

In Situ database Analyses Report

Argo

prepared by the Pi-MEP Consortium

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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 deviation)
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^2	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
$SSS_{in situ}$	In situ SSS data considered for the match-up

SSS _{SAT}	Satellite SSS product considered for the match-up
ΔSSS	Difference between satellite and in situ SSS at colocalized point ($\Delta\text{SSS} = \text{SSS}_{\text{SAT}} - \text{SSS}_{\text{insitu}}$)
SST	Sea Surface Temperature
Std	Standard deviation
Std*	Robust Standard deviation = $\text{median}(\text{abs}(x - \text{median}(x))) / 0.67$ (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

This report presents some characteristics of the Argo in situ dataset used by the Pi-MEP to validate SMOS, SMAP and Aquarius satellite SSS products. A series of plots is proposed showing:

- Number of SSS data as a function of time and distance to coast
- Histogram of shallowest salinity and pressure (if relevant)
- Temporal mean of shallowest salinity and pressure (if relevant)
- Temporal STD of shallowest salinity
- Spatial density of shallowest salinity
- Δ SSS between local in situ data and ISAS analyses sorted as function of geophysical conditions
- Conditional analyses

The conditional analyses proposed in the document, correspond to filter/subdivide the different in situ datasets 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 $> 5^{\circ}\text{C}$ 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 $< 20\text{m}$.
- **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 conditions, the temporal mean (gridded over spatial boxes of size $1^{\circ}\times 1^{\circ}$) and the histogram of the difference Δ SSS between ISAS and in situ SSS value are presented. The use of ISAS (monthly SSS in situ analysed field) 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.

1.1 In situ dataset

1.1.1 Argo

Argo is a global array of 3,000 free-drifting profiling floats that measures the temperature and salinity of the upper 2000 m of the ocean. This allows continuous monitoring of the temperature and salinity of the upper ocean, with all data being relayed and made publicly available within hours after collection. The array provides around 100,000 temperature/salinity profiles per year distributed over the global oceans at an average of 3-degree spacing. Only Argo salinity and

temperature float data with quality index set to 1 or 2 and data mode set to real time (RT), real time adjusted (RTA) and delayed mode (DM) are considered in the Pi-MEP. Argo floats which may have problems with one or more sensors appearing in the [grey list](#) maintained at the Coriolis/GDACs are discarded. Furthermore, Pi-MEP provides an additional [list](#) of ~ 1000 "suspicious" argo salinity profiles that are also removed before analysis. The upper ocean salinity and temperature values recorded between 0m and 10m depth are considered as Argo sea surface salinities (SSS) and sea surface temperatures (SST). These data were collected and made freely available by the international Argo project and the national programs that contribute to it ([Argo \(2000\)](#)).

1.2 Auxiliary geophysical datasets

Additional EO datasets are used to characterize the geophysical conditions at the in situ 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 spatio-temporal 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^{-1} ; 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 in situ SSS value. 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, annual std climatological field from the World Ocean Atlas ([WOA13](#)) at the in situ location are also used to have an a priori information of the local SSS variability.

1.2.1 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 x 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: ftp://ftp.cpc.ncep.noaa.gov/precip/CMORPH_V1.0/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).

1.2.2 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⁻¹ and 20°.

1.2.3 ISAS

The In Situ Analysis System (ISAS), as described in [Gaillard et al. \(2016\)](#) is a data based re-analysis 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°N–70°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.

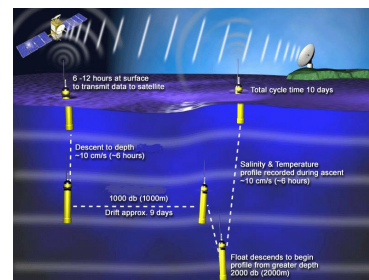
1.2.4 World Ocean Atlas Climatology

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 In Situ Database Analyses

2.1 Introduction

Argo is a global array of 3,000 free-drifting profiling floats that measures the temperature and salinity of the upper 2000 m of the ocean. This allows continuous monitoring of the temperature and salinity of the upper ocean, with all data being relayed and made publicly available within hours after collection. The array provides around 100,000 temperature/salinity profiles per year distributed over the global oceans at an average of 3-degree spacing. Only Argo salinity and temperature float data with quality index set to 1 or 2 and data mode set to real time (RT), real time adjusted (RTA) and delayed mode (DM) are considered in the Pi-MEP. Argo floats which may have problems with one or more sensors appearing in the **grey list** maintained at the Coriolis/GDACs are discarded. Furthermore, Pi-MEP provides an additional **list** of ~ 1000 "suspicious" argo salinity profiles that are also removed before analysis. The upper ocean salinity and temperature values recorded between 0m and 10m depth are considered as Argo sea surface salinities (SSS) and sea surface temperatures (SST). These data



were collected and made freely available by the international Argo project and the national programs that contribute to it (Argo (2000)).

2.2 Number of SSS data as a function of time and distance to coast

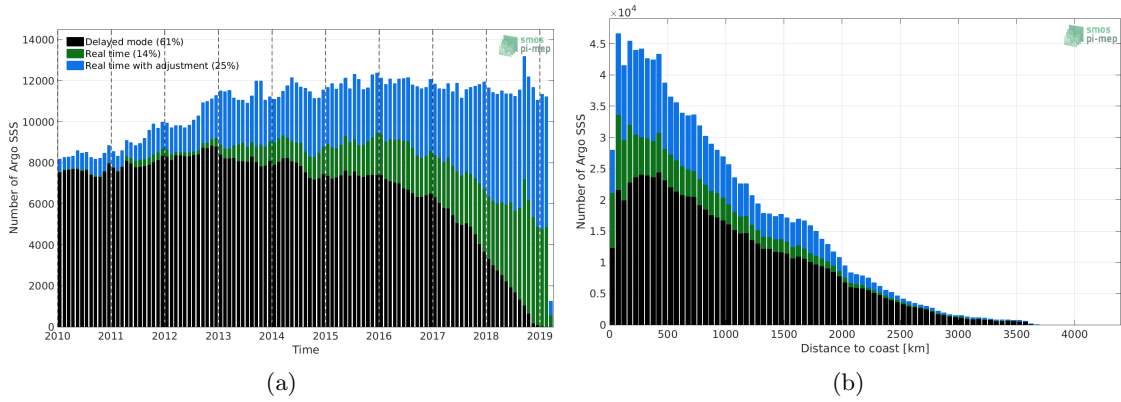


Figure 1: Number of SSS from Argo as a function of time (a) and distance to coast (b).

2.3 Histogram of shallowest salinity and pressure

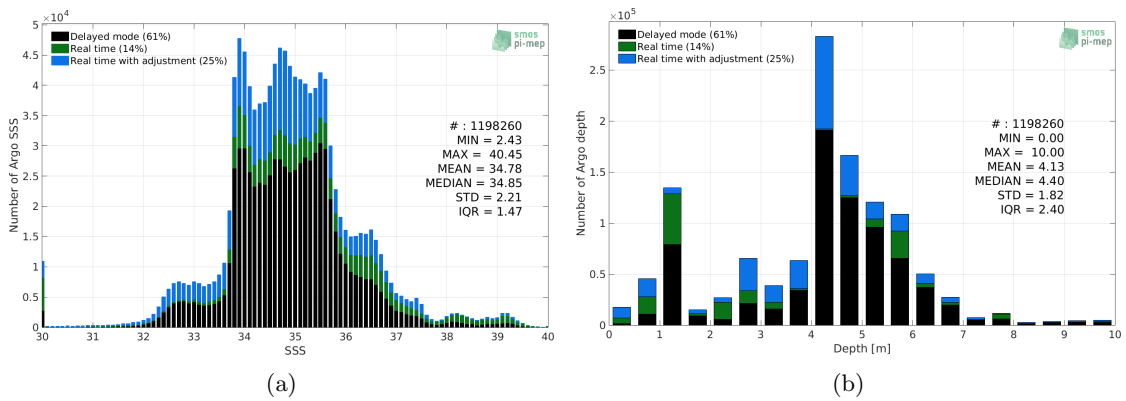


Figure 2: Distribution of SSS (a) and pressure (b) from Argo floats per bins of 0.1 and 0.5, respectively.

2.4 Temporal mean of shallowest salinity and pressure

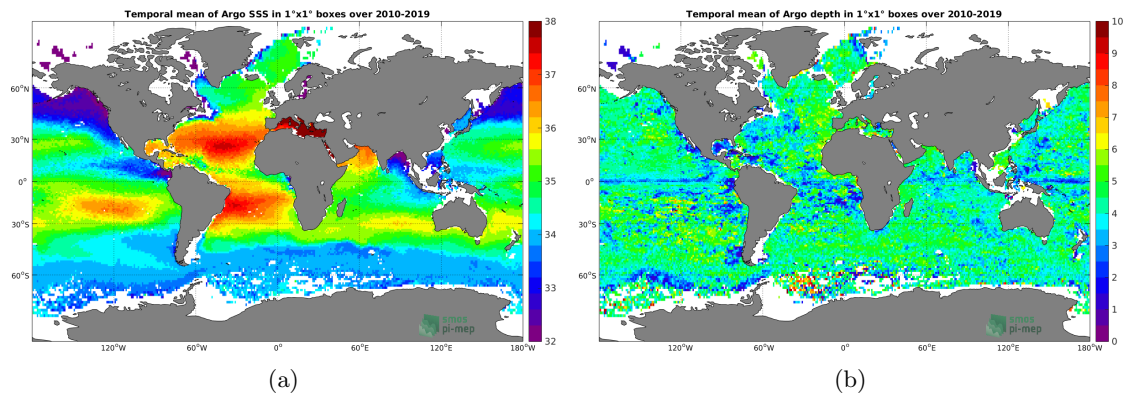


Figure 3: Temporal mean SSS (a) and pressure (b) from Argo floats in 1°x1° boxes.

2.5 Temporal STD of SSS

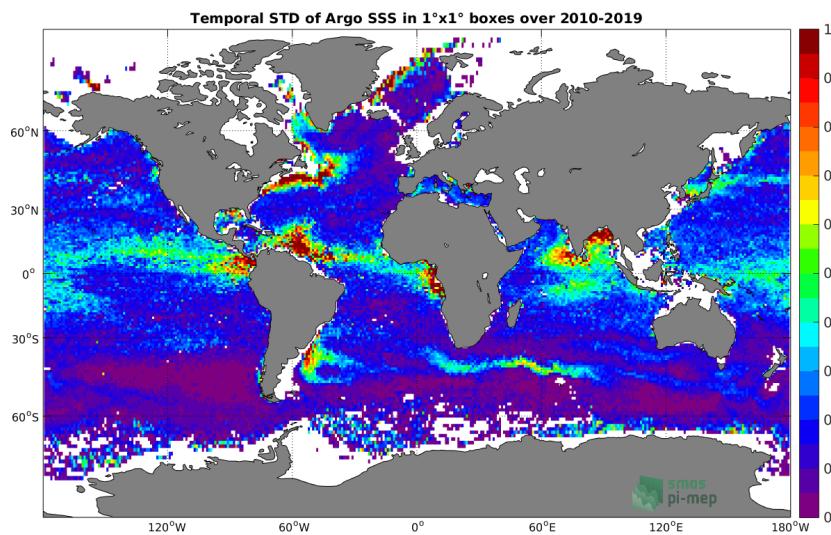
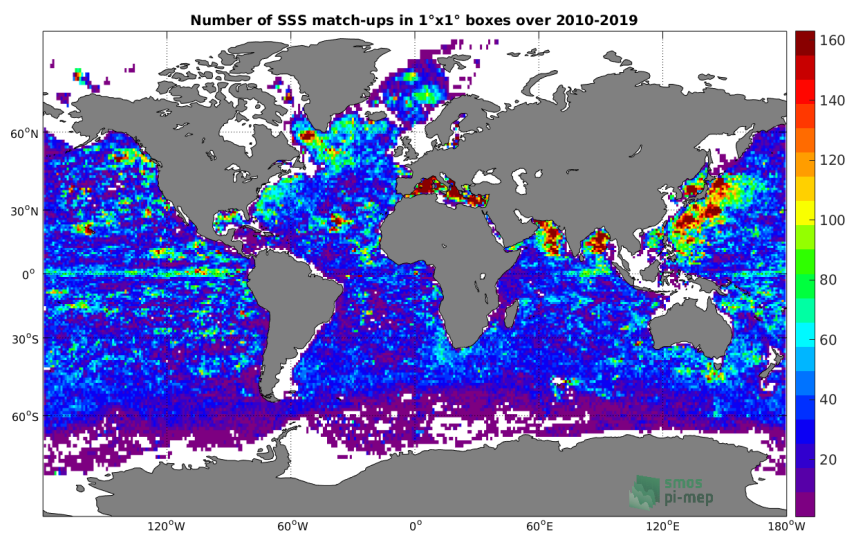


Figure 4: Temporal STD of SSS from Argo in 1°x1° boxes.

2.6 Spatial density of SSS



2.7 Δ SSS sorted as geophysical conditions

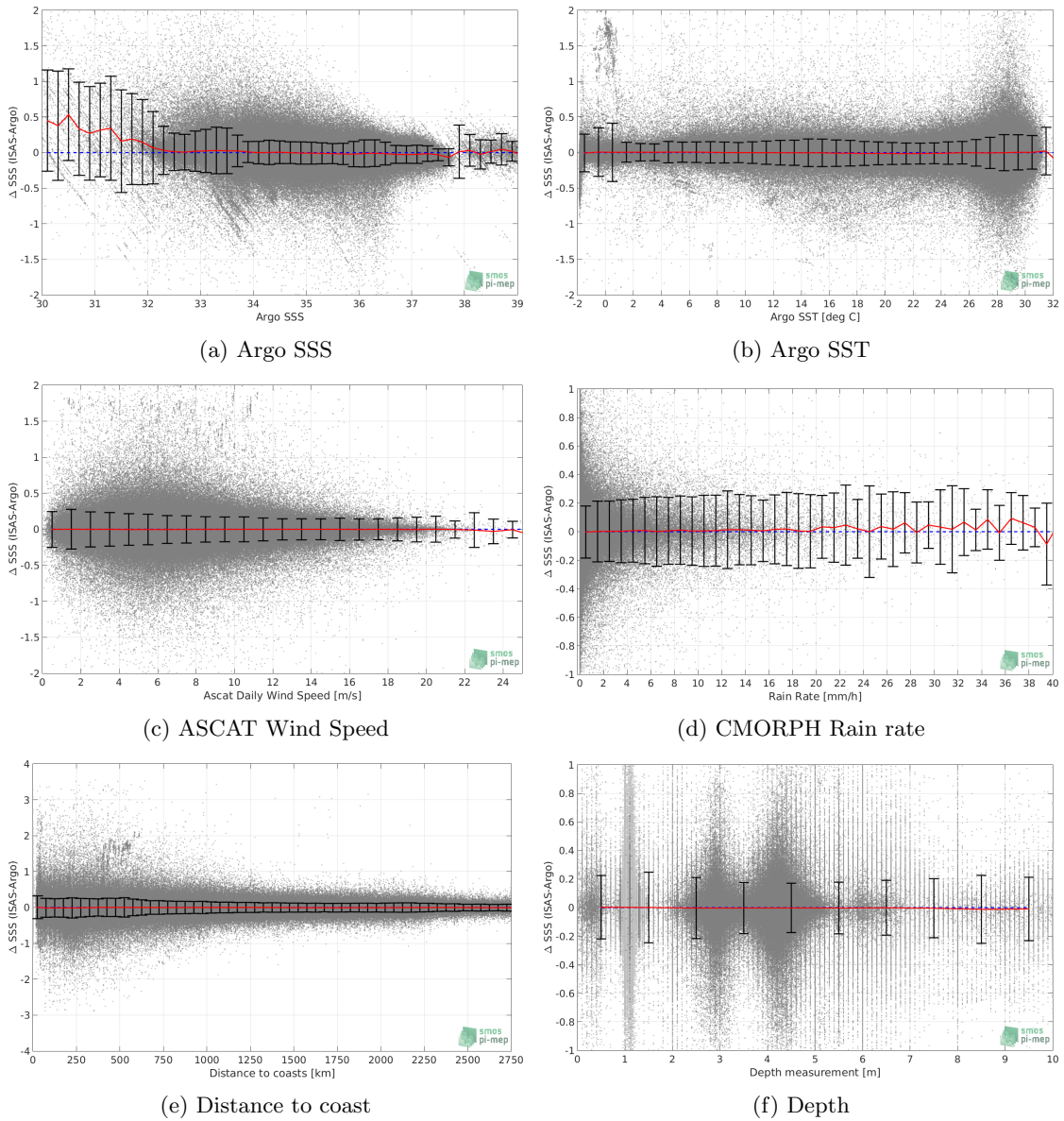


Figure 6: Δ SSS (ISAS - Argo) sorted as geophysical conditions: Argo SSS a), Argo SST b), ASCAT Wind speed c), CMORPH rain rate d), distance to coast (e) and depth measurements (f).

2.8 Conditional analyses

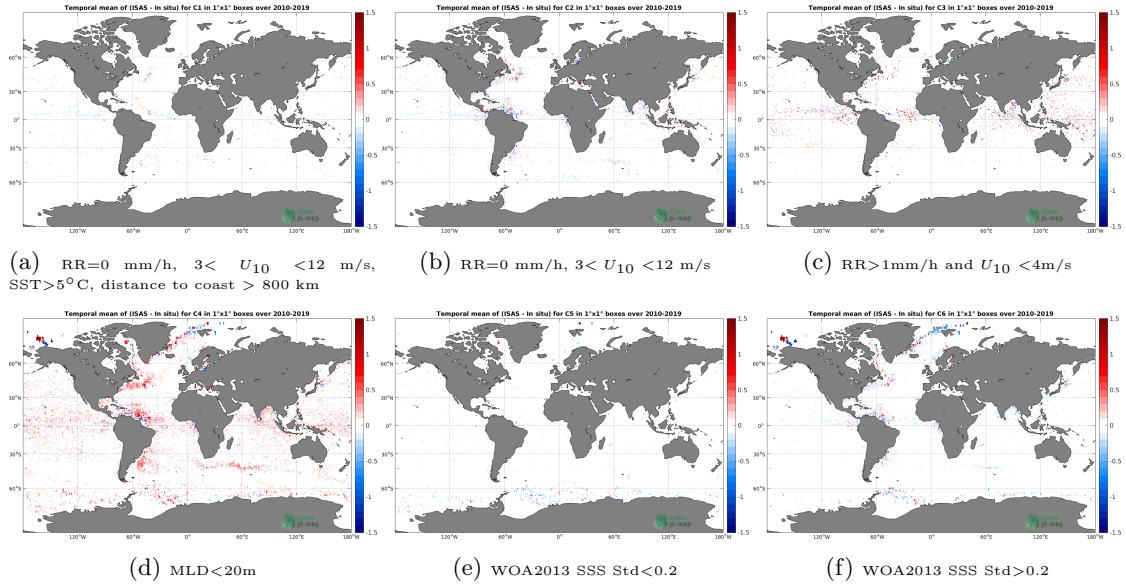


Figure 7: Temporal mean of Δ SSS (ISAS - Argo) for 6 different subdatasets corresponding to C1 (a),..., C6 (f).

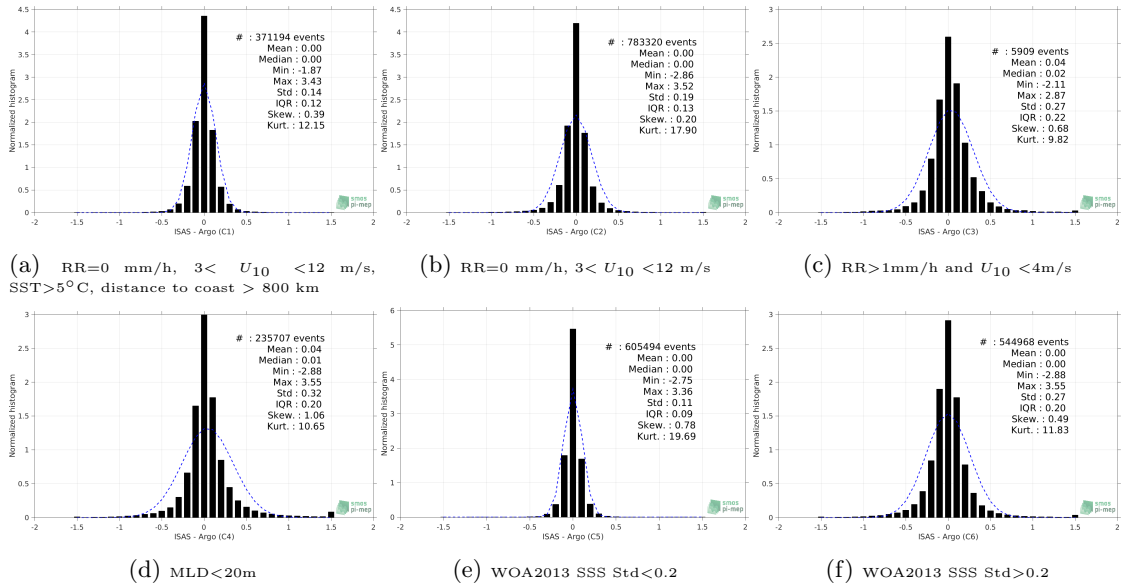


Figure 8: Normalized histogram of Δ SSS (ISAS - Argo) for 6 different subdatasets corresponding to C1 (a),..., C6 (f).

2.9 Summary

Table 1 shows the mean, median, standard deviation (Std), root mean square (RMS), interquartile range (IQR), correlation coefficient (r^2) and robust standard deviation (Std*) of the match-up differences Δ SSS (ISAS - Argo) 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 $U_{10} < 4$ m/s
- C4: only pairs where MLD<20m
- C5: only pairs where WOA2013 SSS Std<0.2
- C6: only pairs where 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°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 Δ SSS (ISAS - Argo)

Condition	#	Median	Mean	Std	RMS	IQR	r^2	Std*
all	1173092	0.00	0.00	0.20	0.20	0.13	0.99	0.09
C1	371194	0.00	0.00	0.14	0.14	0.12	0.98	0.09
C2	783320	0.00	0.00	0.19	0.19	0.13	0.99	0.10
C3	5909	0.02	0.04	0.27	0.27	0.22	0.98	0.16
C4	235707	0.01	0.04	0.32	0.32	0.20	0.99	0.15
C5	605494	0.00	0.00	0.11	0.11	0.09	0.99	0.07
C6	544968	0.00	0.00	0.27	0.27	0.20	0.99	0.15
C7a	112860	-0.01	0.00	0.28	0.28	0.18	1.00	0.13
C7b	496389	0.00	0.00	0.24	0.24	0.13	0.97	0.10
C7c	563843	0.00	0.00	0.14	0.14	0.11	0.98	0.09
C8a	106236	0.00	0.03	0.24	0.24	0.07	0.99	0.05
C8b	247933	0.00	0.00	0.17	0.17	0.09	1.00	0.07
C8c	818439	-0.01	0.00	0.21	0.21	0.15	0.99	0.11
C9a	68933	0.02	0.11	0.45	0.47	0.21	0.99	0.14
C9b	1046224	0.00	-0.01	0.17	0.17	0.12	0.96	0.09
C9c	57935	-0.02	-0.02	0.15	0.15	0.14	0.96	0.10

Table 1 numerical values can be downloaded as a csv file [here](#).

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