DMQC Cookbook for Core Argo parameters

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... items can be added to address other regions

This DMQC cookbook was initiated after the 1st EU DMQC workshop held in Brest in April 2018, under the MOCCA project. Lately, this work has been undertaken under EuroArgo RISE project.

The main objectives of the 1st EU DMQC workshop was to bring all EU countries towards the same level of DMQC knowledge and to start sharing DMQC procedures/tools/methods.

The initial content of this cookbook is then based on presentations made at the 1st EU DMQC workshop. The DMQC cookbook documents the end-to-end processing chain, provides guidelines on existing manuals, and explains best practices through case studies. It could also serve as a basis for any future DMQC workshops.

This cookbook is of course intended to evolve and be extended to other ocean areas over time. Any further contributions would be very welcome.

1. Prerequisites

Contacts: C. Cabanes, G. Notarstefano, C. Coatanoan

Argo data access

Data are available on **GDAC FTP servers** at:

- Coriolis: ftp://ftp.ifremer.fr/ifremer/argo
- US GODAE:

ftp://usgodae.org/pub/outgoing/argo

Fichier : 6902766_Rtraj.nc Fichier : 6902766_meta.nc Fichier : 6902766_prof.nc Fichier : 6902766_tech.nc

FIG 1: Example of files found in the folder /dac/coriolis/6902766/

The trajectory file (traj.nc) contains locations, cycle timing and ocean state measurements performed at various intermediate times during the cycle (e.g. pressure measured at depth during the drift). The **metadata file** (meta.nc) contains information about an Argo float (e.g. sensor information,...). The configuration, technical file (tech.nc) contains technical information from an Argo float for each cycle (e.g. battery, pressure offset measured at surface). Pressure, temperature and salinity vertical profiles from all cycles are merged into the profile file (prof.nc). If the float measures biogeochemical (BGC) parameters, Sprof.nc file will also be included. To perform the DMQC of Argo core parameters (PRES, TEMP, PSAL) the operator modifies the **single-cycle profile files** that are stored in the "profiles" folder.

File naming convention

Naming convention for **single-cycle profile files** can be found on the ARGO user's manual (section 4.1.1). For each cycle, **core parameters** are stored in an R_file (ex R6902766_090.nc) that becomes a D_file (ex D6902766_001.nc) as soon as delayed mode analysis has been performed for this cycle.

Core-Argo single-cycle profile file, format 3.1

Full description of format and variables can be found on the ARGO user's manual (section 2.2).

A **core-Argo profile** contains the CTD sensor parameters (pressure, temperature, salinity, conductivity).

An **Argo single-cycle profile file** may contain several profiles from a single cycle (N_PROF can be greater than 1) that are measured at the same location and time. The **primary profile** is always stored with N_PROF=1. Other profiles (N_PROF>1) contain **core parameters** acquired with another sampling scheme (e.g. near surface data acquired with unpumped CTD). More details can be found in the ARGO user's manual (section 2.6.1.1 and reference table 16).

A 'R'-core file becomes a 'D'-core file only when DMQC has been processed on the primary profile (N_PROF=1).

<PARAM>, <PARAM>_ADJUSTED, and DATA_MODE

<**PARAM>** contains the raw values telemetered from the floats. <**PARAM>_ADJUSTED** contains adjusted values, either in real time (DATA_MODE(N_PROF) = 'A') or in delayed time (DATA_MODE(N_PROF) = 'D'). More details on real time adjustment on vertical profiles can be found in the ARGO quality control manual (section 2.3).

the adjustment lf is equal to zero <PARAM>_ADJUSTED = <PARAM>. lf <PARAM>_ADJUSTED, <PARAM_ADJUSTED_QC and <PARAM>_ADJUSTED_ERROR are all empty (Fill Value), this means that the profile has not gone through any adjustment determination procedure either in real or delayed time $(DATA_MODE (N_PROF) = 'R').$

Real time and near Real Time Quality Checks

<**PARAM>_QC** contains QC flags that pertain to the values in <PARAM>. The <PARAM>_QC flags are first defined in real time after a series of simple automatic tests to detect gross errors. These tests are fully described in the ARGO quality control manual (section 2.1) and the flag scale is explained in the Reference Table 2 (section 3.2). A more complex statistical test is also performed on a daily basis at Coriolis data center. This test, called **"Min/Max test"** uses validity intervals based on local Minimum/Maximum values inferred from historical datasets rather than from more classical (Mean +/- N*Std) values (Gourrion et al, 2020).

Moreover, at Coriolis, all profiles are visually checked by an operator. If necessary, either the <PARAM>_QC flags are modified, if the float belongs to the Coriolis DAC, or a message is sent to the other DACs. Each month, a report synthesizes all the messages sent to other DACs. In particular, this report gives a list of floats for which a suspicious drift has been detected during the month.

Altimetry quality Checks

The dynamic height anomalies (DHA) from the Argo T/S profiles are compared to the co-located sea level anomalies (SLA) from altimetry in order to identify anomalies in the floats' measurements (Guinehut et al, 2008). The main objective is to detect float malfunctions before it goes through DMQC and then flag bad data more quickly.



In addition to real time flags, a comparison to altimetry is performed quarterly. Anomalies detected can be either a spike, an offset or a drift (see for example **Figure 2**). Status on the anomalies detected is distributed through the Argo Information Center (AIC) and stored in the AIC database. The full list of anomalies can be found here. An email is sent for each anomaly to the DAC & DM-operator. Analysis of the DM-operator is required to confirm the alert and flag bad data. Feedback from the DM-operator must be done through the link provided in the email.

Grey List

A grey list (ar_greylist.txt) has been created to have the possibility to **flag real time data** from sensors that are potentially not working correctly. It's the DM-operator responsibility to insert a float parameter in the grey list either because a problem has been detected by some external tests (e.g. altimetry tests) or because you have detected a sensor problem that cannot be corrected in real time for a float that is still active. More details on the grey list can be found in the ARGO quality control manual (section 2.1.2, test 15). Note that a float parameter can be put automatically in the grey list if it fails the MIN/MAX test documented in the Coriolis monthly report.

Delayed-Mode data accuracy

Salinity

For Argo, it is expected to have conductivity sensors capable of making measurements of salinity that are stable to 0.01 PSU over the course of 4 or 5 years (Argo Science Team, 2000). Problems (leakage of biocide into the conductivity cell, faulty electronics components, volume variation of the conductivity cell due to bio-fouling) can lead to measurements that are outside the expected accuracy. Delayed-mode check for salinity drifts and offsets is necessary.

Pressure

Expected accuracy for Argo pressure is 2.4 dbar. Pressure is generally measured within the accuracy, but problems (e.g. oil microleaks) can lead to measurements that are outside the expected accuracy. Delayed-mode check for pressure drifts and offsets is necessary.

Temperature

Expected accuracy for Argo temperature is 0.002 °C (generally measured within the accuracy).

For details on how the accuracies of Argo delayed-mode data have been evaluated, please refer to the Argo data paper, Wong et al (2020).

References:

Argo Science Team, 2000. Report of the Argo Science Team 2 nd Meeting (AST-2) March 7-9, 2000, Southampton Oceanography Centre, Southampton U.K., http://www.argo.ucsd.edu/iast2.pdf

Gourrion, J., T. Szekely, R. Killick, B. Owens, G. Reverdin, and B. Chapron, 2020: Improved Statistical Method for Quality Control of Hydrographic Observations. J. Atmos. Oceanic Technol., **37**, 789–806, https://doi.org/10.1175/JTECH-D-18-0244.1.

Guinehut S., C. Coatanoan, A.-L. Dhomps, P.-Y. Le Traon and G. Larnicol, 2008: On the use of satellite altimeter data in Argo quality control, J. Atmos. Oceanic. Technol, Vol. 26, No. 2, pp 395-402.

Wong, A. P. S., Wijffels, S. E., Riser, S. C., Pouliquen, S., Hosoda, S., Roemmich, D., et al. (2020). Argo data 1999–2019: Two million temperature-salinity profiles and subsurface velocity observations from a global array of profiling floats. Frontiers in Marine Science, 7, 700. https://doi.org/10.3389/FMARS.2020.00700

2. DMQC workflow

Contacts : K. Walicka, C. Cabanes

This workflow is given for DMQC analysis of Argo core data (P,T,S). It provides a list of steps from getting R-files from the GDAC to sending the D-files back. This workflow has the following objectives:

- (1) Verify and change QC flags if necessary. This concerns P,T and S data.
- (2) Apply correction to the data.

- In general T is considered as good and no correction is applied to T.

- The correction applied to P is based on the surface pressure offset for floats that do not apply it onboard.

- For S, two types of corrections are required: possibly thermal mass error and bias+drift correction. For the latter case, the OWC method is recommended.

For each step, more details can be found in this cookbook. Full documentation can be found either in the Argo Quality Control Manual or in the README.doc file of the OWC software.

List of steps

- 1. Download single_cycle netcdf profile files from GDAC ftp servers.
- 2. **Find out about the float** and review previous screening:
 - What type of float is it ?
 - When was the float deployed?
 - Is the float still active?
 - Where is the float and what is the trajectory over its lifetime? Has it crossed through different water masses, changed oceanographic regions, etc...?
 - Has the float ever raised an alert (e.g MIN/MAX tests, altimetry checks)
 - Is the float on the grey list?
 - Does the previous screening indicate any problems or concerns?
 - If DMQC has been done on previous profiles what decisions have been made?

This should give you a good indication of what has already been done and any problems associated with the float.

- Screen your float's data: visually inspect profiles (P,T); (P,S); (P/Rho); (Theta/S). Check date and position. Edit raw QC flags (PRES_QC, TEMP_QC and PSAL_QC), position and date QC flags if necessary.
- 4. If applicable, correct pressure for offset or drift using the surface pressure offset (see Argo Quality Control Manual section 3.3). Fill PRES_ADJUSTED, PRES_ADJUSTED_QC and PRES_ADJUSTED_ERROR in the netcdf file. If necessary, re-compute the salinity with the adjusted pressure (fill PSAL_ADJUSTED and PSAL_ADJUSTED_QC).
- 5. If applicable, **correct salinity for cell thermal mass error** (Johnson et al. 2007) and fill PSAL_ADJUSTED, PSAL_ADJUSTED_QC and PSAL_ADJUSTED_ERROR.
- 6. Create **OWC input mat file** from netcdf files. Make sure you upload the latest reference databases.
- 7. Run OWC software that compares float salinity data with historical reference data. You will get calibration files that can be used to correct salinity for drift or offset, if necessary
- 8. Make decisions based on OWC outputs

The outputs from OWC on the float salinity time series are comparaisons against the CTD and Argo reference databases, and are not a definitive recommended correction. Oceanographic evaluation is needed to discern if any detected salinity differences are due to true ocean signals, or are due to sensor drift. The decision-making process is a sum of the specific knowledge about the water mass properties, ocean circulation and mechanisms, and other supportive reports from specific ocean regions. The scientist then has 2 decision options:

(1) Reject the computed adjustment, as float salinities look stable and do not require any corrections, or because the detected salinity difference is due to true ocean signals and not due to sensor drift.

(2) Accept the computed adjustment, if it is determined that the detected salinity difference is due to sensor drift or offset. Endeavor to refine the computed adjustment by refining the parameters setting in OWC.

- 9. Write a report explaining the reasons for your decisions.
- 10. Write the D-files. You must fill PARAM_ADJUSTED, PARAM_ADJUSTED_QC, PARAM_ADJUSTED_ERROR, calibration and history sections of netcdf files even if you have decided that the parameter does not need to be adjusted.

Available softwares and resources

Here is a non exhaustive list:

- Find out about a float: basic plots, technical and metadata informations (**step 2**):

https://fleetmonitoring.euro-argo.eu/dashboard

- Screening profiles and editing QC flags (**step 3**):https://www.seanoe.org/data/00374/48531/
- OWC software (**step 7**):
- https://github.com/ArgoDMQC/

- Others tools and softwares are shared here: https://github.com/euroargodev

- dm_floats: Create OWC input mat file from netcdf files (step 6) and create core Argo D-files using salinity calibration from OWC software (step 10)
- check_CTD-RDB: hosts some code to perform a first diagnosis of the CTD reference database in a user-defined region.
- matlab_profiles_visualization: reads the Argo NetCDF files, converts the files in MATLAB format, allows Argo profiles selection, produces graphs of temperature and salinity, performs a tailored comparison between the float and reference profiles and provides the main information of float profiles.
- Argopy: python tool to load and manipulate Argo data and Argo reference dataset...
- pyowc is a python implementation of the OWC method.

The AST website also has a page listing Argo related softwares.

3. Checks of QC flags in delayed time

Contact: D. Dobler

The automatic RTQC tests flag measurements through a list of robust tests. They are designed to achieve a good robustness rate with as much performance as possible. Based upon alert systems, some profiles are visually inspected in near-real time and corrected by real-time operators. These two first steps are intended to discard the most obvious and large errors but, firstly, they can't trap every single failure or its entire vertical extent and secondly, automatic tests can flag by mistake. The delayed-mode operator should therefore be critical with automatic tests and edit the already set <PARAM>_QC flags when necessary, for erroneous values missed by real-time and near-real time processes. The following subsections present the most common failure cases you may encounter when screening your float's data. They are sorted by observed occurrence frequencies and indications on how to handle them using QC flags are provided.

Conductivity Sensor drift

The most frequent failure is the drift of the conductivity sensor. Applying the OWC method will give a more accurate estimation of the drift and a calibration correction but beforehand, cycles that are known to be unrecoverable can be flagged with QC4.

In Near real time, these drifts can be detected by comparison with the local distribution envelope (MinMax method. Gourrion et al., 2020), see **Figure 1**, or by comparison with altimetry (step performed by CLS) or of course, by any other means.



FIG 1: Salinity in PSU function of pressure in dbar for Float 4902312 cycle 125 and its surrounding platforms. The orange bold curve is cycle 125. The blue limits are minimum and maximum limits from the MinMax Method (Gourrion et al. 2020). The other curves in between (in green for QC1, yellow for QC2, orange for QC3 and red for QC4) are salinity profiles in the surroundings within 2 degrees and 5 years taken from the Coriolis Database. The map in the bottom-left corner gives the localisation of cycle 125 (green square) and of surrounding profiles (dark red squares).

Spikes

The second most frequent failure is spikes. Temperature and/or salinity profiles can be affected. The spike can clearly show up in the density profiles or in the theta-S diagram. This is most likely due to either a failure during the acquisition (and will impact salinity if temperature is affected) or during the transmission. This kind of failure is guite easy to spot and can be flagged with QC4. Special care must be taken when dealing with hedgehog profiles (see Figure 2). In real-time it is often easier for a given immersion level to flag the of {pressure, salinity whole set and temperature} when one of them is out, then to look back at the remaining measurements in comparison with the local distribution to check whether other measurements are out or not. In delayed mode, more care can be given to pick out only real spikes.

Part I: General Information for DMQC analysis



(top) and salinity in PSU (bottom) function of pressure (in dbar) for Float 3900844 cycle 281.

Erratic temperature or salinity profiles

Erratic profiles rank third in terms of occurrence. These are fairly easy to spot and can sometimes follow a conductivity drift. They must be flagged with QC4 of course.

Transient dirt or pollution events

Let us explain this type of failure in more detail: It is transient because the measurements can recover later, during the same cycle or during the next several cycles. There have also been cases where the measures have recovered after several cycles. This is probably due to some "dirt" that gets into the water pipe and impacts the conductivity measurements. This dirt can be biological, mineral, plastic, etc. Wobbling salinity and density profiles are typical of this failure, with variations in density similar in magnitude to those of salinity (see **Figure 3**). This correlation can be explained by the linearized equation of state:

 $\rho = \rho_0 (1 - \alpha_T (T - T_0) + \beta_S (S - S0) + \gamma_p (p - p_0))$

Let δS be the salinity anomaly due to the transient dirt and $\delta \rho$ be the corresponding density anomaly. This yields:

$$\rho + \delta \rho = \rho_0 (1 - \alpha_T (T - T_0) + \beta_S (S + \delta S - S0))$$

$$+ \gamma_p (p - p_0))$$

$$\delta \rho = \rho_0 \beta_S \delta S$$

Given that:

then

$$ho_0 \# 10^3 kg/m3$$

 $ho_S \# 7.6 (+ / - 0.2) * 10^{-4} PSU^{-1}$

δρ#δS



FIG 3: Salinity in PSU (top) and potential density anomaly (sigma0) in kg/m3 (bottom) function of pressure (in dbar). Float 6901578 cycle 78 is in bold line (in red above 580 dbar and in green below) and the other cycles of float 6901578 are in thin green lines. Blue limits are MinMax method thresholds

In the example given in **Figure 3**, salinity variations above 350 dbar are within the expected variability inferred from previous and next profiles of the same float. Without looking at the density profile which shows that the failure goes up to the surface, an operator might be tempted to flag only the lower part of the profile (350 to 580 dbar). This example shows that it is necessary to visually inspect not only the other salinity profiles of the same float but also the corresponding density profiles to accurately flag this type of failure.

The real-time automatic tests often down-qualify only a part of the affected salinity measurements when they fail the density inversion test. This automatic test also down-qualified the corresponding temperature points. Once a transient dirt has been diagnosed, the corresponding temperature measurements should be put back to QC1 and the affected salinity measurements should be QC4.

Thermal mass error



FIG 4: Temperature in degrees celsius (top) and practical salinity in PSU (bottom) function of pressure (in dbar) for Float 4901797 cycle 45. Blue limits are MinMax method thresholds

The primary source of dynamic errors when calculating salinity are the temperature and the conductivity sensor misalignment (sensors do not sample the same water parcel) and the conductivity cell thermal mass, when conductivity cell temperature does not match the measured seawater temperature (Johnson et al. 2007, Martini et al., 2019). Both errors affect the salinity profile on the thermocline and on the base of the mixed layer. There can be a spike just above the halocline and a decaying exponential on the base of the surface mixed layer (see Figure 4). Please keep in mind that measurements in the halocline are also affected. This problem is often flagged in

real-time (with mainly a QC4). As mentioned in the Argo Quality control document, an algorithm is available to correct thermal mass error and can be asked to G.C. Johnson.

Noisy conductivity sensors

Some conductivity sensors can be very noisy and often trigger the Real-Time QC spike test (**Figure 5**). The biggest spikes should of course be flagged with QC4 (if not already done in RTQC) but it would be a good usage to at least down-qualify the remaining measures to QC2 as they visually disrespect the known accuracy.



FIG 5: Salinity in PSU (top) and potential density anomaly (sigma0) in kg/m3 (bottom) function of pressure (in dbar) for cycles 251 to 289 of Float 5904325. Red segments are QC4 and yellow segments are QC2. Blue limits are MinMax method thresholds.

Frozen temperature profiles

This case is very rare but **Figure 6** gives an illustration of the observed symptoms. The almost "frozen-like" part of the profile should be flagged with QC4.



Weird temperature profiles

This case is also rare: the temperature is weird compared to the surrounding distribution envelope. Most often the salinity profile is also out of bounds. This can be due to a failure in the pressure measurements (Druck pressure sensor "oil microleak" or Incorrect pressure sensor coefficient as explained in the Argo Quality Control Manual) and this will affect both temperature and salinity profiles shape (see **Figure 7**). There is no rule for setting a QC in this case, at least QC2 if pressure can be recovered, or QC4 if pressure can't be recovered.



FIG 7: Temperature in degrees celsius function of pressure in dbar (top) and practical salinity in PSU function of temperature (bottom). Float 3901931 cycle 108 is in bold red dotted curve, surrounding profiles in a 5°/30 days area are in thin green curves. Blue limits are MinMax method thresholds

Position and Date checks

Make sure the positions are reasonable. Pay attention to check interpolated positions, especially when they are missing for many positions in a row and no longer make sense or when 180 degrees of longitude is crossed. The date consistency should also be checked.

References

Johnson, G. C., J. M.Toole, and N. G. Larson, 2007:Sensor corrections for Sea-Bird SBE-41CP and SBE-41 CTDs. J. Atmos. Oceanic Technol., 24, 1117–1130, https://doi.org/10.1175/JTECH2016.1.

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Martini, K. I., D. J. Murphy, R. W. Schmitt, and N. G. Larson, 2019: Corrections for Pumped SBE 41CP CTDs Determined from Stratified Tank Experiments. J. Atmos. Oceanic Technol., **36**, 733–744, https://doi.org/10.1175/JTECH-D-18-0050.1.

4. Pressure corrections

Contacts: B. Klein

The only way to assess the quality and possible bias of the pressure sensor is to use the surface pressure value measured by the float. This information is provided in the technical files (wmoxxx_tech.nc) as the surface pressure offset value. The surface pressure offset can be found under different names depending on how the float stores this information and whether the float auto-corrects the pressure or not. Surface pressure offset is a mandatory variable in the Argo files and the naming of variables is curated and given in a list of technical parameter names. This table also describes actions required in RT or DM.

Corrections of surface pressure for PROVOR/ARVOR floats and SOLO floats

No correction is needed as the surface pressure offset is used onboard to correct pressure values. However, screening the surface pressure offset helps identify failure of the pressure sensor.

Despiking of surface pressure and pressure corrections for APEX and Navis floats

APEX floats return "raw" pressures, which are stored in the variable PRES in the Argo netCDF files. The floats record surface pressure at the end of each surface transmission time but only telemeter the information with the profile data of the next cycle. In real-time pressure adjustment will therefore be applied by using SURFACE PRESSURE (SP) values from the previous cycle returned by the APEX floats (see Argo QC manual section 2.3.1). These SP values are stored in the Argo technical files in specific variables named:

PRES_SurfaceOffsetTruncatedPlus5dbar_dbar or PRES_SurfaceOffsetNotTruncated_dbar. More instructions on how to filter the SP data appropriately for real-time adjustments and how to fill adjusted parameters appropriately is given in section 2.3.1 of the Argo QC manual. Similar to the real-time procedure, pressures from APEX floats need to be adjusted for offsets by using SURFACE PRESSURE (SP) values in delayed-mode. The various steps are explained in detail in section 3.3.1 of the Argo Oc manual. The raw data transmitted by a float (green line in **Figure 1**) need to be despiked by the dmgc operator by comparing the SP values with a smoothed time series derived from a 5-point median filter (blue line in **Figure 1**). Spikes and missing values should be replaced bv interpolations between good neighboring points. Missing values occurring at the end of the time series can be extrapolated from the last good point. The resulting SP time series should then be visually inspected (Figure 1) and the clean SP values for cycle i+1 are used to adjust pressures in cycle i.

PRES_ADJUSTED (cycle *i*) = PRES (cycle *i*) - SP (cycle *i*+1).

After adjustment, delayed-mode operators should check that PRES_ADJUSTED > 0 (see Figure 2). SP and PRES values for resulting negative adjusted pressures should carefully be examined again and be flagged appropriately since they are likely to be erroneous. Salinity needs to be recalculated by using PRES_ADJUSTED and recorded in PSAL_ADJUSTED.







Figure 3 gives an example of a float (WMO 6900564) which showed continuous negative drift of its SP readings reaching negative offsets of -8 dbar at the end of its lifetime. This is due to oil microleak defect in some Druck pressure sensors (see part I.7). The SP time series is used to adjust pressure in delayed time.



How to flag APEX profiles with truncated negative surface pressure values

APEX floats from the early times of the program with Apf-5, Apf-7, or Apf-8 controllers need special treatment by the dm-operators because they truncated their SP values to zero for negative SP values. It is unlikely that dm-operators nowadays will be dealing with such floats unless floats have to be re-examined or reformatted. For completeness, a short paragraph is given below and the reader is referred to the Argo QC manual for more information.

The problem with some of these APEX floats having unknown negative pressure error escalated with the discovery of the oil microleak defect in Druck pressure sensors (see part I.7). If a pressure sensor develops a negative pressure drift on APEX floats with an APF8 or earlier series controller, the reported SP values are always zero. In principle, SP values can also be zero for longer periods due to atmospheric conditions without microleak problems, but in such instances SP values should return to positive values again during the SP time series (see Figure 4). Profiles from continuous periods with zero SP readings are labeled as having "Truncating Negative Pressure Drifts" or TNPD and are not correctable. Argo has performed audits of the treatment of pressure biases in the global data set. TNPD affected profiles can be identified in the profile files through the character string "TNPD" in the SCIENTIFIC_CALIB_COMMENT field for PRES. TNPD data are labeled with PRES_ADJUSTED_QC '2'. The more severe ones = have PRES_ADJUSTED_ERROR = 20db.

The Argo QC manual gives detailed examples and schematic graphics about TNPD float DMQC treatment in section 3.3.2. These examples illustrate how to identify the 'Truncated Negative Pressure Drift' parts of a float's time series, i.e. continuous zero readings and distinguish it from periods when SP is influenced by atmospheric conditions, i.e. reverts back to positive values or contains occasional positive values. It was agreed that the continuous valid zero-reading period needs to span at least 6 months, preferably longer. This captures the microleakers whose oil leak rates are fastest and allows for seasonal variability from half of an annual cycle when surface pressure values may read just below zero.



5. Reference databases for salinity

Contacts: C. Coatanoan

The OWC software uses historical salinity interpolated to the float positions and observed θ levels. Therefore, common reference databases used by all DM-operators and containing only high quality data, in the OWC format are needed.

Content

Two reference databases are supplied to the DM-operators :

The CTD reference database : it is maintained by Coriolis (C. Coatanoan) and contains historical shipboard CTD data obtained from the World Ocean Database (OCL), from the CLIVAR and Carbon Hydrographic Data Office (CCHDO), from the International Council for the Exploration of the Sea (ICES) or directly from individual scientists. Spatial coverage is displayed on **Figure 1**.

The Argo reference database : it is maintained by J. Gilson and contains historical Argo profiles that have been verified in delayed time and have not required any salinity adjustments. Spatial coverage is displayed on **Figure 2.**

Bottle data were originally used in areas where CTD data were too sparse. But because they were of lower quality and the spatial coverage from Argo was growing, it was decided not to maintain such a reference database. You can still use your own bottle data for your analysis as soon as it is put in the same format as CTD and Argo reference databases.



FIG 1: Current spatial coverage of CTD reference database



A full list of criteria for CTD or Argo profiles to be retained in the reference databases are provided in the ARGO quality control manual (Appendix 4.5 and 4.6).

Note that only profiles deeper than 900 dbar (for CTD casts) and 800 dbar (for Argo) are retained in the reference databases. This may be problematic in some shallow areas (e.g , Baltic Sea).

Distribution and format

These two reference databases are distributed on *ftp.ifremer.fr*. You should ask for login/password to codac@ifremer.fr.

As these databases are regularly updated you should **ensure that you are using the latest version available.**

In the OWC format, Argo and CTD reference profiles are stored in mat files - one file per ten-degree latitude-longitude boxes. These boxes are numbered following the World Meteorological Organization (WMO) ten-degree square numbering scheme. You can see the geographical area that corresponds to each WMO number here.

The variables stored in *ctd_****.mat* or *argo_****.mat* files are listed in this readme file (item 2). Note that another variable - **qc_level** (1xn) - has been added but only to the *ctd_****.mat* files. **qc_level** indicates which is the profile provider: COR (Coriolis), CCH (CCHDO), GSH (GO-SHIP), OCL, ICE (ICES), SPI

(individual scientist) or OGS (Argo Italy). This is different from the **source** variable which provides a unique identifier per profile. Knowing the provider gives a general indication of the level of quality that can be expected (better quality for SPI for example).

The file **/data/constants/wmo_boxes.mat** is used by OWC software to check which WMO box has what data available. Therefore, **you must update this file** each time you update the reference databases. More explanations on this file can be found here (item 3)

wmo	CTD	Bottle	Argo
1800	0	0	1
1700	1	0	0
1600	1	0	0
1000	1	0	0
3000	1	0	0

FIG3: Example of the content of wmo_boxes.mat file. *0* = no data, or do not use. 1 = data exists, and use them.

You can also **edit this file to exclude some reference data** from your analysis. If, for example, you do not want to use Argo data, simply set the column "Argo" to all 0s.

Other possibilities to access the **Argo** reference database

Since Argo data included in the reference database are publicly available, Ifremer provides ERDDAP access to this subset of the Argo dataset. It is available here:

http://www.ifremer.fr/erddap/tabledap/ArgoFlo ats-ref.html

This access allows for easier selection and visualisation of reference data.

Argo reference data can furthermore be fetched using the argopy python library, using the 'ref' keyword in the definition of fetchers, for instance:

from argopy import DataFetcher as Fetcher

f = Fetcher(src='erddap', ds='ref')
Then, you can retrieve Argo reference data for a
specific space/time region like this:

ds = f.region([-85, -45, 10, 20, 0, 1000, `2012-01', `2012-02']).to_xarray() This command example will return Argo reference data for the region 85W/45W, 10N/20N, 0-1000db and for January 2012.

Quality controls

Additional quality checks are performed whenever new CTD data are included in the CTD reference database (e.g. visual inspection, plot of theta/S diagram, etc.). This is particularly necessary because the CTD profiles included in the database are on "observed levels" and some data providers (e.g. OCL) only check the quality of their data on "standard levels". Therefore, quality flags provided on the observed levels need to be checked again.



FIG4: CTD data in box 3514 : before quality control (left) and after (right)

Feedback from users

If you are using CTD and Argo reference databases and have found some suspicious data, please send an email to Christine Coatanoan or John Gilson indicating the version of the database (e.g. 2019V01), the wmo box number (e.g. 3514) and profile number of suspicious profiles in the mat file. Any feedback from users is very important to improve the reference data quality. Your input will be taken into account in the following version.

Regional Needs

The work done at global level does not always fit the regional needs. This may be because the region has shallow areas (not covered in the reference database due to the 900 db threshold used to retain CTD profiles for example) or because high variability requires greater spatial and temporal coverage using other CTD sources, through personal contacts or existing regional databases. The additional work done for Mediterannean, Black Sea, and Nordic Seas is fully described in part II of this cookbook. Whenever possible (e.g. unrestricted data), work carried out in specific regions improves the global reference database.

6. Salinity drift or offset corrections

Contacts: B. Owens, A. Wong, C. Cabanes

Background

OWC is a package used for calibrating profiling float conductivity sensor drift. The matlab version can be downloaded here. A python version is under development.

The method was originally developed by Wong et al., 2003 for Argo floats. Bohme and Send (2005) improved the original method by using float observed theta levels, and introduced potential vorticity as a factor for selecting reference data. Owens and Wong (2009), combined the improvements of Bohme and Send (2005) with the original method, and introduced piecewise linear fit to the treatment of the time series. Additional modifications, such as separating data across the Sub Antarctic Front (SAF), have also been added. More recently, modifications suggested in Cabanes et al (2016) have been adopted to better take into account interannual variability and provide more realistic error bars.

The method relies on highly accurate quality-controlled reference databases (Argo and CTD reference databases).

Steps of the algorithm

- Select reference profiles (see find_besthist.m): The objective is to retain the reference profiles that are closest positioned and most contemporaneous to the float profile date. A maximum of N profiles (N=CONFIG_MAX_CAST) are selected among all the reference profiles available within an area that extends over three times the large spatial scales. Note that N/3 reference profiles are randomly selected within the area to ensure that the large-scale mean is well represented.
- Interpolate salinity from reference profiles onto float θ levels (see interp_climatology.m). The algorithm takes into account possible temperature inversions.
- 3. Use objective mapping (Bretherton et al, 1976) to estimate climatological value at

location and time of float observation. This is a 2 step process, large scale estimate, followed by shorter scale mapping of the deviations from the large scale estimate. Uses Gaussian covariances with scales defined by the user. Note that if there is no reference data within defined temporal and spatial scales the salinity estimate is relaxed back to the mean salinity computed from the N reference profiles, hence with larger mapping errors.

- 4. Choose θ levels for carrying out least square fit. The algorithm will choose at most 10 levels with the smallest salinity variance in the float time series (see find_10theta.m).
- 5. Calibration (i.e. fit the time varying correction for salinity): the model assumption is that there is a change in the volume over which the conductivity measurement is made. So the change is modeled as a multiplicative factor (∂r) times the observed conductivity value. Since ∂r can changes with time, a piecewise linear fit is used to treat the time series of ∂r and to filter out the variability inherent in the data.To choose the "best" fit, the AIC statistics is used. The AIC criterion works to mitigate the number of linear segments (or breakpoints) regarding the number of independent observations in the time series (number of degrees of freedom). That somewhat prevents you from overfitting the data and including variability that is not related to a sensor malfunction. In OWC, the number of independent observations is estimated by using the vertical covariance between theta levels and lateral covariance determined by small mapping scales. Model fit and fit errors are therefore particularly sensitive to the choice of small mapping scales.

How to set up the OWC software ?

Full instructions are given in the README.doc file of the OWC software.

You will have to set up the **configuration parameters** used by the algorithms. These parameters are defined in the last section of the configuration file (ow_config.txt). Again, instructions are given in the README.doc file and you can find examples of the configuration parameters used in different regions in this cookbook (Part II or Part III). This step is critical and must include oceanographic judgement, particularly when setting spatial and temporal scales. Note that the objective mapping error is very sensitive to the choices of mapping scales. In set calseries.m you can change the value of 8 variables that are used for calibration (maximum number of breakpoints, set breakpoints if any, split of the time series, constraints on the chosen 10 θ levels,..). Instructions are given in the README.doc file and you can find examples of changing the values of these variables in this cookbook (Part **III**, float **1901227, 5902203**). Note that you don't need to run the objective mapping again if you change the values of the variables in set_calseries.m. Only the calibration part will be impacted by these changes. However, you will manually delete the need to file calseries xxxxx.mat so that the changes in the configuration file are taken into account the next time you run the software. Alternatively, can change the variables you in calseries_xxxxx.mat directly, but make sure you save the mat file with the changes.

OWC outputs

Diagnostic plots are produced by the OWC package. A full description of these plots is given in the README.doc file.



Figure 1 from OWC shows the map of the float migration. You can also check which reference data have been selected for mapping by looking at **Figure 1**. Note that the selected reference

data are within an area that extends over three times the large spatial scales.

Figure 2 from OWC shows the θ /S plots based on the raw salinity data. Large sensor drifts can be seen in **Figure 2** as a gradual shift in the θ /S plots. Objectively estimated reference salinity at the 10 float θ levels that are used in calibration are superimposed. This figure can be used to check that the automatic selection of the 10 theta levels is correct. Examples on how to use this figure are given in **Part III** (see the analyses of floats **6901720**, **3901598** and **1901227**)



estimated reference salinity with their mapping error at the 10 float θ levels that are used in calibration. Two examples are shown: one float with no salinity drift and another float with a large salty drift.

Figure 3 from OWC shows the suggested adjustment (green curve)in conductivity and in salinity. It is important to understand that the prescribed fit must be evaluated by the DM operator. Indeed, the fit may reflect spatial or temporal variability that is not related to a sensor malfunction. There may be many reasons for this: the chosen configuration parameters are not the most appropriate, the float crosses very different water masses, etc... **Figure 3** illustrates some easiest cases where the final decision to correct or not the salinity was consistent with the prescribed adjustment. More complicated cases are illustrated in **Part III.**

Figure 4 from OWC is the same as **Figure 2** but uses the calibrated float salinity instead of the raw float salinity. Figure 4 can be used as a quick check to see how well the calibration is, if used.



with time, as a result of the piecewise linear fit (green curve). The top panel plots the potential conductivity multiplicative adjustment. The bottom panel plots the equivalent salinity additive adjustment. The red line denotes one-to-one profile fit that uses the vertically weighted mean of each profile. Green error bars show the fit error and blue error bars show the doubled fit error.

Figure 5 from OWC (here **Figure 4**) shows float salinity anomalies on θ levels, i.e. the difference between observed float salinity and the mean float salinity along its path. You can visualize where the most stable θ levels are (i.e. levels with the less salinity variation along the float path). A sensor drift will be seen as a change in salinity anomaly at all levels, i.e. an apparent shift by the same amount (or a systematic bias) in several different water masses.

Figure 6 from OWC (here Figure 5) shows the evolution of salinity with time along the two most stable θ levels. The float salinities are shown in blue while the mapped salinities are shown in red along with the mapping errors. If the sensor is drifting, the blue curve will move away from the red curve beyond the error bars.

Figure 7 from OWC is the same as **Figure 5** but uses the calibrated float salinity instead of the original float salinity. Figure 7 can be used as a quick check to see how well the calibration is, if used. A successful calibration will remove the salinity anomalies seen in Figure 5.



FIG 4: (Figure 5 from OWC) Float salinity anomalies along the float path. At each θ level, salinity anomalies are the difference between observed float salinity for profile N and the mean float salinity along the float path.



FIG 5 : (Figure 6 from OWC) evolution of salinity with time along two selected θ levels with minimum salinity variance.

Figure 8 from OWC (here Figure 6) shows the 10 theta levels (green horizontal lines) that have been selected by the algorithm to compute the calibration. You can check that the chosen theta levels are in a tight area of the theta S diagram. If you decide to apply a constraint on theta levels (by setting use_theta_lt, use_theta_gt, use_pres_gt or use_pres_lt in set_calseries.m) to reduce the vertical extent where you perform the calibration, you can check what are the 10 new chosen theta levels on this figure (for an example, see **Part III**, float **1901227**).

If you split the time series (by modifying calseries in set_calseries.m), the software will choose 10 different theta levels for each part of the time series. However, you won't see the effect of splitting the time series on Figure 6. Indeed, to draw this figure, the 10 theta levels are re-calculated using the whole time series.



FIG 6: (Figure 8 from OWC): The ten most stable float θ levels used to compute the fit are displayed in green. The chosen levels are those for which float salinity variance is minimum (see top left plot)

Evaluating the fit

This is a critical step. The computed calibration may not be consistent with our knowledge of how the sensor drifts, for example.

After applying the OWC calibration, the PSAL_ADJUSTED_QC flags should be set according to section 3.5.5 and 3.5.6 of the Argo

Quality Control Manual for CTD and Trajectory Data. Specifically, the QC flags can't be set to 1 anymore when calibration exceeds 0.05 psu and the **grey list** should be used to propagate QC in real-time if the float is still alive.

Summary

The OWC method is a framework to choose how to correct the float salinities.

Significant scientific judgement is still required to make these adjustments, including:

1. A proper choice for the scales used to map the historical data that reflects the spatial and temporal scales of the water masses.

2. The accuracy of the adjustment is only as good as the reference data.

3. The objective mapping formalism probably underestimates the uncertainties. Smaller scale variability can suggest adjustments that are probably not appropriate. Knowledge of how the sensor is likely to drift needs to be used in making the final judgement.

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7. Examples of hydraulic or sensor problems

Contacts: Walicka K., Klein B., Cabanes C., Notarstefano G.

Most of the time, the P, T and S measurements provided by the float are within the expected accuracy. If not, this may be due to some instrument errors and failure modes. The most common problems are listed in the ARGO quality control manual (section 4.4). The following subsections illustrate some of these problems.

Leak in the float Pump

This issue does not directly affect the pressure, temperature and salinity measurements themselves, but it is worth mentioning because it can prevent the float from reaching its programmed depth.

The Argo 6901922 float was deployed in 2016. It is an Apex float equipped with SBE41_V3 (6640) and a Druck pressure sensor (4037675).

The float mission has been initially set to sample up to 1000 m. However, the temperature and salinity time-series recorded by the float shows one profile with a depth reaching around 1000 m, while all other profiles did not exceed 400 m (see report

6901922_DMQCreport_20190930.pdf). After analysis, we found linearly increasing POSITION_PistonProfile_COUNT, suggesting a technical problem of this float (**Figure 1a**). The position piston count was increasing from 17 to 146, which can be caused by (1) wrongly balanced float or (2) a leak. After checking the PRESSURE_InternalVacuum_mbar parameter we found no constant pressure values, which informs us about a leak in this float (**Figure 1b**).



FIG 1: Float 6901922. Time series of (a) position piston counts, (b) pressure of the internal vacuum.

Pressure Sensor problems

Druck pressure sensors : oil microleak

A pathology encountered in some Druck pressure sensors manufactured between approximately 2007 to 2008 is an oil microleak past the glass/metal seal. This oil leak leads to an internal volume loss, which then exhibits itself as an increasing negative offset at all pressures. At the early stages of oil microleak, float measurements are still correctable and usable. However, as more and more oil is leaked, the flexible titanium diaphragm will dip so far down the oil chamber that it will short the electrical parts, causing erratic behaviour in float measurements. This is the end stage of oil microleak, and the data at this point are bad and uncorrectable.

Figure 2 gives an example of a slow microleaker (WMO 6900564) which showed continuous negative drift of its surface pressure readings reaching negative offsets of -8 dbar at the end of its lifetime. For this float, P is correctable using the method explained in section 1.4.



Figure 3 gives an example of a faster microleaker (WMO 6900563) which showed negative drift of its SP readings that accelerates after cycle 54. Before cycle 54, P is correctable but after cycle 54 P, T and S measurements become erratic due to internal shorts and are uncorrectable. P T and S are then flagged with a QC4.



Druck "Snowflakes problem"

"The Druck pressure sensor "snowflakes" problem is due to internal electrical shorting by the growth of titanium oxide particles ('snowflakes') in the oil-filled cavity in the pressure sensor, causing the pressure sensor to report erratic pressure measurements, or going to full scale, i.e. either report PRES ~ 3000 dbar or -3000 dbar" (Argo User's Manual, 2020). A few SBE41 CTDs manufactured in late 2002 through the end of 2003 with Druck pressure sensor have experienced this problem.

Float 49066 is an example of snowflakes issue. The float was deployed in the Irminger Sea at the western side of the Reykjanes Ridge, where further flow was carried northward toward the Denmark Strait by the Irminger Current. This Float is equipped with an SBE41 (211) and a Paine pressure sensor (195966). **Figure 4** shows that the surface pressure became erratic after profile around 53, ranging from 2000 to 6000 dbar. Pressure measurements affected by the "snowflakes" problem are not adjustable in delayed-mode. P, T and S measurements need to be flagged with a QC4.



FIG 4: Sea surface pressure of the float 49066 for which the pressure sensor has experienced the "snowflake" problem. The upper panel is a zoom between -20 20db while the lower panel shows the full range. The red cross indicates the raw pressure before float descent, recorded after

sending data to GDAC. Blue circles indicate pressure value in the real-time. Green rotated cross shows the pressure correction applied from the previous float cycle.

Kistler pressure sensors

In 2016, a defect in the Kistler pressure sensors was detected. The problem - a sudden shift in the pressure span (the calibration slope of pressure) - concerns CTDs built between January and July 2016.

The magnitude of the pressure span shift is 1-30 %, pivoting at 0 pressure, and always one sign – resulting in higher reported pressure than actual pressure. Although the pressure sensors were checked during the routine manufacturing process for the defect, there was a small chance that the check would not catch all the affected sensors. More information can be found in this report.

The Argo 3901931 float was deployed in 2017. It is an Arvor float equipped with an SBE41CP (8497) and a Kistler pressure sensor (4940374), The CTD was built in May 2016. According to e-mail exchanges between R. Cancouet and K.Martini, this float was probably affected by the problem mentioned above.

This float had received a MIN/MAX warning starting around cycle 105 with fresher salinity values (-0.35 psu at depth). After analysis, it appears that there is a problem with the pressure sensor, which reports higher pressure values than the actual values.



FIG 5: Temperature (left) and Salinity (right) for float 3901931 in function of pressure. Cycles 99 to 112



Pressure problem appears clearly on these plots (**Figures 5 and 6**): note the large temperature shift in the thermocline, the salinity minimum shift from 850db to 1150db, the shift in the theta/S diagram with the profiles acquired after cycle 105 that are no longer parallel to the previous profiles.

Pressure does not seem correctable with a simple pressure offset as the magnitude of the pressure error increased with depth.

Because pressure is not correctable, we put this float into the grey list for PRES, PSAL, et TEMP with a QC4 from cycle 104.

Conductivity Sensor problems

Fast salty drift:

In September 2018 Argo had issued a warning to users about fast salty drifters on the internet.



FIG 7: Analysis of CTDs affected by fast salty drift (http://www.argo.ucsd.edu/DM_report_ArgoPositiveDrifters8Mar2018.pdf

Due to a manufacturing problem that occurred prior to 2014, a larger than normal number of SeaBird Scientific CTD cells (SNs > 6000) used in Argo developed a high salinity bias within 2 years of deployment (**Figure 7**). Many of these CTDs are still active in Argo, and as result, a higher portion than normal of Argo real time data are subject to salinity errors larger than Argo's 0.01 accuracy target. The frequency of occurrence of drift is CTD batch dependent.

SeaBird's analysis indicated that this failure mode was a result of seawater intrusion between the glass conductivity cell and the urethane encapsulant, causing a parallel resistance path between signal and ground leads, resulting in a calibration drift toward higher salinity. The problem was identified by SBE in the summer of 2014 and, as an added precaution to the solution, put an extensive screening test in place to keep such hermetic failures out of the Argo fleet.

Additional diagnostic plots are provided by WHOI in form of N2 and salinity anomaly plots to help dm-operators in identifying fast salty drifters. Since the initial analysis, an additional cohort of CTD cells has been identified in the SN range 8000 – 8500 and 10500-11500.

A working group has been established to investigate the behaviour of the fast salty drifters, their temporal behaviour and limits of correctability, including analysis of potential depth dependence. This analysis so far includes examples of fast salty drift in deep floats in stable near bottom water masses of the Pacific. OWC was run on multiple levels (2000, 3000, 4000, 5000 dbar) to establish depth dependence of corrections. In 2000 dbar 'Core Argo floats' examples were selected from areas where tight TS-regions exist (Indian Ocean, Atlantic Ocean central waters) and OWC runs with shallow <1000 m reference levels were compared to those with deep levels >1500m. Delayed-mode operators are reminded that the OWC method applies a depth-independent offset adjustment to correct salinity. Therefore any salinity sensor

drifts that have significant vertical variations are considered unadjustable by the OWC method.



For strong drift (\triangle S>0.2 psu) depth dependence of the salt drift is seen in the examined Deep-Argo floats and shows highest drift values at depth (**Figure 8**).



Similar observations are made for core floats with strong drift (**Figure 9**), but for more moderate drift rates results are less conclusive. To date the anomalous salt drift threshold at which depth dependence occurs remains unclear. In some examples it started soon after the onset of drift. DM-operators are advised to follow existing rules and flag PSAL_ADJUSTED_QC as '4' once the Δ S exceeds +0.05 psu. Any sudden changes or reversal in drift rate or jumps (>0.01 from one cycle to

another) (**Figures 10 and 11**) should be examined carefully because they could indicate sensor failure and thus uncorrectable data.

same format as the spreadsheet or request editing access to the spreadsheet.



FIG 10: Changes in drift rate and reversals in a core Argo float (WMO 3901636).



To monitor the impact of premature CTD failures in Argo, a shared spreadsheet is being maintained by B. Klein. The spreadsheet lists important information on the affected floats, including CTD model and serial number. The floats being entered into the spreadsheet are those with CTD serial number > 6000, and with an estimated salinity adjustment of > 0.01 psu within 2 years of deployment, or salinity data becoming unadjustable within 5 years of deployment. The goal is not to record all floats that drift salty, but to only record floats that drift salty prematurely. You can either report floats that drift salty prematurely to B. Klein, using the

8. How to fill D files and good practices to document DMQC

Contacts: Cabanes C., Maze G., Walicka K.

Documenting decision: why?

There are many good reasons to keep track and document decisions made during DMQC:

- make your work reproductible
- help the data users to understand the behaviour of your float (e.g pathologies you were able to identify)
- help to find common problems in the whole dataset (e.g TNPD floats)
- make machine learning possible (e.g. when you document QC flags change in D files)

Documenting decision : how?

Decisions made during DMQC process should be documented at least:

- In reports
- In D files through the calibration and history sections.

How to fill D files ?

PARAM ADJUSTED variables

Once you have made a decision about the DMQC of a parameter you have to fill the D-file. A list of compulsory variables to be filed in a D-file is given in the Argo Quality Control Manual (section 3.6).

Note that even if no adjustment has been applied you will have to fill:

- PARAM_ADJUSTED (=PARAM),
- PARAM_ADJUSTED_QC (=PARAM_QC)
- and PARAM_ADJUSTED_ERROR.

PARAM_ADJUSTED_ERROR is generally set to the manufacturer specified accuracy for PRES and TEMP (**2.4 db** and **0.002°C** respectively) and **max[(Σadjustment_error**²)^{1/2}, **0.01]** for PSAL. "adjustment_error" is the uncertainty from each type of adjustment applied to PSAL. These can be statistical uncertainty from sensor drift adjustment, uncertainty from conductivity cell thermal mass adjustment, etc. More information on PARAM_ADJUSTED_ERROR can be found in the Argo quality control manual (sections 3.3, 3.4 and 3.5).

WheneverPARAM_ADJUSTED_QCis'4',PARAM_ADJUSTEDandPARAM_ADJUSTED_ERROR should be set to theirFillValue.

Scientific Calibration Section

It is also compulsory to fill the **scientific calibration section** for each profile and each parameter. You can find examples in the Argo Quality Control Manual (section 3.6) for different adjustment cases: pressure adjusted by using the pressure offset at the sea surface, no adjustment required for TEMP or PSAL, PSAL adjusted for drift or unadjustable data.

It can be more complicated to fill in the scientific calibration section when **more than one adjustment have been applied** to a parameter (e.g. salinity has been first corrected for the Conductivity Thermal Mass - CTM - and then for a drift detected by the OWC software). In that case it is possible to use the dimension **N_CALIB** to record the successive steps of the adjustment. An example is given here, showing how to fill the scientific calibration section for PSAL when several adjustments have been applied. Note that an increase in **N_CALIB** is not required when an adjustment is updated.

History Section

A history record should be appended to the HISTORY section of the netcdf file each time:

- a flag has been modified in delayed time
- a delayed mode analysis has been performed on a parameter.

You should refer to the Argo User's Manual (§5 "Using the History section of the Argo netCDF Structure") on usage of the History section.

D-files Compliance

Whenever a D-File is submitted, it is checked by the GDAC to ensure compliance. A description of all tests performed at the GDAC level is available here. If a test fails, the D-file will be rejected.

Writing reports

Examples of DMQC reports are given here:

- example from BODC
- example from Ifremer/Coriolis
- example from Glazeo
- example from ifremer/lops
- example from Argo Spain
- example from csiro
- example from OGS

Work is underway to produce a common DMQC report template for core Argo parameters. A first draft of this template can be found in DMQC report template for core Argo data. Both report template and codes used to generate plots required in the report will be made available in a Euro-Argo ERIC github repository dm-report-template.

1. Subpolar North Atlantic

Contacts: Cabanes C., Thierry V., Herbert G., Buck J.

Introduction

The North Atlantic Subpolar Gyre is a key oceanic region, that lies between the northeastward North Atlantic Current (NAC) to the south and the Nordic Seas to the north (**Figure 1**). It is the northern branch of the thermohaline circulation and a formation region of North Atlantic Deep Water.

There are numerous processes that influence the circulation and water properties including:

- Intense winter heat loss that leads to deep convection up to 2km depth.

- Arctic inputs (Northern Labrador Sea, Greenland Sea, Norwegian Sea).

- Subtropical gyre inputs from the south via the NAC.

- Atmospheric influences on short temporal scales such as passing weather systems and on inter-annual scales such as the North Atlantic Oscillation.



FIG 1: Source: Daniault et al. (2016).

Schematic of the large-scale circulation in the northern North Atlantic . Topographical features and currents of North Atlantic are indicated as follows: Bight Fracture Zone (BFZ), Charlie-Gibbs Fracture Zone (CGFZ), Faraday Fracture Zone (FFZ), Maxwell Fracture Zone (MFZ), Mid-Atlantic Ridge (MAR), Azores-Biscay Rise (ABR), Iberian Abyssal Plain (I.A.P.), Northwest Corner (NWC), Rockall Trough (RT), Rockall Plateau (Rockall P.) and Maury Channel (MC). The main associated water masses are indicated: Denmark Strait Overflow Water (DSOW), Iceland-Scotland Overflow Water (ISOW), Labrador Sea Water (LSW), Mediterranean Water (MW) and Lower North East Atlantic Deep Water (LNEADW). Significant inter-annual and inter-decadal variability is observed in many of these processes. As such, the region presents a challenge to Argo delayed mode operators.

The purpose of this section is not to give a comprehensive description of the processes and water masses in the subpolar region, but rather to focus on some points that can help for analysing floats in delayed mode, in particular the verification of QC flags, the parametrization of OWC software and the analysis of the results. In **Part III**, case studies (floats **6901720** and **5902303**) illustrate some of the points discussed below.

Overflow waters

The submarine ridge that lies between Greenland and Scotland separates the Nordic Seas from the Atlantic Ocean. The dense waters that flow across the sills entrain the surrounding waters and form the Nordic Seas overflow water: The Denmark Strait Overflow Water (DSOW) that flows into the Irminger Sea and Iceland-Scotland Overflow Water (ISOW) that contains waters from two sills east of Iceland and flows into the Iceland Basin (**Figure 1** and **Figure 2**).



FIG 2: Source Yashayaev et al., 2007.

Salinity section (depth/distance) across the subpolar North Atlantic ocean according to measurements made by ship in 1994. Labrador Sea Water (LSW) appears in each of the bassins between 1000 and 2000m depth (Labrador Sea, Irminger Sea, Iberian Basin and Rockall Trough), with a relative minimum of salinity in its core

Argo floats, going down to 2000m, may sample these waters near the sills or on the topography slopes. **Figure 3** shows profiles of a float located in the northern part of the Icelandic basin. Some of the profiles clearly show the ISOW characteristic, which is particularly cold and relatively salty. The ISOW appears here as a hook at the bottom of the temperature, salinity and density profiles. The DM operator must therefore be careful not to flag these hooks as bad.



FIG 3: Example of overflow water (ISOW) sampled by the float 6900640, in the northern part of the Iceland Basin . These dense waters are particularly salty and cold and appear as a hook at the base of the profiles . SIGMA0 is shown on the right panel . TEMP and PSAL are shown on the lower left panels. Example provided by C. Lagadec.

Flow is highly constrained by topography.



FIG 4: Argo satinities in the region of the Reykjanes Ridge at specified theta levels (3.4-3.5°c). Only data below 1000m depth and with a QC=1 are considered. Adjusted values are used when available.

The subpolar circulation is strongly steered by topography. As a major topographic feature, the Reykjanes Ridge influences the spatial pattern of the subpolar gyre circulation (Bower et al., 2002) and water masses (Thierry et al., 2008). The dense, cold and salty Iceland-Scotland Overflow Water (ISOW) is banked to the eastern flank of the Reykjanes Ridge when flowing southward in the Iceland Basin (see **Figure 2**). At intermediate levels, the relatively warm and salty Iceland slope water (ISW), which is formed through a mixing process of ISOW and SPMW near the Faroes (Van Aken, 1995), follows the slope of Iceland and Reykjanes Ridge. A profile obtained near the ridge would therefore sample saltier water than one obtained further inside the Icelandic basin (see **Figure 4**).

OWC software includes an option (MAP_USE_PV) that can be enabled to account for the cross-isobath separation. Figure 5 gives an example of adding this constraint when selecting the reference profiles. A large cross-isobath scale $\Phi_1 = 0.1$ is efficient to select reference data following the isobath. Note that the reference data is selected on each side of the Reykjanes ridge, which can be an issue because the salinity on the eastern flank is noticeably higher than on the western flank at the same theta level (see Figure 4). The OWC software does not provide an easy way to select the reference data on the same side of the ridge as the float profile. You should therefore be careful when analyzing the OWC results and eventually try to reduce the spatial scales to minimize the weight of reference data on the opposite side of the ridge.



FIG 5: Example of the reference data selectionned within the ellipsis (axis 3*Lx, 3*Lx) by the OWC software for an Argo profile (magenta) located close to the Reykjanes Ridge. (left:) cross-isobath scale is not used. (right) cross-isobath scale is set to 0.1. Lx and Ly are the longitude and latitude scales respectively.

Deep convection

In the North Atlantic, dense water formation occurs through deep convection in both the Nordic Seas and the subpolar gyre (Labrador and Irminger Seas). **Figure 6** shows some Argo profiles sampled in the Irminger Sea that illustrate a deep convection event down to 1000 m depth.



potential temperature (°C) (c) profiles from floats 4901163 (red), 4901165 (green), 4901166 (blue) and 5902298 (yellow) located in the Irminger Sea, with an MLD of about 1000 m.

Labrador Sea Water (LSW) generally forms in late winter in the Labrador Sea and Irminger Sea when severe weather conditions cause strong and deep mixing (Piron et al, 2016, 2017). This deep mixing tends to homogenize water properties from the surface to 1000-2000 m.

The newly formed LSW moves out of the Labrador Sea and Iceland Basin and part of it feeds into intermediate layers of the subpolar region with a characteristic minimum of salinity (**Figure 2**).

Profiles shown in **Figure 7**, which are very homogenous in temperature and salinity, are typical of the Labrador Sea region.



float 6901754). Theta/S diagram is shown on the right panel . TEMP and PSAL are shown on the lower left panels.

Homogeneity of the temperature profiles can be an issue when analyzing the float with the OWC software. Because reference data are mapped onto float theta levels it can happen that reference data with the same theta but with very different depths are used. It is possible to avoid this problem by reducing the parameter MAP_P_DELTA in the configuration file. A value of 50-100db is generally suitable in the subpolar region.

Temperature inversions on the float profile can also be an issue. Indeed, several depths are associated with a single theta value. For example, the level theta=3.1°C in Figure 7 shows up in a surface layer and in a deep layer. The algorithm that selects the 10 best theta levels with less salinity variance (find_10thetas.m) will possibly pick out salinity value in the deepest layer for one cycle and salinity value in the upper layer for another cycle to calculate the salinity variance at theta=3.1°C. This gives artificially high salinity variability and prevents the algorithm to choose this theta level to perform the analysis. In this case, it is recommended to exclude the upper levels from the analysis. It can be done in two ways: either set the parameter MAP_P_EXCLUDE in the configuration file to exclude the first xxxx db of the water column or set use pres gt in set_calseries.m. In the first case, the mapping will be faster, while in the second case you will be able to quickly test different values. Note that you can't have use_pres_gt smaller than MAP_P_EXCLUDE. Use_pres_gt= 1000 db is generally suitable in the Labrador Sea region.

High temporal variability at depth

Figure 8 shows the difference between ISAS-13 (In Situ Analysis System, Gaillard et al., 2009) and the WOA05 salinity climatology (Antonov et al., 2006). It therefore highlights the broad-scale decadal salinity changes observed at 1500 m depth in the North Atlantic between the pre-2005 period and 2004-2012.

At 1500m depth, an increase of salinity is generally observed in the western Subpolar Gyre while a slight decrease is observed in the eastern part. Similar salinity changes were also observed along repeated hydrographic sections in the North Atlantic. For example, four occupations of the repeated zonal transatlantic section along 59.5-60°N (from the Scottish shelf to Cape Farewell) showed that the deep Labrador Sea Water (dLSW), which was found around 1500m in the Irminger sea, became saltier by 0.04 on average between 1997 and 2006 (Sarafanov et al., 2007).



More recent changes in salinity have been documented, including a widespread surface freshening (Tesdal et al, 2017) during 2005-2015, which is particularly visible in the eastern subpolar North Atlantic from 2005 to 2018 (Johnson et al, 2019). This freshening trend is also observed at depth in the Labrador Sea over the period 2010-2015 (Figure 9 in Tesdal et al, 2017) and seems to persist and extend into the Irminger Basin after 2015 (see **Figure 9**).

Such salinity changes at depth, make the analysis of the OWC results challenging. Indeed, a lack of recent or contemporaneous reference data for the float being analyzed can lead to a spurious offset or trend that may be difficult to distinguish from a real offset or a sensor drift (Cabanes et al, 2016). To avoid interpretation errors, it is important to have a precise idea of the temporal coverage of the reference data used by the software. It is also recommended analysis be that the OWC performed successively using CTD reference data (whose spatial and temporal coverage may be sparse) and Argo reference data (whose coverage is denser and more recent). Configuration parameters (MAPSCALE LONGITUDE LARGE, MAPSCALE LATITUDE LARGE, MAPSCALE AGE LARGE) must be set to account for large scale interannual salinity changes (see the next section). Ideally, OWC results should be cross-validated by the comparison of the float salinity with independent and recent shipboard

CTD data, at least for some profiles in the float time series.



FIG 9: Difference at 1500 m depth between monthly salinity fields produced by the Near-Real-Time Objective Analysis (https://resources.marine.copernicus.eu/) and averaged over a year with the ISAS-13 climatology that covers the 2004-2012 period. These plots were obtained thanks to the ISAS viewver.

Beyond these large-scale changes that take place in the deepest layers sampled by classical Argo floats, important salinity variations are also observed locally and on shorter time scales. **Figure 10** highlights the salinity variability recorded by 7 moorings deployed between 2015 and 2017 from West (IRW) to East (ICE) of the Reykjanes ridge as part of the RREX project (Thierry et al.).



FIG 10: Upper panel (left): Mean 2002 – 2010 salinity section along part of the Ovide line and localized above the Reykjanes Ridge and position of the 7 RREX moorings. (right) : Standard deviation of salinity for each mooring at each vertical level, from daily averaged data. Lower panel: Example of time series of daily averaged salinity (psu) around 2000m at mooring ICE.

At 1500 m, the standard deviation of salinity reaches 0.01 psu and the day-to-day variability can exceed 0.02 psu during particular events

(see e.g. bottom panel of **Figure 10**). This short time scale variability may be an issue when comparing the first float profile with the reference hydrographic cast made at float launch.

OWC Configuration parameters in the Subpolar North Atlantic.

The following configuration parameters are generally used in the subpolar North Atlantic. Spatial scales are set according to Boehme and Send (2005) and MAPSCALE_AGE_LARGE is set according to Cabanes et al., (2016).

CONFIG_MAX_CASTS: 250 MAP_USE_PV: 1 MAP_USE_SAF: 0 MAPSCALE_LONGITUDE_LARGE: 3.2 MAPSCALE_LONGITUDE_SMALL: 2 MAPSCALE_LATITUDE_LARGE: 2 MAPSCALE_LATITUDE_SMALL: 1 MAPSCALE_PHI_LARGE: 0.1 MAPSCALE_PHI_SMALL: 0.02 MAPSCALE_AGE_LARGE: 2 MAPSCALE_AGE_SMALL: 0.69 MAP_P_EXCLUDE: 0 - 1000 MAP_P_DELTA: 50-100, depending on the water masses sampled by the float.

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2. Medditeranean and Black Seas

Contacts: Notarstefano G.

Reference datas in MED Sea

This section describes the work done at regional level to try to improve the official CTD reference dataset with other new and more updated CTD data.

1. Regional needs

The Mediterranean Sea is characterized by a complex bathymetry, where the existing shallow areas represent a threshold in the selection criteria for the CTD profiles to be retained in the official reference database (only profiles that sampled deeper than 900 dbar are selected). Moreover, some local research institutes that collect CTD data on a regular basis don't share their data because they are not part of dedicated infrastructures or international projects. This can cause the CTD reference dataset not to be updated and scarce in temporal and spatial coverage in some areas. Since the Mediterranean Sea is characterized by several water masses that can change properties dramatically over the years, it is crucial to have the best co-location (in space and time) between the CTD reference dataset and the Argo CTD profiles in order to separate differences between the two datasets due to sensor drift or to the change of water mass properties. For these reasons, OGS, as responsible for the DMQC activities in the Mediterranean and Black Sea, tries to collect CTD data in complement of the official CTD reference dataset using mainly two approaches: personal contacts from one side and regional data services from another side.

2. Improving of the CTD reference dataset

Since the DMQC activity requires the availability of a good reference dataset, the work consists of exploring the possibility to fill some gaps (in time and space) in the CTD reference dataset.

2.1 CTD profiles obtained through personal contact

The collection of CTD profiles through personal contacts started in 2008 and since then several profiles have been used to improve the CTD reference dataset. European colleagues from different research institutes kindly provide us with CTD data acquired during regular cruises or in the framework of projects. A lot of work has been done in finding the right contacts, email exchanging and gathering the data. Dozens of datasets were collected in this way spanning from 1997 to 2017 and from the Alboran to the Levantine Seas. The CTD profiles used to build the MEDAR-MEDATLAS climatology have also been added to these datasets and it consists of data from 1972 to 2000.

The last CTD data collection was done in the second part of 2018 under the MOCCA project activity and it consists of CTD profiles from 2013 to 2017 in the Adriatic, Alboran, Algerian, Ionian, Tyrrhenian Seas, Sicily Channel and Cretan Passage.

The files were usually received in different formats and hence file-reading MatLab scripts were prepared accordingly. The data were supposed to be already of good quality but a light additional quality control has been applied in order to remove any residual outliers and spikes.

Many CTD data collected were policy free and hence they have been shared with the Coriolis in-situ Service and integrated in the "official" CTD reference dataset. The data policy is discussed with the owner of the data and as soon as they are declared "not restricted", they become part of the "official" dataset.

The CTD profile locations of this dataset is shown in **Figure 1** and the respective temporal distribution is in **Figure 2**.



FIG 1: spatial distribution, color-coded for time, of the CTD profiles collected and used as a complement of the CTD reference dataset.



2.2 CTD profiles obtained through dedicated services

Another CTD data source taken into consideration is the one connected to the marine monitoring services. The Copernicus Environment Monitoring Marine System (CMEMS) has been chosen because it provides a great quantity of data that follow a multiple level quality control procedure. These data are not integrated in the CTD reference dataset by the Coriolis in-situ Service. The CMEMS files are in NetCDF format and are available through a dedicated FTP server. The CTD files have to be extracted by a common folder reading the file name that is coded per platform and profile types. MatLab scripts have been built to convert the files from NetCDF to MatLab format. The procedure has been done twice in two different data repositories: the first time to collect the CTD data in the Mediterranean Sea (Figure 3 and 4) and the second time for the Black Sea (Figure 5 and 6).

The last CTD data collection has been done in 2018 in the framework of the MOCCA project and the following two CMEMS products were used:

 INSITU_MED_TS_REP_OBSERVATIONS_01 3_041 INSITU_BS_TS_REP_OBSERVATIONS_013_ 042

for the Mediterranean and Black Sea, respectively.



collected through the CMEMS portal and used as a complement of the CTD reference dataset of the Mediterranean Sea.



FIG 4: temporal distribution of the CTD profiles collected through the CMEMS portal and used as a complement of the CTD reference dataset of the Mediterranean Sea.



FIG 5: spatial distribution, color-coded for time, of the CTD profiles collected through the CMEMS portal and used as a complement of the CTD
reference dataset of the Black Sea. # historical CTD casts per year 1400 1300 1200 1100 1000 900 # CTD casts 800 700 600 500 400 300 200 100 0 1995 1997 1999 2001 2003 2005 2007 2009 2011 2013 2015 2017 years

FIG 6: temporal distribution of the CTD profiles collected through the CMEMS portal and used as a complement of the CTD reference dataset of the Black Sea.

3. Merger of the dataset 3.1 Checking for duplicates

Once the files are converted from their original format into MatLab format, a further step is requested to make them compatible to be used by the OWC software for calibration purposes. The CTD data are then compared to the CTD reference dataset and checked to remove duplicates taking into account thresholds of 10 minutes and 100 meters for time and location respectively. CTD profiles whose difference in time and space is less than the above predefined thresholds considered are duplicates and hence removed from the dataset.

3.2 Subset of the CTD data and merger

The CTD data are first separated into 10° X 10° WMO boxes. Then, due to the different nature of the existing water masses and to the geography of the Mediterranean Sea, the CTD data within the WMO boxes are grouped according to the dimension of various climatological sub-basins, as defined by the EU/MEDAR-MEDATLA II project (**Figure 7**).



The new CTD data are eventually merged into the CTD reference dataset and this final version is summarized in **Figure 8** and **9**. The dataset consists of about 56000 CTD profiles. Data before 1995 were discarded because they were considered too old for quality control purposes.



FIG 8: spatial distribution, color-coded for time, of the CTD profiles in the final version of the CTD reference dataset of the Mediterranean and Black Seas.





3. Nordic Seas

Contacts: Angel-Benavides I.M.

Reference data in the Nordic Seas

During the process of the DMQC on Argo floats operating in the Nordic Seas, which in most cases is the responsibility of the German Federal Maritime and Hydrographic Agency (BSH), the lack of recent profiles in the Iceland Sea became apparent. Therefore, and as part of the MOCCA project, we performed a thorough check of the 2018v02 version of the CTD reference database in the Nordic Seas region. It consisted of an assessment of its spatial and temporal coverage and a verification of its conformity with the selection criteria described in the Argo quality control manual (Appendix 4.5). Code developed to perform this diagnosis in a user-defined region is publicly available at https://github.com/euroargodev/check_CTD-RD B. Figure 1 shows the WMO boxes that cover the Nordic Seas are shown in Figure 1. For completeness, the boxes surrounding the deep basins and the ones in the Arctic region were also included.



Status of the 2018v02 version

After removing the profiles in the North Atlantic region of boxes 7602 and 7601, these boxes contained a total of 9460 profiles, which position and year are shown in **Figure 2**.



FIG 2: Spatial distribution of the profiles in the 2018v02 version of the CTD reference database. The year of sampling is color-coded.

We identified two main issues:

a) a large number of profiles (1158, 12% of the total) had a maximum recorded pressure shallower than 900 dbar, most of which (1086) were located in box 7600 (n = 1086). Feedback on this issue was given to C. Coataonan, who traced the presence of these shallow profiles back to an error occurred during the preparation of the 2012v01 version of the database. This error, which also affected boxes 1700 and 7700, implied that many profiles were stored with wrong metadata.

b) an absence of recent profiles (**Figure 2 and 3**), with 2011 being the last year with a relatively large number of profiles (252) followed by a gap of four years with no data and 2 profiles collected in 2016. Only 15% of the profiles present in the database were collected after 2005.



Actions for the 2019v01 update

We took following actions to locally improve and update the CTD reference database:

a) Fix the 2018v02 versions of boxes 1700, 7600, and 7701. We rebuilt the boxes by taking their 2011v01 versions as starting points and adding the updates prepared by C. Coatonan from 2012 on.

b) Improve temporal coverage by adding profiles from two data sources: the Unified Database for Arctic and Subarctic Hydrography – UDASH (Behrendt et al., 2018), from which profiles north of 65°N and collected between 1995 and 2015 were selected; and the International Council for the Exploration of the Sea – ICES, from which C. Coatanoan selected profiles north of 60°N that were collected between 2015 and 2018.

Profile Quality control

While the profiles in UDASH were subjected to strict quality control through which quality flags were assigned to each sample (see Behrendt et al., 2018 for details), the ICES profiles are distributed without any quality flagging. Therefore, it was necessary to inspect them to verify their quality. First, we visualized each profile together with other profiles collected by the same ship in the same WMO to provide context. In this way we identified and deleted suspicious and bad quality profiles. The most common cause for removal was the presence of large multidirectional spikes in the temperature profiles. We then examined the remaining profiles between 900 and 2000 dbar, to flag and remove bad samples (outliers).

Merging and duplicate checks

The profiles from UDASH and ICES were merged with the corrected version of the 2018v02 CTD reference database and were assigned to their corresponding WMO boxes. Afterwards, we excluded bad and incomplete samples (i.e. samples were either temperature or salinity was missing). Since this procedure could affect the maximum recorded pressure of the profiles, we reevaluated the 900 dbar criterium and deleted those profiles that did not fulfill it.

Then we performed an exhaustive duplicate check, which was necessary due to the inherent redundancy of the data sources. For example, the UDASH database contains data from both the World Ocean Database and ICES which, at least partially, were already included in the 2018v02 version of the CTD reference database. Therefore, it is expected that many profiles are present in more than one of our three data sources.

It is important to remove duplicated profiles to avoid data redundancy and hence skewed statistics about the number of profiles available for the objective interpolation of salinity in the OWC method. The implications of the presence of duplicated profiles for the objective interpolation itself are negligible because the method accounts for redundant information, unless one of the profiles contains bad quality data (outliers). Thus, it is also important to select the best quality profile when removing duplicates that have gone through different subsampling and quality screenings, to preserve the highest amount of information and avoid the presence of bad quality data. We use two criteria to decide which profile should be kept in the database: the information content and the information about the origin of the profiles, giving priority to the first. For the assessment of the information content of the profiles we used the following criteria, which are listed in order of preference: Maximum recorded pressure, the salinity resolution (number of decimal digits) and the vertical resolution (number of samples divided by the pressure range). For the profile origin we preferred the profiles with the higher quality control and better traceability. Thus, profiles from UDASH and ICES, which were subjected to detailed quality control, are preferred to those with gclevel COR and OCL.

While the identification of metadata exact and near duplicates (same or very similar position timestamp) is straightforward, and the identification of content duplicates is more complicated since often the same profile has been subsampled or interpolated to different vertical resolutions, or trimmed to different pressure ranges. We used a sample-by-sample test (Figure 4) based on the implementation of the Gronell and Wijffels (2008) algorithm by Behrendt et al. (2018): a) the profile with highest vertical resolution is interpolated to the pressure levels of the one with lowest resolution at the overlapping pressure levels, accounting for the different sampling pressure levels; and

b) the precision of the temperature and salinity values is degraded. The test output is a percentage of the number of temperature and salinity samples, of the preprocessed profiles, that are identical.



If more than 95% of the samples are equal, the profiles are automatically labeled as content duplicates. If more than 75% are equal, the operator must confirm the duplicate by examining the profiles visually. The workflow is shown in Figure 5.



Following checks were consecutively performed:

a) Check for exact metadata duplicates in each box. If the pair is also a content duplicate we deleted the worst profile. If the pair is not a content duplicate, we deleted both profiles because their metadata/content are uncertain.

b) Check for metadata near duplicates in each box. Here we compare the truncated variables down to one decimal digit for latitude and longitude, and 1 day for the timestamp. If the pair is also a content duplicate, we deleted the worst profile. Otherwise, we kept both profiles.

c) Check for content duplicates in all boxes. Given that the content duplicate checks are this computationally costly we divided procedure in two parts: First we found profile pairs that were likely to be content duplicates by running the Gronell and Wijffels (2008) exact content duplicate test, that compares the sum of all temperatures and salinities, on simplified versions of all profiles, which were obtained by interpolating them to common pressure levels and reducing their resolution to 1 and 2 decimal digits for temperature and salinity, respectively. Then, the content duplicates were either confirmed or refuted with the procedure summarized in Figure 5. For content duplicates that are near in time and space (distance smaller than 3km and time difference shorter than 3 days) we deleted the worst profile. If the profiles are far in time or space, we deleted both profiles because their metadata uncertain.

Final quality check

To check for any remaining outliers, we interpolated the salinity to 900 dbar inside each one of the four deep basins, which limits were defined using a combination of geographical constraints and their characteristic f/H ratio, following Latarius and Quadfasel (2010). The f/H threshold is 0.079 for the Icelandic Plateau and 0.045 for the Greenland Sea, the Lofoten Basin, and the Norwegian Basin.

Figure 6 shows the time series of the interpolated values for the Norwegian Basin. The data points highlighted with the red circles were considered outliers and the profiles from which they originated were excluded. Similar

outliers were found, and excluded, in the Icelandic Plateau and the Lofoten Basin.



Status of the 2019v01 version

The 17 WMO boxes of the 2019v01 version of the CTD reference database contain 15319 profiles of which 14340 are located in the Nordic Seas. This represents an increase of 4880 profiles when compared with those in the 2018v02 version. The spatial distribution of the profiles is shown in **Figure 7**.



The temporal distribution of the profiles is considerably improved, as seen in **Figures 7 and 8**, the latter showing the temporal distribution of the profiles. While in the 2018v02 only 2 profiles were collected after 2012, a total

of 1592 profiles are present in the 2019v01 version. Still, a small temporal lag persists with the most recent profile collected in November of 2017.



Outlook

Given that the reference databases are centrally maintained by single individuals, it is crucial that the DMQC operators take an active role in the verification of its quality at a local level, as well as in the contribution of profiles from alternative sources. Aiming to further improve the CTD reference database at the global level, the scripts used for duplicate and other quality checks will be implemented by C. Coatonan for the next global updates. This work will be part of the EA-RISE project and will be shared with the Argo community via the Euro Argo collaborative framework in Github.

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4. Southern Ocean

Contacts: Walicka K.

Introduction

The Southern Ocean is a very challenging region for DMQC analysis due to complex ocean circulations pathways, various water masses and deep water mass formation, sea ice formation, and a limited amount of reference data to compare with the Argo float.

The main oceanographic feature in this region is the Antarctic Circumpolar Current (ACC), which flows continuously eastward, encircling Antarctica (**Figure 1**). ACC is dynamically connected with the Meridional Overturning Circulation (MOC), which ventilates deep and bottom portions of the Pacific, Atlantic, and Indian Oceans (Lumpkin and Speer 2007; Johnson 2008; Marshall and Speer 2012). This current is strongly constrained by complex bathymetry and wind forcing (Talley et al. 2011).



FIG 1: Source: Llort, (2015). A schematic view of the major ocean currents of the Southern Hemisphere oceans south of 201°S. Depths shallower than 3500m are shaded. C, current; G, gyre; F, front; ACC, Antarctic Circumpolar Current.

Subantarctic Front (SAF)

The ACC strongly interacts with the southward flowing subtropical western boundary currents (Brazil Current, Agulhas, and East Australian Current), blending water masses from different basins (Rintoul et al. 2001; Van Sebille et al. The northern part of the ACC is 2013). accompanied by a strong front formed by meridional density gradients called the Subantarctic Front (SAF), separating the ACC from warmer and saltier subtropical waters (Figure 1). This front is reflected in steeply sloping isopycnals at all depths. The SAF is identified as a maximum horizontal gradient between the 3 and 5°C isotherms at 300 m. To prevent the selection of the historical data from different regimes, the algorithm (frontalConstraintSAF.m) separates historical data depending on whether it falls north or south of the SAF. The DMQC operator can decide to use the SAF parameter to select data in the objective mapping (MAP_USE_SAF=1 or 0). Figure 2 shows differences in the amount of selected historical data for setting the SAF parameter. The use of the SAF parameter can reduce the variability of the historical data and improve the comparison with Argo float data.



FIG 2: Trajectory map of float 3901889 plotted with the CTD (2019v01) and Argo (2020v03) reference data. Historical data selected using (a) SAF=0, (b) SAF=1

Water masses

The Argo floats driven by significantly varying over time ACC fronts are often crossing different water masses in the Southern Ocean. **Figure 3** shows a schematic representation of water masses and frontal zones in the Southern Ocean. Presence of water masses with substantial changes in temperature and salinity properties over the float life can make it very difficult to identify the most appropriate theta levels in the DM analysis.



FIG 3: A schematic meridional section of water masses, meridional circulation, fronts, and most zones in the Southern Ocean. Acronyms: Continental Shelf Water (CSW), Antarctic Surface Water (AASW), Subantarctic Mode Water (SAMW), Subantarctic Surface Water (SASW), Subtropical Surface Water (STSW), Antarctic Slope Front (ASF), Southern Boundary (SB), Southern ACC Front (SACCF), Polar Front (PF), Subantarctic Front (SAF), and Subtropical Front (STF). (Talley et al. 2011)

Figure 4 shows the time series of salinity and T/S diagram, where initial profiles were in the Argentine Basin, between the SAF and STF (Subtropical Front). These profiles show characteristics of Subantarctic Surface Water in the upper layer, below that is Antarctic Intermediate Water with the salinity minimum at around 500 m and the lowest part of profile represent upper Circumpolar Deep Water (CDW). Further, float flowed eastward crossing the SAF to the Polar Frontal Zone, with Antarctic Surface Water (AASW) in the upper layer and larger contribution of CDW in the lower part of the profile. Profiles along the Southwest Indian Ridge indicate the Antarctic Zone, with a thin layer of cold and low saline AASW and thicker upper and lower CDW. In DM analysis, the algorithm that selects the 10 best theta levels could select levels for which salinity values come alternately from upper and bottom layers, which can lead to enormous high salinity variability and for some profiles may prevent choosing the theta level to perform the analysis. The DM operator can consider to split the time series in the set calseries.m program:



FIG 4: Example float (1901869) crossing through different water masses and fronts in the Southern Ocean. Upper panel- time series of salinity; lower panel (left)- trajectory map of Argo float with historical data (combined CTD and Argo reference data), (right) theta/S diagram of float data.

calseries = [ones(1,50) 2*ones(1,90-50)
3*ones(1,n-90)]; % example split of float
profiles

This setting will split the time series into three parts and estimate the salinity error for these parts separately. This will help to better represent the variability of salinity data for each part of the float and compare it with surrounding reference data.

Status of the reference data

The key challenge to perform the DMQC analysis in the Southern Ocean is very limited spatial and temporal coverage of CTD reference data (**Figure 5**), which can lead to large uncertainties, spurious offset or trend that may be difficult to distinguish from a real offset or a sensor drift. The regions with relatively poor data coverage with complex ocean dynamics are, for instance, the Drake Passage, the Weddell Sea and southern Agulhas Basin. The majority of profiles in the CTD version 2019v01 reference database exceed around 25 years (9000 profiles). Since 1995 the number of CTD profiles per year was below 1100, with a

relatively strong drop in the number of profiles after 2011. The DM operator needs to therefore have a good understanding of spatial and temporal coverage of reference data and be careful in analyzing the OWC results. It is recommended to firstly perform the OWC analysis separately for CTD and Argo reference data and further to more precisely error and drift correction estimate use the combined CTD and Argo reference data. Moreover, in regions where reference data are not sufficient, DM operators can try to expand the spatial and temporal scales parameters (MAPSCALE_ LONGITUDE_LARGE, MAPSCALE_LATITUDE_ LAR-GE, MAPSCALE_AGE_LARGE) in objective mapping. The recommended settings are presented in the next section.



FIG 5: Upper panel- spatial distribution and lower panelnumber of CTD profiles per year in the Southern Ocean in 2019v01 version of the reference database. The year of sampling is color-coded.

OWC Configuration parameters in the South Atlantic and Southern Ocean.

The following configuration parameters are generally used in this region.

CONFIG_MAX_CASTS: 310 MAP_USE_PV: 1 MAP_USE_SAF: 1 MAPSCALE_LONGITUDE_LARGE: 6 MAPSCALE_LONGITUDE_SMALL: 3 MAPSCALE_LATITUDE_LARGE: 4 MAPSCALE_LATITUDE_SMALL: 2 MAPSCALE_PHI_LARGE: 0.1 MAPSCALE_PHI_SMALL: 0.02 MAPSCALE_AGE_LARGE: 20 MAPSCALE_AGE_SMALL: 10 MAP_P_EXCLUDE:100 MAP_P_DELTA: 200

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6901720

North Atlantic/ Subpolar Gyre

Contacts : Cabanes C., Herbert G., Thierry V.



Float Path

This ARVOR float was deployed in July 2016, close to the Bight Fracture Zone (**Figure 1**). It first crossed the Reykjanes Ridge going westward, then it came back and recirculated into the Iceland Basin. Finally, it crossed again the Ridge and started to flow northwestward following the western flank of the Reykjanes Ridge.

DMQC steps

Checking of RT flags

RT flags were checked, no profile needed flag modifications.

Running OWC software

OWC was run using the configuration parameters suggested for the North Atlantic (see **Part II.1**) and using successively Argo reference database (2018v1) and CTD reference database (2018v2).

Analysis of results

We first looked at the results obtained when OWC is run using the Argo reference database. If you are not familiar with the diagnostic plots of the OWC software, it is recommended to first read **Part I.6**. **Figure 2** shows that the 10 theta

levels (green horizontal lines) used to estimate the salinity correction are automatically chosen above and below the Labrador Sea Waters (LSW). Some of the theta levels are at depths shallower than 1000m. It should be fine since these levels are those with the less salinity variance along the float path.



To check that the automatic selection of the 10 theta levels is correct, we can look at **Figure 3**



FIG 3: Figure 2 from OWC (zoom on the deepest theta levels), REF ARGO

This figure plots the mapped salinities and their objective errors on the 10 theta levels, superimposed on the float theta/S diagram. Here, the choice of the 10 theta levels seems fine because the mapping errors are fairly homogeneous from one theta level to another and are comparable to the salinity variability observed along the float's path.



FIG 4: Number of observations selected by find_besthist.m (CONFIG_MAX_CASTS=250) within large spatial scales (upper panel) and small spatial scales (lower panel) for all the profiles of float 6901720. The time scale is represented on the vertical axis. "All" means that all data within the defined spatial scales are considered; "10" means that only data within 10 years and at the defined spatial scales are considered. The average number of observations available over all cycles is given on the left side of the graph.

Interannual variability can be high in subpolar North Atlantic even at depths greater than 1000m. The MAP_AGE_LARGE configuration parameter, which is equal to 2 years, will give priority to the most contemporary reference salinity profiles to estimate the mapped salinity. However, to better interpret the results of the OWC analysis, it is important to know the availability of reference data within the spatial and temporal scales that are defined in the configuration parameters.

Figure 4 indicates that some reference data are available for most of the profiles of this float within large spatial scales and within 2 years. Note that there is no reference data available within 1 year for the last 40 cycles. To this date, the float is still active and even the latest version of the Argo reference database does not contain such recent data. Within the small spatial and temporal scales (MAP_AGE = 0.69 yr), very few reference data are available.



Figure 5 shows that the salinity of the float 6901720 compares generally well with the salinity of surrounding Argo reference data. The variability observed on the red curve is expected in this region. The correction proposed is a small linear trend that lies within the 0.01 instrument accuracy threshold. It is however questionable whether the high positive red curve values observed during the first few cycles could reflect a failure of the salinity sensor, measuring too fresh values at the beginning of the float's mission.



FIG 6 : Figure 6 from OWC, REF ARGO. Float salinities are plotted against mapped salinities and their objective errors at each cycle and at different theta levels.

The analysis of Figure 6 can somewhat rule out this point because it shows that these fresher measurements are not observed at every theta level. At theta equal to 4.02°C float salinities of the first few cycles are indeed lower than the mapped salinities but this is not observed at a deeper theta level (3.48°C), where float salinities and mapped salinities are similar.

Whenever possible, it is recommended to make a reference hydrographic profile at float launch and to compare it to the first float profile.



reference hydrographic profile made at float launch (BOCATS campaign)

For Provor and Arvor floats, we used either the first descending profile recorded when the float dive to reach its parking depth or the first ascending profile. The first descending profile of float 6901720 and the reference hydrographic profile are obtained less than one day apart and are similar (Figure 7). The average salinity difference on theta levels is 0.0052, confirming that the float salinity sensor is working well at the beginning of the float's mission.

The OWC run using the CTD reference database is interesting to independently validate float salinity data, but it is important to first ensure that there is sufficient contemporary reference data in the vicinity of the float profiles. This condition is met for the float 6901720, thanks to recent data from OVIDE and RREX hydrographic campaigns that are included in the CTD reference database.

The correction proposed by this second OWC run (Figure 8) is very similar to the one obtained when Argo reference database is used. This confirms our previous analyses.



FIG 8: Figure 3 from OWC, REF CTD

Applied corrections

PSAL ADJUSTED=PSAL

The results of the two OWC runs are very similar and both propose a correction that is below the 0.01 PSU threshold. The similarity with the CTD made at the launch indicates that the salinity sensor is working well at the beginning of the float's mission. As a result, we consider that to date, the salinity measurements of the float 6901720 are not affected by any instrument errors, such as sensor drift or calibration offset.

PSAL_ADJUSTED_QC='1'

QC flags for adjusted salinity data are set to 1.

PSAL_ADJUSTED_ERROR = MAX (OWC uncertainties, 0.01)



FIG 9: Vertically averaged PSAL correction, QC flags (green=1, yellow=2, magenta=3 and red=4) and PSAL ADJUSTED ERROR written into the D-files.

5902303

North Atlantic/ Subpolar Gyre

Contacts : Cabanes C., Herbert G., Thierry T.



Float Path

This PROVOR float was deployed in june 2010, in the south-eastern part of the Icelandic basin (**Figure 1**). It then flowed northward, reached the North of the basin and finally started to flow southwestward, along the eastern flank of the Reykjanes Ridge.

DMQC steps

Preliminary checks



Before running OWC software, simple plots were analysed to get a first idea of the water mass sampled and the behavior of the sensors. Theta/S diagram and section charts that are displayed on the Argo Floats monitoring website show that the float sampled quite different water masses along its path especially after cycle 30, where it encountered saltier waters at depth (see **Figure 2**). This is because the float started to flow along the eastern flank of the Reykjanes Ridge where it encountered saltier water than in the inner Iceland Basin (**Figure 3**).



Argo salinities in the surrounding area at specified theta levels(3.4-3.5°c). Only RT data with QC=1 are selected and adjusted values are used if available.. Data from float 5902303 are circled with magenta.

This float is auto correcting pressure so no additional DM adjustment is required for PRES. Surface pressure corrections, which can be visualized on the Argo Floats monitoring website (Technical plots, other technical parameters) indicate that the pressure sensor is stable along the float life.

RT flags were finally checked, no profile needed flag modifications.

Running OWC software

OWC was run using the configuration parameters suggested for the North Atlantic (see **Part II.1**) and using successively Argo reference database (2018v1) and CTD reference database (2018v2).

Analysis of results

First OWC run

We first looked at the results obtained when OWC is run using the Argo reference database. These results were consistent with those obtained with the CTD reference database, which will not be discussed further. If you are not familiar with the diagnostic plots of the OWC software, it is recommended to first read **Part 1.6**. The correction proposed by the OWC software is shown on *Figure 3*. The correction suggests that a small fresh bias was present during the first 30 cycles and then the sensor has started to drift salty.



However, these first OWC results can be questioned. Indeed, **Figure 4** does not show any evidence of a salty drift in upper theta levels (7,72°C): the float salinities are comparable to the climatologies within error bars after cycle 30.



Figure 5 and **6** can help to understand what happened. **Figure 5** shows the 10 theta levels that have been selected by the software to compute the correction. Theta levels were automatically selected between 3.4°C and 5°C. We can see that the salinity of the float is highly variable at these levels: we're not really in a tight zone of theta/S diagram.





FIG 6: Figure 5 from OWC, REF: ARGO, first run

Figure 6 provides a complementary picture, showing the float salinity anomalies on theta

levels along its path. Anomalies are computed relative to the time averaged salinities of the float. While salinity is fairly homogeneous in the 3-4°C layers during the first thirty cycles , it is not the case after, where salinity seems more stable in upper layers.



Second OWC run : splitting the time series

A second OWC run was then performed using the same configuration parameters as for the first run but splitting the time series in two distinct parts. To split the time series it is necessary to edit the set_calseries.m function. For example, if you want to split the time series at cycle 32 you must change the following line: calseries= [ones(1,n)];

by:

calseries = [ones(1,32) 2*ones(1,n-32)];

Figure 7 shows the theta levels that have then been chosen by the software for cycles 1-32 and for cycles 33-44. They are different and range between 3-4°C before cycle 32 and 5-8°C after. The correction proposed by the software is less variable particularly after cycle 32 and indicates a fresh offset very close to 0.01 PSU (**Figure 8**). This fresh offset is consistent with the one obtained by the comparison of the first descending profile recorded when the float dive to reach its parking depth and the reference hydrographic profile made at float launch (**Figure 9**)



FIG 8 : Figure 3 from OWC, REF ARGO, second run.



FIG 9: Comparison of the first descending profile of float 5902303with the reference hydrographic profile made at float launch (OVIDE 2010 campaign)

Conclusions

The results of the second OWC run and the comparison to the reference hydrographic profile made at float launch are consistent and indicate that the salinity sensor is slightly fresh biased. We have then decided to apply the correction proposed by the second OWC run.

PSAL_ADJUSTED_QC='1'

QC flags for adjusted salinity data are set to 1.

PSAL_ADJUSTED_ERROR	=	MAX	(OWC
uncertainties, 0.01)			

3901598 and 3901988

Nordic Seas

Contacts : Klein B. and Angel-Benavides I.M.



FIG 1: Topography and surface currents in the Nordic Seas, from Mork et al. 2019

3901598

This Arvor float was deployed in 09.05.2017 in the Noridc Seas in the Lofoten Basin. Because the flow in the Nordic Sea is so closely guided by topography the float trajectory follows basin contours. The small scales of variability in the Nordic Seas require much smaller search radii than in the subpolar Atlantic. The selection shown in **Figure 2** has been achieved by multiplying the recommended NA settings of Cabanes et al. by 0.5. It is mandatory to use the f/H criterion to limit the reference data to the topographic contours and avoid data from surrounding basins.

The selection of reference levels should focus on the deep layers. In the deep Norwegian, Lofoten and Greenland Basin one should select theta levels deeper than 1000 m, in the shallower Iceland Sea where maximum water depth is less than 1500 m a compromise has to be found and depth greater than 800 m should be considered. In this case the reference levels were evenly spread between 1000- 2000 m and cover the temperature range from -0.2 °C to -0.9 °C (**Figure 3**). As can be also seen from **Figure 3** the hydrographic properties converge to a very narrow range below 1000 m and the upper layers have a much larger variability due to inflow of Atlantic waters from the subpolar Atlantic.



FIG 2: Float trajectory for 3901958 and selected reference data in blue

Analysis of results

Because of the low levels of variability in the Nordic Seas the cycle to cycle deviations of float salinity measurements compared to the reference climatology have little variation (**Figure 4**) and differ markedly from similar OWC diagnostic plots in the SPG (see **Part III**, float**6901720**). The cycle-to-cycle variations in corrections are largest in the first 60 cycles when the float is in closer proximity to boundary current with inflowing Atlantic waters. Proposed corrections are well within the uncertainty limits of the method and therefore the Argo Qc manual suggests that no corrections should be performed.



reference levels in the stable deep layers.

The distributions on isopycnals (**Figure 5**) shows the extreme stability of hydrographic properties in the deep layers of the Nordic Seas. Float measurements are always with the standard deviations of the reference data set, even though they are consistently at the lower range of the reference data distributions in the first half of the time series.

In contrast to the stable deep layers the water column down to 1000 m depth shows clear signs of long-term trends associated with climatic changes upstream in the subpolar gyres and these signals propagate from surface to larger depth over time (**Figure 6**). In the Norwegian and Lofoten basin they have reached 1000 m depth.



FIG 4: Modified Fig. 3 from OWC. The light green band between -0.01 to 0.01 indicates the expected uncertainty range for the OWC method in the global ocean.



It is therefore essential that the temporal coverage of the reference data in the Nordic

Seas is up-to-date in order to reflect the climatic trends and the progression of these signals to larger depth. This is especially true for the shallower Iceland Sea where trends have affected most of the water column. An update of the reference database has been performed in 2019 (see section 5) and additional data from sources UDASH and ICES have been added. **Figure 7** shows the evolution of salinity at a level of 900 m and shows distinct trends in the Greenland Basin and Iceland Sea and to a lesser extent for the Norwegean Basin. The Lofoten Basin stands out with its elevated variability levels.



FIG 6: Salinity and temperature trends in the upper 1000 m of the Norwegian and Loftoten basin, from Mork et al. 2019.



FIG 7: Salinity trends at 900 m depth in the Nordic Seas

3901988

This APEX float was deployed on 28.02.2018 in the Iceland Sea has remained in the basin. With the same settings of OWC as described above the selected reference data are confined to the Iceland Sea and the East Greenland current along the coast (**Figure 8**).



FIG 8: trajectory of float until cycle 176 and reference data in blue



FIG 9: Fig. 3 from OWC from DMQC performed until cycle 176

In this case the selected reference levels are distributed over the depth range 800-1100 m and the comparison to the selected reference data (**Figure 9**) shows no signs of salinity drift except for the end of the time period spanned at the dmqc performed in August 2019.

Comparing **Figure 9** to **Figure 10** it appears as if the float itself is reporting very stable salinities. For this float which is still alive it has to be checked at following dmqc sessions if the trends continue or are related to hydrographic variability or distribution of reference data in particular parts of the float trajectory.



References:

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Part III: Use cases

1901227

Southern Ocean

Contacts : Walicka K.

Float Path

In December 2008, the analysed Apex float was deployed in the Southern Ocean region, in the Drake Passage (**Figure 1**). This float was driven eastward by the Antarctic Circumpolar Current, where after 7.34 years it reached the Australian Antarctic Basin.



FIG 1: (Figure 1 from OWC, REF:ARGO) Float 1901227. Location of the float profiles (red line with coloured numbers) and the CTD and Argo reference data selected for mapping (blue dots).

DMQC steps

Checking of RT flags

Float shows few profiles with density inversion issues at the pycnocline depths (profiles: 116-117, 222-232) and salty hooks at the bottom part of the profiles (233-242, 248-250). These parts of the profiles were flagged as bad data, 4.

Running OWC software

OWC was run using the configuration parameters suggested for the Southern Ocean (see **Part II.4**) for CTD and Argo reference database (2018v1) (see **Part I.5**). The DMQC analysis was performed for both CTD and Argo reference data, due to relatively low coverage by CTD casts. This analysis has been performed for two different constraints of theta levels. In the

first run of OWC, we did not constrain the selection of theta levels in set_calseries.m. In the second iteration, the theta levels were constrained to below 500 dbar. This configuration allowed us to avoid high variable mode water masses from the upper layers and density inversion that occurred below 3 °C.

Analysis of results

The first OWC run



FIG 2: (Figure 8 from OWC, REF:ARGO) Float 1901227. Plots including the theta levels chosen for calibration: Top left: Salinity variance at 10 theta levels. Top right: T/S diagram of all profiles of Argo oat. Bottom left: potential temperature plotted against pressure. Bottom right: salinity plotted against pressure.

Figure 2 shows 10 theta levels used to estimate the salinity corrections, automatically selected by the OWC method. The selected theta levels represent the upper and mid-layer corresponding to Antarctic Intermediate Water. The tightness relationship between the salinity variance and potential temperature is relatively weak of 0.05. The T/S diagram shows that these theta levels were selected from the range of water mass inversion, with a large range of variability in salinity data. This result shows that selected levels are not the best for comparison with Argo float.



oat salinity and the objectively estimated reference salinity at the 10 float the tale used in calibration.

The T/S diagram from **Figure 3** helps to distinguish between different water masses regimes. For the first around 100 profiles, where the float is between the Drake Passage and the Mid-Atlantic Ridge, the water masses are relatively cold, below 2°C. Further, when the float moved eastward, float temperature markedly increased, which is characteristic for this region. The selected theta levels are associated with high error and capture mostly profiles from the second half of float life.

Figure 4 demonstrates very high anomalies between the Argo float salinity and reference data. For most of the float life, these differences exceed ±0.02. The estimated error is very low of 0.005, however, this can be biased by a very long time series (268 profiles). To reduce the variability of this float and to obtain a more representative error estimate, another run of OWC with different theta levels constraints is recommended.



FIG 4: (Figure 3 from OWC, REF:ARGO) Float 1901227. Evolution of the suggested adjustment with time. The top panel plots the potential conductivity multiplicative adjustment. The bottom panel plots the equivalent salinity additive adjustment. The red line denotes one-to-one profile fit that uses the vertically weighted mean of each profile. The red line can be used to check for anomalous profiles relative to the optimal fit.



FIG 5: (Figure 6 from OWC, REF:ARGO) Float 1901227. Plots of the evolution of salinity with time along with selected theta levels with minimum salinity variance

Figure 5 reveals many very fresh spikes, almost for the entire time series, these are because OWC software is also selecting salinity data from

shallow depths due to temperature inversion. Another OWC analysis, run with constrained theta levels to deeper layers should reduce the spikes. However, Argo float data are within the variability of the reference data, showing no indications of an issue with the float.

The second OWC run

To apply a constraint on depth when selecting theta levels for the analyses, you must modify the set_calseries.m program:

use_pres_gt = 500;

use_pres_lt = [];

will select theta levels whose pressure is greater than 500 dbar.

After applying the theta level depth constraint to below 500 dbar, all theta levels were selected below 1500 m (**Figure 6**). The salinity variance at these theta levels showed a very tight relationship, reaching below 0.0025, which confirms the well-selected range of data for comparison.



FIG 6: (Figure 8 from OWC, REF:ARGO) Float 1901227. Plots including the theta levels chosen for calibration: Top left: Salinity variance at 10 theta levels. Top right: T/S diagram of all profiles of Argo oat. Bottom left: potential temperature plotted against pressure. Bottom right: salinity plotted against pressure.

Figure 7 presents the T/S diagram for the float data with the selected theta levels with the associated errors including both the early profiles and those from the end of the float life.

This result ensures we correctly selected the 10 theta levels for DMQC analysis.



FIG 7: (Figure 2 from OWC, REF:ARGO) Float 1901227. Plots the original oat salinity and the objectively estimated reference salinity at the 10 float theta levels that are used in calibration.



FIG.8: (Figure 5 from OWC, REF:ARGO) Float 1901227. Evolution of the suggested adjustment with time. The top panel plots the potential conductivity multiplicative adjustment. The bottom panel plots the equivalent salinity additive adjustment. The red line denotes one-to-one profile fit that uses the vertically weighted mean of each profile. The red line can be used to check for anomalous profiles relative to the optimal fit.

The evaluation of the suggested adjustment presented in **Figure 8** informs that the Argo

float data are in relatively good agreement compared with surrounding reference data. Some temporal variability recorded over float life can be an effect of the local eddies and very different and complex hydrographic regimes. The corrections suggested by the OWC method shows a slight linear trend. However, this trend lies within the 0.01 salinity differences that is an uncertainty threshold suggested by the manufacturer.

Figure 9 demonstrates reduction of spikes and variability at the theta levels. Similar to results from the first OWC run, the Argo float salinity data lie within the variability of the reference data. In this iteration, for some profiles (Profiles 150-240) the selected theta levels are not available, however, by considering the previous iteration of this float we can confirm good fit to reference data and that this float is behaving well.



FIG 9: (Figure 6 from OWC, REF:ARGO) Float 1901227. Plots of the evolution of salinity with time along with selected theta levels with minimum salinity variance.

Applied corrections

PSAL_ADJUSTED=PSAL

The results from the OWC outputs show no indications of offset of drifts in this float. The associated error has been estimated based on

the second OWC output, due to lower salinity anomalies. The error of salinity data is below 0.01.

PSAL_ADJUSTED_QC='2'

The QC flag of salinity data has been set to 2, due to the TNPD issue of the pressure data (see **Part I.4**).

PSAL-ADJUSTED_ERROR=MAX (OWC uncertainties, 0.01

3901494

Southern Ocean

Contacts : Walicka K.

Float Path

Float 3901494 was deployed in April 2014 in the Falkland Plateau (**Figure 1**). This float was driven westward by the Antarctic Circumpolar Current (ACC). Initially float entered the Argentine Basin, then it reached the region of the Scotia Arc, to finally flow along the American-Antarctic Ridge.



FIG 1: (Figure 1 from OWC, REF: ARGO) Float 3901494. Location of the float profiles (red line with coloured numbers) and the CTD and Argo reference data selected for mapping (blue dots).

DMQC steps

Checking of RT flags

The visual inspection of this float did not show any issues with the profiles.

Running OWC software

OWC was run using the configuration parameters from **Part II.4**. Due to relatively poor time and spatial data coverage in this region (**Part II**, Figure 5) in analysis both CTD (2019v01) and Argo (2020v03) reference databases were used. The review of the temperature and salinity profiles in Figure 2 shows that the analysed float was crossing through different fronts and zones of the ACC with distinct water mass properties. The initial part of the float presents relatively warmer water masses in the entire water column, whereas with moving south-eastward it cools significantly. Figure 3 (top left) shows the T/S diagram reflecting three different properties of water masses through which the float was crossing. This variety of water mass properties can lead to difficulties in selecting the theta levels for time series of the entire float. Additional difficulty with this float is the presence of the temperature inversion, with very low temperature in the upper and lower part of the profiles, which could cause that in OWC analysis the code can select the salinity data from various depths, leading to huge spikes along the float time series.



FIG 2: Float 3901494. Time series of vertical distribution of (a) potential temperature (°C) and (b) salinity (PSS-78).

Analysis of results

The first OWC run

The first run of OWC was performed without selecting particular levels in set_calseries.m code (**Figure 3**). The theta levels selected in this run are therefore from both upper and lower parts of the profiles (**Figure 3**, top left) leading to presence of many spikes and large differences between float profiles and reference data (**Figure 3**, bottom).



To prevent selection of the theta levels from different water masses in set_calseries.m code the theta levels were set to below 500 dbar. Then, to better represent the changes in water masses variability and salinity error the float time series was separated into three parts:

calseries = [ones(1,20) 2*ones(1,44-20) 3*ones(1,n-44)]; % split of float profiles

The second OWC run

In the second run the theta levels selected to comparison with Argo float come from the deepest part of the profiles (**Figure 4**) with relatively low objective error associated. The salinity variance on the selected theta levels are

in order of 10^{-5} , representing the well selected levels.



FIG 4: (Figure 8 from OWC, REF: CTD+ARGO) Float 3901494. Plots including the theta levels chosen for calibration: Top left: Salinity variance at 10 theta levels. Top right: T/S diagram of all profiles of Argo oat. Bottom left: potential temperature plotted against pressure. Bottom right: salinity plotted against pressure.

Figure 5 shows relatively high variability of salinity data for the first around 20 profiles, resulting in differences between the float and reference data exceeding 0.03. This variability is associated with location of float in a very dynamic region with strong influence of eddies and fronts. The time series of further profiles shows that the salinity difference is not exceeding 0.01, suggesting a good agreement between float profiles and reference data.



FIG 5: (Figure 3 from OWC, REF: CTD+ARGO) Float 3901494. Evolution of the suggested adjustment with time. The red line denotes one-to-one profile fit that uses the vertically weighted mean of each profile. The red line can be used to check for anomalous profiles relative to the optimal fit.

The time series of Argo at three selected theta levels (**Figure 6**) shows a good fit of referenced data from CTD and Argo database. The initial part of the float time series is not displayed because these theta levels are not available there. However, by analyzing the rest of the float variability the OWC analysis showed no evidence of salinity drift of offset.





Applied corrections

The OWC outputs show no evidence of the salty drift or offset for the entire float life. No correction was needed.

PSAL_ADJUSTED_QC='1'

QC flags for adjusted salinity data are set to 1.

PSAL_ADJUSTED_ERROR = MAX (OWC uncertainties, 0.01)

3901852

Black Sea

Contacts: Notarstefano G.

Status of the float

The float was deployed in the Black Sea in December 2016 (**Figure 1**) and performed 129 cycles at the time of the analysis. The salinity and potential temperature profiles are depicted in **Figures 2 and 3**, respectively.







Surface pressure

The adjusted surface pressure is plotted in **Figure 4**. Surface pressure is extracted from the Argo technical file: the variable name is "PRES_SurfaceOffsetCorrectedNotResetNegative _1cBar Resolution_dbar". No further adjustment of the CTD pressure profiles is required because the data is auto-corrected on board the float.



FIG 4: Adjusted surface pressure values versus profile number.

Reference dataset

The reference dataset used in the DMQC method, is composed of the following CTD and Argo historical datasets:

CTD:

CMEMS: INSITU_BS_TS_REP_OBSERVATIONS_013_042 Coriolis: CTD_for_DMQC_2018V01 **Argo**: ARGO_for_DMQC_2018V01

The analysis is performed using both the two datasets, due to the not homogeneous coverage (both in time and space) of the CTD reference dataset.

Analysis before the OWC approach

Regional characteristics

The main water masses of the Black Sea are highlighted in the TS diagram of **Figure 5**: the surface water (BSSW, 2% del volume totale), the cold intermediate water (CIL, sub-surface, 2% del volume totale), the intermediate water (BSIW, 100-1100 m, 55% del volume totale), the deep water (BSDW, 40% del volume totale). The BSDW is a water mass with stable TS characteristics, with vertical homogeneity of T and S from 1700 m to the bottom, where TS values collapse to a single point (8.90 °C; 22.32).



When OWC is applied, the part of the TS diagram to be used is the one characterized by the tightest relationship between T and S and hence in the area of the BSDW. So, "set_calseries" and "ow_config" files have to be configured accordingly. In particular, in "set_calseries" the parameter "use_theta_gt" was

set equal to 8.855 °C (that means use theta greater than 8.855 °C) and in the "ow_config" the "MAP_P_EXCLUDE" was set equal to 900 (that means exclude the top 900 dbar).

Before running OWC, the theta-salinity (θ -S) diagram of the float is analyzed and in particular the area where the θ -S relationship is the tightest (**Figure 6**). The analysis of this portion of the θ -S curve can help in detecting sensor salinity anomalies. No significant salinity drift is observed.



DMQC: configuration and results

The parameters used for the objective mapping are listed hereafter. A maximum of 4 break points is allowed in the piecewise linear fit.

```
CONFIG_MAX_CASTS: 300
MAP_USE_PV: 1
MAP_USE_SAF: 0
MAPSCALE_LONGITUDE_LARGE: 4
MAPSCALE_LONGITUDE_SMALL: 1.33
MAPSCALE_LATITUDE_SMALL: 1.33
MAPSCALE_LATITUDE_SMALL: 1.33
MAPSCALE_PHI_LARGE: 0.5
MAPSCALE_PHI_SMALL: 0.1
MAPSCALE_AGE: 10
MAP_P_EXCLUDE: 900
MAP_P_DELTA: 100
```

In set_calseries.m: use_theta_gt = 8.855 In **Figure 7** the float trajectory and the historical CTD locations selected by the OWC method are shown.



The results of the OWC method are presented in **Figures from 8 to 10.** The 10 θ -levels chosen for the correction are reported in **Figure 8**. The corrected and uncorrected float salinity and the mapped salinity on two selected θ -levels are depicted in **Figure 9**. The correction proposed is presented in **Figure 10**.





FIG 9: Comparison between the float salinity data and the mapped salinity, on θ -levels.



The analysis of the θ -S diagram of profile segments deeper than 900 dbar (**Figure 11**) shows that the OWC method was run where the θ -S relationship is the tightest. The mapped historical data are depicted as red lines in **Figure 11** whilst the uncalibrated float data as black lines.



Conclusions

The correction proposed by OWC (**Figure 10**) is quite small, below the Argo requested accuracy (0.01) and within the sensor accuracy (0.005). The one-to-one fit (red line in **Figure 10**) is stable and this means that the fit is realistic. **Figure 9** shows that the float salinity is quite constant on selected θ -levels during the float's lifetime. In the most uniform section of the θ -S curve (**Figure 6 and 11**) no systematic shift in time of the θ -S profiles is observed. We can conclude that there is not any salinity drift/offset in the float measurements. Hence, the salinity data of Float WMO 3901852 are accurate and don't need a delayed mode correction:

PSAL_ADJUSTED=PSAL

The quality flags applied are the following:

PSAL_ADJUSTED_QC='1' from cycle 1 to 129

3901908

Mediterranean Sea

Contacts : Notarstefano G.

Status of the float

The float was deployed in the Central Mediterranean (Ionian sub-basin, **Figure 1**), in January 2017 and performed 220 cycles at the moment of this analysis. The salinity and potential temperature profiles are depicted in **Figures 2 and 3**, respectively.



FIG 1: Float trajectory color-coded per cycle number (the black dot represents the last float position).





Surface pressure

The adjusted surface pressure is plotted in **Figure 4**. Surface pressure is extracted from the Argo technical file: the variable name is "PRES_SurfaceOffsetCorrectedNotResetNegative _1cBar Resolution_dbar". No further adjustment of the CTD pressure profiles is required because the data is auto-corrected on board the float.



FIG 4: Adjusted surface pressure values versus profile number.

Reference dataset

The reference dataset used in the DMQC method, is composed of the following CTD and Argo historical datasets:

CTD:

CMEMS:

INSITU_MED_TS_REP_OBSERVATIONS_013_041 Coriolis: CTD_for_DMQC_2019V01 Historical CTD profiles provided through personal contact **Argo**: ARGO_for_DMQC_2019V03

The analysis is performed using both the two datasets, due to the not homogeneous coverage (both in time and space) of the CTD reference dataset.

Analysis before the OWC approach

Before running OWC, the theta-salinity (θ -S) diagram of the float (**Figure 5**) is analyzed and in particular the area where the θ -S relationship is the tightest (**Figure 6**). The analysis of this portion of the θ -S curve can help in detecting sensor salinity anomalies. A large positive salinity drift is observed after about the first 20 profiles (blue profiles circled in red in **Figure 6**). A huge negative salinity offset occurs after cycle 132 (group of red profiles in **Figure 5**).





FIG 6: Area of the θ -S diagram (color-coded per cycle number) where the θ -S relationship is more uniform.

DMQC: configuration and results

OWC was applied to the float WMO 3901908 operating in the Mediterranean Sea. The parameters used for the objective mapping are listed in hereafter. A maximum of 4 break points is allowed in the piece-wise linear fit.

CONFIG_MAX_CASTS: 300 MAP_USE_PV: 1 MAP_USE_SAF: 0 MAPSCALE_LONGITUDE_LARGE: 4 MAPSCALE_LONGITUDE_SMALL: 1.33 MAPSCALE_LATITUDE_LARGE: 4 MAPSCALE_LATITUDE_SMALL: 1.33 MAPSCALE_PHI_LARGE: 0.5 MAPSCALE_PHI_SMALL: 0.1 MAPSCALE_AGE: 10 MAP_P_EXCLUDE: 700 MAP_P_DELTA: 250

In **Figure 7** the float trajectory and the historical CTD locations selected by the OWC method are shown.



The results of the OW method are presented in **Figures from 8 to 10**. The 10 θ -levels chosen for the correction are reported in **Figure 8**. The corrected and uncorrected float salinity and the mapped salinity on two selected θ -levels are depicted in **Figure 9**. The correction proposed is presented in **Figure 10**.





FIG 9: Comparison between the float salinity data and the mapped salinity, on θ -levels.



The analysis of the θ -S diagram of profile segments deeper than 700 dbar (**Figure 11**) shows that the OW method was run where the θ -S relationship is the tightest. The mapped historical data are depicted as red lines in **Figure 11**, whilst the uncalibrated float data as black lines.



Conclusions

The correction proposed (Figure 10) is negative up to profile 132 and a strong positive drift is observed from profile 23; the correction is larger than -0.5 at profile 132. Then, the correction proposed becomes largely and suddenly positive. Figure 9 shows that there is an offset in salinity at profile 23 followed by a constant drift, where the float salinity on selected θ-levels strongly exceeds the climatological estimates. This is an indication of a conductivity sensor malfunctioning. In the most uniform section of the θ -S curve (**Figure 6**) and 11) the variability of the float salinity is extremely large (about 0.5) and a systematic salinity offset in time is observed: this is a confirmation that salinity measurements from this Argo float are inaccurate. We can conclude that there is evidence of a salinity drift in the float measurements. After profile 132 there is a suddenly huge negative offset (Figure 9) that states the ultimate deterioration of the conductivity sensor or other serious problems. Since the observed salinity drift and offset are extremely large, we consider the salinity data of Float WMO 3901908 unadjustable:

PSAL_ADJUSTED=PSAL from cycle 1 to 220

The quality flags applied are the following:

PSAL_ADJUSTED_QC='1' from cycle 1 to 22 PSAL_ADJUSTED_QC='4' from cycle 23 to 220

Since the float is still alive at the moment of this analysis, it has been decided to assign a QC flag 3 to salinity in the real time files (Rfiles) and to put this float into the grey list.

3901907

Mediterranean Sea : an example of salty drift

Contacts : Notarstefano G.

Status of the float

The float was deployed in the Western Mediterranean (Algerian sub-basin), north of the Algerian coast (**Figure 1**), in January 2017 and performed 120 cycles at the moment of this analysis. The salinity and potential temperature profiles are depicted in **Figures 2 and 3** respectively.







Surface pressure

The adjusted surface pressure is plotted in **Figure 4**. Surface pressure is extracted from the Argo technical file: the variable name is "PRES_SurfaceOffsetCorrectedNotResetNegative _1cBar Resolution_dbar". No further adjustment of the CTD pressure profiles is required because the data is auto-corrected on board the float.





Manual inspection and identification of major spikes in temperature and salinity

One spike was detected in salinity profile 85 at the pressure level of 645.5 dbar (**Figure 5**). The quality flag associated with this salinity value was changed to 4.



Reference dataset

The reference dataset used in the DMQC method, is composed of the following CTD and Argo historical datasets:

CTD:

CMEMS: INSITU_MED_TS_REP_OBSERVATIONS_013_041 Coriolis: CTD_for_DMQC_2018V01 Historical CTD profiles provided through personal contact **Argo:** ARGO_for_DMQC_2018V01

The analysis is performed using both the two datasets, due to the not homogeneous coverage (both in time and space) of the CTD reference dataset.

Analysis before the OWC approach

Before running the Owens and Wong method, referred to as OWC hereafter, the theta-salinity (θ -S) diagram of the float is analyzed (**Figure 6**) and in particular the area where the θ -S

relationship is the tightest (**Figure 7**). The analysis of this portion of the θ -S curve can help in detecting sensor salinity anomalies. A large positive salinity drift is observed after about profile 100.



FIG 6: *θ* -S diagram color-coded per cycle number.



FIG 7: Area of the θ -S diagram (color-coded per cycle number) where the θ -S relationship is more uniform.

Three salinity float profiles are selected to perform a comparison (in time and space) with the historical data. The salinity float profile is depicted in black while other colours represent the salinity reference profiles in **Figures 8, 9, 10.** The red colour means that the historical data are more recent with respect to the float ones, while magenta states that the float data are more recent than the historical ones (the maximal difference is 3 years). A time difference between 3 and 6, 6 and 9 and larger than 9
years is depicted in green, cyan and blue, respectively.







data (upper panel) and the respective salinity profiles (bottom panel).



The comparison of these 3 selected salinity float profiles with the closest (in space) salinity reference profile is shown in **Figures from 11 to 13.** The temporal difference between the two datasets is quite large for profile number 2, whilst it is about one year for profiles 60 and 120. The agreement between the float salinity profiles and the historical salinity profiles is good for profile 2, whilst a small difference is observed for profile 60 in the intermediate and deeper layers, where the water column is more stable. The salinity of the float profile 120 is in strong disagreement with the selected historical profile.



FIG 11: The salinity float profile number 2 (black dots in upper panel) is compared to the nearest in space reference profile (red dots in upper panel). The locations of the two profiles and their distance is given in the bottom panel.



FIG 12: The salinity float profile number 60 (black dots in upper panel) is compared to the nearest in space reference profile (red dots in upper panel). The locations of the two profiles and their distance is given in the bottom panel.



compared to the nearest in space reference profile (red dots in upper panel). The locations of the two profiles and their distance is given in the bottom panel.

A comparison with another float deployed in the same area is also performed. The θ -S diagram of the float WMO 6901513 is superimposed to the one of the Argo float WMO 3901907 in **Figure 14.** A large positive salinity drift of float WMO 3901907 seems to be confirmed after about the first 100 profiles.



FIG 14: The θ -S diagram of the uncalibrated float WMO 3901907 (black lines) compared to the float WMO 6901513 (red lines).

DMQC: configuration and results

We applied the OWC DMQC method to the float WMO 3901907 operating in the Mediterranean Sea. The parameters used for the objective mapping are listed hereafter. A maximum of 4 break points is allowed in the piece-wise linear fit.

CONFIG_MAX_CASTS: 300 MAP_USE_PV: 1 MAP_USE_SAF: 0 MAPSCALE_LONGITUDE_LARGE: 4 MAPSCALE_LONGITUDE_SMALL: 1.33 MAPSCALE_LATITUDE_LARGE: 4 MAPSCALE_LATITUDE_SMALL: 1.33 MAPSCALE_PHI_LARGE: 0.5 MAPSCALE_PHI_SMALL: 0.1 MAPSCALE_AGE: 10 MAP_P_EXCLUDE: 700 MAP_P_DELTA: 250

In **Figure 15** the float trajectory and the historical CTD locations selected by the OWC method are shown.



the historical CTD data (blue dots).

The results of the OWC method are presented in **Figures from 16 to 19.** The 10 θ -levels chosen for the correction are reported in **Figure 16**. The corrected and uncorrected float salinity and the mapped salinity on two selected θ -levels are depicted in **Figure 17.** The float salinity data corrected by the OWC method are presented in **Figure 18**. The correction proposed (**Figure 19**) is always negative with values that exceed -0.1.





FIG 17: Comparison between the float salinity data and the mapped salinity, on θ -levels.



FIG 18: θ -S diagram of the corrected salinity data (color-coded per time in the upper panel and with the mapped data in red superimposed in the bottom panel).



The analysis of the θ -S diagram of profile segments deeper than 700 dbar (**Figure 20**) shows that the OWC method was run where the θ -S relationship is the tightest. The mapped historical data are depicted as red lines in **Figure 25**, whilst the uncalibrated float data as black lines.





Conclusions

The correction proposed (Figure 19) is negative and a small positive drift is observed up to profile 96; then, a strong positive drift is evident up to the last analyzed profile (120), where the correction proposed is larger than -0.1. Figure **17** shows that the float salinity is not constant on selected θ -levels and values strongly exceed the climatological estimates after profile 96. This is an indication of a conductivity sensor malfunctioning (drift). Moreover, in the most uniform section of the θ -S curve (**Figure 7 and** 20) the variability of the float salinity is extremely large (larger than 0.1) and a systematic salinity offset in time is observed (Figure 7): this is a confirmation that salinity measurements from this Argo float are inaccurate. The comparison between selected float salinity profiles and the historical profiles (Figures from 11 to 13) shows the lowering of the conductivity sensor stability in the first 100 profiles followed by a strong deterioration. The conductivity measurements drift is also observed by comparing the θ -S curve of the float to the one of float 6901513 (Figure 14) that is guite close in space. We can conclude that there is evidence of a salinity drift in the float measurements. Hence, the salinity data of Float WMO 3901907 need a delayed mode correction, that is the following:

PSAL_ADJUSTED=PSAL+ Δ S from cycle 1 to 120

The quality flags applied are the following:

PSAL_ADJUSTED_QC='1' from cycle 1 to 96 PSAL_ADJUSTED_QC='4' from cycle 97 to 120

The delayed-mode files (Dfiles) have been created accordingly and sent to the Coriolis GDAC. Since the float is still alive at the moment of this analysis, it has been decided to assign a QC flag 3 to salinity in the real time files (Rfiles) and to put this float into the grey list, due to this large salinity drift.