Report on the suitability of the actual reference data sets for deep Argo DMQC

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v0.2	26/09/2022	Kamila Walicka	Introduction, summary, assessment of the reference data from the Southern Ocean
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v1.0	26/10/2022	Kamila Walicka	Final version

EXECUTIVE SUMMARY

This report provides an assessment of the availability and quality of the CTD reference data for Argo DMQC analysis from the specific regions of deployment of the European deep Argo fleets. The review was undertaken for the areas such as the North Atlantic, Mediterranean Sea, South Atlantic and Nordic Seas. In the North Atlantic, the CTD reference data are sufficient to perform a reliable DMQC analysis of deep Argo floats. However, in terms of other analysed regions, the report highlights a concerning issue of relatively old and sparse representation of these data. It is advised to the entire Argo community for a more strategically and coordinated plan of deployments of the deep Argo floats and the associated ship-based CTD measurements.

Moreover, this report points out various issues related to the data delivery of the ship-based CTD data to Coriolis for DMQC analysis submitted by both data centres and Principal Investigators (PI's). It has been recommended to both European and International partners to work on improving the collaboration to identify potential sources of the CTD data and ensure a clear flow of these data to Ifremer.

The ship-based CTD data submitted to Coriolis requires various time-consuming additional quality checks before their incorporation into the CTD reference data for Argo. Increasing the team of permanent CTD data operators is strongly recommended to sustain timely publications of the most updated versions of the CTD reference data for DMQC analysis.

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1. Introduction

The ship-based CTD reference database for Argo is a collection of high-accuracy climatology data. Usually, the profiles are obtained via downstream services: the updates of the Ocean Climate Laboratory/NODC to the World Ocean Database WOD (OCL), and data from the International Council for the Exploration of the Sea ICES (ICE), the CLIVAR and Carbon Hydrographic Data Office CCHDO (CCH) and their product GO-SHIP Easy Ocean dataset (Katsumata K., 2022) and data directly submitted from the research cruises by Principal Investigators. The origin of each profile is recorded in the variable QCLEVEL using a three-letter code.

The CTD reference data for Argo are formatted for direct use with the OWC software, necessary for delayed-mode quality control (DMQC) to verify the quality of the Argo floats. The DMQC analysis of Argo floats needs to be done one year from the time when the float has been deployed. The DMQC process is repeated annually, including the profiles from the new currently available profiles, until the float stops working. Therefore, it is crucial to continue a regular collection and submission of the ship-based CTD profiles for DMQC analysis.

The ship CTD reference database for Argo is updated yearly by a team at Coriolis or more often when there is enough new data to justify an upgrade. As this database includes CTDs that are not freely accessible, access is restricted. This database is available on a password-protected FTP site. This ensures that any new ship CTD data which are still under the embargo period will not be used for any other reason than DMQC of Argo floats.

However, the maintenance and development of the CTD reference database for Argo is not trivial and requires continuous additional checks to ensure their high quality. The CTD data submitted by the international groups requires very detailed and careful review before it will be merged into the main dataset for DMQC use. These mostly include a variety of visual inspections and checks to capture and eliminate any duplicates and remove spikes and bad and noisy profiles. A zoom on deep waters is also performed to visualise possible drifts. In recent years, there has been an effort to try to keep metadata information in the source field to better enforce duplicate checking.

The works undertaken by the Euro-Argo RISE partners to improve the quality and update the existing CTD reference database have been carried out at various levels as a part of the WP2 and WP5 work packages. For the WP2 Deliverable 2.7, works have been done to establish high-quality reference datasets and perform regional updates (Marginal seas such as Nordic Seas, the Mediterranean Sea and the Black Sea). Specifically, data from the Unified Database for the Arctic and Subarctic Hydrography (UDASH) were added for the Arctic region. Moreover, in order to identify possible errors, suspicious data or large temporal gaps a diagnosis using the check_CTD-RDB toolbox was performed. As a part of the WP5 Deliverable 5.3, BSH made their efforts in the assessment of the temperature and salinity of data in the Southern Ocean and South Atlantic by adding the additional profiles from the PANGAEA dataset that were not previously integrated into this sector.

2. Assessment and progress review in the reference data for Deep Argo

2.1. GO-SHIP Easy Ocean data product

The GO-SHIP Easy Ocean product includes a collection of ship-based hydrographic sections with high spatial and vertical resolution measurements of physical, chemical, and biological parameters over the full water column essential for physical, chemical, and biological oceanography and climate science. This dataset spans four decades and consists of more than 40 cross-ocean transects. (Figure 2.1) (Katsumata, 2022). GO-SHIP Easy Ocean dataset gives access to a gridded, machine-readable hydrographic ocean dataset, readily available for scientific use.

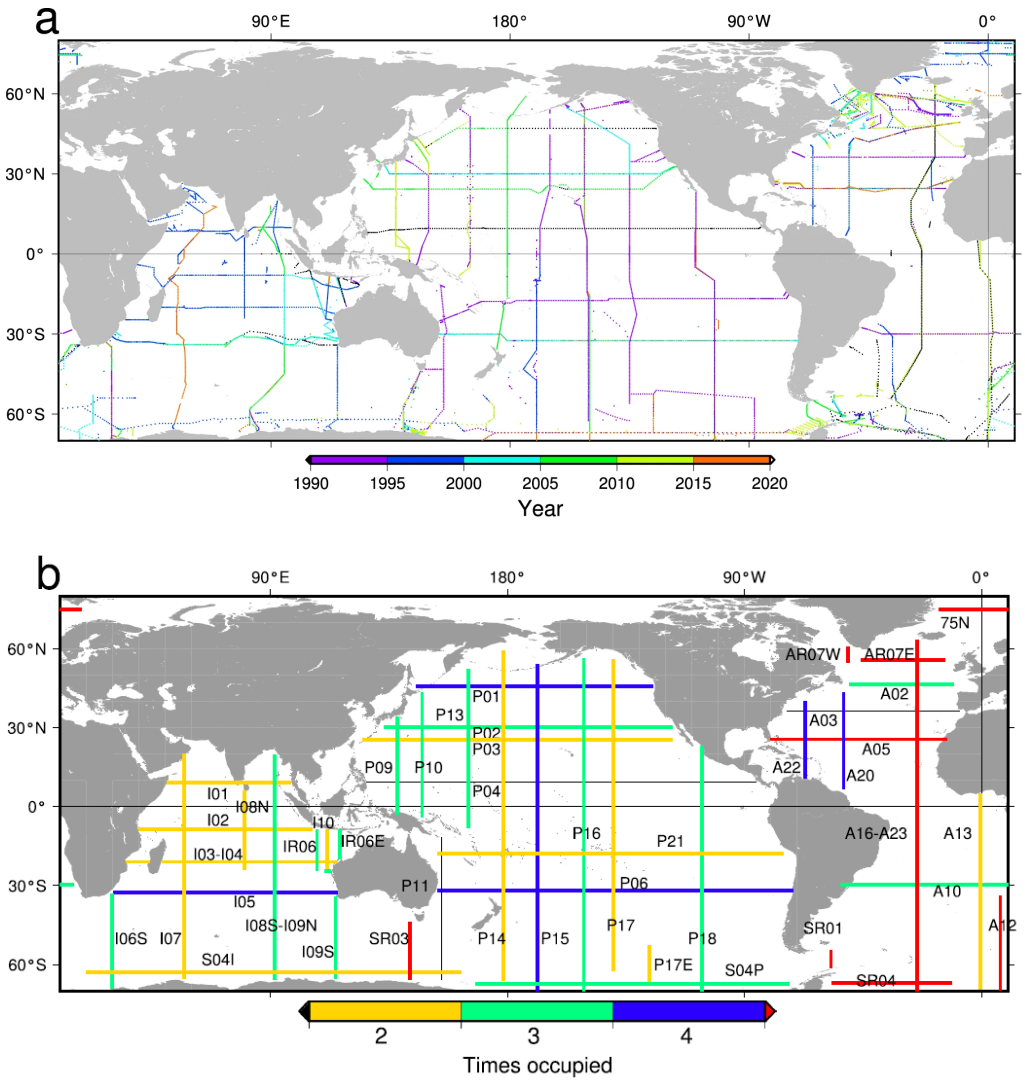


Figure 2.1: a) A map of hydrographic stations included in the section data used to produce the gridded GO-SHIP Easy Ocean data product. The colour shows the year of occupation. b) Approximate locations of GO-SHIP Easy Ocean gridded sections with section names. The colour shows how many times (at least partially) the sections have been occupied as of September 2021 (Katsumata, 2022).

The temperature and salinity from this dataset are used by the team at Coriolis to feed to the CTD reference data for Argo. The GO-SHIP Easy Ocean product is used in the CTD reference data for Argo from 2021. Before that, the GO-SHIP dataset was used.

Before the GO-SHIP Easy Ocean product was implemented to the CTD-referenced data for Argo the data went through a very detailed check to avoid any potential issues in assimilated data. During the initial checks, European partners detected some bad data still present in the GO-SHIP Easy Ocean product (Figures 2.2 and 2.3). They found, for instance, some suspicious profile casts, data points with flags (QC=>2) not appropriate for the DMQC analysis and large spikes. All identified issues have been reported to the GO-SHIP Easy Ocean team and also presented at the annual Argo Data Management Team (ADMT) meetings.

Overall, European partners verified and implemented the CTD reference data for Argo of 16231 hydrographic stations from the uninterpolated format. Any bad measurements were removed from the reference database. The CTD reference data for Argo can be identified in the WMO boxes files with the field QCLevel: GSD (GO-SHIP Deep Argo). If the GO-SHIP profile from CCHDO already existed in the CTD reference, it has been replaced with the easy ocean product's version.

With an increase of the new CTD data from the GO-SHIP Easy Ocean and continuation of performing, additional checks of quality for these data is strongly recommended. However, these additional activities are often very time and resource-consuming and require additional support and funding for the team working on ensuring the best quality of the CTD reference data for Argo is needed.

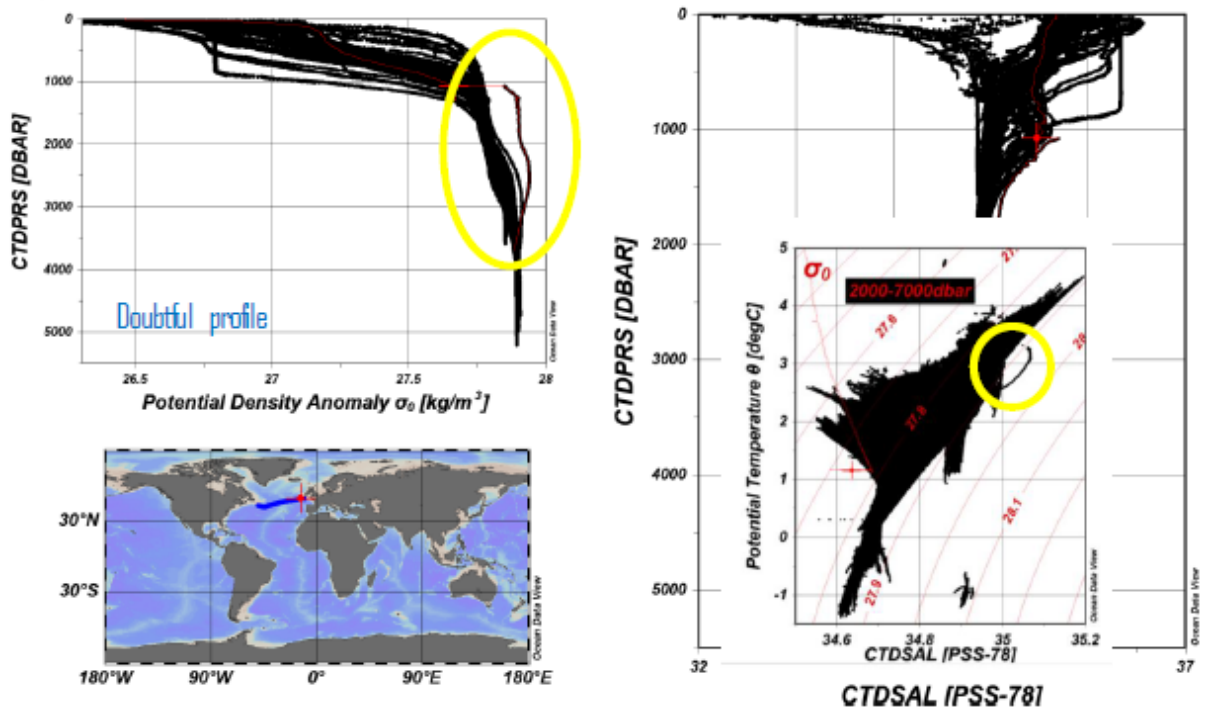


Figure 2.2: Example of identified suspicious bad salinity cast in the GO-SHIP Easy Ocean product.

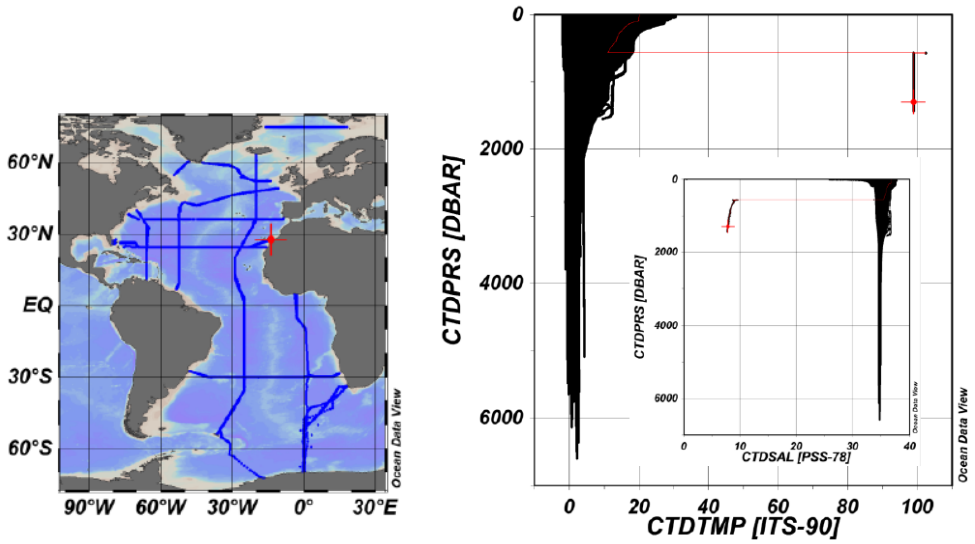


Figure 2.3: Example of identified bad values of temperature in the GO-SHIP Easy Ocean product.

2.2. The North Atlantic

The CTD reference database for Argo is supplied to delayed mode operators and updated on a yearly basis by the Coriolis team. The data quality of this database is crucial for verifying the quality of the salinity measurements of deep Argo floats. As a part of the extension to the deep ocean Euro Argo RISE project, Ifremer/LOPOS team scrutinised historical CTDs profiles in the North Atlantic, with special attention given to the deepest layers. This will ensure the highest quality of the CTD reference data for Argo used for the DMQC analysis.

The review of the currently available CTD reference data for argo (CTD_for_DMQC_2021V02) helped to identify and remove any suspicious profiles. The example with doubtful profiles has been presented in Figure 2.4. The analysis was performed by comparing salinity observed on deep and stable theta levels to the salinity of neighbour profiles, in space and in time. Theta/S diagrams of these suspicious profiles were also checked. More than 500 profiles have been reported to the Coriolis team and excluded from the CTD reference for the Argo database.

The common activity undertaken by the European partners is also acquiring the newest CTD data directly from the Principal Investigations from the research cruises and adding them to the CTD reference data for Argo. Most of these data come from European partners. Very crucial data for the deep DMQC analysis are the CTD casts collected during the float deployment. These data allow the deep DMQC operator to compute the optimised compressibility constant term (CPcor) used to calculate the salinity from the conductivity collected by the deep CTD sensors and correct a bias resulting from the conductivity cell compressibility with increased pressure (more information can be found in Deliverable 3.4). Figure 2.5 shows the example data obtained from the research cruise regularly collecting data at the OVIDE transect.

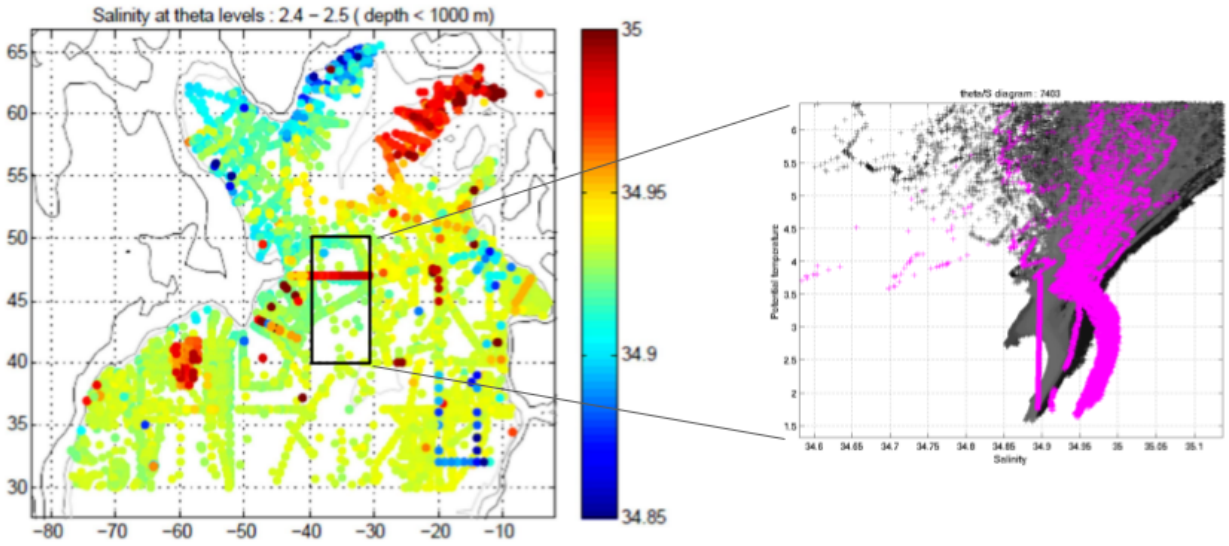


Figure 2.4: Salinity observed at a deep theta level from historical CTD profiles (left panel). Suspicious values were identified (in particular along ship tracks) and the corresponding CTD profiles were compared to neighbouring profiles in a 10°x10° area (right panel). All bad profiles have been excluded from the CTD reference database.

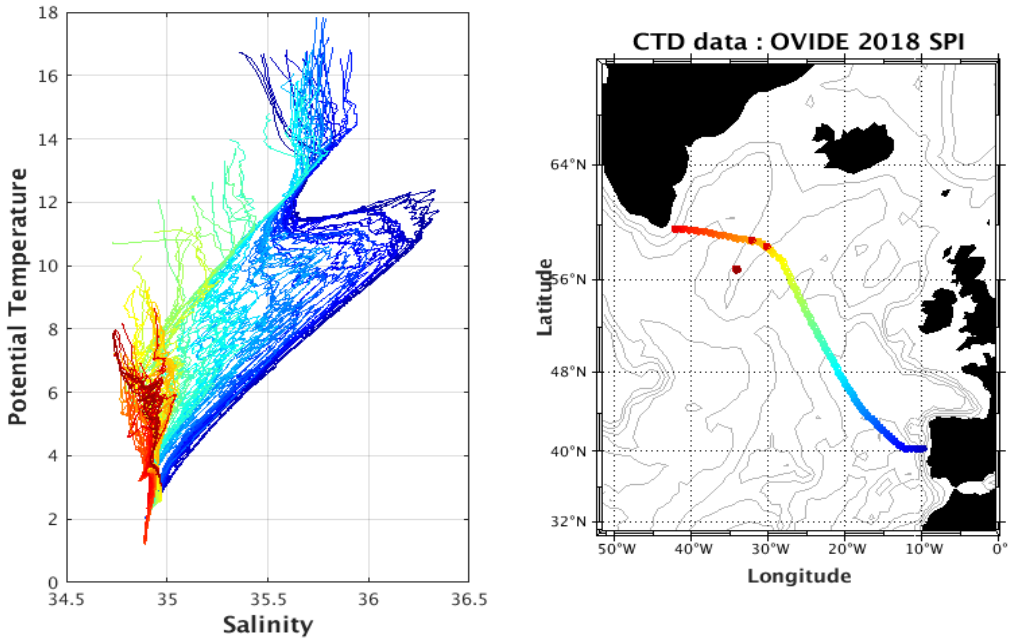


Figure 2.5: Example data acquired CTD casts from the PI during the research cruise at the OVIDE section in the North Atlantic.

The assessment of the temporal and spatial distribution of the currently available CTD reference data for Argo in the North Atlantic (CTD_for_DMQC_2021V02) of data suitable for DMQC analysis of the deep Argo floats shows a relatively good representation of the data (Figure 2.6). The DMQC analysis performed by the European partners in the North Atlantic (more details in Deliverable 3.4) showed that the CTD reference dataset for Argo from this region has been verified as an appropriate source of data to compare with the deep Argo floats. That can make the DMQC analysis of deep floats relatively accurate and efficient in this region. However, the limitation is the relatively small availability of CTD profiles in the central part of the North Atlantic. These gaps in data can be observed in the subtropical gyre. The lack of CTD data cast and high natural variability in the North Atlantic may lead to higher uncertainty in quality checks of deep Argo floats. It is recommended to the DMQC operators to very carefully review the availability, temporal and spatial coverage of the reference data selected for their DMQC analysis of the deep Argo floats.

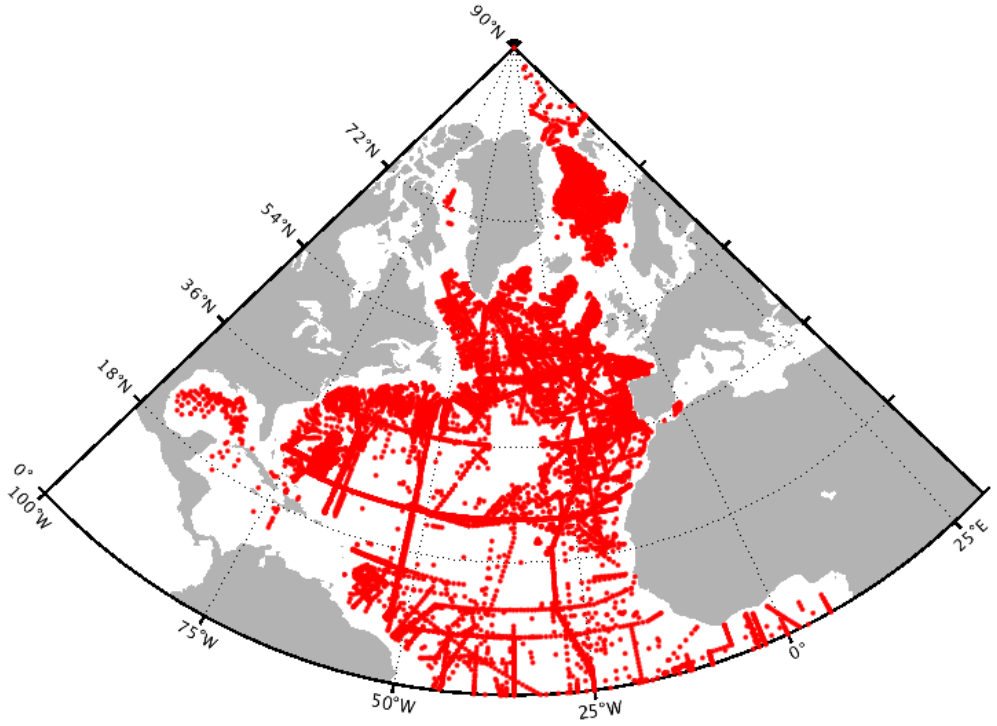


Figure 2.6: Spatial distribution of the profiles in the North Atlantic Ocean which represent data deeper than 2000 dbar.

2.3. The Mediterranean Sea

OGS, responsible for the DMQC activities in the Mediterranean and Black Seas, revised and improved on a regular basis the availability of high-quality ship-based CTD reference data for the quality control of the core and deep Argo physical data, as described in the Deliverable 2.7. In addition to the historical reference dataset provided by Coriolis Global Data Assembly Centre (GDAC), data are

collected from the main European Marine Services and several research institutes at the regional level.

Figure 2.7 shows the time and spatial redistribution of the CTD reference for Argo data used for the DMQC analysis of deep Argo floats from the Mediterranean Sea. The dataset eligible for the deep DMQC analysis consists of 2251 ship-based CTD profiles deeper than 2000 dbar. However, this database is full of gaps in temporal and spatial scales, for instance, the Southern-Central Lonian and the Levantine, represent high scarcity and the oldest CTD data. The assimilated data includes CTD casts from 1995, however, these relatively old data are not efficient for the DMQC analysis of deep Argo floats. This is due to natural changes in properties and extreme climatological events (like the Eastern Mediterranean Transient, Schröder et. al, 2006) that affects the deep layers. The critical issue for the CTD reference data for Argo in the Mediterranean Sea is a lack of available CTD cast after 2019. This is related to very limited research cruises during the COVID-19 pandemic period.

The lack of recent and contemporaneous data on the Deep float mission is a key limitation of the DMQC analysis in the Mediterranean Sea. Without sufficient CTD reference data deep enough at the deployment location, the evaluation of the best CPcor and the OWC results becomes less reliable.

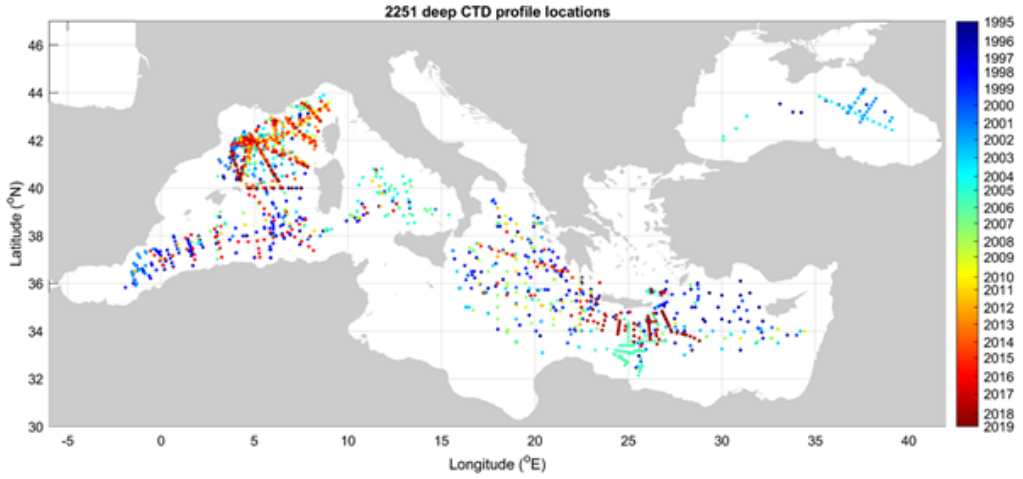


Figure 2.7: *Spatial distribution, colour-coded for time, of the CTD profiles deeper than 2000 dbar in the CTD reference dataset of the Mediterranean Sea (CTD_for_DMQC_2021v2).*

2.4. The South Atlantic

The initial review of the CTD reference database in the South Atlantic (SA) and the Southern Ocean (SO) shows that most of the available data are very old, representing years before the Argo program started (Figure 2.8). Moreover, the spatial distribution of the data shows large areas with almost no reference profiles available such as the central part of the South Atlantic Subtropical Gyre. The most recent reference data in the SO comes mostly from the frequently revisited cruise lines, which seem to be deteriorating over the years.

The efforts made within the Euro-Argo RISE WP5 allowed for some improvement in the availability of CTD reference data for Argo. The works were mostly focused on removing the duplicated profiles and adding profiles from the PANGAEA dataset that were not previously present in the SO sector. The removal of duplicates in the database is necessary to avoid data redundancies, which lead to an artificially high number of profiles available for DMQC and therefore improves the selection of the reference profiles. Although recently collected profiles were made available, the number of profiles per cycle in the Weddell Gyre is low and still, there are large areas without any CTD reference data coverage. A more detailed review of the CTD reference data in the SO can be found in the Deliverable 5.3 report.

A limited and sparse amount of the CTD reference data in this region prevents performing the accurate DMQC analysis in this region leading to a significant drop in the availability of the deep Argo floats in delayed mode. It is recommended to the European and International partners to ensure that there is a clear flow of reference data supplied to the CTD reference database for Argo managed by Ifremer.

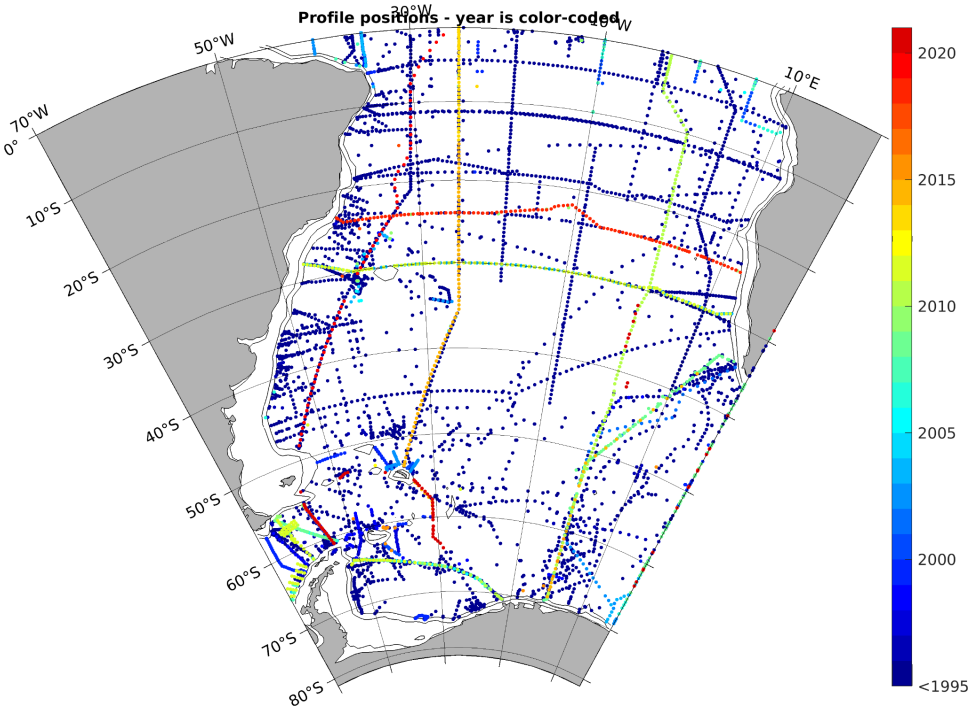


Figure 2.8 Position of the profiles in the South Atlantic and the Southern Ocean colour-coded by year based on the reference data CTD_for_DMQC_2021v2. The CTD profiles represent data deeper than 2000 dbar.

2.5. The Nordic Seas

The improvement of the quality and accessibility of the CTD reference data in the Nordic Seas have been mostly carried out as a part of the MOCCA (Angel-Benavides et al., 2020) and Euro-Argo RISE Deliverable 2.7 projects.

The key improvements made in the Nordic Seas by European partners were to include profiles from Unified Database for the Arctic and Subarctic Hydrography (UDASH) (Behrendt et al. 2018) and from the International Council for the Exploration of the Sea (ICES). These works, however, extended beyond the Nordic Seas and included the entire Arctic Ocean. The CTD data obtained from these sources were carefully quality controlled to ensure the appropriate quality control flags on these data, any duplicates in data were removed and the metadata information was appropriately saved to the source field. Moreover, to improve the status of the reference database the European partners from BSH also added to the CTD reference data for Argo data acquired from alternative sources such as PANGAEA and NABOS (Nansen and Amundsen Basins Observational System). PANGAEA data centre does not deliver its data directly into the WOD. The assimilated data were successively added to the CTD reference data for Argo starting from the CTD_for_DMQC_2020v1 following onward releases of the version of this reference data.

The Euro-Argo RISE partners have developed the shared software allowing the merging of all new datasets and performing additional checks using the Matlab scripts available on GitHub (clean_CTD-RDB_for2021v01release). The diagnosis of the CTD reference data can be performed using the shared software check_CTD-RDB, available on GitHub.

Despite all the efforts to improve the quality of existing data in the CTD reference database and add previously unavailable historical data there, the most concerning issue in the Nordic Seas is the lack of the most recent reference data in this region. The most recent data in the Nordic Seas in the CTD reference data for Argo comes from 2018 (Figure 2.9). This makes the outputs of the OWC analysis procedure potentially unreliable.

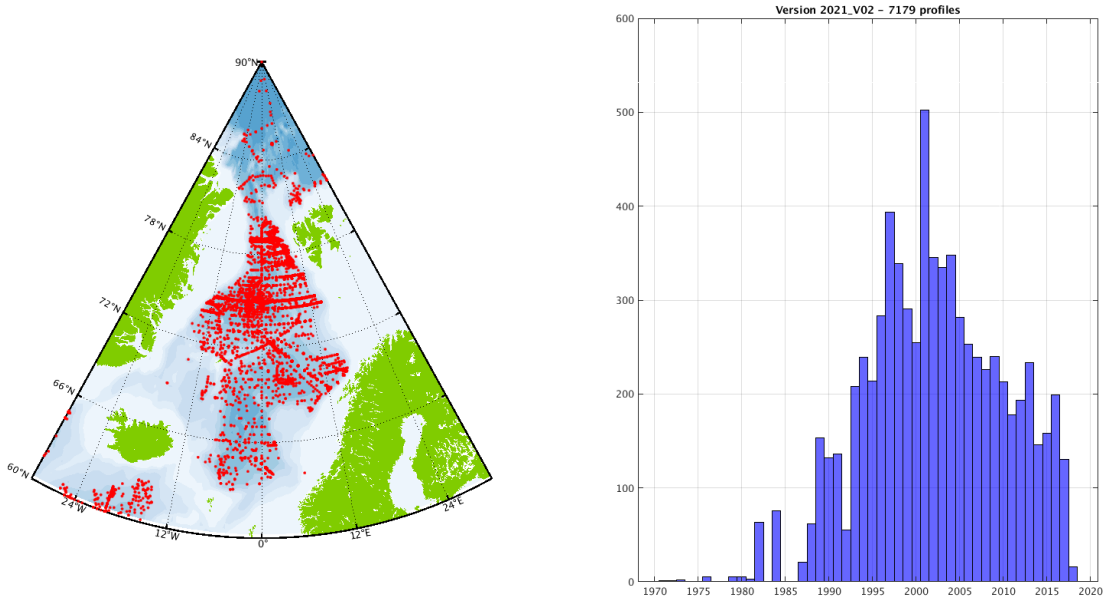


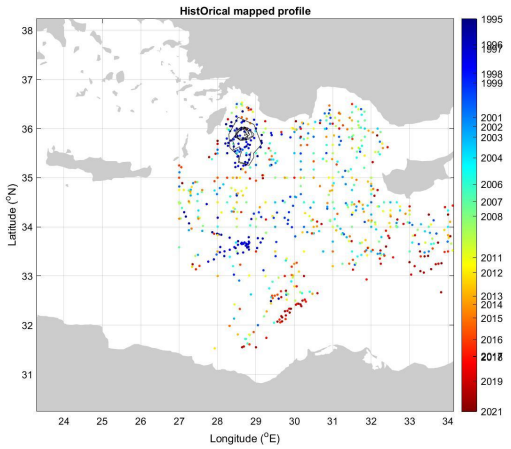
Figure 2.9: Spatial distribution of the profiles in the Arctic Ocean which represent data deeper than 2000 dbar and a corresponding number of profiles by year, based on the reference data CTD_for_DMQC_2021v2.

3. Importance of the CTD reference data and OWC configurations in the quality control analysis

In the DMQC analysis of deep Argo floats, the density distribution of the CTD reference data below 2000 dbar plays a crucial role in the objective salinity mapping calculations. The age, spatial length and time scale configurations selected in the OWC software configurations need to be appropriate to the availability of reference data for the specific regions in the deep ocean. For regions where reference data are sparse in the deep ocean, it is likely that mapping scales in the OWC codes will need to be modified (e.g. extended) to correspond with the reference data distribution. The DMQC operators of deep Argo floats need to have extensive awareness about the reference data coverage in areas of deep float operation and pay special attention to selecting decorrelation length scales there.

Figure 3.1 shows an example of the DMQC analysis of floats in the Mediterranean Sea demonstrating significant differences in the results due to the selection of the reference data from two different ranges of pressure with the reference data during two separate iterations of the OWC software. These two-run allowed an additional check of potential salinity drift at different water masses and also allowed the possibility to determine different offsets at different pressures, which would be characteristic of a badly determined CpCor. For the first iteration, the selected thickness between 700 and 2500 dbar (upper panel) includes a larger amount and more recent CTD reference data for analysis. While, in the second iteration, where a thickness between 2000 and 2500 dbar was used (lower panel), the reference data are very limited and sparse. The results show that the use of the thicker range of the pressure level with the reference data shows a salty salinity offset of about 0.007 with relatively low associated error bars of ~ 0.003 (Figure 3.1 B). There the use of reference data from below 2000 dbar shows salty offset reaching or around 0.01 with much larger uncertainty errors of around 0.008 (Figure 3.1 D). These results indicated that the use of the thicker range of pressure with the reverence data (700-2500 dbar) allowed for more reliable estimates of the quality of this deep Argo float.

A)



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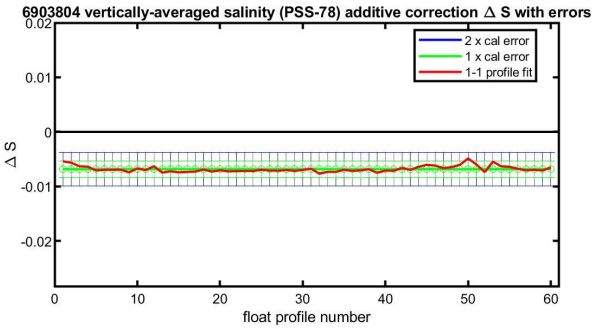
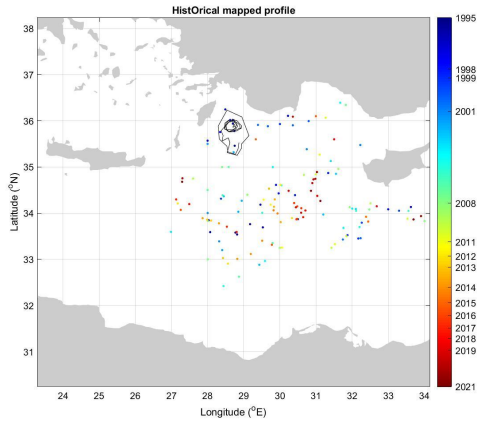


C)



D)

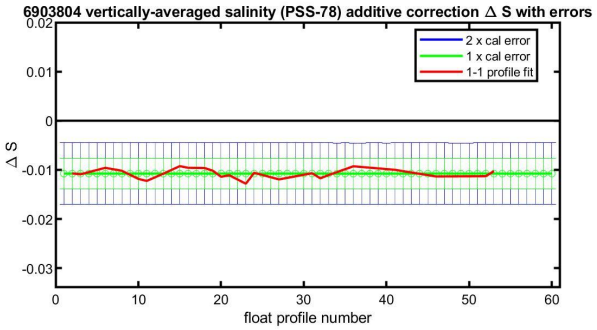


Figure 3.1: Float 6903204. Results from the OWC software using: upper panel- A) the reference data from 700 to 2500 dbar and B) the evolution of the suggested adjustment with time. Bottom panel - C) the reference data from 2000 to 2500 dbar and D) the evolution of the suggested adjustment with time.

4. Summary and recommendations

4.1. Regions with limited reference data

The review of the regions where the European deep Argo fleet is deployed reveals a concerning issue of very limited availability of CTD reference data for the DMQC analysis of deep Argo data. The key areas of the poor density of data coverage are the regions of the South Atlantic and the Southern Ocean as well as the Nordic Seas and the Mediterranean Sea. Except for a very sparse spatial coverage of the CTD reference data for Argo in these regions, the issue is also relatively old data

there. The limited availability of the CTD reference data for Argo can cause a huge problem to perform reliable DMQC analysis of deep Argo floats.

This issue could be overcome by strengthening cooperation between both European and International partners in regular sharing of the CTD reference dataset with Coriolis and providing support in quality control of these data.

Another recommendation to improve the temporal and spatial coverage of the ship-based CTD data is more coordination in the deployment of deep Argo floats and CTD measurements across the Argo community.

4.2. Issues with data delivery to CTD reference data for Argo from external database data identification with quality

One of the key limitations in performing a sustainable development of the CTD reference database for Argo is a huge issue with the availability of CTD data for some regions, from the last few years. These lead to a lack of sufficient data to be used to verify the quality of deep Argo floats in delayed mode.

It has been observed that European and International Data Centres are struggling to timely deliver to Ifremer the CTD observational data. Some data centres are currently working to restore their pipelines to the key external data centres such as ICES and WOD, where when ready, data will be sent in reverse chronological order (i.e. most recent first). These will be further available to be pulled by Ifremer to the CTD reference data for Argo. While others don't send data to external databases and reference data operators need to regularly investigate potential sources of data.

Another limitation for data centres which causes a delay in data submission to the external databases can be an issue during the internal processing procedures due to a delay in sending data from PIs to data centres or an issue with sending data with incomplete metadata. This prevents a further redistribution of CTD datasets until all data information will be obtained.

Some data centres or PI's might also be late in the submission of the ship-based CTD to Ifremer due to the embargo period. It would be worth more widely reminding that all of the CTD data submitted to Ifremer are used to compile the CTD reference data for Argo. These data are well secured, access is password restricted and these data are only used for DMQC analysis of Argo floats.

We also found that some DM operators seem to use their own reference databases which are a combination of the CTD reference database for Argo maintained by Coriolis and data coming from different sources (embargoed CTD, CTD data from datasets such as Copernicus, etc). It would be very beneficial for more knowledge and experience exchange between DM and CTD data operators and that the DM operators could provide the Argo community with possible data deemed useful for data calibration.

Over the last two years during the period of the Covid-19 pandemic, a majority of research cruises performing the CTD measurements have been postponed. This gap in the availability of the CTD will also have a significant effect on the DMQC analysis of deep Argo floats.

The key role for European Argo partners is to ensure a clear flow of climatology data supplied to the ship CTD reference database managed by Ifremer. European Argo partners should work to enhance the amount of data included in this dataset. This could be achieved by initiating much closer collaboration with the European and International PI's and data centres.

Additionally, a very helpful step to increase the number of submitted reference data to Ifremer would be that the Euro-Argo partners could start to build up the list of existing but not submitted cruises with CTD and request them specifically from the identified data centres of PI more individually.

4.3. Maintenance effort of the reference data

Each year, the new CTDs available (GO-SHIP Easy Ocean program and others) on the CCHDO website are downloaded to be added to the reference database as well as data updated from the WOD database and directly from PI's. Before the data will be assimilated into the CTD reference data for Argo, any new data have to go through a series of additional quality control checks to remove any bad data or duplicates in measurements and actively identify the new potential sources of CTD data. Hence there is a constant need for an additional audit of data submitted to Ifremer. Moreover, due to continuous developments, growth of the amount of data to analyse and technical improvements of the CTD reference data for Argo, the CTD data operator has to continuously upskill and expand its accountabilities.

Currently, in Ifremer, there is only one person working full-time on this database. This person is collaboratively working with the CCHDO and indirectly with the US-NODC. This single person is responsible for all of the work with the adoption of the CTD data and is most knowledgeable and skilled in this mission. A lack of any additional dedicated team is creating a very high risk for the potential single point of failure. This could lead to further issues in knowledge transfer and failure in the sustainable long-term development of the CTD reference data for Argo, which is used by the entire International Argo community.

Some temporary support in improving the CTD reference data for Argo have been obtained from the European partner (BSH) as a part of the MOCCA and the Euro-Argo RISE WP2 project. This support allowed us to perform some quality checks on both metadata and CTD data itself. This collaboration led also to create and improve the availability of shared software at GitHub for some initial quality checks of CTD data.

All of these works require a tremendous amount of time and attention to detail from the CTD reference data operator which exceeds the capacity of one full-time. **It is strongly recommended to increase the team of permanent CTD reference data operators.**

A potential group which could more permanently support the development of the CTD reference database for Argo from the specific ocean regions could be the Argo Regional Centres. European partners are well placed to facilitate this as coordinating members of Argo Regional Centres in the Atlantic Ocean, the Southern Ocean and the Mediterranean Sea. This collaboration could be extended also to other Argo Regional Centres operating in the Pacific and Indian Oceans.

5. References

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