positive and many plan to contribute. However the timeline for publication by mid-February was considered not achievable. In addition, there was a call to explore other publication journals such as the EGU open source online journal Ocean Science.

5.7 Status of XBT data in Southwestern Atlantic Ocean. Marcela Charo

Marcela presented a summary of MBT and XBT data available in the Navy Hydrographic Service, in Argentina. Metadata of these records are analyzed in order to apply bias depth and temperature corrections.

Most of this data is already in the WOD13.

5.8 XBT status in India. Uday Bhaskar

India started its XBT program way back in 1990 with the support from Department of Science and Technology (DST) as a part of International TOGA program. Subsequently it is funded by Department of Ocean Development (DOD) and Ministry of Earth Sciences (MoES) through INCOIS. Recently this program finished 25 years of its existence and is termed as the longest and most sustained observational program in the Indian Ocean initiated by Govt of India.

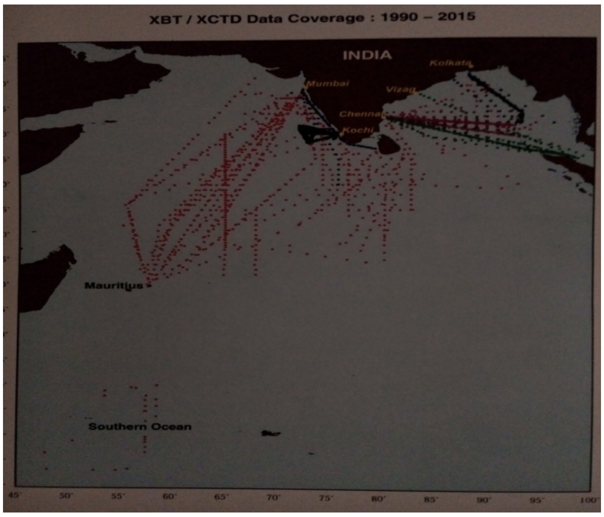
Under the Indian XBT program data collection and processing is done as follows:

- Temperature profiles up to 760 m were collected using M/s Sippican Inc, USA make personal computer based
  - MK 12/ MK 21/ MK 150 data acquisition
  - LM 3A hand held launcher
  - T-7 XBT probes.
- Temperature and depth accuracies of the probes are
  - ± 0.20C and 2% of the probe depth
- Data are collected at a spatial resolution as follows:
  - 50 Km apart close to Indian coast
  - 100 Km apart in the open ocean.

The following are the transects along with the data is collected:

- XBT data is collected along the following transects:
  - (1) Chennai – Port Blair
  - (2) Port Blair – Kolkata
  - (3) Chennai – Singapore
  - (4) Mumbai – Mauritius
  - (5) Mumbai – Colombo
  - (6) Kochin – Kavaratti – Minicoy – Kochi.
- Of late due to non-availability of ships data are collected only along lanes 1, 2, 6 only.

Figure below shows the total XBT transects along which data is collected during the past 25 years.



Utilization of data for scientific studies: The XBT data is used for the following scientific objectives.

- Atlas of XBT thermal structures in the Northern Indian Ocean for period 1993 – 2003 was prepared.
- Study of Warm Pool in the South Eastern Arabian Sea and its relation to monsoon onset vortex.
- Surface layer temperature inversions in the Arabian Sea and Bay of Bengal.
- Barrier Layer variability in the Bay of Bengal and Arabian Sea.
- Intra and inter-annual variability of near surface thermal structure.

5.9 Discussion.

Discussion was held during and after each presentation, and mostly centred on XBTs, however, MBTs were also discussed. Shoichi suggested that the Japanese MBT manufacturer is different from other MBT manufacturers. Viktor is not sure how many manufacturers there are. The Soviet Union only used USSR manufactured MBTs. Viktor has documentation on the USSR manufactured MBTs. The USA had their own manufacturer also. How important is it? The MBT was not mass manufactured, therefore the manufacture process is not as important for the MBT as XBT.

The aim of our XBT Science group with respect to IQuOD is to come to consensus as to correction and bias estimates. We will ideally continue development of schemes, assess all schemes and determine best scheme. Finally, we can then provide uncertainty estimates to IQuOD.

We need to involve the SOOPIP (JCOMMOPS) coordination group (Martin Kramp) to organize meetings and help with planning. They will be able to help with publicising the metadata requirements for XBTs and with coordination of XBT/CTD tests, perhaps incorporating GO-Ship.

Janet and Gustavo (and many others) are helping with an XBT review paper. All agreed to help with the paper where possible.

XBT action items:

1. Bec and Martin to find people to give them their deployment heights for historical data. Need this going forward as well.
2. Start a communication with JCOMMOPS to coordinate yearly XBT/CTD comparisons between XBT group and GO-SHIP group. Bec/Martin. Can we start a list?
3. Correction schemes that can be updated yearly, should be. Supply the correction scheme updates to WOD for publication. Should be done in the first quarter of every year. Viktor, Bec, Tim, Lijing, Ishii, Hamon method? (Christine to ask Loic). Can use the EN bathymetry method as a validation tool.
4. Communication of launch heights from SOOP ships to JCOMMOPS from Australia, AOML, SCRIPPS, WHOI, etc, etc. Communicate essential metadata requirements to JCOMMOPS, (Bec, Martin)
5. Strip chart recorder testing – Franco undertaking tests on 16 December. Ann to send timing box to Franco ASAP. Does Argentine Navy still use strip-chart recorders? Will they allow testing of the recorders on board? Marcela.
6. Can we perform lab tests on temperature error variation with water temperature? Time available?
7. Launch height tests – Gustavo and Francis have collected some data, Bec has some. Can Bec try adding Francis' correction to the data collected on the Investigator, 2015?
8. Franco has some 2008 probes that he is deploying (40 boxes). T5 (4 boxes, 2008), T4 (2 boxes 1994/95).
9. Bec will deploy old T5's next year – probably XBT vs XBT while underway.

10. All will help with XBT review headed up by Gustavo.
11. Next XBT meeting – Japan, 2016, September. Next SOOP Panel meeting potentially April 2017, London. Should we coordinate an XBT science meeting with SOT?
12. Ask authors of corrections to do a sensitivity test similar to Viktor's to assess the radius of the XBT/CTD pair selection. What effect does the radius/time selection have on the temperature bias/depth error? Tim, Lijing, Ishii?, Hamon?
13. Bec to talk with Natalia about XBT/CTD pairs in the Southern Ocean.
14. Bec to provide a list of required metadata to Uday to help him get the metadata from historical Indian XBTs.

5.10 Future Plans, 6th Workshop

We would like to have a side meeting in association with next IQuOD meeting. We need a science meeting in coordination with other groups. Maybe we can have an XBT science meeting at SOT/SOOP IP meeting in April 2017?

6 Appendix 1. Words to introduce IQuOD to the public.

Words by John Gould encouraged by Steve Diggs. We may be able to use/develop this text to attract the attention of the public for crowd-sourcing, for funding and other purposes.

Earth's heat store: past, present – and future.

Making it clear

There are many ways in which the oceans make life on earth possible – they contain a large part of the biosphere and so act as earth's lungs exchanging oxygen and carbon dioxide with the atmosphere. More fundamentally they are the earth's major heat reservoir, moderating climate extremes and sharing with the atmosphere the task of moving heat away from the equator and towards the poles.

Knowing where that ocean heat is stored and how that storage has changed is one of the keys to understanding how earth's climate will evolve.

Measurements of the oceans' temperature started in a small way in the late 19^{th} century and have grown as technologies have developed and as the importance of the oceans has grown. There are now around 15 million measurements of how temperatures changes with depth but they are of varying quality.

A crucial task is to re-examine these 15 million observations and, using present day knowledge and computer power to eliminate errors so as to produce the best possible knowledge of temperature change – not just for the past but encompassing new observations presently growing at a rate of ¼ million per year.

This work is being done through a project called IQuOD producing an **I**nternational **Qu**ality-controlled **O**cean **D**atabase.

<u>Practical steps – what is being done now and what is planned?</u>

Scientists and computing experts have developed prototype schemes that are being applied to large ocean data sets so as to identify anomalies, duplicated and to eliminate observations that are believed to be erroneous. A next step will be, based on our knowledge of how the measurements were taken and processed to assign to each an estimate of uncertainty (i.e. how good is the measurement as a representation of the temperature of the ocean at the time and location of the observation).

These techniques will be applied to the data holdings of World Ocean Database and made available to anyone interested in using the data and the reactions of the user community will guide future activities of IQuOD and the application of the quality control of future observations.

In the longer term similar quality control will be applied to other ocean properties starting with salinity (an indicator of changes in the global hydrological cycle).

What will be the benefits from the project?

Ocean heat content – the summation of all ocean temperature data - is used to calculate the amount of sea level rise associated with warming of the oceans. Past calculations of such change are a guide to how sea-level will change in the future. IT is expected that the work of IQuOD will lead to improvements of our knowledge of past and future sea-level changes.

The ocean biosphere – is influenced in complex ways by ocean temperatures and in turn this affects the transfer, generation and absorption of gases that play key roles in regulating climate. Also from a purely physical standpoint the solubility of gases is sea water is temperature dependent. These again point to the importance of improving the quality of the ocean temperature record.

At high latitude the temperature of seawater in contact with both seasonal sea-ice and more permanent ice fields has been implicated in the rapid decrease in artic sea-ice. The comparatively sparseness of high latitude temperature measurements adds importance to ensuring that erroneous measurements are removed from the data record in these areas.

I'd like to see the project succeed - How can I help?

Ocean observing scientists – if you have made ocean observations that are in the World Ocean Database you are the best person to know the uncertainties associated with those observations. We need your help to ensure that the uncertainties that we assign to your data are consistent with your views. This is particularly important for observations from many years ago where we re in danger of losing this information.

Present-day ocean observing programmes. As your measurements enter WOD they will automatically be handled and tested by the IQuOD process. However, your researchers are the best people to apply state-of-the-art best practice to ensure their data are of the highest quality consistent with the needs of your project. We encourage you to do this and also to build on the experience gained by projects that have already applied considerable resources to data quality assurance

Users of ocean temperature data - you are the ultimate beneficiaries of this project. We encourage you to enter a dialogue with the project, to use the IQuOD QC's database in your research and to provide IQuOD with feedback on how much the data set has been improved and whether there is other work that IQuOD

Funding agencies - Many agencies have already made heavy commitments to the funding of programmes that collected the data that IQuOD will process and, indeed, to the quality control of those data. However, much data has not undergone detailed QC. Those data supplement and complement the existing high quality by allowing the infilling of gaps in both space and time. Comparisons of coincident high- and low-quality data have the potential for us to assign realistic uncertainties to all data. The assignment of these uncertainties increases the value and comprehensiveness of the ENTIRE data set.

Thus funding of IQuOD activities does not repeat, but instead expands, the DQ assurance process for ALL data and for a small fraction of the original cost of data collection and QC.

The exercise is truly international in that all countries that have collected and submitted data to WOD are therefore involved in the project. Indeed the benefits of the success of IQuOD will have a positive impact on all nations and institutions with and interest in a better understanding of earth's climate. Our hope is that this may result in a very wide range of funding opportunities.

7 Appendix 2. Participant list

Name	Affiliation
Bhaskar, TVS Udaya	INCOIS, India
Boyer, Tim	NCEI, NOAA, USA
Charo, Marcela	SHN, Argentina
Cheng, Lijing	Chinese Academy of Sciences, China
Coatanoan, Christine	IFREMER, France
Cowley, Rebecca*	CSIRO, Australia
Demidov, Alexander	Moscow State University
Diggs, Steve	UCSD, USA
Galibert, Guillaume	IMOS, Australia
Good, Simon	Met Office, UK
Gould, John	NOC, Southampton
Gouretski, Viktor**	University of Hamburg
Jandt, Simon	BSH, Germany
King, Edward	CSIRO, Australia
Kizu, Shoichi	Tohoku University, Japan
Klein, Birgit	BSH, Germany
Kozyr, Alex	CDIAC/ORNL
Macdonald, Alison	WHOI
Mills, Bill	Independent
Palmer, Matthew*	Met Office, UK
Reseghetti, Franco	ENEA, Italy
Sato, Kanako	JAMSTEC, Japan
Sprintall, Janet	UCSD, USA
Suzuki, Toru	MIRC, Japan
Thresher, Ann*	CSIRO, Australia
Castelao, Guilherme	Instituto Oceanografico - USP
Domingues, Catia*	ACE CRC, Australia
Fonseca, Carlos	CPTEC/INPE Center for Weather and Climate Forecast
Hidas, Marty	IMOS, Australia
Ribeiro, Natalia	Federal Uni of Rio Grande
Kramp, Martin	JCOMMOPS
Warren, Rachel	Met Office, UK

* Organizers, ** Local organizer

8 Appendix 3. Summary of Action items

8.1 Uncertainties/Formats Tasks

No.	Item	Who	When
1	Provide a definition of uncertainty for IQuOD purposes.	Bec, Rachel, John, others?	June, 2016
2	Provide uncertainties for temperature to the instrument level and available country/institution level. Use the hierarchy table structure presented by Tim Boyer.	John Gould, Bec, Tim, Viktor	June, 2016
4	A readable table will be made available on line (WOD)	Tim	June, 2016
5	Develop a template for feedback from those who collected data – table or document. Include salinity uncertainties.	John, Bec, Viktor	
6	Add to the existing list of experts (eg Fabien, Loic). Gliders, seal data, etc.	Viktor, Alexander, Bec, Alison, Seb Swart?	
7	Approach experts with the template and ask for feedback.	John	
8	Define a format for our files (eg, based on Argo, IMOS, GTSPP). How the data is stored/served could have a big impact on the choice. Get a task team together to start assessing formats with the aim of documenting a netcdf format for IQuOD.	Bec	June, 2016
9	Decide on QC flag standards. This decision will be dependent upon QC tests and will need more interaction with AutoQC and ManualQC groups. Get a task team together to start assessing flags. Do this in the next few months	?	
10	Produce a journal paper on uncertainties, how far we can take the hierarchy of estimation of uncertainty (eg, instrument, manufacturer, country, institute, cruise levels) and how they are applied to IQuOD	John, Bec, ?	Start by end 2016

8.2 Auto QC tasks

No.	Item	Who	When
1	A number of datasets were identified as good test candidates for validating AutoQC performance (QuOTA for the 3 or 4 months that were fully manually QCed, seal data, North Sea data, Argo D mode data + others?) CORA was also mentioned but this is in an Argo-like netCDF format so it would make more sense for us to implement a netCDF reader than for Tim to spend time converting the data. Bec to ensure Simon and Bill have the versions given to CSIRO earlier with the QC flags. Conversion to WOD format, including originator flags to be done by Tim.	Bec, Simon, Bill, Tim	May, 2016
2	Bec/Ann to identify to Auto QC group the 4 months in Quota that have every profile visually QC'd.	Bec/Ann	ASAP, January, 2016
3	We also identified a number of further QC tests to implement; Bill and Simon to assist with CSIRO (Bec) and ICDC (Viktor) tests. Implementation either with Bill's help or do it yourself in this repo: https://github.com/IQuOD/AutoQC	All with autoQC tests available, Viktor, Bec	September 2016
4	Ann, Bec, and anyone else interested to provide examples of profiles that are flagged in expert/manual QC. Examples to be sent to Bill Mills and Guilherme Castelao	Ann, Bec, anyone	March 2016
5	Simon, Bill + all to implement as many QC tests as possible (May).	Simon, Bill	May 2016
6	Simon, Bill to use test datasets to determine performance of tests and the best set to use, and check consistency across datasets (June)	Simon, Bill	June 2016
7	Simon, Bill to distribute files containing results of applying the best set of tests to interested people (Viktor, Ann, others?) to calculate statistics/check that the results look sensible (in time for the next IQuOD workshop – September?)	Simon, Bill, Viktor, Ann	Before next workshop

No.	Item	Who	When
8	Simon, Bill + other contributors to draft paper (September onwards)	Simon, Bill, others	After September 2016
9	Regarding the AutoQC benchmarking work – the geographic distribution of false positives should be investigated		
10	There may be computational and storage resources available from Amazon – perhaps this should be investigated further?		
11	Post the AutoQC "Quick Start" guide to the IQuOD website (Simon/Bec)	Simon, Bec	January 2016
12	Investigate the appropriate license for the IQuOD dataset. Eg: creative commons. Will have to work with NCEI requirements.	Simon, Bill, Tim	September, 2016

8.2.1 Manual/Expert QC tasks

No.	Item	Who	When
1	Ann to describe what the expert QC software interface should look like and discuss with Bill Mills & Guilherme Castelao	Ann, Bill, Gui	
2	Bill to enquire about crowd sourcing activities, e.g. with Zooinverse	Bill	
3	Alison to look into crowd source funding for IQuOD. Note that this is different to the crowd sourcing that Bill will investigate	Alison	
4	Come up with a list of well QC-ed databases, including Hydrobase and the WOCE database	All	Done already?
5	Matt (Catia?) to come up with funding strategy for IQuOD expert QC – e.g. tapping into H2020 proposals or similar	Matt, Catia	

9 Appendix 4. Action Items from 2nd Workshop, 2014

No.	Item	Who	When
1	Scientific Implementation plan V0.1. Incorporate a timeline. Get feedback from IQuOD members during development. Get feedback from community on version 1.0. Incorporate Simon/Viktors tables, Tim's data flow and Manual QC costing into the plan. Also plots of OHC with and without QC'd data, or with/without XBT biases or with /without selected data.	Matt Palmer, Catia Domingues & task group leaders	June 30, 2014. Final (1.0) version December, 2014 ROLLED OVER FROM LAST WORKSHOP
2	Make a summary of lessons learned from SST, ICOADS, GTSPP, GOSUD, etc efforts. Talk to Peter Thorne (and about crowd sourcing). Talk to Kate Willett.	Catia Domingues, Bec Cowley, Simon Good, Tim Boyer	Next week, June 30 ROLLED OVER FROM LAST WORKSHOP
3	Create a list of regional/instrumental experts who will be willing to contribute to the Manual QC aspect of the project.	Viktor	August, 2014 ROLLED OVER FROM LAST WORKSHOP
4	Start a list of users and user requirements, encourage user requirement feedback.	Simon Good	August, 2014 ROLLED OVER FROM LAST WORKSHOP
5	Group leaders to maintain regular meetings between workshops. Conference calls.	Catia Domingues, Bec Cowley, Tim Boyer, Ann Thresher and Simon Good	ROLLED OVER FROM LAST WORKSHOP
6	Organise a manual QC workshop in conjunction with IQUOD workshop 3. Identify experts to be involved and pin down QC requirements prior to the workshop.	Ann Thresher	June 2015 ROLLED OVER FROM LAST WORKSHOP
7	Investigate how 2-way communication/feedback between users and IQUOD might work (using ESGF/ESCOG)	Matt Palmer, Catia Domingues	June 2015 ROLLED OVER
8	Talk with WOD/Jim Potemra about Quota-style QC'd Pacific data for auto QC benchmarking	Bec/Catia	August, 2014 ROLLED OVER
9	Viktor to maintain a table of data types (as shown in his presentation) that will be incorporated into IQUOD, their priorities etc, and allow others to contribute to it. Put it on the website.	Viktor	ROLLED OVER
10	Identify already highly QCd databases and start collecting them	Tim (collection), everyone else for input & information	Ongoing ROLLED OVER
11	Plot up a dataset gridded dataset with and without data QC. Aim is to show that the QC of data and presence of metadata is important.	Gustavo/Marlos, Simon, Bec, Tim/Melissa.	July 1 ROLLED OVER

No.	Item	Who	When
12	When anyone becomes aware of funding opportunities let everyone know.	All	Ongoing ROLLED OVER
13	Investigate crowd sourcing for funding.	Alison and Steve	December, 2014? ROLLED OVER
14	Set up a mailing list that is useable to everyone. Make sure the steering team has a generic email address.	Bec, Ricardo, Olga.	ROLLED OVER?
15	Set up some webinars during the year. Webex?	Catia and Bec and steering team	June, 2015 DELETE??
16	See if we can assign a set amount of time to IQUOD. Then we can present this information to a funder to show what manpower we already have.	Everyone	August 2014 ROLLED OVER
17	Investigate crowd sourcing for manual QC	Volunteer from wider community	June, 2015 ROLLED OVER