International Quality-controlled Ocean Database (IQuOD)

Quantification of uncertainties in global ocean temperature observations

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Background/Methodology

Ocean observations are crucial for climate research and forecasting activities such as climate monitoring, ocean reanalysis and seasonal-to-decadal forecasts.

The IQuOD effort has enhanced this crucial data set with measurement uncertainty estimates for each type of observation (figure 2), quality control software (references), global coordination, and comunity building.

IQuOD task teams are now working to add best estimates of representation uncertainties (figures 3 and 4), as well as extend the previous effort to salinity measurements.

IQuOD also provides a platform to integrate with other IODE-supported efforts focused on collecting and distributing ocean T/S data sets (WOD, GTSPP, GOSUD).

In November 2024, the joint IQUOD/SOOP/GTSPP/XBT meeting sponsored by IODE took place in Bologna, Italy (picture 1). This gave us a very fruitful opportunity to review progress made, plan ahead for the coming years, and connect with ODIS.

Topics covered at the meeting included :
- automatic quality control
- duplicate data handling
- salinity data uncertainties
- representation uncertainty
- ocean reanalysis as a use case
- IODE Quality Flag Schemes

Measurement Uncertainties

Derivation of measurement uncertainties in IQuOD followed the Guide to Measurement of Uncertainty (GUM, 2008). Figure 4 shows the workflow concept used to calculate measurement uncertainties.

IQuOD v0.1 (2018) release contains 'Type B' measurement uncertainties determined from manufacturer specifications and other publications , which are reported in Table 1.

Measurement uncertainty changes over time depending on the main components of the observing system, measurement methods, and instrumental platforms being used. Improvements to measurement uncertainties in future IQuOD releases will include rescue of information from sources such as voyage reports and calculation of uncertainty budgets.

IQuOD also plans to publish uncertainty budget templates and a software code base with sample calculations for uncertainty budgets.

Figure 2: Uncertainty quantification flow chart.

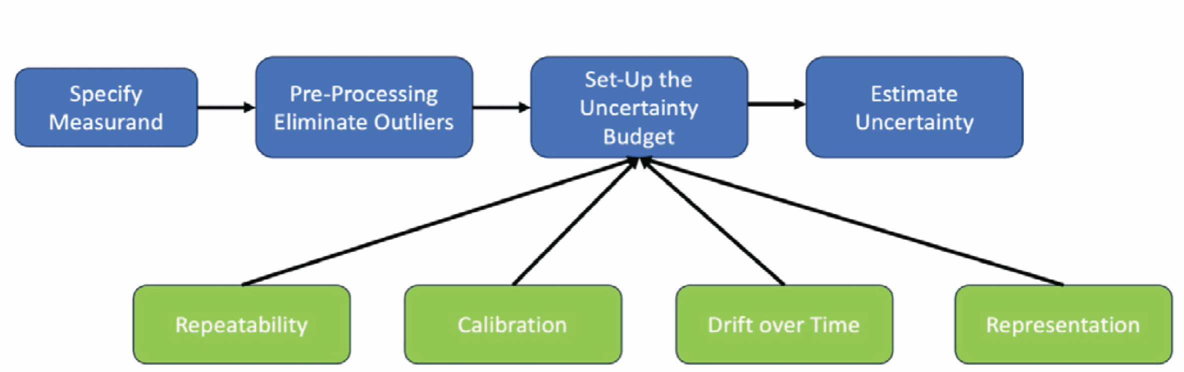


Table 1: Uncertainty estimates for a selection of instrumentation in the WOD as described in Cowley et al, 2021. See https://www.iquod.org/specifications.html for full information.

Instrument type	Temperature (°C)	Depth/Pressure	Approx. First Year of Routine Use
Bottle/reversing thermometer	0.02	5%	1900
Conductivity-Temperature-Depth (CTD) uncalibrated and calibration status unknown	0.01	0.08%	1964
CTD calibrated	0.002	0.015%	1964
CTD animal mounted	0.005	-	2004
Glider	0.002	-	2002
Profiling floats (pre-Argo)	0.005	-	1994
Profiling floats (Argo***)	0.002	2.4 dbar	2000
Expendable Bathythermograph (XBT) Sippican manufacturer	0.1	<=230 m: 4.6 m; >230 m: 2%	1967
Mechanical Bathythermograph (MBT)	0.3	3%	1938

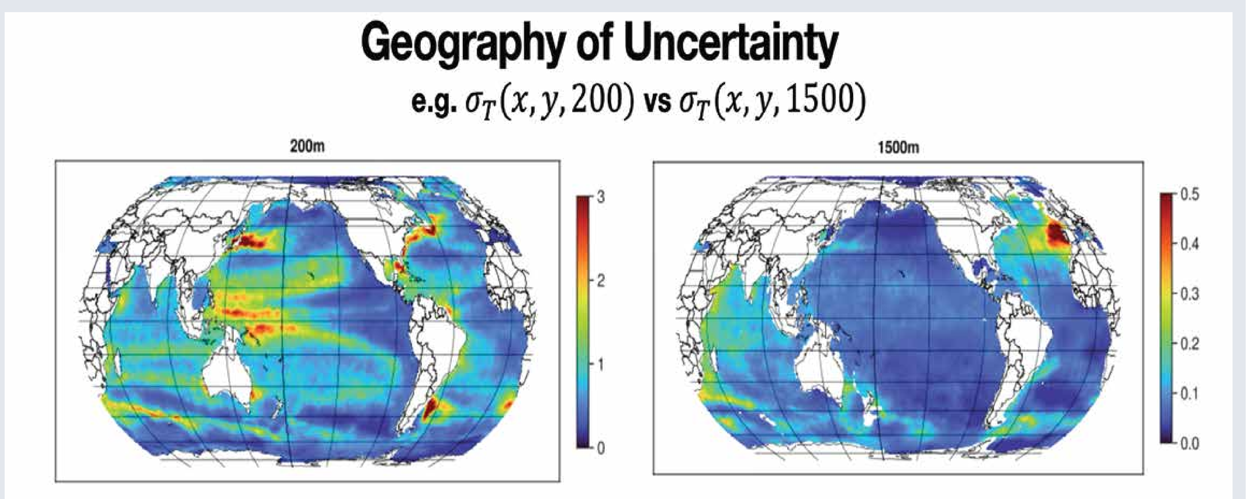
An important consideration in IQuOD is the mapping trough space and time of global warming and changes in Earth's water cycle from sparse ocean T/S observations collected in the field (IQuOD, WOD, ...).

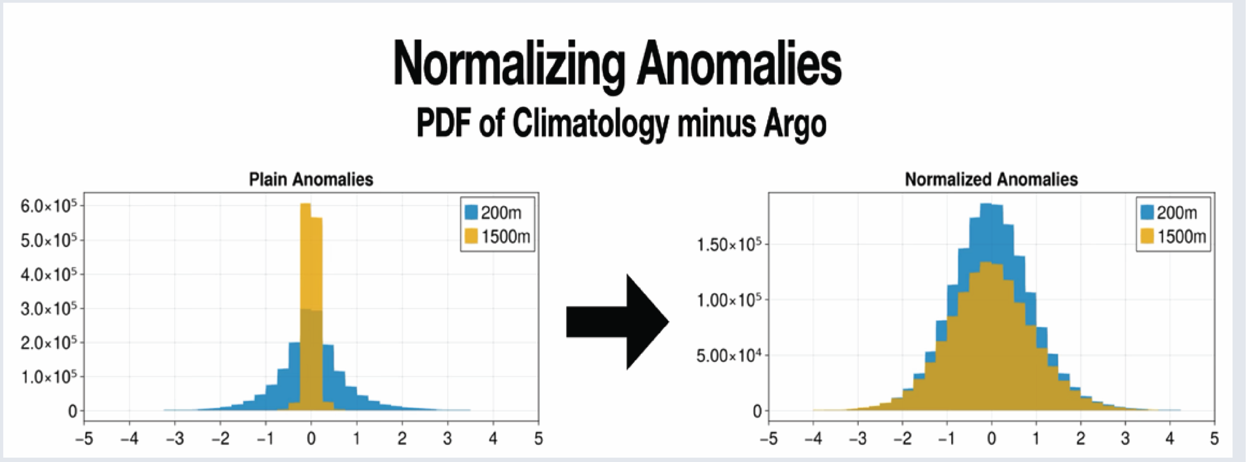
Uncertainties in such gap-filled data products must reflect the sparsity of ocean data as well the amount of geophysical noise that affects T/S profile measurements (i.e., representation uncertainty).

Representation Uncertainties

Definition: When considering incorporating measurements into model applications (e.g., optimal interpolation, ocean reanalyses), representation error describes the uncertainty of using a pointwise measurement to represent spatio-temporal averages. As per Forget and Wunsch (2007), or Oke and Sakov (2008), representation uncertainty for temperature and salinity is known to show large spatial heteogeneity. It is most often larger than measurement uncertainty in magnitude.

Estimation: We bin quality-controlled observations into temporal-spatial grids (e.g. 1° grid, 1 month), subtract a monthly mean climatology or a smooth data assimilation product, and finally calculate standard deviations of all these anomalies (figure 3a).





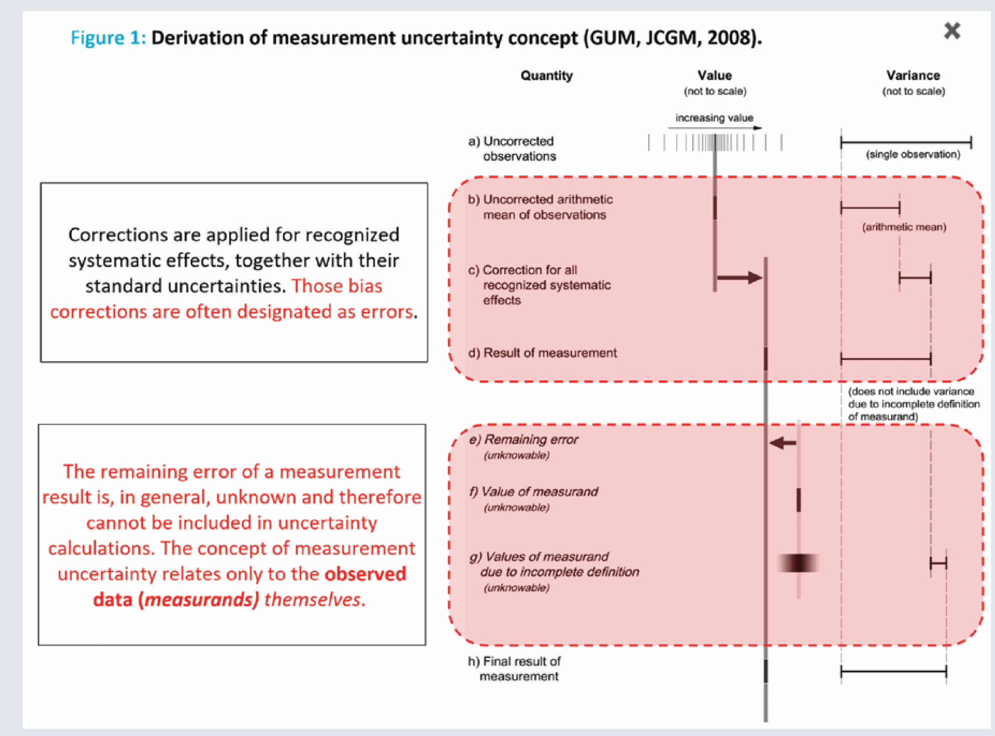
Preliminary results: representation uncertainty estimated on a 1° grid tends to reflect the geography of meso- and submeso-scale activity. It is generally intensified in places where T/S gradients are large, such that ocean motions can generate large T/S variance (e.g. the thermocline).

Hence, representation uncertainty sharply decreases with depth (Figure 3a). Normalizing model-data misfits is therefore a crucial step (Figure 3b) when evaluating the quality of the fit between pointwise profiles and climatologcal estimates (Forget & Wunsch 2007, Forget et al 2015).

Plans for IQuOD include supplying gridded uncertainty maps for typical applications, including publication of a set of algorithms for different use cases to calculate representation uncertainty.

What's next in IQuOD?

- seasonal representation uncertainties
- IQuOD for salinity, then oxygen
- deeper integration with ODIS
- cloud-ready file formats
- WOD/NOAA integration
- IQuOD & WOD backup



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