Integrated Marine Observing System

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Animal Tracking

Best Practice Manual for SMRU CTD Satellite Relay Data Loggers: Instrument Calibration, Near Real-Time and Delayed Mode Data QA/QC

Version 1.0

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Australia's Integrated Marine Observing System (IMOS) is enabled by the National Collaborative Research Infrastructure Strategy (NCRIS). It is operated by a consortium of institutions as an unincorporated joint venture, with the Univeristy of Tasmania as Lead Agent.

IMOS acknowledges the Traditional Custodians and Elders of the land and sea which we work and observe, and recognise their unique connection to land and sea. We pay our respects to Aboriginal and Torres Strait Islander people past and present.

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Contents

1. Introduction

This document is the IMOS Animal Tracking Facility's Best Practice manual for near real-time and delayed-mode processing of physical and behavioural observations collected using Sea Mammal Research Unit CTD Satellite Relay Data loggers (SMRU CTD-SRDL). The IMOS Animal Tracking Facility deploys SMRU CTD-SRDL's on southern elephant seals (*Mirounga leonina*) and Weddell seals (*Leptonychotes weddellii*) in the Southern Ocean and on olive ridley sea turtles (*Lepidochelys olivacea*) and flatback sea turtles (*Natator depressus*) in the Timor and Arafura Seas. The data transmitted by these instrumented animals contributes to the study of ocean structure and dynamics by supplying temperature and salinity observations within the upper ocean in high latitude, shallow coastal and tropical regions that are historically under-sampled by traditional observing platforms.

This document describes the calibration methods used by the IMOS Animal Tracking Facility prior to instrument deployment and the quality analyses/quality control (QA/QC) methods for both near real-time and delayed-mode data.

2. Background

Animals collecting hydrographic observations have advanced our understanding of the world's oceans and the behaviour of its top predators (Roquet *et al.*, 2013; Roquet *et al.*, 2014; Williams *et al.*, 2016; McMahon *et al.*, 2017; McMahon *et al.*, 2019; Harcourt et al. 2019; Hindell *et al.*, 2020). Technological advancements in instrument design, data compression and data transmission have made accessible data previously unavailable (Fedak *et al.*, 2002; Boehme *et al.*, 2009; Fedak, 2013), but crucially important to oceanographic, climate and ecological studies and to the oceanographic operational and forecasting communities through the Global Telecommunications System (GTS).

The Animal Borne Ocean Sensors (AniBOS) network, of which the IMOS Animal Tracking Facility is a core member, coordinates the collection and delivery of marine measurements collected by platforms deployed on animals into the broader Global Ocean Observing System (GOOS). AniBOS provides a cost-effective and complementary capability to existing GOOS networks to monitor essential ocean variables (EOV), essential climate variables (ECV) and essential biodiversity variables (EBV) (McMahon *et al.* 2021). AniBOS was formally recognized in 2020 as a GOOS network by the Observation Coordination Group (OCG). The Temperature-Salinity observations the network contributes to GOOS greatly improves our ability to more comprehensively monitor the oceans and animals that live in them, thereby improving our understanding of the global ocean and climate processes for societal benefit (UN Sustainability Goals 13 & 14: Climate & Life below Water).

Since the first oceanographic instruments were attached to animals in 2002, over 650,000 conductivity-temperature-depth (CTD) profiles have been made freely available to the global community via the Global Telecommunications System (GTS) (McMahon *et al.* 2021). The animal-borne ocean observing community started as a series of independent programs to collect animal behaviour and oceanographic data. However, the vast amount of generated data required some level of international coordination to provide standardized, quality-controlled data to the oceanographic community (Roquet *et al.* 2014). To facilitate and coordinate this effort, the Marine Mammals Exploring the Oceans Pole to Pole (MEOP) was established as part of the International Polar Year (Roquet *et al.*, 2017; Treasure *et al.*, 2017) and ensured that these animal-derived physical data were readily and publicly available for operational and scientific applications. However, as the community has grown it has become increasingly apparent that instrument calibration and data quality control procedures need to be decentralised.

In the following sections we outline the procedures used to overcome technology-related limitations of animal-borne observations (*e.g.* sensor drift, errors related to thermal mass and density inversion, etc.) and maximise the accuracy and precision of hydrographic profiles and their positions.

3. Animal-borne SMRU CTD-SRDL tags

The SMRU CTD-SRDL tags use a Valeport CTD miniaturized sensor head (see Supplementary Information 8.1 for details) to measure conductivity, temperature, and pressure. Tags are deployed on seals and sea turtles while the animals are hauled out on land. Once back in the water, the tags continuously record pressure at a 4-s sample rate (Fig. 1).

As both seals and turtles dive frequently, the time-linked pressure measurements provide detailed behavioural information on diving activity. During the ascent phase (upcast) of deeper dives, the tags measure conductivity and temperature at 1 Hz to construct CTD profiles that are stored in onboard memory. These high-resolution data can be downloaded from the tag should it be recovered, however relatively few tags are recovered. For this reason, the tags rely on the Argos satellite system for both data transmission and 2-D location fixes. Bandwidth limitations imposed by the Argos system, each transmission ‘message’ is limited to 247 bits, require that high-resolution tag data be summarized prior to transmission. The SMRU CTD-SRDL tags discretize the CTD profiles to 17 pairs of conductivity and temperature values (Roquet et al. 2011, Photopoulou et al. 2015), which are sent to the tag’s transmission buffer along with the corresponding pressure measurements. The transmission of CTD and other behavioural data temporarily stored in the tag transmission buffer occurs when the tag’s wet/dry and pressure sensors indicate the animal-borne tag is at the surface. Communication between the tag and Argos satellite is unidirectional so there is no guarantee that all data, packaged in 247-bit ‘pages’, will be received. Furthermore, to optimize battery life over long deployments (e.g., 9-12 months), this process typically yields 4 – 12 CTD profiles per day (Photopoulou et al. 2015) although alternate tag programming schemes can yield more profiles when desired.

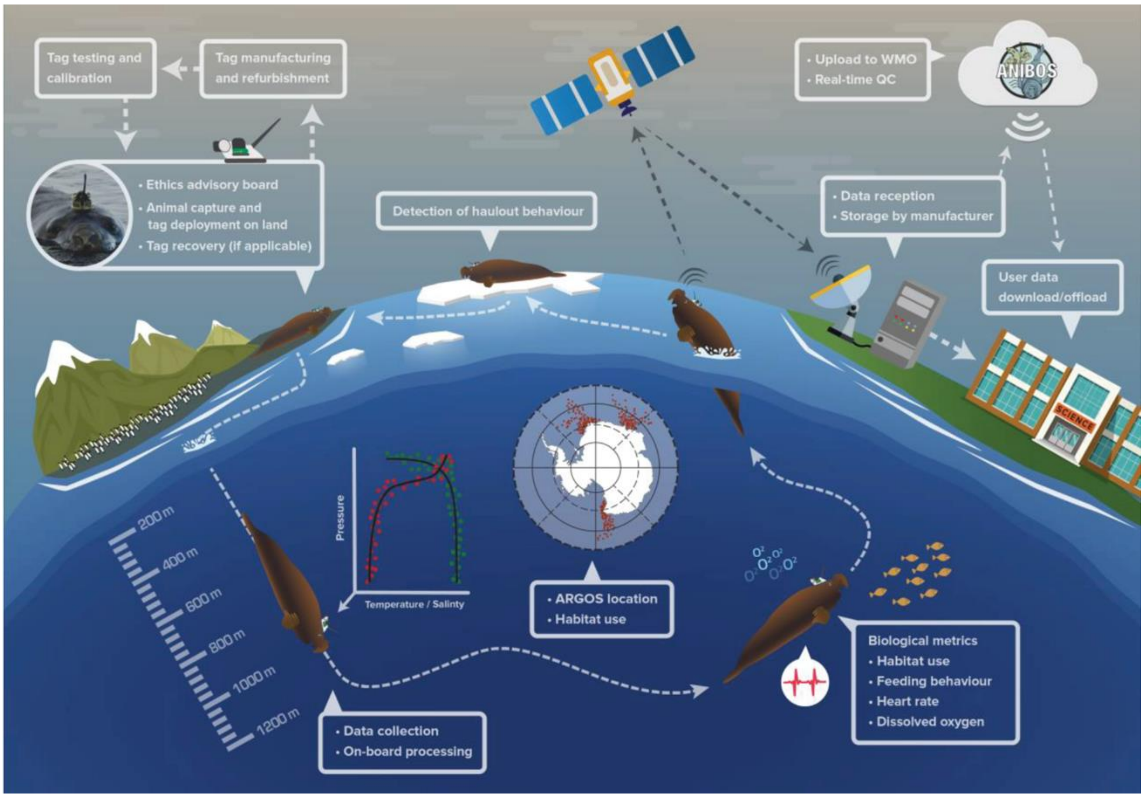

Figure 1. Schematic of a typical SMRU CTD-SRDL tag deployment on a southern elephant seal. Data collection, transmission and processing are also depicted. Reproduced from McMahon et al. 2021.

SMRU accesses transmitted data from CLS Argos in real-time, pre-processes the FV00 raw data (decodes the data using tag-specific parameters, conducts sanity checks). SMRU then distributes the FV00 raw CTD profile data to the British Oceanographic Data Centre (BODC) where the profiles are made available to end-users via the Global Telecommunication System (GTS) (Figure 2). The complete FV00 data are stored on a secure SMRU server as Microsoft Access Database files (.mdb) and are updated daily. The IMOS Animal Tracking Facility accesses these .mdb files daily to conduct a near real-time QC process (section 5) and annually to conduct delayed-mode QC processes (sections 5 and 6).

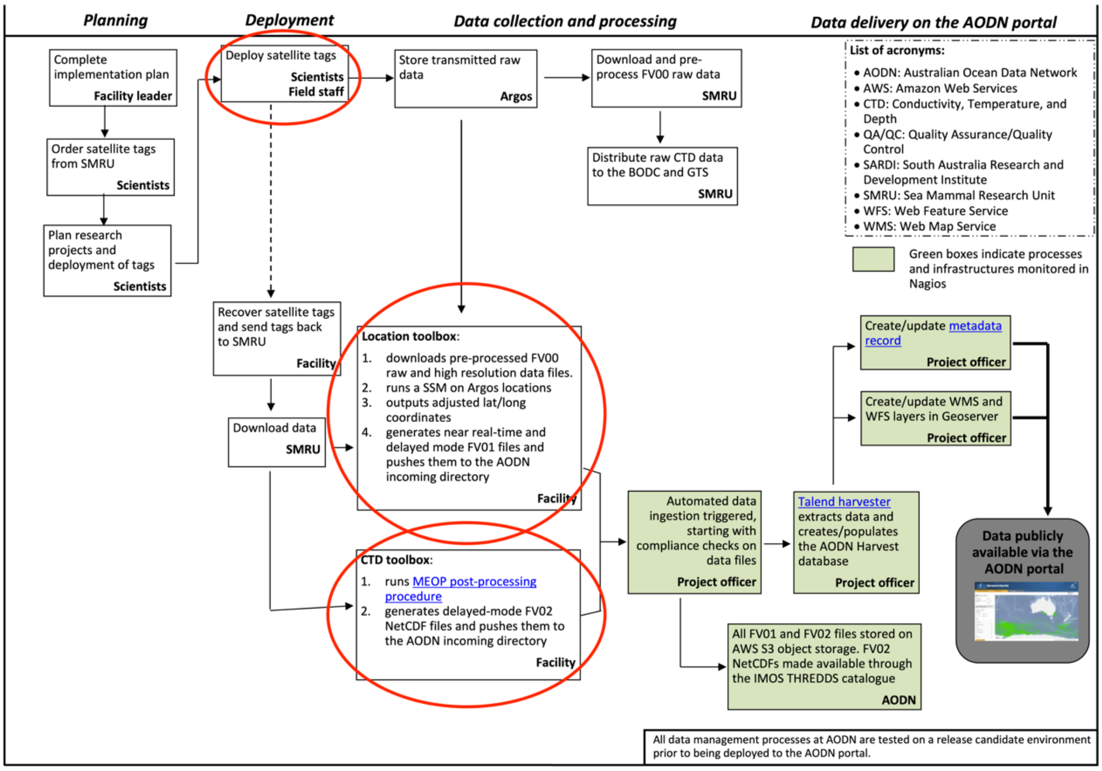

Figure 2. Workflow of IMOS Animal Tracking – Satellite Tracking data. Red circles indicated steps covered in this document. IMOS Data Workflows, 2024.

4. Instrument calibration

To ensure that hydrographic measurements collected by animals are of high quality *i.e.* they are accurate and precise, instruments require calibration prior to deployment. To capture the variation across the range of temperatures instruments are likely to encounter it is desirable to derive calibration coefficients from a quadratic fit from a broad suite of calibration points such as that done at SHOM (Service Hydrographique et Océanographique de la Marine, Brest, France). At this hydrographic facility, animal-borne tags are calibrated by changing the temperature of calibration baths to four points: -1°C, 6 °C, 12 °C, 20 °C. Typically tags are brought close to the bath's sensor and allowed to record for 90 seconds, a process that must be done for each tag at a time to prevent interference between sensors. Following immersions, sensor data from tags are offloaded before calculating average and standard deviation for each temperature to ensure that measurements recorded are precise. Once all calibrations points have been completed a quadratic model is fit in the form described below to estimate three coefficients (β_0, β_1, and β_2) that can be subsequently entered via the tag configuration software:

$$T = \beta_0 + \beta_1 T_{obs} + \beta_2 T_{obs}^2$$

Where T is the calibration (or corrected) temperature and T_{obs} is the temperature measured by the tag. Once tags have been re-configured using the estimated coefficients, calibrated tags should be re-immersed in all calibration baths to ensure that the corrected temperatures they record are accurate.

An alternative approach is to calibrate animal-borne sensor tags during oceanographic voyages. Measurements from ship-based CTD sensors are used to compare with SMRU CTD-SRDL observations using the following workflow:

1. Pressure offset in the tag configuration software is corrected against the ship-based CTD using at least four points, across multiple ascending profiles.
2. Apply offset at different sections of profile using a high pass filter for automated pressure offset correction.
3. Interpolate SMRU CTD-SRDL measurements to match ship-based CTD measurements.
4. Use a linear regression between temperature and salinity differences between ship-based CTD and SMRU CTD-SRDL measurements, averaging to remove variability.

5. Argos location QC

When at the surface, tag locations are derived via the polar-orbiting Argos satellite system. The system uses the Doppler shift in received tag transmitter frequency to estimate locations via a Kalman filter algorithm (Lopez et al. 2015). This geolocation approach is much less accurate than GPS (Jonsen et al. 2020) but uses less tag battery as none of the associated processing is done by the tag. Due to the imprecision in Argos-derived locations, the IMOS Animal Tracking Facility uses a quality control process to estimate more precise locations associated with all data records.

5.1 Data and metadata formats

The SMRU CTD-SRDL tag data is accessed from .mdb files on SMRU's data portal. The files contain data for all tags under a single deployment campaign – typically, these are tags deployed on the same species, in the same locality (e.g., Iles Kerguelen), over a relative narrow time-period (e.g., 2-3 weeks). Each .mdb file contains up to 10 tables, depending on the particular tag type and transmission programming (see http://www.smru.st-andrews.ac.uk/protected/specs/DatabaseFieldDescriptions.pdf for full details). In this document, and for QC purposes, we focus on the following 6 tables:
diag, **gps** (when present, see below), **ctd**, **dive**, **haulout**, and **summary**.

The **diag** and **gps** tables contain Argos and GPS locations, respectively, and associated diagnostic information. The **gps** table is present in sea turtle deployments as these tags include a GPS chipset. The **ctd** table includes the temperature, conductivity, calculated salinity, and pressure profiles each grouped as single records. The **dive** table includes broken stick (typically 4 inflection points, including the maximum depth) summaries of all transmitted dives below a pre-programmed threshold. The **haulout** table includes time periods when the tag's wet/dry sensor is continuously dry for at least 10 minutes, indicating the animal is "hauled out" on land or ice. The **summary** table includes summary statistics of behavioural events (dives and haulouts) typically calculated over 6 h. Each of the records in these tables is associated with a time, which can be the start time or end time of the event. For example, the time associated with each CTD profile in the **ctd** table is the end time of the CTD upcast.

Deployment metadata comprise information provided by SMRU and the field researchers. The metadata files are .csv files with mandatory attributes outlined in Table 1.

5.2 Location QC process

Since 2020, the IMOS Animal Tracking Facility uses a state-space modelling approach to filter the Argos locations provided by the SMRU CTD-SRDL tags (Jonsen et al. 2020). State-space models (SSMs) are a widely used statistical time-series method that can estimate the state (true locations at discrete points in time) of an unobserved process (tagged animal movement) from which only error-prone measurements (Argos-derived locations) can be obtained (Jonsen et al. 2005, Patterson et al. 2008).

Jonsen et al. (2020) presented a correlated random walk SSM that quality-controls Argos-satellite-derived locations provided by the SMRU CTD-SRDL tags. The SSM uses Argos location error ellipse estimates (Lopez et al. 2015; Fig. 3) provided with each measurement to filter out measurement error and estimate the true tag locations at specified points in time (Fig 4). Comparison of these SSM-estimated locations to contemporaneous GPS locations implies that the SSM-based approach yields locations with a median accuracy of 3.24 (6.15 SE) km for southern elephant seals and 1.69 (3.61 SE) km for sea turtles (Jonsen et al. 2020).

This QC process is conducted in both near real-time (NRT) on daily downloads of the latest data from active deployments, and in delayed-mode (DM) once all tags from a deployment have ceased transmitting data.

Table 1. IMOS Animal Tracking Facility metadata for SMRU CTD-SRDL tag deployments. Multiple examples are separated by semi-colons.

Attribute name	Description	Example(s)
sattag_program	SMRU campaign name	ct180
device_id	SMRU reference ID	ct180-156-BAT-15
ptt	Argos platform terminal transmitter ID	14156
body	SMRU tag ID	196997
device_wmo_ref	WMO ID	Q9902018
tag_type	SMRU tag type designation	CTD_QUOT_23A
common_name	Deployment animal common name	Southern elephant seal
species	Deployment animal scientific name	*Mirounga leonina*
release_longitude	Tag deployment coordinate	70.218
release_latitude	Tag deployment coordinate	-49.3496
release_site	Tab deployment locality	Iles Kerguelen
release_date	Tag deployment date	2023-12-21T00:00:00Z
recovery_date	Tag recovery date	NA
age_class	Animal age class	Juvenile; adult; NA
sex	Animal sex	m; f; NA
length	Animal length (m)	2.36
estimated_mass	Animal mass (kg) researcher estimated	250; NA
actual_mass	Animal mass (kg) measurement	255.5; NA
state_country	Country of deployment	French Overseas Territory
qc_start_date	Time of first data record included in QC	2024-01-02T12:00:00Z
qc_end_date	Time of last data record included in QC	2024-01-06T18:00:00Z

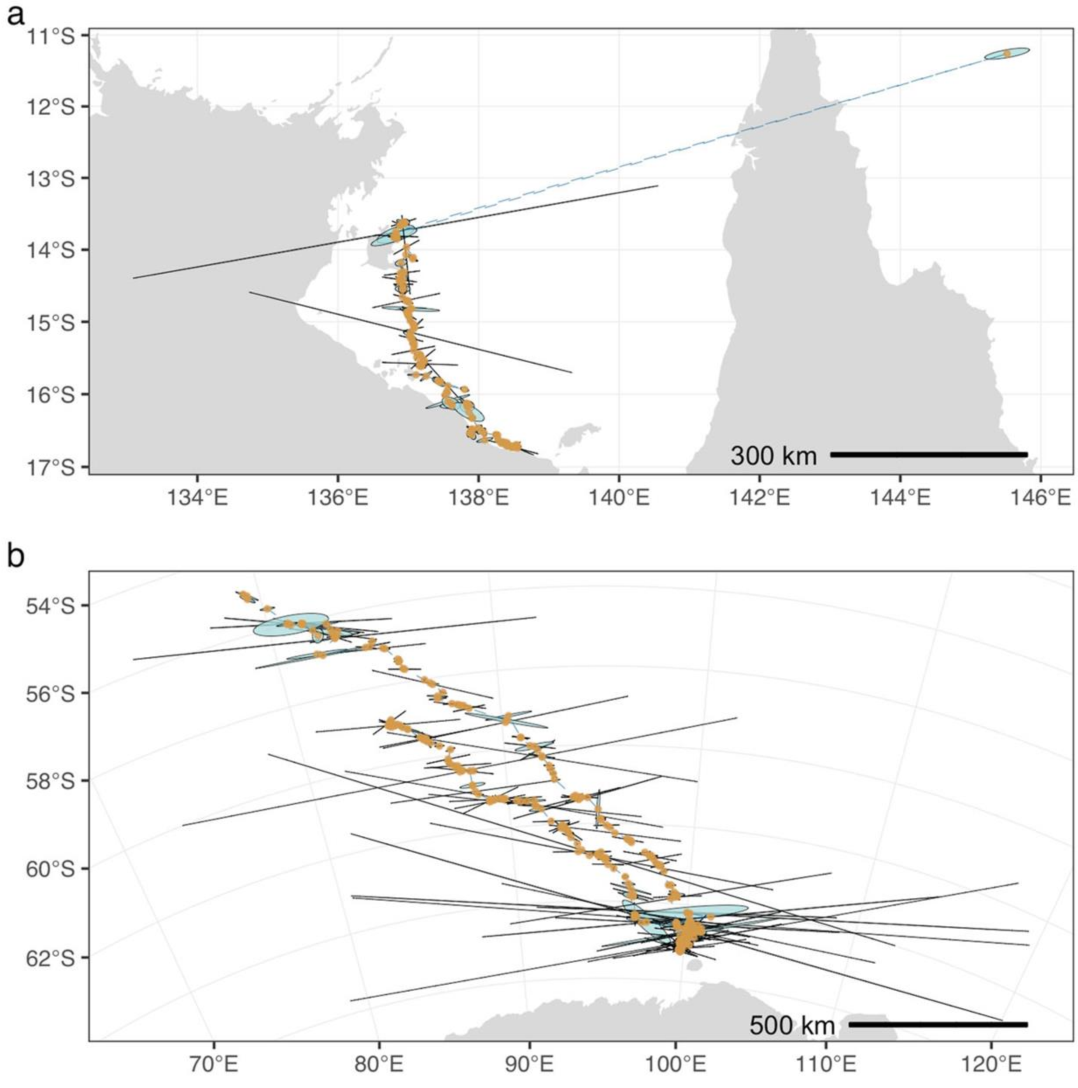

Figure 3. Unprocessed Argos Kalman filter locations (gold points) and error ellipses (pale blue with black borders) for (a) Hawksbill sea turtle and (b) southern elephant seal. Error ellipses can frequently span over 600 km in the longitudinal direction (b). Note, the highly implausible location at the upper right (a). Extreme locations such as this are not uncommon in Argos satellite-derived location data. Reproduced from Jonsen et al. 2020.

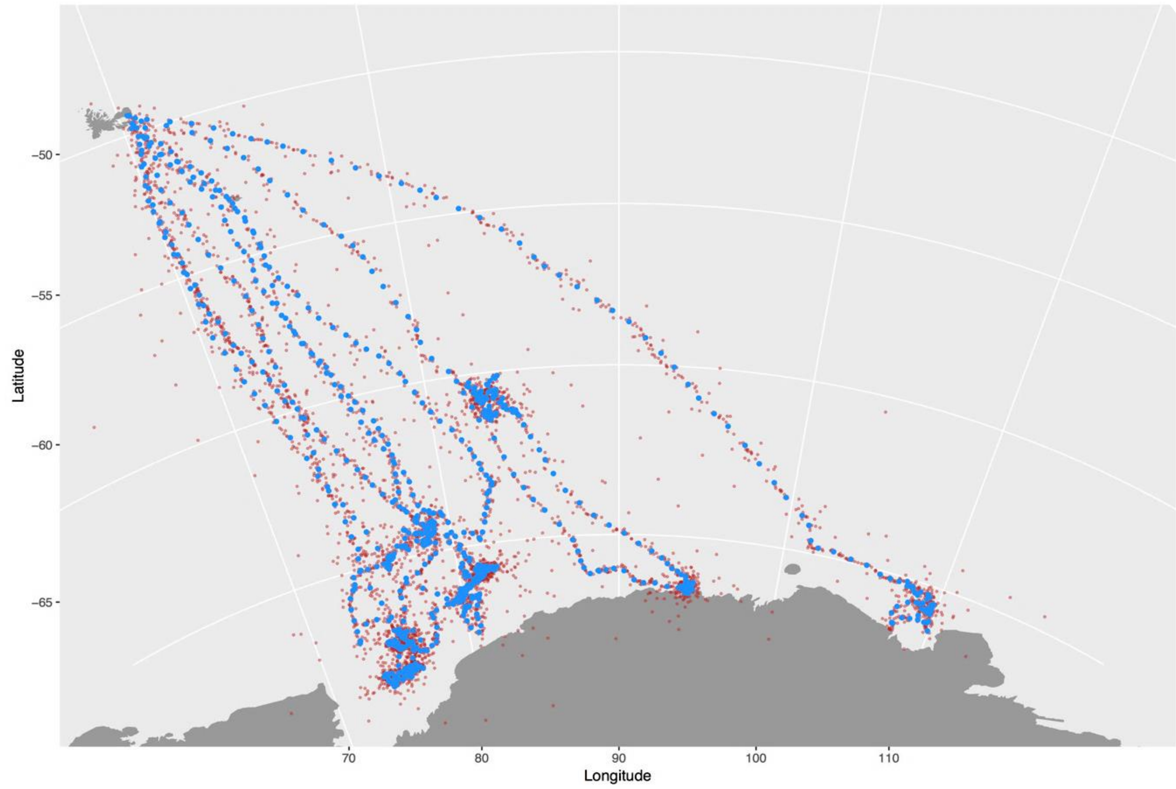

Figure 4. State-space model-estimated locations (blue) overlaid on Argos-satellite-derived locations (red) for four southern elephant seals carrying SMRU CTD-SRDL tags deployed on Iles Kerguelen (upper left). Note how the SSM-estimated locations smooth through the error-prone Argos locations.

5.2.1 Near real-time (NRT) QC process

The near real-time QC is conducted on an unsupervised basis every 24 h, using the R statistical computing environment (R Core Team 2024). The QC is initiated once the deployment metadata are made available by the field researchers (typically 4-6 weeks after all deployments are completed).

The NRT QC workflow (Figure 5) automatically performs the following essential tasks:

1. Downloads the latest .mdb file from the SMRU server
2. Collates & restructures SMRU tag and researcher deployment metadata
3. Determines QC start and end times for each deployed tag based on the times of the first and last transmitted CTD profiles from each tag
4. Fits the Argos location SSM (Jonsen et al. 2020) to all transmitted Argos locations (and GPS locations if present) within the QC start and end times for each tag
5. Appends SSM-estimated locations to the records in the **diag**, **gps** (if present), **ctd**, **dive**, **haulout**, and **summary** tables.

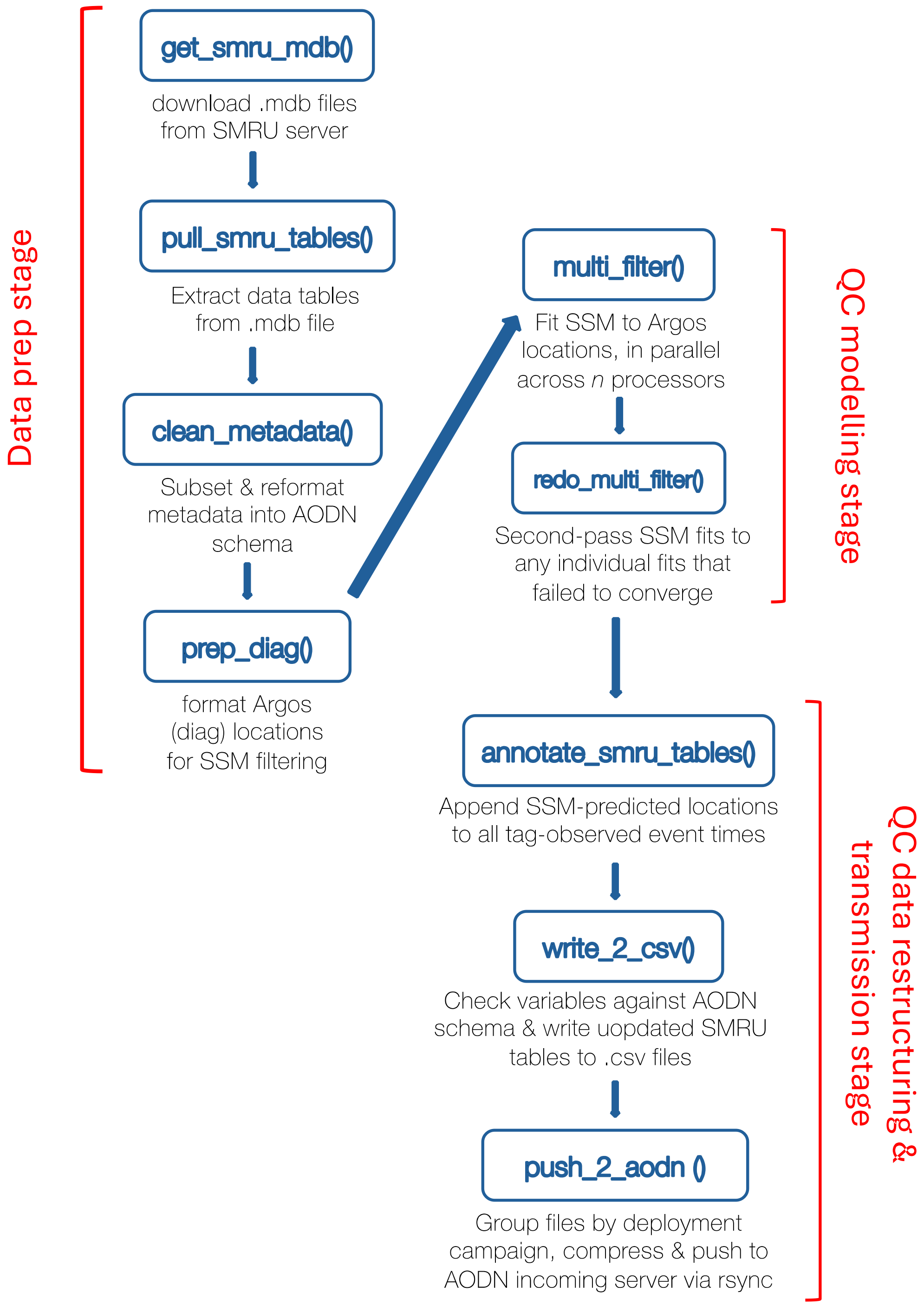

Figure 5. Schematic of NRT and DM location QC process. Boxes correspond to functions in the Argos QC R package.

6. Performs a sanity check on all table values to ensure they are in the expected format and value range.
7. Writes each table, metadata, and SSM outputs to deployment specific .csv files and pushes to the AODN incoming server.

This workflow is run on a NECTAR VM instance with 16 VCPU's and 32 GB RAM, running an RStudio server on Ubuntu 22.04 LTS. The above tasks are encoded in a series of R functions and documented in the open-access R package, **ArgosQC**, published at https://github.com/ianjonsen/ArgosQC. The ArgosQC package leverages the aniMotum R package (Jonsen et al. 2023; https://github.com/ianjonsen/aniMotum) for fitting the SSM to location data.

5.2.2 Delayed mode (DM) QC process

The DM QC is conducted on a supervised basis after all deployed tags cease transmitting (typically 9-12 months after deployment). The QC workflow consists of the same 7 tasks as the NRT workflow (Figure 5), with the following exceptions:

1. QC start and end times for each tag are determined manually by examining a combination of the **dive**, **ctd**, **diag** and **gps** (if present) tables to ascertain when the tag first started transmitting at sea after the recorded deployment date, and when the tag ceased transmitting useful data prior to any prolonged periods of no transmissions (data gaps).

2. Various SSM diagnostic plots (see Jonsen et al. 2023 for details) are examined to determine whether any SSM fits could be improved through refinements to the SSM parameterization or through the manual removal of problematic and likely erroneous observed locations (typically much less than 1% of the data). If so, the SSM is refit to all relevant tag datasets and new diagnostic plots are examined to confirm an improvement in fit.

5.3 Magnitude of location corrections

In general, the QC-imposed corrections to CTD profile, dive, and haulout locations improve accuracy over the "raw" Argos locations (Jonsen et al. 2020). The magnitudes of improvement differed between the SMRU .mdb tables. The CTD profiles had the largest median correction distance (3.9 km) and haulout events had the smallest (1.2 km) (Figure 6). The smaller correction distances for haulout events are due to the averaging that SMRU conducts over the multiple locations tied to each haulout, whereas all other events are associated with a single location. Note that the 95 % interval for CTD locations extends to nearly 20 km, with extreme values (not displayed) extending further.

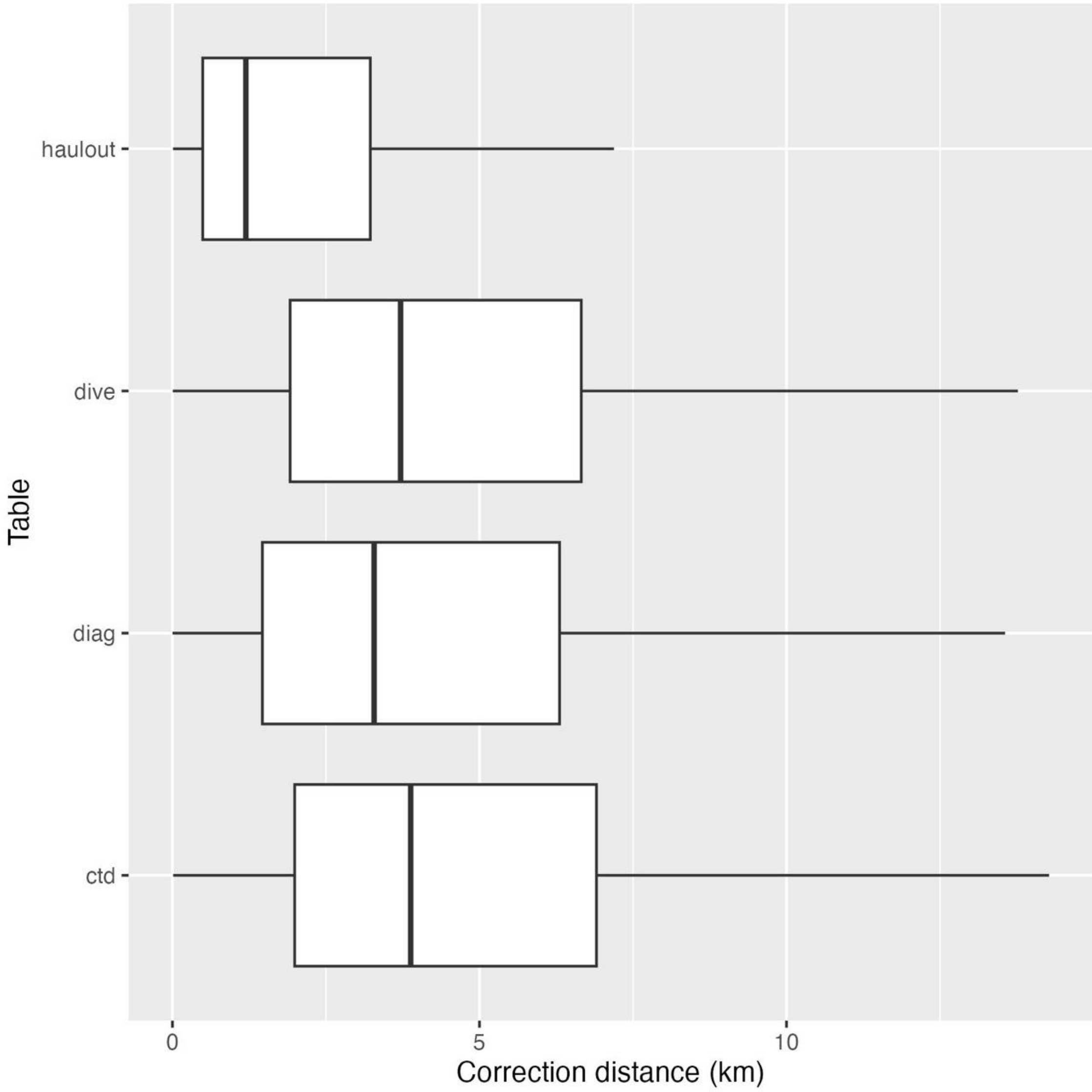

Figure 6. Distributions of correction distances (km) imposed by the location QC on ct170 deployments (25 southern elephant seals tagged on Iles Kerguelen in 2023) by data table. The white boxes denote the inner quartile range, the vertical bars are medians, whiskers denote the 95% interval. Extreme values > 20 km are not displayed.

5.4 QC'd data on the AODN portal

The NRT and DM data with quality-controlled locations are available on the AODN portal, under `Platform = Biological platform/land-sea mammals`, in 2 separate collections: "Near real-time data with quality-controlled locations" and "Delayed mode data with quality-controlled locations" (Figure 7). Currently, these data extend back to the 2019/20 deployments.

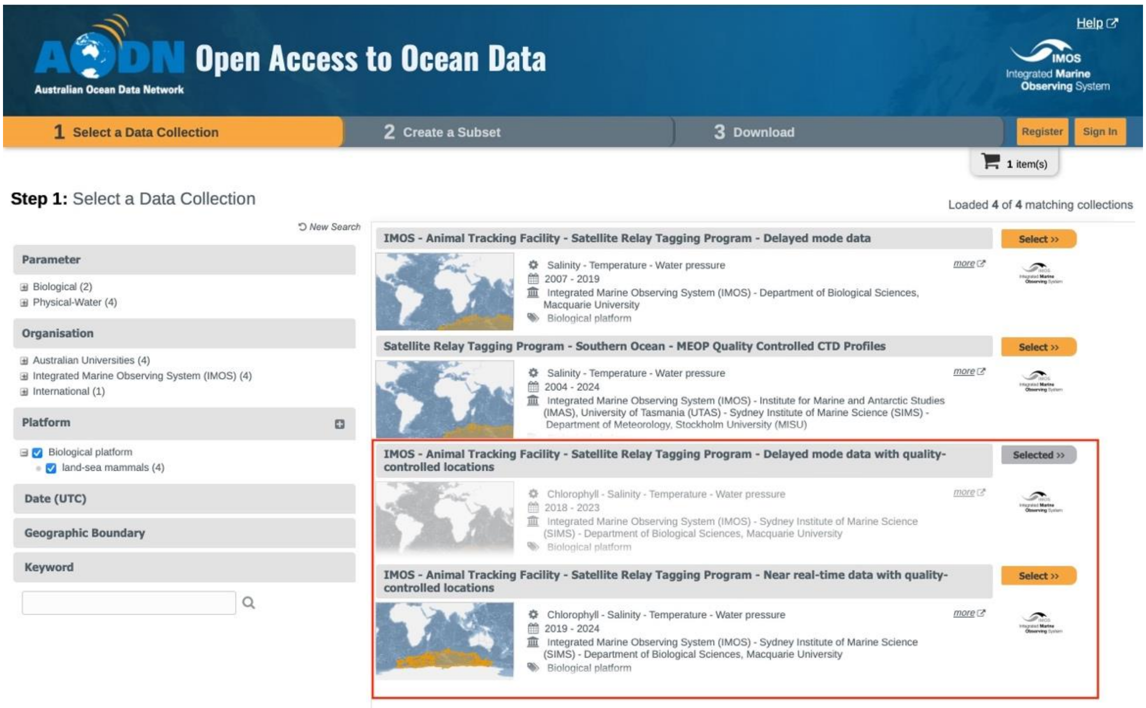

Figure 7. Screenshot of AODN Portal highlighting the NRT and DM quality-controlled location data. The individual tables can be downloaded separately as .csv files.

6. Delayed mode CTD profile QC

6.1 CTD data and metadata

The QC'd CTD profile data and metadata are provided in netCDF format as FV02 files. The file standard is Marine Mammals NetCDF Format v 1.2 (http://www.meop.net/database/data-format.html), an adaptation of the Argo format (Roquet et al. 2014, Carval et al. 2014). The global attributes relevant to MEOP/IMOS animal-borne CTD data are listed in Table 2. At the time of writing this document, the global attributes for the IMOS subset of MEOP QC'd data are undergoing revision. This document will be updated once all QC'd IMOS CTD netCDF are appended with revised metadata. The key variables used in the QC are outlined in Table 3.

As of 2023, the entire MEOP/IMOS DM CTD QC is conducted on a secure MEOP server, located at the University of Gothenburg, Sweden. This approach ensures that the QC of IMOS CTD profile data is aligned with MEOP, using the latest Matlab & Python code (https://github.com/fabien-roquet/MEOP_process). The IMOS Animal Tracking Facility accesses this server to conduct the DM QC on its own schedule rather than relying on MEOP personnel.

The first stage of the MEOP/IMOS DM CTD QC is to obtain the latest SMRU CTD-SRDL tag data and metadata. SMRU's tag metadata is pushed to the MEOP server in a .JSON file on a regular basis, and all SMRU tag data are downloaded off the SMRU data server.

Table 2. Global attributes of MEOP/IMOS netCDF files.

Attribute Name	Description
pi_name	Name of principal investigator
species	Character string with species scientific name
platform_code	Unique identifier number for the tag dataset
wmo_platform_code	WMO identifier
smru_platform_code	SMRU reference ID (used in filename)
deployment_code	SMRU deployment code
distribution_statement	"Follow MEOP data policy standards, cf. http://www.meop.net/the-dataset/data-access.html. Data available free of charge. User assumes all risk for use of data. User must display citation in any publication or product using data. User must contact PI prior to any commercial use of data"
citation	"The marine mammal data were collected and made freely available by the International MEOP Consortium and the national programs that contribute to it (http://www.meop.net)"
positioning_system	"argos" or "gps"
number_of_ts_profiles	…
number_of_t_profiles	…

Table 3. Key variables used in MEOP/IMOS netCDF files.

Name	Dimension	Description
SMRU_NAME	N_PROF	CTD-SRDL unique identifier
PI_NAME	N_PROF	Principal investigator name
JULD_LOCATION	N_PROF	Julian date since 1950-01-01
LATITUDE	N_PROF	Estimated latitude
LONGITUDE	N_PROF	Estimated longitude
PRES	N_PROF X N_LEVELS	Raw pressure (dbar)
PRES_ADJUSTED	N_PROF X N_LEVELS	Adjusted pressure (dbar)
PRES_ADJUSTED_QC	N_PROF X N_LEVELS	Pressure QC flag*
PRES_ADJUSTED_ERROR	N_PROF X N_LEVELS	Estimate of uncertainty (1 value per tag)
TEMP	N_PROF X N_LEVELS	Raw temperature (°C)
TEMP_ADJUSTED	N_PROF X N_LEVELS	Adjusted temperature (°C)
TEMP_ADJUSTED_QC	N_PROF X N_LEVELS	Temperature QC flag
TEMP_ADJUSTED_ERROR	N_PROF X N_LEVELS	Estimate of uncertainty (1 value per tag)
PSAL	N_PROF X N_LEVELS	Raw practical salinity (psu)
PSAL_ADJUSTED	N_PROF X N_LEVELS	Adjust practical salinity (psu)
PSAL_ADJUSTED_QC	N_PROF X N_LEVELS	Practical salinity QC flag
PSAL_ADJUSTED_ERROR	N_PROF X N_LEVELS	Estimate of uncertainty (1 value per tag)
SCIENTIFIC_CALIB_EQUATION	N_PROF x 2	Calibration equation used to adjust T and S data
SCIENTIFIC_CALIB_COEFFICIENT	N_PROF x 2	Coefficients of calibration used to adjust T and S data

*QC flags follow the Argo convention (Carval et al. 2014)

6.2 Delayed mode QC process

All CTD profiles transmitted by SMRU CTD-SRDL tags undergo a rigorous QC process to improve the quality of the hydrographic data. The automated portion of this process, applied to the raw temperature, T, and calculated salinity, S, data is summarized in Figure 8. The QC description below follows this organization.

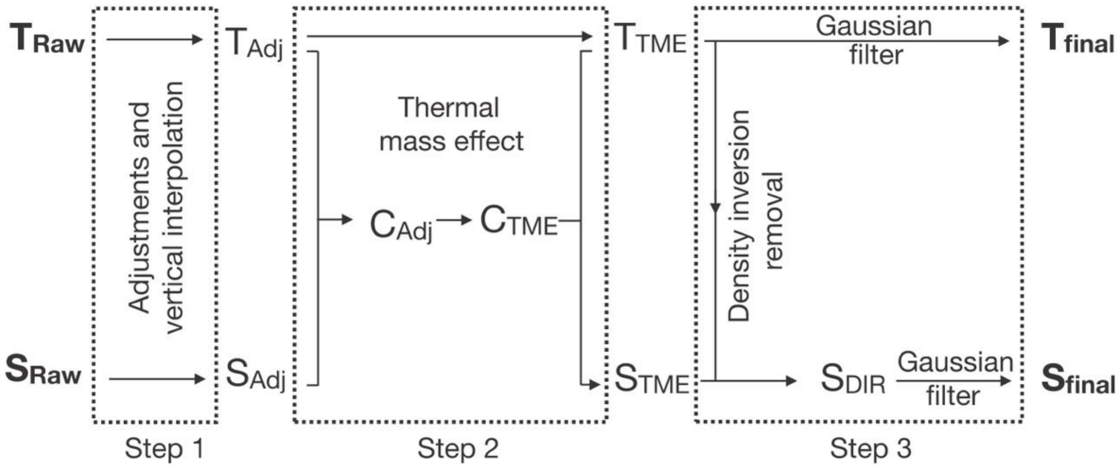

Figure 8. Schematic summarising the automated correction procedure implemented on all SMRU CTD-SRDL tags. From Seigelman et al. 2022. Step 1 is described in Roquet et al. 2011. Steps 2 and 3 are detailed in Seigelman et al. 2022.

6.2.1 Delayed mode QC Step 1

The initial QC step corrects temperature and salinity for pressure-induced linear biases (Figure 8) based on a comparison of the SMRU CTD-SRDL profile data and ship-based CTD measurements (described in Roquet et al. 2011). The pressure-effect correction for temperature is:

$$T_c = T - \alpha_t P - \beta_t$$

Where T_c is the corrected temperature, *T* is the tag-measured temperature, *P* is tag-measured pressure, and α_t and β_t are the linear correction parameters from Roquet et al. (2011). The salinity correction accounts for both pressure and external field effects:

$$S_c = S - A_S P - B_S$$

Where S_c is the corrected salinity, *S* is the calculated salinity (from tag-measured conductivity), and A_S and B_S are correction parameters from Roquet et al. (2011). Here, B_S is an additional offset for the external field effect.

The linear corrections in T and S provide both offset (β_t , B_S) and trend (α_t , A_S) adjustments to account for the pressure-induced change in biases in tag-measured T and S (Figure 9).

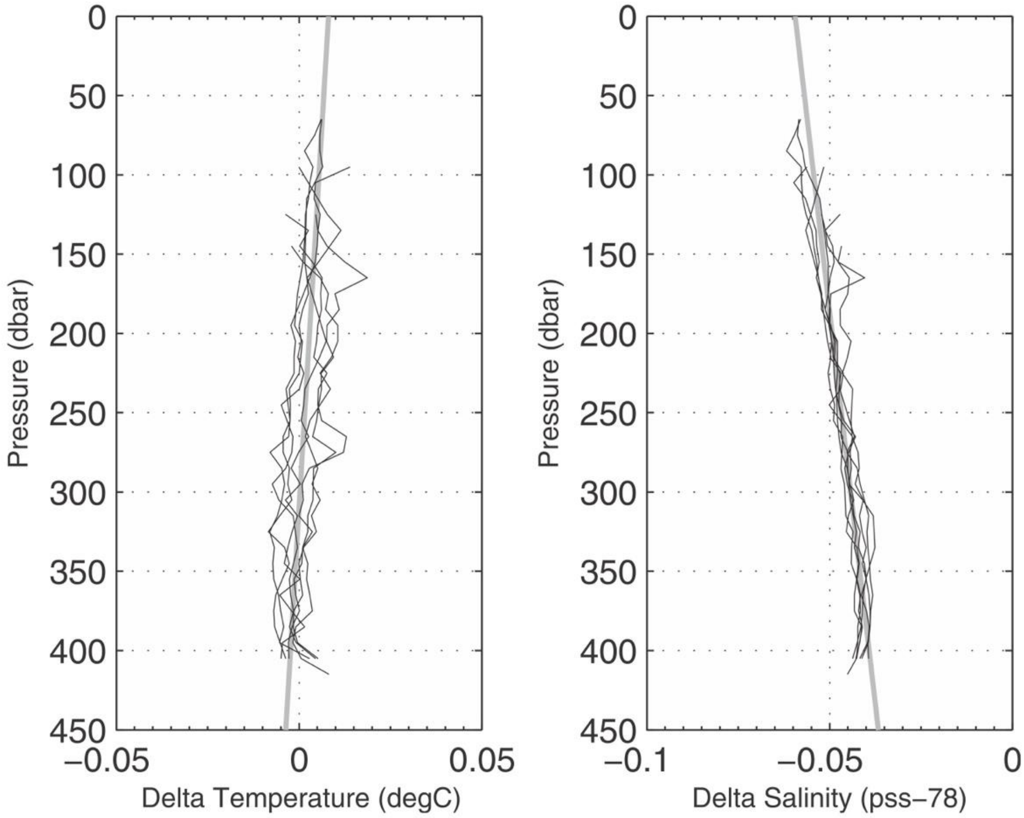

Figure 9. Differences between a SMRU CTD-SRDL tag and SBE25 CTD for 7 temperature (left) and salinity (right) profiles. Linear fits are grey straight lines. From Roquet et al. (2011).

Finally, the low-resolution CTD profiles are vertically interpolated using the corrected T and S to 1 m resolution.

6.2.2 Delayed mode QC Step 2

The second QC step corrects temperature and conductivity for a thermal mass effect (Figure 8) that results from the transfer of heat from the sensor wall to the sample being measured (Siegelman et al. 2019). This effect leads to significant error in salinity estimates from SMRU CTD-SRDL's as the conductivity cell is unpumped.

Conductivity is corrected following Lueck and Picklo (1990) via the formula:

$$C_T(n) = \Gamma_C \alpha_C (1 - 0.5\beta\Delta_t)^{-1} T_{\text{hp}}(n)$$

Where C_T is the conductivity correction added to the n^{th} sample, $T_{\text{hp}}(n)$ is the high-pass filtered sample temperature, Γ_C is the coefficient of sensitivity of conductivity to temperature at fixed salinity and pressure, and Δ_t is the sampling time interval (2 s for SMRU CTD-SRDL's) (see Mensah et al. 2018, Siegelman et al. 2019 for further details). Salinity is recalculated from the corrected conductivity.

The thermal mass correction for temperature is like that for conductivity, following Morison et al. (1994):

$$T_T(n) = \alpha_T(1 - 0.5\beta\Delta_t)^{-1}T_{\text{hp}}(n)$$

Appropriate values for the parameters α_T, α_C, and β are detailed in section 4 of Siegelman et al. (2019).

6.2.2 Delayed mode QC Step 3

The third QC step removes density inversions (Figure 8), following Barker and McDougall (2017). Density inversions can arise from instrument noise or salinity spikes. The procedure adjusts the profiles so that they do not exceed a minimum N^2 threshold (by default $N = 1 \times 10^{-9}$ s^{-2} – the Brunt-Väisälä frequency). This minimally adjusts absolute salinity (SA) and leaves conservative temperature (CT) unchanged. Finally, a Gaussian filter with a 1-dbar window is applied to both CT and SA to remove noise (sharp, localized jumps). This noise is introduced to SA by the density inversion removal process and is also present in CT. See Siegleman et al. (2019) for further details.

Complete assessment of the efficacy of this 3-step QC process is detailed in Roquet et al. (2011), Mensah et al. (2018), and Siegelman et al. (2019). Using high-resolution profile data (from recovered SMRU CTD-SRDL's), Siegleman et al. (2019) found that the largest corrections from QC steps 2 and 3 occurred between the surface and 300 m, where stronger temperature gradients typically occur in the Southern Ocean (Figure 10). Overall, the step 2 QC has a stronger contribution to final CT, and both steps 2 and 3 QC's have a significant contribution to final SA.

6.2.3 Delayed mode QC Step 4 – Manual corrections

The final stage of the QC process (not outlined in Figure 8) are manual corrections to the CT-SA profiles. Diagnostic plots for each CTD-SRDL deployment are produced that display CT-SA diagrams for all transmitted profiles (both raw and corrected). Overlaid on these diagrams are co-located profiles obtained from 1) the World Ocean Database (Boyer et al. 2018) and 2) the CORA database (Cabanes et al. 2013) (Figure 10). Adjustment coefficients (offset and slope) for CT and SA are selected visually to match the CTD-SRDL profiles to the historical data. In the example, an SA offset of 0.2 is applied to shift the CTD-SRDL profiles to the left (lower SA values) so they better align with the co-located historical profile data (Figure 11, compare upper left vs right panels).

Once manual corrections are completed, the raw and adjusted profiles for each SMRU CTD-SRDL tag (along with QC flags) are written to a unique netCDF file with global attributes and variables per Tables 2 and 3.

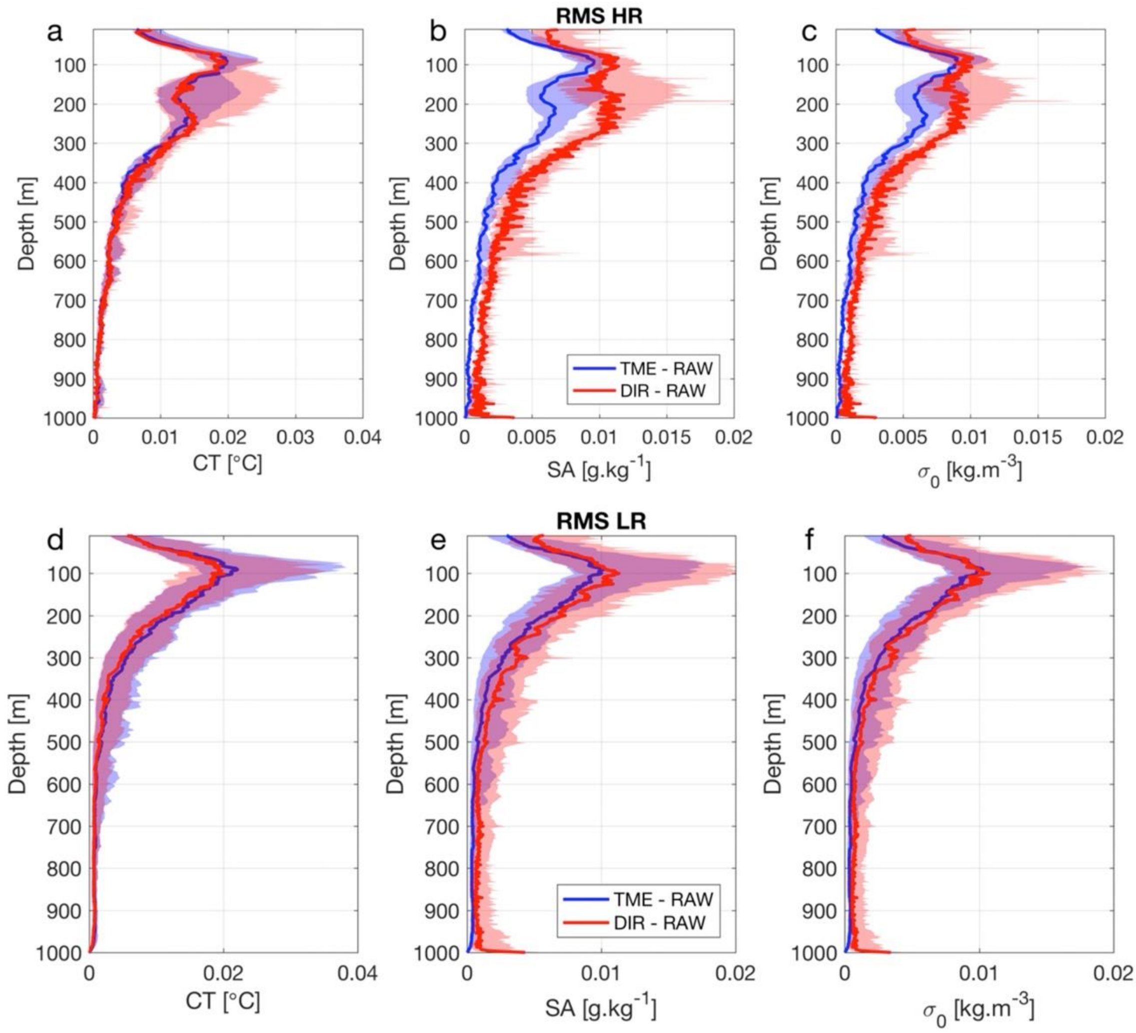

Figure 10. Mean RMS between raw and corrected CT and SA data for both high-resolution (recovered tags, top) and low-resolution (Argos transmitted tag data, bottom) data. TME = thermal mass effect correction (QC step 2). DIR = density inversion removal (QC step 3). Shading denotes the 80th percentiles. From Siegelman et al. (2019).

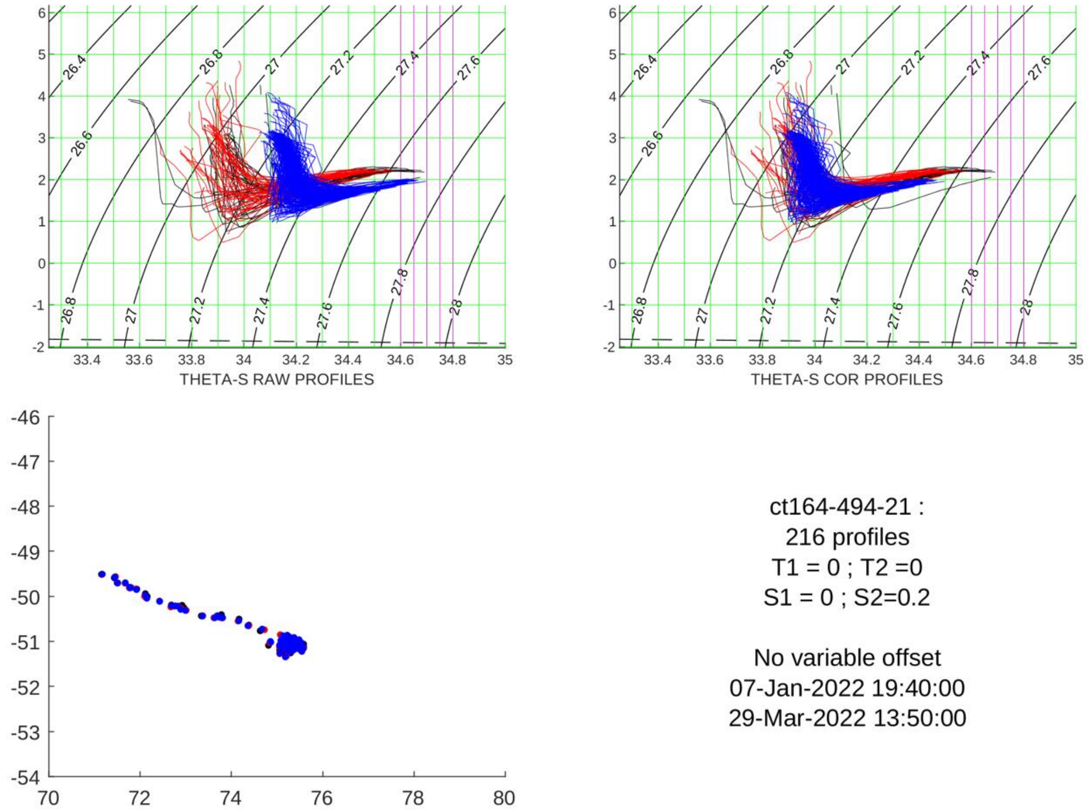

Figure 11. SMRU CTD-SRDL tag calibration plot example. The 216 CT - SA profiles (with density, θ, isopleths) for raw (left, upper) and adjusted (right, upper). The CTD-SRDL profiles (blue) are overlaid on co-located historical profile observations (co-location displayed at lower left) – World Ocean Database, WOD, (black) and from other CTD-SRDL tags, (red). In this example (CTD-SRDL ct164-494-21), a salinity offset of 0.2 is applied to shift the blue profiles toward lower θ and SA values that better match the historical observations (compare upper left vs right panels).

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8. Supplementary Information

8.1 CTD-SRDL general specifications

Incorporates many of the features of the SMRU SRDL tag plus:

- Oceanographic quality temperature & salinity profiles (4 - 12 profiles per day)
- CTD data automatically submitted to the GTS in near real-time
- Up to 50,000 full length Argos data transmissions
- pressure-proof to 2000m

Valeport CTD sensor head

- Temperature
  - range: -5° to 35°C
  - accuracy: +/- 0.005°C
  - resolution: 0.001°C
- Conductivity
  - range: 0 to 80mS/cm
  - accuracy: +/- 0.01mS/cm
  - resolution: 0.002mS/cm
- Pressure (depth)
  - range: 0 to 2000 dBar
  - accuracy: 2 dBar +/- (0.3 + 0.035%*reading)/°K
  - resolution: 0.05 dBar

TDR capability

- Retains a continuous record of depth readings (4 sec sample rate), which can be retrieved by bluetooth link if the tag is recovered.
- Also records all individual temperature and salinity measurements (1 Hz) made during profiling.

General specifications

- Longevity up to one year
- Size: 10.5 x 7 x 4 cm
- Weight: 545 g
- Volume: ~250 cm^3