







# Match-up database Analyses Report

SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG

Sea mammals

Southern Ocean

prepared by the Pi-MEP Consortium

March 15, 2019

# Contents

1	Ove	erview							
2	The	MDB file datasets							
	2.1	Satellite SSS product							
		2.1.1 SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG							
	2.2	In situ SSS dataset							
	2.3	Auxiliary geophysical datasets							
		2.3.1 CMORPH							
		2.3.2 ASCAT							
		2.3.3 ISAS							
		2.3.4 World Ocean Atlas Climatology							
	2.4	Overview of the Match-ups generation method							
		2.4.1 In Situ/Satellite data filtering							
		2.4.2 In Situ/Satellite Co-localization							
		2.4.3 MDB pair Co-localization with auxiliary data and complementary infor-							
		mation							
		2.4.4 Content of the Match-Up NetCDF files							
	2.5	MDB characteristics for the particular in situ/satellite pairs							
		2.5.1 Number of paired SSS data as a function of time and distance to coast							
		2.5.2 Histograms of the SSS match-ups							
		2.5.3 Distribution of in situ SSS depth measurements							
		2.5.4 Spatial Distribution of Match-ups							
		2.5.5 $$ Histograms of the spatial and temporal lags of the match-ups pairs							
3	MD	B file Analyses							
	3.1	Spatial Maps of the Temporal mean and Std of in situ and satellite SSS and of							
		the difference ( $\Delta SSS$ )							
	3.2	Time series of the monthly averaged mean and Std of in situ and satellite SSS and							
		of the ( $\Delta SSS$ )							
	3.3	Zonally-averaged Time-mean and temporal Std of in situ and satellite SSS and of							
		the $\Delta SSS$							
	3.4	Scatterplots of satellite vs in situ SSS by latitudinal bands							
	3.5	Time series of the monthly averaged mean and Std of the $\Delta$ SSS sorted by latitu-							
		dinal bands							
	3.6	$\Delta$ SSS sorted as function of geophysical parameters							
	3.7	$\Delta$ SSS maps and statistics for different geophysical conditions							
4	Sun	nmary							
L	ist	of Figures							
	1	Number of match-ups between Sea mammals and SMOS-L4-CATDS-CECOS-							
		IFREMER-V2-WEEKLY-0.5DEG SSS as a function of time (a) and as function							
		of the distance to coast (b) over the Southern Ocean Pi-MEP region and for the							
		full satellite product period							

2	Histograms of SSS from Sea mammals (a) and SMOS-L4-CATDS-CECOS-IFREMER V2-WEEKLY-0.5DEG (b) considering all match-up pairs per bins of 0.1 over the	₹-
	Southern Ocean Pi-MEP region and for the full satellite product period	20
3	Histograms of the depth of the upper level SSS measurements from Sea mammals	
•	in the Match-up DataBase for the Southern Ocean Pi-MEP region (a) and tempo-	
	ral mean spatial distribution of pressure of the in situ SSS data over 1°x1° boxes	
		20
4	and for the full satellite product period (b)	20
4	Number of SSS match-ups between Sea mammals SSS and the SMOS-L4-CATDS-	
	CECOS-IFREMER-V2-WEEKLY-0.5DEG SSS product for the Southern Ocean	
	Pi-MEP region over 1°x1° boxes and for the full satellite product period	21
5	Histograms of the spatial (a) and temporal (b) lags between the time of the Sea	
	mammals measurements and the date of the corresponding SMOS-L4-CATDS-	
	CECOS-IFREMER-V2-WEEKLY-0.5DEG SSS product	22
6	Temporal mean (left) and Std (right) of SSS from SMOS-L4-CATDS-CECOS-	
	IFREMER-V2-WEEKLY-0.5DEG (top), Sea mammals (middle), and of $\Delta$ SSS	
	(Satellite - Sea mammals). Only match-up pairs are used to generate these maps.	23
7	Time series of the monthly averaged mean SSS (top), mean $\Delta$ SSS (Satellite - Sea	
	mammals) and Std of $\Delta$ SSS (Satellite - Sea mammals) over the Southern Ocean	
	Pi-MEP region considering all match-ups collected by the Pi-MEP platform	24
8	Left panel: Zonally averaged time mean SSS from SMOS-L4-CATDS-CECOS-	
	IFREMER-V2-WEEKLY-0.5DEG (black) and from Sea mammals (blue). Right	
	panel: zonally averaged time-mean $\Delta$ SSS (Satellite - Sea mammals) for all the	
	collected Pi-MEP match-up pairs estimated over the full satellite product period.	25
9		20
9	Contour maps of the concentration of SMOS-L4-CATDS-CECOS-IFREMER-V2-	
	WEEKLY-0.5DEG SSS (y-axis) versus Sea mammals SSS (x-axis) at match-up	
	pairs for different latitude bands. For each plot, the red line shows x=y. The	
	black thin and dashed lines indicate a linear fit through the data cloud and the	
	$\pm 95\%$ confidence levels, respectively. The number match-up pairs $n$ , the slope	
	and R <sup>2</sup> coefficient of the linear fit, the root mean square (RMS) and the mean	
	bias between satellite and in situ data are indicated for each latitude band in each	
	plots	26
10	Monthly-average mean (red curves) $\Delta$ SSS (Satellite - Sea mammals) and $\pm 1$ Std	
	(black vertical thick bars) as function of time for all the collected Pi-MEP match-	
	up pairs estimated over the Southern Ocean Pi-MEP region and for the full satellite	
	product period are shown for different latitude bands: (a) Latitude band 80°S-	
	80°N, (b) latitude band 20°S-20°N, (c) Mid Latitude bands 40°S-20°S and 20°N-	
	40°N and (d) Latitude bands 60°S-40°S and 40°N-60°N	27
11	$\Delta$ SSS (Satellite - Sea mammals) sorted as function of Sea mammals SSS values a),	
	Sea mammals SST b), ASCAT Wind speed c), CMORPH rain rate d) and distance	
	to coast (e). In all plots the mean and Std of $\Delta$ SSS for each bin is indicated by	
	the red curves and black vertical thick bars $(\pm 1 \text{ Std}) \dots \dots \dots$	28
12	Temporal mean gridded over spatial boxes of size $1^{\circ}x1^{\circ}$ of $\Delta SSS$ (SMOS-L4-	20
12	CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG - Sea mammals) for 6 differ-	
	ent subdatasets corresponding to:RR=0 mm/h, $3 < U_{10} < 12$ m/s, SST>5°C, dis-	
	tance to coast $> 800 \text{ km}$ (a), RR=0 mm/h, $3 < U_{10} < 12 \text{ m/s}$ (b), RR>1mm/h and $U_{10} < 4\text{m/s}$ (c),MLD $< 20\text{m}$ (d),WOA2013 SSS Std $< 0.2$ (e),WOA2013 SSS Std $> 0.2$	
		90
	(f)	29



13	Normalized histogram of $\Delta$ SSS (SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKL	Y-
	0.5DEG - Sea mammals) for 6 different subdatasets corresponding to: RR=0	
	mm/h, $3 < U_{10} < 12$ m/s, SST>5°C, distance to coast > 800 km (a), RR=0	
	mm/h, $3 < U_{10} < 12$ m/s (b), RR>1mm/h and $U_{10} < 4$ m/s (c), MLD<20m (d),	
	WOA2013 SSS Std<0.2 (e), WOA2013 SSS Std>0.2 (f)	30



# Acronym

Aquarius NASA/CONAE Salinity mission

ASCAT Advanced Scatterometer

ATBD Algorithm Theoretical Baseline Document

BLT Barrier Layer Thickness CMORPH CPC MORPHing technique

CTD Instrument used to measure the conductivity, temperature, and pressure of

seawater

DM Delayed Mode
EO Earth Observation
ESA European Space Agency
FTP File Transfer Protocol

GOSUD Global Ocean Surface Underway Data GTMBA The Global Tropical Moored Buoy Array

Ifremer Institut français de recherche pour l'exploitation de la mer

IPEV Institut polaire français Paul-Émile Victor

IQR Interquartile range ISAS In Situ Analysis System

Kurt Kurtosis (fourth central moment divided by fourth power of the standard de-

viation)

L2 Level 2

LEGOS Laboratoire d'Etudes en Géophysique et Océanographie Spatiales

LOCEAN Laboratoire d'Océanographie et du Climat : Expérimentations et Approches

Numériques

LOPS Laboratoire d'Océanographie Physique et Spatiale

MDB Match-up Data Base

MEOP Marine Mammals Exploring the Oceans Pole to Pole

MLD Mixed Layer Depth

NCEI National Centers for Environmental Information

NRT Near Real Time

NTAS Northwest Tropical Atlantic Station

OI Optimal interpolation

Pi-MEP Pilot Mission Exploitation Platform

PIRATA Prediction and Researched Moored Array in the Atlantic

QC Quality control

 $R_{sat}$  Spatial resolution of the satellite SSS product

RAMA Research Moored Array for African-Asian-Australian Monsoon Analysis and

Prediction

r<sup>2</sup> Square of the Pearson correlation coefficient

RMS Root mean square

RR Rain rate

SAMOS Shipboard Automated Meteorological and Oceanographic System

Skew Skewness (third central moment divided by the cube of the standard deviation)

SMAP Soil Moisture Active Passive (NASA mission)
SMOS Soil Moisture and Ocean Salinity (ESA mission)
SPURS Salinity Processes in the Upper Ocean Regional Study

SSS Sea Surface Salinity

 $SSS_{insitu}$  In situ SSS data considered for the match-up



 $SSS_{SAT}$  Satellite SSS product considered for the match-up

 $\Delta$ SSS Difference between satellite and in situ SSS at colocalized point ( $\Delta$ SSS =

 $SSS_{SAT}$ -  $SSS_{insitu}$ )

SST Sea Surface Temperature Std Standard deviation

Std\* Robust Standard deviation = median(abs(x-median(x)))/0.67 (less affected by

outliers than Std)

Stratus Surface buoy located in the eastern tropical Pacific

Survostral SURVeillance de l'Océan AuSTRAL (Monitoring the Southern Ocean)

TAO Tropical Atmosphere Ocean

TSG ThermoSalinoGraph

WHOI Woods Hole Oceanographic Institution
WHOTS WHOI Hawaii Ocean Time-series Station

WOA World Ocean Atlas



# 1 Overview

In this report, we present systematic analyses of the Match-up DataBase (MDB) files generated by the Pi-MEP platform within the following Pi-MEP region and for the below pair of Satellite/In situ SSS data:

- Pi-MEP region: Southern Ocean (download the corresponding mask here)
- SSS satellite product (SSS<sub>SAT</sub>): SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG
- In situ dataset ( $SSS_{Insitu}$ ): Sea mammals (download the corresponding report here)

In the following,  $\Delta SSS = SSS_{SAT}$ -  $SSS_{Insitu}$  denotes the difference between the satellite and in situ SSS at the colocalized points that form the MDB.

This report presents successively:

The MDB file DataSets (Section 2)

- A short description of the satellite SSS product considered in the match-up (2.1)
- A short description of the In situ SSS dataset considered in the match-up (2.2)
- A short description of the auxiliary geophysical datasets co-localized with SSS pairs (2.3)
- An overview of how the Match-ups were evaluated (2.4)
- An overview of the MDB characteristics for the particular in situ/satellite pairs (2.5)

The major results of the MDB file Analyses (Section 3)

- Spatial Maps of the Time-mean and temporal Std of in situ and satellite SSS and of the  $\Delta$ SSS (3.1)
- Time series of the monthly averaged mean and Std of in situ and satellite SSS and of the  $\Delta$ SSS (3.2)
- Zonally-averaged Time-mean and temporal Std of in situ and satellite SSS and of the  $\Delta$ SSS (3.3)
- Scatterplots of satellite vs in situ SSS by latitudinal bands (3.4)
- Time series of the monthly averaged mean and Std of the  $\Delta$ SSS sorted by latitudinal bands (3.5)
- $\Delta$ SSS sorted as function of geophysical parameters (3.6)
- $\Delta$ SSS maps and statistics for different geophysical conditions (3.7)

All analyses are conducted over the Pi-MEP Region specified above and over the full satellite SSS product period.



### 2 The MDB file datasets

## 2.1 Satellite SSS product

#### 2.1.1 SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG

The version V02 of the SMOS L4a salinity Ifremer research product from the CATDS/CEC Expertise center includes reprocessed data from May 2010 to December 2017 with a weekly temporal window at  $0.5^{\circ}$  resolution. Level 4a include weekly SMOS SSS biased-corrected at large scale  $(10^{\circ} \times 10^{\circ})$  using monthly in situ OI (ISAS) fields.

In addition, this L4a product also includes an ensemble of geophysical parameters derived from well-acknowledged products in the scientific communities that are useful for synergistic science applications using SMOS data. These include:

- Sea Surface Temperature (ECMWF)
- surface currents (OSCAR)
- rain rate (TRMM and CMORPH)
- evaporation (OAFLUX)
- surface wind stresses (ASCAT)
- mixed-layer depth from Argo OI (APDRC)
- surface salinity from in situ OI (ISAS)
- salinity at the base of the mixed-layer depth estimated also from in situ OI (ISAS)

These fields are averaged or cummulated in time -or interpolated- over the week of the SMOS L4a SSS and gridded at the same 0.5° spatial resolution.

Table 1: Satellite SSS product characteristics

SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG						
Spatial resolution	$0.5^{\circ}$					
Temporal resolution	Weekly					
Temporal coverage	From 2010-05-01 to 2017-12-31					
Data Provider	CATDS					
Release Date	2017-09-08					
Version	2					
Data access	ftp://ftp.ifremer.fr/Ocean_products/L4a/Weekly/					
Documentation	<pre>ftp://ftp.ifremer.fr/Ocean_products/documentation/</pre>					

These weekly Composite, half degree resolution SMOS SSS data were obtained from the Ocean Salinity Expertise Center (CECOS) of the CNES-IFREMER Centre Aval de Traitemenent des Donnees SMOS (CATDS), at IFREMER, Plouzane (France).



#### 2.2 In situ SSS dataset

Instrumentation of southern elephant seals with satellite-linked CTD tags proposes unique temporal and spatial coverage. This includes extensive data from the Antarctic continental slope and shelf regions during the winter months, which is outside the conventional areas of Argo autonomous floats and ship-based studies. The use of elephant seals has been particularly effective to sample the Southern Ocean and the North Pacific. Other seal species have been successfully used in the North Atlantic, such as hooded seals. The marine mammal dataset (MEOP-CTD database) is quality controlled and calibrated using delayed-mode techniques involving comparisons with other existing profiles as well as cross-comparisons similar to established protocols within the Argo community, with a resulting accuracy of  $\pm 0.03$  °C in temperature and  $\pm 0.05$ in salinity or better (Treasure et al. (2017)). 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). This dataset is updated once a year and can be downloaded here (Roquet et al. (2018)). A preprocessing stage is applied to the database before being used by the Pi-MEP which consist to keep only profile with salinity, temperature and pressure quality flags set to 1 or 2 and if at least one measurement is in the top 10 m depth. Marine mammal SSS correspond to the top (shallowest) profile salinity data provided that profile depth is 10 m or less.

# 2.3 Auxiliary geophysical datasets

Additional EO datasets are used to characterize the geophysical conditions at the in situ/satellite SSS pair measurement locations and time, and 10 days prior the measurements to get an estimate of the geophysical condition and history. As discussed in Boutin et al. (2016), the presence of vertical gradients in, and horizontal variability of, sea surface salinity indeed complicates comparison of satellite and in situ measurements. The additional EO data are used here to get a first estimates of conditions for which L-band satellite SSS measured in the first centimeters of the upper ocean within a 50-150 km diameter footprint might differ from pointwise in situ measurements performed in general between 10 and 5 m depth below the surface. The spatiotemporal variability of SSS within a satellite footprint (50–150 km) is a major issue for satellite SSS validation in the vicinity of river plumes, frontal zones, and significant precipitation. Rainfall can in some cases produce vertical salinity gradients exceeding 1 pss m<sup>-1</sup>; consequently, it is recommended that satellite and in situ SSS measurements less than 3-6 h after rain events should be considered with care when used in satellite calibration/validation analyses. To identify such situation, the Pi-MEP test platform is first using CMORPH products to characterize the local value and history of rain rate and ASCAT gridded data are used to characterize the local surface wind speed and history. For validation purpose, the ISAS monthly SSS in situ analysed fields at 5 m depth are collocated and compared with the satellite SSS products. The use of ISAS is motivated by the fact that it is used in the SMOS L2 official validation protocol in which systematic comparisons of SMOS L2 retrieved SSS with ISAS are done. In complement to ISAS, monthly std climatological fields from the World Ocean Atlas (WOA13) at the match-up pairs location and date are also used to have an a priori information of the local SSS variability.

#### 2.3.1 **CMORPH**

Precipitation are estimated using the CMORPH 3-hourly products at  $1/4^{\circ}$  resolution (Joyce et al. (2004)). CMORPH (CPC MORPHing technique) produces global precipitation analyses at very high spatial and temporal resolution. This technique uses precipitation estimates that have been derived from low orbiter satellite microwave observations exclusively, and whose



features are transported via spatial propagation information that is obtained entirely from geostationary satellite IR data. At present NOAA incorporate precipitation estimates derived from the passive microwaves aboard the DMSP 13, 14 and 15 (SSM/I), the NOAA-15, 16, 17 and 18 (AMSU-B), and AMSR-E and TMI aboard NASA's Aqua, TRMM and GPM spacecraft, respectively. These estimates are generated by algorithms of Ferraro (1997) for SSM/I, Ferraro et al. (2000) for AMSU-B and Kummerow et al. (2001) for TMI. Note that this technique is not a precipitation estimation algorithm but a means by which estimates from existing microwave rainfall algorithms can be combined. Therefore, this method is extremely flexible such that any precipitation estimates from any microwave satellite source can be incorporated.

With regard to spatial resolution, although the precipitation estimates are available on a grid with a spacing of 8 km (at the equator), the resolution of the individual satellite-derived estimates is coarser than that - more on the order of  $12 \times 15$  km or so. The finer "resolution" is obtained via interpolation.

In effect, IR data are used as a means to transport the microwave-derived precipitation features during periods when microwave data are not available at a location. Propagation vector matrices are produced by computing spatial lag correlations on successive images of geostationary satellite IR which are then used to propagate the microwave derived precipitation estimates. This process governs the movement of the precipitation features only. At a given location, the shape and intensity of the precipitation features in the intervening half hour periods between microwave scans are determined by performing a time-weighting interpolation between microwave-derived features that have been propagated forward in time from the previous microwave observation and those that have been propagated backward in time from the following microwave scan. NOAA refer to this latter step as "morphing" of the features.

For the present Pi-MEP products, we only considered the 3-hourly products at 1/4 degree resolution. The entire CMORPH record (December 2002-present) for 3-hourly, 1/4 degree lat/lon resolution can be found at: <a href="ftp://ftp.cpc.ncep.noaa.gov/precip/CMORPH\_V1.">ftp://ftp.cpc.ncep.noaa.gov/precip/CMORPH\_V1.</a>
O/RAW/. CMORPH estimates cover a global belt (-180°W to 180°E) extending from 60°S to 60°N latitude and are available for the complete period of the Pi-MEP core datasets (Jan 2010-now).

### 2.3.2 ASCAT

Advanced SCATterometer (ASCAT) daily data produced and made available at Ifremer/CERSAT on a 0.25°x0.25° resolution grid (Bentamy and Fillon (2012)) since March 2007 are used to characterize the mean daily wind at the match-up pair location as well as the wind history during the 10-days period preceding the in situ measurement date. These wind fields are calculated based on a geostatistical method with external drift. Remotely sensed data from ASCAT are considered as observations while those from numerical model analysis (ECMWF) are associated with the external drift. The spatial and temporal structure functions for wind speed, zonal and meridional wind components are estimated from ASCAT retrievals. Furthermore, the new procedure includes a temporal interpolation of the retrievals based on the complex empirical orthogonal function (CEOF) approach, in order to enhance the sampling length of the scatterometer observations. The resulting daily wind fields involves the main known surface wind patterns as well as some variation modes associated with temporal and spatial moving features. The accuracy of the gridded winds was investigated through comparisons with moored buoy data in Bentamy et al. (2012) and resulted in rms differences for wind speed and direction are about 1.50 m.s<sup>-1</sup> and 20°.



#### 2.3.3 ISAS

The In Situ Analysis System (ISAS), as described in Gaillard et al. (2016) is a data based reanalysis of temperature and salinity fields over the global ocean. It was initially designed to synthesize the temperature and salinity profiles collected by the Argo program. It has been later extended to accommodate all type of vertical profile as well as time series. ISAS gridded fields are entirely based on in-situ measurements. The methodology and configuration have been conceived to preserve as much as possible the data information content and resolution. ISAS is developed and run in a research laboratory (LOPS) in close collaboration with Coriolis, one of Argo Global Data Assembly Center and unique data provider for the Mercator operational oceanography system. At the moment the period covered starts in 2002 and only the upper 2000 m are considered. The gridded fields were produced over the global ocean  $70^{\circ}N-70^{\circ}S$  on a  $1/2^{\circ}$  grid by the ISAS project with datasets downloaded from the Coriolis data center (for more details on ISAS see Gaillard et al. (2009)). In the Pi-MEP, the product in used is the INSITU\_GLO\_TS\_OA\_NRT\_OBSERVATIONS\_013\_002\_a v6.2 NRT derived at the Coriolis data center and provided by Copernicus (www.marine.copernicus.eu/documents/ PUM/CMEMS-INS-PUM-013-002-ab.pdf). The major contribution to the data set is from Argo array of profiling floats, reaching an approximate resolution of one profile every 10-days and every 3-degrees over the satellite SSS period (http://www.umr-lops.fr/SNO-Argo/Products/ ISAS-T-S-fields/); in this version SSS from ship of opportunity thermosalinographs are not used, so that we can consider SMOS SSS validation using these measurements independent of ISAS. The ISAS optimal interpolation involves a structure function modeled as the sum of two Gaussian functions, each associated with specific time and space scales, resulting in a smoothing over typically 3 degrees. The smallest scale which can be retrieved with ISAS analysis is not smaller than 300–500 km (Kolodziejczyk et al. (2015)). For validation purpose, the ISAS monthly SSS fields at 5 m depth are collocated and compared with the satellite SSS products and included in the Pi-MEP Match-up files. In addition, the "percentage of variance" fields (PCTVAR) contained in the ISAS analyses provide information on the local variability of in situ SSS measurements within  $1/2^{\circ} \times 1/2^{\circ}$  boxes.

### 2.3.4 World Ocean Atlas Climatology

The World Ocean Atlas 2013 version 2 (WOA13 V2) is a set of objectively analyzed (1° grid) climatological fields of in situ temperature, salinity and other variables provided at standard depth levels for annual, seasonal, and monthly compositing periods for the World Ocean. It also includes associated statistical fields of observed oceanographic profile data interpolated to standard depth levels on 5°, 1°, and 0.25° grids. We use these fields in complement to ISAS to characterize the climatological fields (annual mean and std) at the match-up pairs location and date.

#### 2.4 Overview of the Match-ups generation method

The match-up production is basically a three steps process:

- 1. preparation of the input in situ and satellite data, and,
- 2. co-localization of satellite products with in situ SSS measurements.
- 3. co-localization of the in situ/satellite pair with auxiliary information.

In the following, we successively detail the approaches taken for these different steps.



#### 2.4.1 In Situ/Satellite data filtering

The first step consist in filtering Sea mammalsin situ dataset using the quality flags as described in 2.2 so that only valid salinity data remains in the produced match-ups.

For high-spatial resolution in situ SSS measurements such as the Thermo-SalinoGraph (TSG) SSS data from research vessels, Voluntary Observing Ships (VOS) or sailing ships, as well as SSS data from surface drifters, an additional spatial-filtering step is performed on the in situ data that will be in fine compared to the satellite SSS products. If  $R_{sat}$  is the spatial resolution of the satellite SSS product (L2 to L3-L4), we keep the in situ data at the original spatial resolution but we also estimate for all spatio-temporal samples a running median filtered SSS applied to all neighbouring in situ SSS data acquired within a distance of  $R_{sat}/2$  from a given in situ acquisition. Both the original and the filtered data are finally stored in the MDB files.

Only for satellite L2 SSS data, a third step consist in filtering spurious data using the flags and associated recommendation as provided by the official data centers and described in 2.1.

#### 2.4.2 In Situ/Satellite Co-localization

In this step, each SSS satellite acquisition is co-localized with the filtered in situ measurements. The method used for co-localization differ if the satellite SSS is a swath product (so-called Level 2-types) or a time-space composite product (so-called Level 3/level 4-types).

#### • For L2 SSS swath data :

If  $R_{sat}$  is the spatial resolution of the satellite swath SSS product, for each in situ data sample collected in the Pi-MEP database, the platform searches for all satellite SSS data found at grid nodes located within a radius of  $R_{sat}/2$  from the in situ data location and acquired with a time-lag from the in situ measurement date that is less or equal than  $\pm$  12 hours. If several satellite SSS samples are found to meet these criteria, the final satellite SSS match-up point is selected to be the closest in time from the in situ data measurement date. The final spatial and temporal lags between the in situ and satellite data are stored in the MDB files.

#### • For L3 and L4 composite SSS products :

If  $R_{sat}$  is the spatial resolution of the composite satellite SSS product and D the period over which the composite product was built (e.g., periods of 1, 7, 8, 9, 10, 18 days, 1 month, etc..) with central time to, for each in situ data sample collected in the Pi-MEP database during period D, the platform searches for all satellite SSS data of the composite product found at grid nodes located within a radius of  $R_{sat}/2$  from the in situ data location. If several satellite SSS product samples are found to meet these criteria, the final satellite SSS match-up point is chosen to be the composite SSS with central time to which is the closest in time from the in situ data measurement date. The final spatial and temporal lags between the in situ and satellite data are stored in the MDB files.

# 2.4.3 MDB pair Co-localization with auxiliary data and complementary information

MDB data consist of satellite and in-situ SSS pair datasets but also of auxiliary geophysical parameters such as local and history of wind speed and rain rates, as well as various information (climatology, distance to coast, mixed layer depth, barrier layer thickness, etc) that can be derived from in situ data and which are included in the final match-up files. The collocation of auxiliary parameters and additional information is done for each filtered in-situ SSS measurement contained in the match-up files as follows:



If  $t_{insitu}$  is the time/date at which the in situ measurement is performed, we collect:

- The ASCAT wind speed product of the same day than  $t_{insitu}$  found at the ASCAT  $1/4^{\circ}$  grid node with closest distance from the in situ data location and the time series of the ASCAT wind speed at the same node for the 10 days prior the in situ measurement day.
- If the in situ data is located within the 60°N-60°S band, we select the CMORPH 3-hourly product the closest in time from tin situ and found at the CMORPH 1/4° grid node with closest distance from the in situ data location. We then store the time series of the CMORPH rain rate at the same node for the 10 days prior the in situ measurement time.

For the given month/year of the in situ data, we select the ISAS and WOA fields for the same month (and same year for ISAS fields) and take the SSS analysis (monthly mean, std) found at the closest grid node from the in situ measurement.

The distance from the in situ SSS data location to the nearest coast is evaluated and provided in km. We use a distance-to-coast map at  $1/4^{\circ}$  resolution where small islands have been removed.

When vertical profiles of salinity (S) and temperature (T) are made available from the in situ measurements used to build the match-up (Argo or sea mammals), the following variables are included into each satellite/in situ match-up file:

- 1. The vertical distribution of pressure at which the profile were measured,
- 2. The vertical S(z) and T(z) profiles,
- 3. The vertical potential density anomaly profile  $\sigma_0(z)$ ,
- 4. The Mixed Layer Depth (MLD). The MLD is defined here as the depth where the potential density has increased from the reference depth (10 meter) by a threshold equivalent to 0.2°C decrease in temperature at constant salinity:  $\sigma_0 = \sigma_{010m} + \Delta \sigma_0$  with  $\Delta \sigma_0 = \sigma_0(\theta_{10m} 0.2, S_{10m}) \sigma_0(\theta_{10m}, S_{10m})$  where  $\theta_{10m}$  and  $S_{10m}$  are the temperature and salinity at the reference depth (i.e. 10 m) (de Boyer Montégut et al. (2004), de Boyer Montégut et al. (2007)).
- 5. The Top of the Thermocline Depth (TTD) is defined as the depth at which temperature decreases from its 10 m value by  $0.2^{\circ}\text{C}$ .
- 6. The Barrier Layer if present, is defined as the intermediate layer between the top of the thermocline and the bottom of the density mixed-layer and its thickness (BLT) is defined as the difference between the MLD and the TTD.
- 7. The vertical profile of the buoyancy frequency  $N^2(z)$

The resulting match-ups files are serialized as NetCDF-4 files whose structure depends on the origin of the in-situ data they contain.

#### 2.4.4 Content of the Match-Up NetCDF files

netcdf pimep-mdb\_smos-l4-catds-ifr-v2-1w\_mammal\_20100116\_v01 { dimensions:

```
N_prof = 1;

N_LEVELS = 27;

N_DAYS_WIND = 10;

N_3H_RAIN = 80;
```



```
STRING = 8;
    TIME\_Sat = UNLIMITED; // (1 currently)
float DATE_MAMMAL(N_prof);
    DATE_MAMMAL:long_name = "Date of marine mammal profile";
    DATE_MAMMAL:units = "days since 1990-01-01 00:00:00";
    DATE_MAMMAL:standard_name = "time";
    DATE\_MAMMAL:\_FillValue = -999.f;
float LATITUDE_MAMMAL(N_prof);
    LATITUDE_MAMMAL:long_name = "Latitude of marine mammal profile";
    LATITUDE_MAMMAL:units = "degrees_north";
    LATITUDE\_MAMMAL:valid\_min = -90.;
    LATITUDE_MAMMAL:valid_max = 90.;
    LATITUDE\_MAMMAL: standard\_name = "latitude" \ ;
    LATITUDE\_MAMMAL:\_FillValue = -999.f;
float LONGITUDE_MAMMAL(N_prof);
    LONGITUDE_MAMMAL:long_name = "Longitude of mammal profile";
    LONGITUDE_MAMMAL:units = "degrees_east";
    LONGITUDE\_MAMMAL:valid\_min = -180.;
    LONGITUDE_MAMMAL:valid_max = 180.;
    LONGITUDE_MAMMALS:standard_name = "longitude";
    LONGITUDE_MAMMAL:_FillValue = -999.f;
float SSS_DEPTH_MAMMAL(N_prof);
    SSS_DEPTH_MAMMAL:long_name = "Sea water pressure at marine mammal location
(equals 0 at sea level)";
    SSS_DEPTH_MAMMAL:units = "decibar";
    SSS_DEPTH_MAMMAL:standard_name = "sea_water_pressure";
    SSS_DEPTH_MAMMAL:_FillValue = -999.f;
float SSS_MAMMAL(N_prof);
    SSS_MAMMAL:long_name = "Mammals SSS";
    SSS\_MAMMAL:units = "1";
    SSS_MAMMAL:salinity_scale = "Practical Salinity Scale(PSS-78)";
    SSS_MAMMAL:standard_name = "sea_water_salinity";
    SSS\_MAMMAL:\_FillValue = -999.f:
float SST_MAMMAL(N_prof);
    SST_MAMMAL:long_name = "Mammals SST";
    SST_MAMMAL:units = "degree Celsius";
    SST_MAMMAL:standard_name = "sea_water_temperature";
    SST_MAMMAL:_FillValue = -999.f;
float DISTANCE_TO_COAST_MAMMAL(N_prof) ;
    DISTANCE_TO_COAST_MAMMAL:long_name = "Distance to coasts at marine mammal
    DISTANCE_TO_COAST_MAMMAL:units = "km";
    DISTANCE_TO_COAST_MAMMAL:_FillValue = -999.f;
float PLATFORM_NUMBER_MAMMAL(N_prof);
    PLATFORM_NUMBER_MAMMAL:long_name = "Mammals unique identifier";
    PLATFORM_NUMBER_MAMMAL:conventions = "WMO float identifier: A9IIIII";
    PLATFORM_NUMBER_MAMMAL:units = "1";
    PLATFORM_NUMBER_MAMMAL:_FillValue = -999.f;
```



```
float PSAL_MAMMAL(N_prof, N_LEVELS);
    PSAL\_MAMMAL:long\_name = "Mammals salinity profile";
    PSAL\_MAMMAL:units = "1";
    PSAL_MAMMAL:salinity_scale = "Practical Salinity Scale (PSS-78)";
    PSAL_MAMMAL:standard_name = "sea_water_salinity";
    PSAL\_MAMMAL:\_FillValue = -999.f;
float TEMP_MAMMAL(N_prof, N_LEVELS);
    \label{eq:temp_mammals} TEMP\_MAMMAL: long\_name = "Mammals temperature profile" \ ;
    TEMP_MAMMAL:units = "degree Celsius";
    TEMP_MAMMAL:standard_name = "sea_water_temperature";
    TEMP\_MAMMAL:\_FillValue = -999.f:
float PRES_MAMMAL(N_prof, N_LEVELS);
    PRES_MAMMAL:long_name = "Mammals pressure profile";
    PRES\_MAMMAL: units = "decibar" \; ;
    PRES_MAMMAL:standard_name = "sea_water_pressure";
    PRES\_MAMMAL:\_FillValue = -999.f;
float RHO_MAMMAL(N_prof, N_LEVELS);
    RHO_MAMMAL:long_name = "Mammals in-situ density profile";
    RHO_MAMMAL:units = "kg/m";
    RHO_MAMMAL:_FillValue = -999.f;
float SIGMA0_MAMMAL(N_prof, N_LEVELS);
    SIGMA0\_MAMMAL:long\_name = "Mammals potential density anomaly profile" \; ;
    SIGMA0\_MAMMAL:units = "kg/m^3";
    SIGMA0\_MAMMAL:\_FillValue = -999.f;
float N2_MAMMAL(N_prof, N_LEVELS);
    N2_MAMMAL:long_name = "Mammals buoyancy frequency profile";
    N2\_MAMMAL:units = "1/s^2";
    N2\_MAMMAL:\_FillValue = -999.f;
float MLD_MAMMAL(N_prof);
     MLD_MAMMAL:long_name = "Mixed Layer Depth (MLD) calculated from marine mam-
mal profile (depth where \sigma_0 = \sigma_{010m} + \Delta \sigma_0 with \Delta \sigma_0 = \sigma_0(\theta_{10m} - 0.2, S_{10m}) - \sigma_0(\theta_{10m}, S_{10m})
)";
    MLD\_MAMMAL:units = "m";
    MLD\_MAMMAL:\_FillValue = -999.f;
float TTD_MAMMAL(N_prof);
    TTD_MAMMAL:long_name = "Top of Thermocline Depth (TTD) calculated from marine
mammal profile (depth where \theta = \theta_{10m} - 0.2)";
    TTD\_MAMMAL:units = "m";
    TTD\_MAMMAL:\_FillValue = -999.f;
float BLT_MAMMAL(N_prof);
    BLT_MAMMAL:long_name = "Barrier Layer Thickness (TTD-MLD)";
    BLT\_MAMMAL:units = "m";
    BLT\_MAMMAL:\_FillValue = -999.f;
float DATE_Satellite_product(TIME_Sat);
    DATE_Satellite_product:long_name = "Central time of satellite SSS file";
    DATE_Satellite_product:units = "days since 1990-01-01 00:00:00";
    DATE_Satellite_product:standard_name = "time";
float LATITUDE_Satellite_product(N_prof);
    LATITUDE_Satellite_product:long_name = "Satellite product latitude at marine mammal
```



```
location";
        LATITUDE_Satellite_product:units = "degrees_north";
         LATITUDE_Satellite_product:valid_min = -90.;
        LATITUDE_Satellite_product:valid_max = 90.;
        LATITUDE\_Satellite\_product:standard\_name = "latitude" \ ;
        LATITUDE_Satellite_product:_FillValue = -999.f;
float LONGITUDE_Satellite_product(N_prof);
        LONGITUDE\_Satellite\_product:long\_name = "Satellite\_product longitude at marine mamber of the product longitude a
mal location";
        LONGITUDE_Satellite_product:units = "degrees_east";
         LONGITUDE_Satellite_product:valid_min = -180. :
        LONGITUDE_Satellite_product:valid_max = 180.;
        LONGITUDE_Satellite_product:standard_name = "longitude";
        LONGITUDE_Satellite_product:_FillValue = -999.f;
float SSS_Satellite_product(N_prof);
         SSS_Satellite_product:long_name = "Satellite product SSS at marine mammal location";
        SSS_Satellite_product:units = "1";
         SSS_Satellite_product:salinity_scale = "Practical Salinity Scale(PSS-78)";
         SSS_Satellite_product:standard_name = "sea_surface_salinity";
         SSS\_Satellite\_product:\_FillValue = -999.f;
float SST_Satellite_product(N_prof);
         SST_Satellite_product:long_name = "Satellite product SST at marine mammal location";
         SST_Satellite_product:units = "degree Celsius";
        SST_Satellite_product:standard_name = "sea_surface_temperature";
         SST_Satellite_product:_FillValue = -999.f;
float Spatial_lags(N_prof);
         Spatial_lags:long_name = "Spatial lag between marine mammal location and satellite SSS
product pixel center";
         Spatial\_lags:units = "km";
         Spatial_lags:_FillValue = -999.f;
float Time_lags(N_prof);
         Time_lags:long_name = "Temporal lag between marine mammal time and satellite SSS
product central time";
         Time\_lags:units = "days";
         Time_lags:_FillValue = -999.f;
float ROSSBY_RADIUS_at_MAMMAL(N_prof);
         ROSSBY_RADIUS_at_MAMMAL:long_name = "Baroclinic Rossby radius of deformation
(Chelton et al., 1998) at marine mammal location";
        ROSSBY_RADIUS_at_MAMMAL:units = "km";
        ROSSBY_RADIUS_at_MAMMAL:_FillValue = -999.f;
float Ascat_daily_wind_at_MAMMAL(N_prof);
         Ascat_daily_wind_at_MAMMAL:long_name = "Daily Ascat wind speed module at marine
mammal location";
         Ascat_daily_wind_at_MAMMAL:units = "m/s";
         Ascat_daily\_wind_at\_MAMMAL:_FillValue = -999.f;
float CMORPH_3h_Rain_Rate_at_MAMMAL(N_prof);
        CMORPH_3h_Rain_Rate_at_MAMMAL:long_name = "3-hourly CMORPH rain rate at ma-
rine mammal location";
         CMORPH_3h_Rain_Rate_at_MAMMAL:units = "mm/3h";
```



```
CMORPH_3h_Rain_Rate_at_MAMMAL:_FillValue = -999.f;
float Ascat_10_prior_days_wind_at_MAMMAL(N_prof, N_DAYS_WIND);
        Ascat_10_prior_days_wind_at_MAMMAL:long_name = "Prior 10 days time series of Ascat
wind speed module at marine mammal location";
        Ascat_10\_prior_days\_wind_at\_MAMMAL:units = "m/s";
        Ascat_10_prior_days_wind_at_MAMMAL:_FillValue = -999.f;
float CMORPH_10_prior_days_Rain_Rate_at_MAMMAL(N_prof, N_3H_RAIN);
       CMORPH\_10\_prior\_days\_Rain\_Rate\_at\_MAMMAL:long\_name = "Prior 10 days times series" and the series of the prior of the series of
of 3-hourly CMORPH Rain Rate at marine mammal location";
        CMORPH\_10\_prior\_days\_Rain\_Rate\_at\_MAMMAL:units = "mm/3h" ;
        CMORPH_10_prior_days_Rain_Rate_at_MAMMAL:_FillValue = -999.f;
float SSS_ISAS_at_MAMMAL(N_prof);
       SSS_ISAS_at_MAMMAL:long_name = "ISAS SSS (5m depth) at marine mammal location"
        SSS\_ISAS\_at\_MAMMAL:units = "1";
       SSS\_ISAS\_at\_MAMMAL: salinity\_scale = "Practical Salinity Scale (PSS-78)" \ ;
       SSS_ISAS_at_MAMMAL:standard_name = "sea_water_salinity";
        SSS_ISAS_at_MAMMAL:_FillValue = -999.f;
float SSS_PCTVAR_ISAS_at_MAMMAL(N_prof);
       SSS_PCTVAR_ISAS_at_MAMMAL:long_name = "Error on ISAS SSS (5m depth) at marine
mammal location (% variance)";
        SSS_PCTVAR_ISAS_at_MAMMAL:units = "%";
        SSS\_PCTVAR\_ISAS\_at\_MAMMAL:\_FillValue = -999.f;
float SSS_WOA13_at_MAMMAL(N_prof);
        SSS_WOA13_at_MAMMAL:long_name = "Annual WOA 2013 (DECAV-1deg) SSS (0m
depth) at marine mammal location";
        SSS_WOA13_at_MAMMAL:units = "1";
        SSS_WOA13_at_MAMMAL:salinity_scale = "Practical Salinity Scale(PSS-78)";
        SSS\_WOA13\_at\_MAMMAL:standard\_name = "sea\_surface\_salinity";
        SSS_WOA13_at_MAMMAL:_FillValue = -999.f;
float SSS_STD_WOA13_at_MAMMAL(N_prof);
        SSS_STD_WOA13_at_MAMMAL:long_name = "Annual WOA 2013 (DECAV-1deg) SSS
STD (0m depth) at marine mammal location";
        SSS\_STD\_WOA13\_at\_MAMMAL:units = "1":
        SSS\_STD\_WOA13\_at\_MAMMAL:\_FillValue = -999.f;
float SSS_ISAS15_at_MAMMAL(N_prof);
        SSS_ISAS15_at_MAMMAL:long_name = "Monthly ISAS-15 SSS (5m depth) at marine
mammal location";
       SSS_ISAS15_at_MAMMAL:units = "1";
       SSS_ISAS15_at_MAMMAL:salinity_scale = "Practical Salinity Scale (PSS-78)";
        SSS_ISAS15_at_MAMMAL:standard_name = "sea_water_salinity";
        SSS_ISAS15_at_MAMMAL:_FillValue = -999.f;
float SSS_PCTVAR_ISAS15_at_MAMMAL(N_prof) ;
        SSS_PCTVAR_ISAS15_at_MAMMAL:long_name = "Error on monthly ISAS-15 SSS (5m
depth) at marine mammal location (% variance)";
        SSS\_PCTVAR\_ISAS15\_at\_MAMMAL: units = "\%";
        SSS_PCTVAR_ISAS15_at_MAMMAL:_FillValue = -999.f;
float SSS_WOA18_at_MAMMAL(N_prof);
        SSS_WOA18_at_MAMMAL:long_name = "Monthly WOA 2018 (DECAV-1deg) SSS (0m
```



```
depth) at marine mammal location";
        SSS_WOA18_at_MAMMAL:units = "1";
        SSS_WOA18_at_MAMMAL:salinity_scale = "Practical Salinity Scale (PSS-78)";
        SSS_WOA18_at_MAMMAL:standard_name = "sea_surface_salinity";
        SSS_WOA18_at_MAMMAL:_FillValue = -999.f;
float SSS_STD_WOA18_at_MAMMAL(N_prof);
        SSS_STD_WOA18_at_MAMMAL:long_name = "Monthly WOA 2018 (DECAV-1deg) SSS
STD (0m depth) at marine mammal location";
        SSS_STD_WOA18_at_MAMMAL:units = "1";
        SSS\_STD\_WOA18\_at\_MAMMAL:\_FillValue = -999.f;
float SEA_ICE_CONCENTRATION_at_MAMMAL(N_prof);
        SEA_ICE_CONCENTRATION_at_MAMMAL:long_name = "Daily sea ice area fraction
(EUMETSAT OSI-SAF OSI-450) at marine mammal location (%)";
        SEA_ICE_CONCENTRATION_at_MAMMAL:units = "1";
        SEA_ICE_CONCENTRATION_at_MAMMAL:standard_name = "sea_ice_area_fraction";
        SEA_ICE_CONCENTRATION_at_MAMMAL:_FillValue = -999.f;
float CCMP_6h_Wind_Speed_at_MAMMAL(N_prof) ;
        CCMP_6h_Wind_Speed_at_MAMMAL:long_name = "6-hourly CCMP wind speed at ma-
rine mammal location";
        CCMP_6h_Wind_Speed_at_MAMMAL:units = "m s-1";
        \label{lem:comp_hammal}  \mbox{CCMP\_6h\_Wind\_Speed\_at\_MAMMAL:standard\_name} = "wind\_speed" \ ;
        CCMP_6h_Wind_Speed_at_MAMMAL:_FillValue = -999.f;
float CCMP_10_prior_days_Wind_Speed_at_MAMMAL(N_prof, N_DAYS_WIND_CCMP);
        CCMP_10_prior_days_Wind_Speed_at_MAMMAL:long_name = "Prior 10 days time series
of CCMP wind speed at marine mammal location";
        CCMP_10_prior_days_Wind_Speed_at_MAMMAL:units = "m s-1";
        \label{lem:comp_10_prior_days_Wind_Speed_at_MAMMAL:standard_name = "wind_speed"} \\ ;
        CCMP_10_prior_days_Wind_Speed_at_MAMMAL:_FillValue = -999.f;
float CDM_GLOBCOLOUR_at_MAMMAL(N_prof) ;
        CDM_GLOBCOLOUR_at_MAMMAL:long_name = "8-day Coloured dissolved and detrital
organic materials - mean of the binned pixels at marine mammal location";
        CDM_GLOBCOLOUR_at_MAMMAL:units = "m-1";
        CDM\_GLOBCOLOUR\_at\_MAMMAL: standard\_name = "volume\_absorption\_coefficient\_of\_radiative\_flux\_in\_sea\_topic flux\_in\_sea\_topic flux\_in\_sea\_to
        CDM_GLOBCOLOUR_at_MAMMAL:_FillValue = -999.f;
float CHL1_GLOBCOLOUR_at_MAMMAL(N_prof);
        CHL1_GLOBCOLOUR_at_MAMMAL:long_name = "8-day Chlorophyll concentration - mean
of the binned pixels at marine mammal location";
        CHL1\_GLOBCOLOUR\_at\_MAMMAL:units = "mg m-3";
        CHL1\_GLOBCOLOUR\_at\_MAMMAL: standard\_name = "mass\_concentration\_of\_chlorophyll\_a\_in\_sea\_water"
        CHL1_GLOBCOLOUR_at_MAMMAL:_FillValue = -999.f;
float EVAPORATION_OAFLUX_at_MAMMAL(N_prof) ;
        EVAPORATION_OAFLUX_at_MAMMAL:long_name = "Daily mean evaporation rate (OAFlux)
at marine mammal location";
        EVAPORATION_OAFLUX_at_MAMMAL:units = "cm year-1";
        EVAPORATION_OAFLUX_at_MAMMAL:_FillValue = -999.f;
float SSS_SCRIPPS_at_MAMMAL(N_prof);
        SSS_SCRIPPS_at_MAMMAL:long_name = "Argo gridded monthly mean SSS (0m depth)
```



```
from SCRIPPS (Roemmich-Gilson) at marine mammal location";
    SSS\_SCRIPPS\_at\_MAMMAL:units = "1";
    SSS_SCRIPPS_at_MAMMAL:salinity_scale = "Practical Salinity Scale (PSS-78)";
    SSS_SCRIPPS_at_MAMMAL:standard_name = "sea_water_salinity";
    SSS\_SCRIPPS\_at\_MAMMAL:\_FillValue = -999.f;
float SSS_IPRC_at_MAMMAL(N_prof);
    SSS_IPRC_at_MAMMAL:long_name = "Argo gridded monthly mean SSS (0m depth) from
IPRC at marine mammal location";
    SSS_IPRC_at_MAMMAL:units = "1";
    SSS_IPRC_at_MAMMAL:salinity_scale = "Practical Salinity Scale (PSS-78)";
    SSS_IPRC_at_MAMMAL:standard_name = "sea_water_salinity";
    SSS_IPRC_at_MAMMAL:_FillValue = -999.f;
float SST_AVHRR_at_MAMMAL(N_prof);
    SST_AVHRR_at_MAMMAL:long_name = "Daily OI AVHRR-only v2 SST (Reynolds et al.,
2007) at marine mammal location";
    SST_AVHRR_at_MAMMAL:units = "degree Celsius";
    SST_AVHRR_at_MAMMAL:standard_name = "sea_water_temperature";
    SST_AVHRR_at_MAMMAL:_FillValue = -999.f;
float U_EKMAN_GLOBCURRENT_at_MAMMAL(N_prof);
    U_EKMAN_GLOBCURRENT_at_MAMMAL:long_name = "15m depth Ekman current ve-
locity: zonal component at marine mammal location";
    U_EKMAN_GLOBCURRENT_at_MAMMAL:units = "m s-1";
    U_EKMAN_GLOBCURRENT_at_MAMMAL:_FillValue = -999.f;
float V_EKMAN_GLOBCURRENT_at_MAMMAL(N_prof);
    V_EKMAN_GLOBCURRENT_at_MAMMAL:long_name = "15m depth Ekman current ve-
locity: meridian component at marine mammal location";
    V_EKMAN_GLOBCURRENT_at_MAMMAL:units = "m s-1";
    V_EKMAN_GLOBCURRENT_at_MAMMAL:_FillValue = -999.f;
float U_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL(N_prof);
    U_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:long_name = "Absolute geostrophic
velocity: zonal component at marine mammal location";
    U_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:units = "m s-1";
    U_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:_FillValue = -999.f;
float V_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL(N_prof);
    V_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:long_name = "Absolute geostrophic
velocity: meridian component at marine mammal location";
    V_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:units = "m s-1";
    V_GEOSTROPHIC_GLOBCURRENT_at_MAMMAL:_FillValue = -999.f;
  // global attributes:
    :Conventions = "CF-1.6";
    :title = "Marine Mammals Match-Up Database";
                                                   :Satellite\_product\_name = "SMOS-"
L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG";
    :Satellite_product_spatial_resolution = "0.5 deg";
    : Satellite\_product\_temporal\_resolution = "Weekly" \ ; \\
    :Satellite_product_filename = "L4a/Weekly/CECOS_SMOS_L4aSSS_0.5deg_2010.120_2010.126_V02.nc";
    :Match-Up_spatial_window_radius_in_km = 27.5;
    :Match-Up_temporal_window_radius_in_days = 3.5;
    :start_time = "20100114T000005Z";
```



```
:stop\_time = "20100118T235026Z";
     :northernmost_latitude = 77.676f;
     :sourthenmost_latitude = -66.423f;
     :westernmost_longitude = -179.219f;
     :easternmost_longitude = 179.199f;
     :geospatial_lat_units = "degrees north";
     :geospatial_lat_resolution = "0.5 deg"
     : geospatial\_lon\_units = "degrees\ east"
     :geospatial_lon_resolution = "0.5 deg";
     :institution = "ESA-IFREMER-ODL";
     :project_name = "SMOS Pilote Mission Exploitation Platfrom (Pi-MEP) for salinity";
     : project\_url = "https://pimep-project.odl.bzh" \ ; \\
     :license = "Pi-MEP data use is free and open";
     :product_version = "1.0";
     :keywords = "Oceans > Ocean Salinity > Sea Surface Salinity";
     :acknowledgment = "Please acknowledge the use of these data with the following statement:
These data were provided by SMOS Pilote Mission Exploitation Platfrom (Pi-MEP) for salinity"
     :Source = "L4a/Weekly/CECOS_SMOS_L4aSSS_0.5deg_2010.120_2010.126_V02.nc";
     :references = "https://pimep-project.odl.bzh";
     :history = "Processed on 2018-04-18 using MDB_generator";
     : date\_created = "2018-04-18\ 17:09:30";
}
```

### 2.5 MDB characteristics for the particular in situ/satellite pairs

### 2.5.1 Number of paired SSS data as a function of time and distance to coast

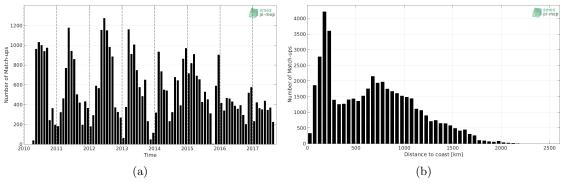


Figure 1: Number of match-ups between Sea mammals and SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG SSS as a function of time (a) and as function of the distance to coast (b) over the Southern Ocean Pi-MEP region and for the full satellite product period.



### 2.5.2 Histograms of the SSS match-ups

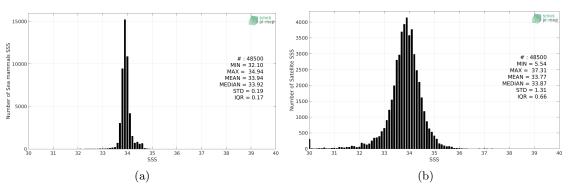


Figure 2: Histograms of SSS from Sea mammals (a) and SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG (b) considering all match-up pairs per bins of 0.1 over the Southern Ocean Pi-MEP region and for the full satellite product period.

## 2.5.3 Distribution of in situ SSS depth measurements

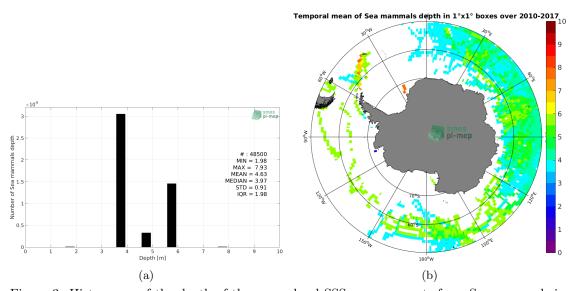


Figure 3: Histograms of the depth of the upper level SSS measurements from Sea mammals in the Match-up DataBase for the Southern Ocean Pi-MEP region (a) and temporal mean spatial distribution of pressure of the in situ SSS data over  $1^{\circ}x1^{\circ}$  boxes and for the full satellite product period (b).



# 2.5.4 Spatial Distribution of Match-ups

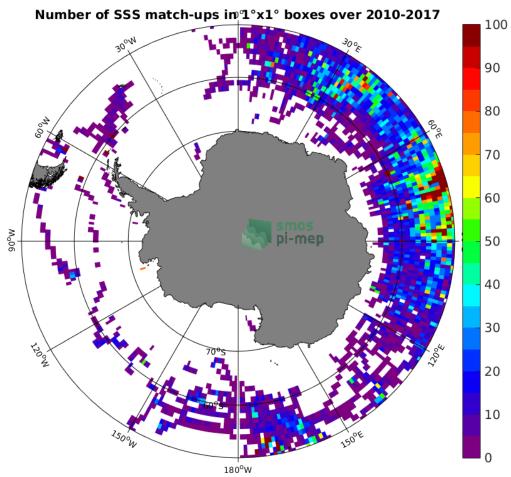


Figure 4: Number of SSS match-ups between Sea mammals SSS and the SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG SSS product for the Southern Ocean Pi-MEP region over  $1^{\circ}x1^{\circ}$  boxes and for the full satellite product period.



### 2.5.5 Histograms of the spatial and temporal lags of the match-ups pairs

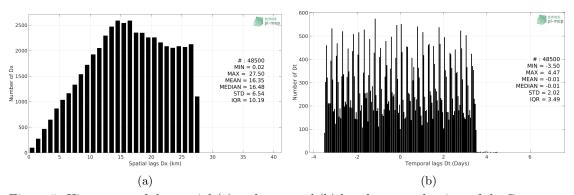


Figure 5: Histograms of the spatial (a) and temporal (b) lags between the time of the Sea mammals measurements and the date of the corresponding SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG SSS product.

# 3 MDB file Analyses

# 3.1 Spatial Maps of the Temporal mean and Std of in situ and satellite SSS and of the difference ( $\Delta$ SSS)

In Figure 6, we show maps of temporal mean (left) and standard deviation (right) of the SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG satellite SSS product (top) and of the Sea mammals in situ dataset at the collected Pi-MEP match-up pairs. The temporal mean and std are gridded over the full satellite product period and over spatial boxes of size 1°x1°.

At the bottom of Figure 6, the temporal mean (left) and standard deviation (right) of the differences between the satellite SSS product and in situ data found at match-up pairs, namely  $\Delta SSS(Satellite$ -Sea mammals), is also gridded over the full satellite product period and over spatial boxes of size 1°x1°.



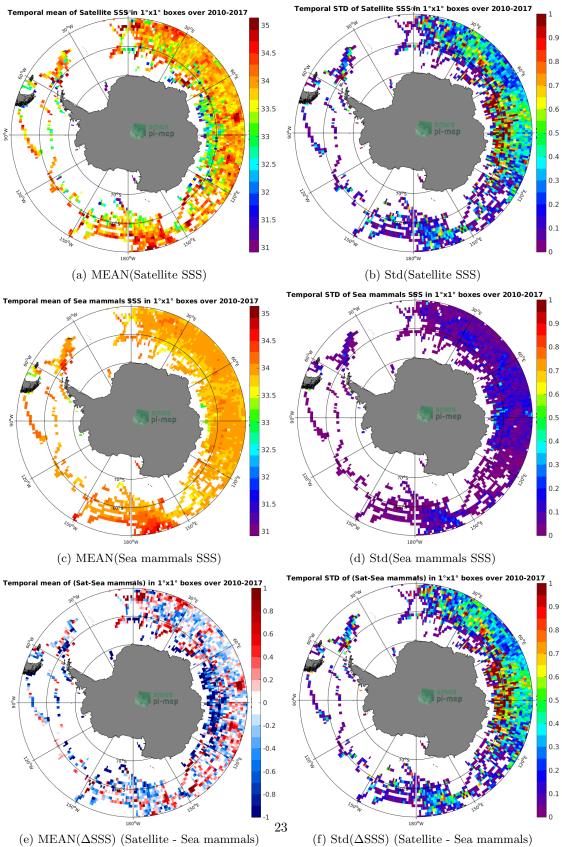


Figure 6: Temporal mean (left) and Std (right) of SSS from SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG (top), Sea mammals (middle), and of  $\Delta$ SSS (Satellite - Sea mammals). Only match-up pairs are used to generate these maps.



# 3.2 Time series of the monthly averaged mean and Std of in situ and satellite SSS and of the ( $\Delta$ SSS)

In the top panel of Figure 7, we show the time series of the monthly averaged SSS estimated over the full Southern Ocean Pi-MEP region for both SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG satellite SSS product (in black) and the Sea mammals in situ dataset (in blue) at the collected Pi-MEP match-up pairs.

In the middle panel of Figure 7, we show the time series of the monthly averaged  $\Delta$ SSS (Satellite - Sea mammals) for the collected Pi-MEP match-up pairs and estimated over the full Southern Ocean Pi-MEP region.

In the bottom panel of Figure 7, we show the time series of the monthly averaged standard deviation of the  $\Delta$ SSS (Satellite - Sea mammals) for the collected Pi-MEP match-up pairs and estimated over the full Southern Ocean Pi-MEP region.

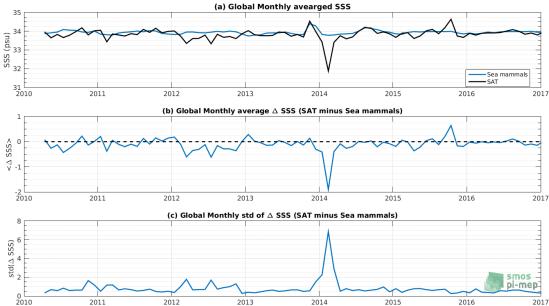


Figure 7: Time series of the monthly averaged mean SSS (top), mean  $\Delta$ SSS (Satellite - Sea mammals) and Std of  $\Delta$ SSS (Satellite - Sea mammals) over the Southern Ocean Pi-MEP region considering all match-ups collected by the Pi-MEP platform.

# 3.3 Zonally-averaged Time-mean and temporal Std of in situ and satellite SSS and of the $\Delta$ SSS

In Figure 8 left panel, we show the zonally averaged time-mean SSS estimated at the collected Pi-MEP match-up pairs for both SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG satellite SSS product (in black) and the Sea mammals in situ dataset (in blue). The time mean is evaluated over the full satellite SSS product period.

In the right panel of Figure 8, we show the zonally averaged time-mean  $\Delta$ SSS (Satellite - Sea mammals) for all the collected Pi-MEP match-up pairs estimated over the full satellite product period.



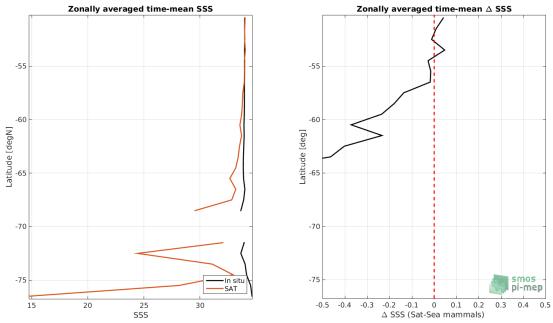


Figure 8: Left panel: Zonally averaged time mean SSS from SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG (black) and from Sea mammals (blue). Right panel: zonally averaged time-mean  $\Delta$ SSS (Satellite - Sea mammals) for all the collected Pi-MEP match-up pairs estimated over the full satellite product period.



# 3.4 Scatterplots of satellite vs in situ SSS by latitudinal bands

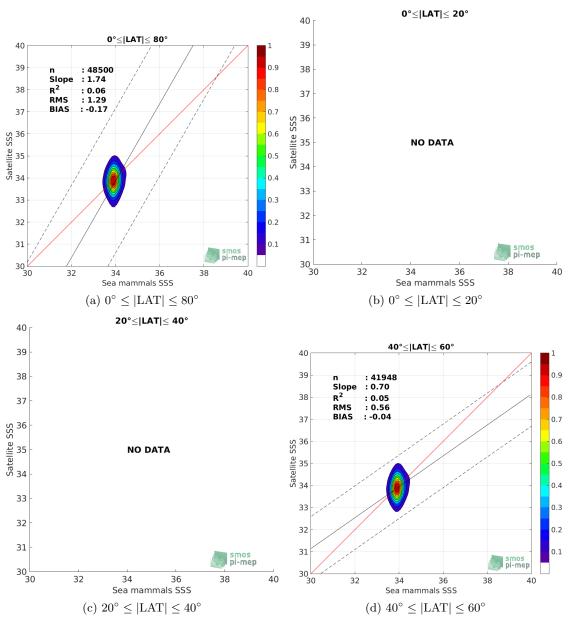


Figure 9: Contour maps of the concentration of SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG SSS (y-axis) versus Sea mammals SSS (x-axis) at match-up pairs for different latitude bands. For each plot, the red line shows x=y. The black thin and dashed lines indicate a linear fit through the data cloud and the  $\pm 95\%$  confidence levels, respectively. The number match-up pairs n, the slope and  $R^2$  coefficient of the linear fit, the root mean square (RMS) and the mean bias between satellite and in situ data are indicated for each latitude band in each plots.



# 3.5 Time series of the monthly averaged mean and Std of the $\Delta SSS$ sorted by latitudinal bands

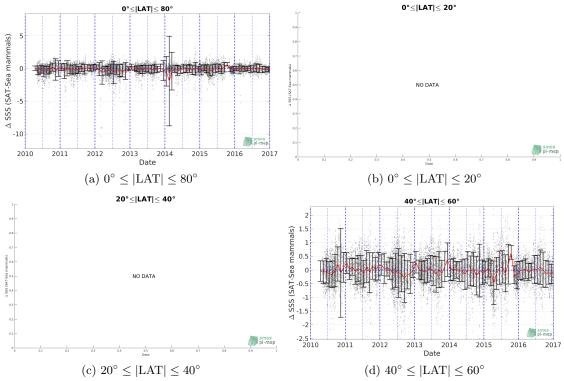


Figure 10: Monthly-average mean (red curves)  $\Delta$ SSS (Satellite - Sea mammals) and  $\pm 1$  Std (black vertical thick bars) as function of time for all the collected Pi-MEP match-up pairs estimated over the Southern Ocean Pi-MEP region and for the full satellite product period are shown for different latitude bands: (a) Latitude band 80°S-80°N, (b) latitude band 20°S-20°N, (c) Mid Latitude bands 40°S-20°S and 20°N-40°N and (d) Latitude bands 60°S-40°S and 40°N-60°N.

# 3.6 $\Delta$ SSS sorted as function of geophysical parameters

In Figure 11, we classify the match-up differences  $\Delta SSS$  (Satellite - in situ) between SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG and Sea mammals SSS as function of the geophysical conditions at match-up points. The mean and std of  $\Delta SSS$  (Satellite - Sea mammals) is thus evaluated as function of the

- in situ SSS values per bins of width 0.2,
- in situ SST values per bins of width 1°C,
- ASCAT daily wind values per bins of width 1 m/s,
- CMORPH 3-hourly rain rates per bins of width 1 mm/h, and,
- distance to coasts per bins of width 50 km.



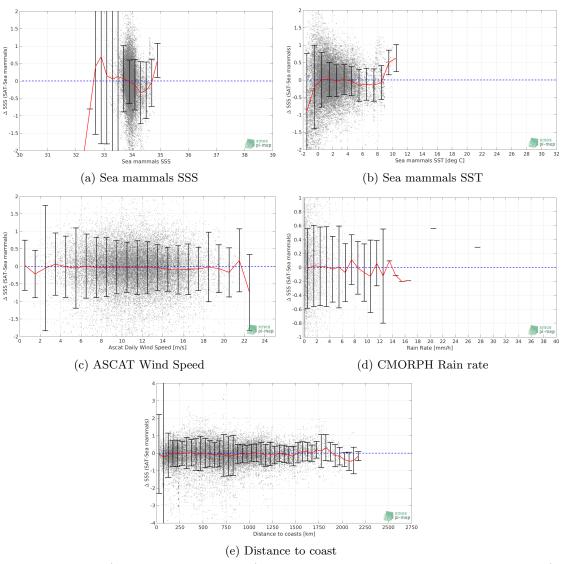


Figure 11:  $\Delta$ SSS (Satellite - Sea mammals) sorted as function of Sea mammals SSS values a), Sea mammals SST b), ASCAT Wind speed c), CMORPH rain rate d) and distance to coast (e). In all plots the mean and Std of  $\Delta$ SSS for each bin is indicated by the red curves and black vertical thick bars ( $\pm 1$  Std)

## 3.7 $\Delta$ SSS maps and statistics for different geophysical conditions

In Figures 12 and 13, we focus on sub-datasets of the match-up differences  $\Delta$ SSS (Satellite - in situ) between SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG and Sea mammals for the following specific geophysical conditions:

- C1:if the local value at in situ location of estimated rain rate is zero, mean daily wind is in the range [3, 12] m/s, the SST is > 5°C and distance to coast is > 800 km.
- C2:if the local value at in situ location of estimated rain rate is zero, mean daily wind is



in the range [3, 12] m/s.

- C3:if the local value at in situ location of estimated rain rate is high (ie. > 1 mm/h) and mean daily wind is low (ie. < 4 m/s).
- C4:if the mixed layer is shallow with depth <20m.
- C5:if the in situ data is located where the climatological SSS standard deviation is low (ie. above < 0.2).
- C6:if the in situ data is located where the climatological SSS standard deviation is high (ie. above > 0.2).

For each of these conditions, the temporal mean (gridded over spatial boxes of size  $1^{\circ}x1^{\circ}$ ) and the histogram of the difference  $\Delta SSS$  (Satellite - in situ) are presented.

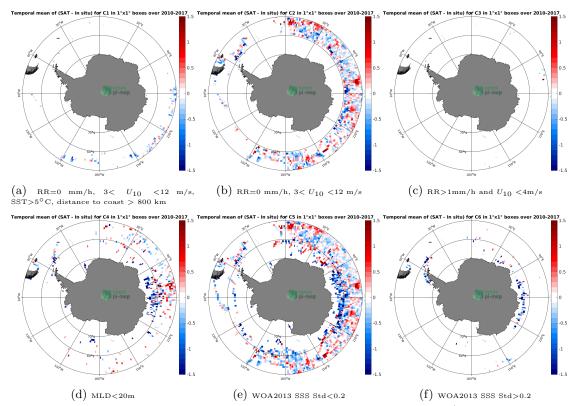


Figure 12: Temporal mean gridded over spatial boxes of size 1°x1° of  $\Delta$ SSS (SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG - Sea mammals) for 6 different subdatasets corresponding to:RR=0 mm/h, 3<  $U_{10}$  <12 m/s, SST>5°C, distance to coast > 800 km (a), RR=0 mm/h, 3<  $U_{10}$  <12 m/s (b), RR>1mm/h and  $U_{10}$  <4m/s (c),MLD<20m (d),WOA2013 SSS Std<0.2 (e),WOA2013 SSS Std>0.2 (f).



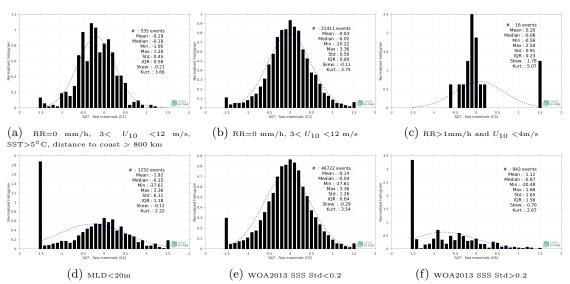


Figure 13: Normalized histogram of  $\Delta$ SSS (SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG - Sea mammals) for 6 different subdatasets corresponding to: RR=0 mm/h,  $3 < U_{10} < 12$  m/s, SST>5°C, distance to coast > 800 km (a), RR=0 mm/h,  $3 < U_{10} < 12$  m/s (b), RR>1mm/h and  $U_{10} < 4$ m/s (c), MLD<20m (d), WOA2013 SSS Std<0.2 (e), WOA2013 SSS Std>0.2 (f).

# 4 Summary

Table 1 shows the mean, median, standard deviation (Std), root mean square (RMS), interquartile range (IQR), correlation coefficient ( $\rm r^2$ ) and robust standard deviation (Std\*) of the match-up differences  $\Delta \rm SSS$  (Satellite - in situ) between SMOS-L4-CATDS-CECOS-IFREMER-V2-WEEKLY-0.5DEG and Sea mammals derived over the Southern Ocean Pi-MEP region and for the full satellite product period and for the following conditions:

- all: All the match-up pairs satellite/in situ SSS are used to derive the statistics
- C1: only pairs where RR=0 mm/h,  $3 < U_{10} < 12$  m/s, SST>5°C, distance to coast > 800 km
- C2: only pairs where RR=0 mm/h,  $3 < U_{10} < 12$  m/s
- C3: only pairs where RR>1mm/h and  $U_{10}$  <4m/s
- C4: only pairs where MLD<20m
- C5: only pairs where WOA2013 SSS Std<0.2
- $\bullet$  C6: only pairs at WOA2013 SSS Std>0.2
- C7a: only pairs where distance to coast is < 150 km.
- C7b: only pairs where distance to coast is in the range [150, 800] km.
- C7c: only pairs where distance to coast is > 800 km.



- C8a: only pairs where in situ SST is  $< 5^{\circ}$ C.
- C8b: only pairs where in situ SST is in the range [5, 15]°C.
- C8c: only pairs where in situ SST is > 15°C.
- C9a: only pairs where in situ SSS is < 33.
- C9b: only pairs where in situ SSS is in the range [33, 37].
- C9c: only pairs where in situ SSS is > 37.

Table 1: Statistics of  $\Delta$ SSS (Satellite - Sea mammals)

Condition	#	Median	Mean	Std	RMS	IQR	$\mathbf{r}^2$	$\mathbf{Std}^{\star}$
all	48500	-0.05	-0.17	1.28	1.29	0.65	0.06	0.49
C1	535	-0.18	-0.19	0.45	0.48	0.58	0.06	0.43
C2	21411	-0.02	-0.03	0.56	0.56	0.60	0.05	0.45
C3	16	-0.08	0.20	0.91	0.90	0.23	0.09	0.18
C4	1252	-0.15	-1.92	6.11	6.41	1.18	0.35	0.78
C5	46722	-0.04	-0.14	1.26	1.27	0.64	0.07	0.48
C6	943	-0.87	-1.12	1.65	2.00	1.56	0.04	1.11
C7a	4968	-0.16	-0.59	3.24	3.29	0.53	0.21	0.40
C7b	25264	-0.04	-0.15	0.86	0.87	0.69	0.03	0.51
C7c	18256	-0.03	-0.08	0.64	0.64	0.64	0.01	0.48
C8a	44345	-0.05	-0.17	1.33	1.34	0.66	0.06	0.49
C8b	4155	-0.10	-0.10	0.49	0.50	0.61	0.35	0.45
C8c	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C9a	53	-27.20	-18.74	11.79	22.08	24.40	0.33	0.34
C9b	48447	-0.05	-0.15	1.05	1.06	0.65	0.04	0.49
C9c	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN

For the same conditions, Table 2 presents statistics of  $\Delta$ SSS (Satellite - ISAS). Only ISAS SSS values with PCTVAR<80% are used to derive the statistics.

Table 2: Statistics of  $\Delta$ SSS (Satellite - ISAS)

Condition	#	Median	Mean	$\widehat{\mathbf{Std}}$	RMS	IQR	$\mathbf{r}^2$	$\mathbf{Std}^{\star}$
all	45480	-0.04	-0.15	1.29	1.29	0.63	0.08	0.47
C1	530	-0.23	-0.18	0.42	0.46	0.53	0.10	0.38
C2	20392	-0.01	-0.02	0.56	0.56	0.59	0.06	0.44
C3	15	-0.11	0.23	0.91	0.91	0.18	0.28	0.13
C4	1169	-0.16	-2.06	6.32	6.64	1.17	0.43	0.77
C5	43931	-0.03	-0.12	1.27	1.27	0.62	0.08	0.46
C6	831	-0.74	-1.07	1.71	2.01	1.73	0.04	1.14
C7a	4824	-0.15	-0.58	3.29	3.34	0.51	0.24	0.38
C7b	24132	-0.02	-0.12	0.82	0.83	0.66	0.04	0.49
C7c	16524	-0.03	-0.06	0.58	0.59	0.63	0.00	0.47
C8a	41355	-0.04	-0.16	1.34	1.35	0.64	0.07	0.48
C8b	4125	-0.08	-0.07	0.47	0.48	0.59	0.39	0.44
C8c	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN
C9a	53	-27.30	-19.02	11.50	22.17	23.79	0.71	0.50
C9b	45427	-0.04	-0.13	1.04	1.05	0.63	0.05	0.47
C9c	0	NaN	NaN	NaN	NaN	NaN	NaN	NaN



Numerical values can be downloaded as csv files for Table 1 and Table 2.

# References

- Abderrahim Bentamy and Denis Croize Fillon. Gridded surface wind fields from Metop/ASCAT measurements. *Int. J. Remote Sens.*, 33(6):1729–1754, March 2012. ISSN 1366-5901. doi: 10.1080/01431161.2011.600348.
- Abderrahim Bentamy, Semyon A. Grodsky, James A. Carton, Denis Croizé-Fillon, and Bertrand Chapron. Matching ASCAT and QuikSCAT winds. *J. Geophys. Res.*, 117(C2), February 2012. ISSN 0148-0227. doi: 10.1029/2011JC007479. C02011.
- Jaqueline Boutin, Y. Chao, W. E. Asher, T. Delcroix, R. Drucker, K. Drushka, N. Kolodziejczyk, T. Lee, N. Reul, G. Reverdin, J. Schanze, A. Soloviev, L. Yu, J. Anderson, L. Brucker, E. Dinnat, A. S. Garcia, W. L. Jones, C. Maes, T. Meissner, W. Tang, N. Vinogradova, and B. Ward. Satellite and In Situ Salinity: Understanding Near-Surface Stratification and Sub-footprint Variability. Bull. Am. Meterol. Soc., 97(8):1391–1407, 2016. ISSN 1520-0477. doi: 10.1175/bams-d-15-00032.1.
- Clément de Boyer Montégut, Gurvan Madec, A. S. Fischer, A. Lazar, and D. Ludicone. Mixed layer depth over the global ocean: An examination of profile data and a profile-based climatology. *J. Geophys. Res.*, 109(C12):C12003, December 2004. ISSN 0148-0227. doi: 10.1029/2004jc002378.
- Clément de Boyer Montégut, Juliette Mignot, Alban Lazar, and Sophie Cravatte. Control of salinity on the mixed layer depth in the world ocean: 1. General description. *J. Geophys. Res.*, 112(C6):C06011, June 2007. ISSN 0148-0227. doi: 10.1029/2006jc003953.
- Ralph R. Ferraro. SSM/I derived global rainfall estimates for climatological applications. *J. Geophys. Res.*, 1021:16715–16736, 07 1997. doi: 10.1029/97JD01210.
- Ralph R. Ferraro, Fuzhong Weng, Norman C. Grody, and Limin Zhao. Precipitation characteristics over land from the NOAA-15 AMSU sensor. *Geophys. Res. Lett.*, 27(17):2669–2672, 2000. doi: 10.1029/2000GL011665.
- Fabienne Gaillard, E. Autret, V. Thierry, P. Galaup, C. Coatanoan, and T. Loubrieu. Quality Control of Large Argo Datasets. *J. Atmos. Oceanic Technol.*, 26(2):337–351, 2012/10/10 2009. doi: 10.1175/2008JTECHO552.1.
- Fabienne Gaillard, Thierry Reynaud, Virginie Thierry, Nicolas Kolodziejczyk, and Karina von Schuckmann. In Situ-Based Reanalysis of the Global Ocean Temperature and Salinity with ISAS: Variability of the Heat Content and Steric Height. *J. Clim.*, 29(4):1305–1323, February 2016. ISSN 1520-0442. doi: 10.1175/jcli-d-15-0028.1.
- Robert J. Joyce, John E. Janowiak, Phillip A. Arkin, and Pingping Xie. CMORPH: A Method that Produces Global Precipitation Estimates from Passive Microwave and Infrared Data at High Spatial and Temporal Resolution. *J. Hydrometeorol.*, 5(3):487–503, June 2004. ISSN 1525-7541. doi: 10.1175/1525-7541(2004)005(0487:camtpg)2.0.co;2.
- Nicolas Kolodziejczyk, Gilles Reverdin, and Alban Lazar. Interannual Variability of the Mixed Layer Winter Convection and Spice Injection in the Eastern Subtropical North Atlantic. *J. Phys. Oceanogr.*, 45(2):504–525, Feb 2015. ISSN 1520-0485. doi: 10.1175/jpo-d-14-0042.1.



Christian Kummerow, Y. Hong, W. S. Olson, S. Yang, R. F. Adler, J. McCollum, R. Ferraro, G. Petty, D-B. Shin, and T. T. Wilheit. The Evolution of the Goddard Profiling Algorithm (GPROF) for Rainfall Estimation from Passive Microwave Sensors. *J. Appl. Meteorol.*, 40(11): 1801–1820, 2001. doi: 10.1175/1520-0450(2001)040(1801:TEOTGP)2.0.CO;2.

Fabien Roquet, Christophe Guinet, Jean-Benoit Charrassin, Daniel P. Costa, Kit M Kovacs, Christian Lydersen, Horst Bornemann, Marthan N. Bester, Monica C. Muelbert, Mark A. Hindell, Clive R. McMahon, Rob Harcourt, Lars Boehme, and Mike A. Fedak. MEOP-CTD in-situ data collection: a Southern ocean Marine-mammals calibrated sea water temperatures and salinities observations, 2018. doi: 10.17882/45461.

Anne Treasure, Fabien Roquet, Isabelle Ansorge, Marthán Bester, Lars Boehme, Horst Bornemann, Jean-Benoît Charrassin, Damien Chevallier, Daniel Costa, Mike Fedak, Christophe Guinet, Mike Hammill, Robert Harcourt, Mark Hindell, Kit Kovacs, Mary-Anne Lea, Phil Lovell, Andrew Lowther, Christian Lydersen, Trevor McIntyre, Clive McMahon, Mônica Muelbert, Keith Nicholls, Baptiste Picard, Gilles Reverdin, Andrew Trites, Guy Williams, and P.J. Nico de Bruyn. Marine Mammals Exploring the Oceans Pole to Pole: A Review of the MEOP Consortium. Oceanography, 30(2):132–138, jun 2017. doi: 10.5670/oceanog.2017.234.