scirocco

scatterometer instrument competence centre

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1. Introduction

This document provides a detailed summary on the verification and validation strategy applied for soil moisture data records derived from ERS-2 ESCAT [RD-4, RD-5]. The objective of verification is to prove the successful accomplishment of soil moisture outputs by means of completeness and the integrity of model parameters estimated and utilized in the retrieval. The main purpose of validation is to evaluate the accuracy of the products and to assess the compliance against predefined requirements. Apart from that, validation is carried out to investigate the physical reliability of the products as well as the characterization of random and systematic errors generated by differences in sampling, retrieval algorithms, observation time, spatial resolution, etc. [Zeng et al., 2015]. One of the most commonly used validation strategy is the comparison between soil moisture products derived from satellite measurements, in situ instruments and land surface models. Despite the fact that the validation can be performed either on a global or on a local scale, preprocessing steps are required to execute an objective validation. In order to compare the different data sets, performance metrics are computed for benchmarking. The results of the validation are statistical parameters characterizing discrepancies or similarities of the involved data sets. The accuracy of the validated products is assessed according to predefined requirements expressed as thresholds for the statistical metrics.

1.1. Scope

This document gives an overview of verification and validation procedures carried out in order to quantify the quality of ESCAT soil moisture products with respect to others. In the framework of the SCIRoCCo project, several soil moisture products with different spatial resolutions, formats (e.g. time series, swath orbit geometry) are generated and distributed to users. A list of available soil moisture products, as well as other SCIRoCCo products (such as wind vector fields) can be looked up on the SCIRoCCo website [http://scirocco.sp.serco.eu/]. The following Table 1.1 gives an overview of the instances of soil moisture products related to this PVR.

ID	Product Name
ERS2-ASPS-N-SSM-Ts	ERS-2 ESCAT nominal resolution SSM time series (12.5 km sampling)
ERS2-ASPS-H-SSM-Ts	ERS-2 ESCAT high resolution SSM time series (12.5 km sampling)
ERS2-ASPS-N-SSM-Or	ERS-2 ESCAT nominal resolution SSM orbits (12.5 km sampling)
ERS2-ASPS-H-SSM-Or	ERS-2 ESCAT high resolution SSM orbits (12.5 km sampling)

Table 1.1: List of soil moisture products related to this PVR.

Targeted audience

This document mainly targets:

1. Remote sensing experts interested in soil moisture from active microwave data sets.
2. Users of remotely sensed soil moisture data sets.

1.2. Applicable and Reference Documents

Applicable Documents

The following documents are related to this document:

ID	Reference	Document Title	Issue	Date
AD-1				
AD-2				
AD-3				

Reference Documents

The following documents provide further reference information:

ID	Reference	Document Title	Issue	Date
RD-1	SCI-TNO-16-0044-v02	Algorithm Theoretical Baseline Document (ATBD)	v0.2	-
RD-3	SCI-TNO-16-0045-v02	WARP 5 grid	v0.2	-
RD-4	SCI-MAN-16-0047-v02	Product User Manual - TS Product	v0.2	-
RD-5	SCI-MAN-16-0048-v02	Product User Manual - Orbit Product	v0.2	-

2. Product Verification

A summary of the performed product verification activities is outlined in this section of the document. Product verification aims to prove the completeness and the compliance of the derived ESCAT soil moisture products and its model parameters. Furthermore, performed integration test of the WARP orbit processor are discussed with reference to the standalone WARP processor. The objective of these tests was to verify that both processor instances provide the same output results.

2.1. Model Parameters

Model parameters have been computed and used separately in the generation of the ESCAT nominal and high resolution soil moisture products. A comprehensive statistical model parameter verification was performed in order to guarantee the spatial completeness of the individual estimated model parameters and to investigate the reliability of the parameters with respect to soil moisture retrieval. The verification consists of basic statistical analyses of each model parameter complemented with a frequency distribution plot. In addition, a map plot of the individual parameters was created to inspect the spatial distribution and completeness. A summary of this verification exercise is given in the following with reference to the verification results presented in the Annex section A.

Computed statistics (see Table 2.1) highlight that all model parameters are in the expected ranges assuring high-quality soil moisture retrievals based on nominal and high resolution ESCAT data. Moreover, the created global maps (see Annex A) confirm the spatial completeness of each individual parameter. Missing or invalid model parameters were mainly detected for the Azimuth Coefficients over regions with an insufficient amount of data, caused by the shared operation time of ESCAT with the on-board SAR instrument and limitations in the tape storage system. The impact of these missing model parameter values, especially over Europe and central Asia, is anticipated to be negligible on the final soil moisture retrieval. Verification of the Surface State Flag (SSF), included in both ERS ESCAT product formats, is not included in this report. Though, a comprehensive overview of verification and validation activities of the SSF estimated from ERS ESCAT with in the SCIRoCCo project can be found in Pfeil [2016].

In conclusion, the verification exercise confirms that the investigated model parameters for ERS ESCAT nominal and high resolution soil moisture retrievals are in an excellent shape, with values in the expected range and spatially complete.

2.2. Integration Tests

Integration tests of the WARP orbit processor were performed with reference to the outputs of the WARP processor. The objective of these integration tests was to prove that both processors generate the same soil moisture output values. Both processor instances follow the same algorithms and underlying assumptions, as outlined in the Algorithm Theoretical Baseline Document [RD-1], but differ with respect to the domain of application to estimate soil moisture values. WARP interpolates the Level 1 orbit data to a fixed Earth grid (WARP 5 grid [RD-3]), where model parameters are computed, stored and directly applicable, while, conversely, WARP orbit interpolates the pre-computed parameters to the orbit grid, in order to obtain soil moisture estimates in orbit geometry. Three test scenarios have been defined to confirm the integration of WARP orbit with respect to WARP. In the following, the three scenarios are outlined in detailed with the obtained test results. The integration tests are included in the WARP orbit processor package implemented in Python.

MP	Mean	Median	StdDev	MAD	Min	Max	nValid	nNAN	nOutliers
ESCAT nominal resolution parameter									
Azim. Correction Fore ASC [dB]	-0.096	-0.102	0.195	0.084	-2.368	2.072	806714	29638	33112
Azim. Correction Mid ASC [dB]	-0.117	-0.142	0.237	0.085	-2.618	2.322	805288	29638	34538
Azim. Correction Aft ASC [dB]	-0.006	0.007	0.228	0.079	-2.970	2.668	806854	29638	32972
Azim. Correction Fore DESC [dB]	0.134	0.141	0.300	0.096	-3.893	3.778	798141	29638	41685
Azim. Correction Mid DESC [dB]	0.074	0.062	0.271	0.098	-3.187	3.185	796376	29638	43450
Azim. Correction Aft DESC [dB]	0.215	0.228	0.330	0.104	-4.204	4.214	799128	29638	40698
ESD [dB]	0.186	0.164	0.078	0.023	0.094	0.944	831455	9	8371
Slope [dB/deg]	-0.120	-0.109	0.0037	0.0348	-0.7685	0.4710	307284896	66612	158039
Curvature [dB/deg^2]	0.00230	0.00188	0.00001	0.00208	-0.04069	0.04814	307302432	66612	140507
Dry Reference [dB]	-12.630	-12.345	9.865	1.892	-49.439	23.134	307305600	67710	138438
Wet Reference [dB]	-9.888	-9.067	7.794	1.153	-28.263	8.040	307308608	67710	135420
Wet Correction [dB]	1.324	0.000	2.324	0.000	0.000	18.263	839826	0	0
ESCAT high resolution parameter									
Azim. Correction Fore ASC [dB]	-0.090	-0.099	0.236	0.094	-2.923	2.604	806985	29662	32841
Azim. Correction Mid ASC [dB]	-0.105	-0.134	0.271	0.093	-2.933	2.650	805808	29662	34018
Azim. Correction Aft ASC [dB]	-0.039	-0.022	0.268	0.090	-3.665	3.210	807206	29662	32620
Azim. Correction Fore DESC [dB]	0.147	0.156	0.351	0.109	-4.569	4.389	799582	29662	40244
Azim. Correction Mid DESC [dB]	0.094	0.079	0.306	0.108	-3.605	3.614	797870	29662	41956
Azim. Correction Aft DESC [dB]	0.194	0.212	0.382	0.118	-5.023	4.873	800444	29662	39382
ESD [dB]	0.237	0.215	0.074	0.021	0.153	0.968	829429	28	10397
Slope [dB/deg]	-0.1195	-0.1077	0.0041	0.0353	-0.8026	0.5044	306014016	1301862	2664153
Curvature [dB/deg^2]	0.00231	0.00192	0.00002	0.00210	-0.04050	0.04741	306018912	1301862	2659271
Dry Reference [dB]	-12.662	-12.343	11.017	2.003	-51.853	25.134	306050560	1304790	2630531
Wet Reference [dB]	-9.908	-9.042	8.522	1.168	-30.122	-0.093	306071520	1304790	2609580
Wet Correction [dB]	1.347	0.000	2.425	0.000	0.000	20.122	839826	0	0

Table 2.1: Verification statistics of the computed model parameters.

Test Case 1: NN-search

ERS ESCAT Level 1 orbit products are the input data set of the WARP orbit processor to compute soil moisture estimates in orbit grid geometry. Therefore, model parameters have to be interpolated into the orbit grid by utilizing a nearest-neighbor search and a Hamming window filter. The nearest-neighbor search functionality was tested by simulating an orbit grid with known Latitude/Longitude coordinates originating from grid points of the WARP 5 grid [RD-3] where model parameters are stored. The expected outcome of this test is that grid points found by the NN-search method are equal to the input coordinates of the simulated orbit.

Test PASS.

Test Case 2: Compute Soil Moisture

The computation of the final soil moisture values was tested by injecting known input data to the WARP orbit processor. The input data were extracted from the data sets (Level 1 backscatter time series, model parameters) derived with WARP and passed to the WARP orbit soil moisture compute function. The expected result of this test is that WARP orbit produces the same soil moisture values as WARP with an accuracy of at least 2 decimals.

Test PASS.

Test Case 3: Compute Surface State Flag

The computation of the Surface State Flag (SSF) was tested by injecting known input data to the WARP orbit processor. The input data were extracted from the data sets (Level 1 backscatter time series, model parameters) derived with WARP and passed to the WARP orbit SSF compute function. The expected result of this test is that WARP orbit produce the same Surface State Flag values as WARP.

Test PASS.

In conclusion, the WARP orbit processor and the WARP processor produce equivalent soil moisture retrievals by considering the same input data, hence they are compliant.

3. Soil Moisture Validation

3.1. Reference data sets

The validation of space-based soil moisture products is typically based on the comparison to other space-based soil moisture data sets, in situ data observations, land surface models or other parameters related to surface soil moisture (e.g. precipitation). The following data sets are used, depending on spatial and temporal availability, for validation purposes.

ISMN

Worldwide in situ soil moisture observations are gathered, harmonized and made available to users through the International Soil Moisture Network (ISMN)[1]. This data hosting facility provides standardized ground based soil moisture measurements in volumetric units (m^3m^{-3}) together with other significant meteorological data [Dorigo et al., 2011]. Even though the data providers are spread globally, most of the networks are concentrated in North America and Eurasia. However, this collection of in situ observations is representative for different climate regions, soil types and textures [Su et al., 2015], which makes it suitable not only for local but also for global validations.

Passive ESA CCI Soil Moisture

The ESA CCI Soil Moisture project[2] is part of the ESA Programme on Global Monitoring of Essential Climate Variables (ECV), better known as the Climate Change Initiative (CCI). The CCI Programme aims to contribute to data bases collecting ECVs required by GCOS (Global Climate Observing System) and other international parties. The objective of the ESA CCI Soil Moisture project is to produce the most complete and most consistent global soil moisture data record based on active and passive microwave sensors. The project focuses on C-band scatterometers (ERS-1/2 scatterometer, Metop ASCAT) and multi-frequency radiometers (SMMR, SSM/I, TMI, AMSR-E, Windsat, AMSR2) as these sensors are characterized by their high suitability for soil moisture retrieval and their long technological heritage [Wagner et al., 2012].

The passive ESA CCI Soil Moisture product is derived by merging soil moisture retrievals of various passive microwave instruments. Level 2 soil moisture retrieval of individual missions is performed by utilizing the Land Parameter Retrieval Model (LPRM) developed by the VU University Amsterdam in collaboration with NASA. [Chung et al., 2015; Owe et al., 2008]. Soil moisture retrievals of the passive microwave mission from Nimbus 7 SMMR, DMSP SSM/I, TRMM TMI, Aqua AMSR-E, Coriolis WindSat, and GCOM-W1 AMSR2 are merged into a single long-term passive soil moisture time series sampled at a regular 0.25 degree grid expressed in volumetric units (m^3m^{-3}) spanning a period from 1978–2014.

ERA-Interim

The ERA-Interim re-analysis data set produced by ECMWF[3] (European Centre for Medium-Range Weather Forecasts) incorporates global atmospheric, ocean and land-surface analysis based on the Integrated Forecast System (IFS) model release Cy31r2 from 2006. The data set covers the period from 1979 to present

[1] http://ismn.geo.tuwien.ac.at
[2] http://www.esa-soilmoisture-cci.org
[3] http://www.ecmwf.int

with a T255 horizontal resolution (~79 km spacing on a reduced Gaussian grid) [Dee et al., 2011]. The re-analysis data set is updated on a regular basis and can be downloaded from the ECMWF dataserver[4].

Daily soil moisture estimates are provided in volumetric units (m^3m^{-3}) in four depth layers at 00:00, 06:00, 12:00 and 18:00 UTC. Furthermore, ERA-Interim contains soil temperature and snow depth data used for masking of invalid soil moisture measurements during the validation process. Volumetric soil moisture estimates of the first soil layer (0.00–0.07 m) are used in this validation study.

GLDAS NOAH

The NOAH model provided by the Global Land Data Assimilation System (GLDAS) contains atmospheric and land surface parameters stored on a regular global grid (spacing 0.25°). The GLDAS NOAH data set provides soil moisture estimates at a 3-hourly temporal resolution (daily at 00:00, 03:00, 06:00, 09:00, 12:00, 15:00, 18:00 and 21:00 UTC) [Rodell et al., 2004]. The data is publicly available at GES DISC[5] (Goddard Earth Sciences Data and Information Services Center). Soil moisture estimates are evaluated in kg m^{-2} and need to be converted into volumetric units for this validation study. Soil characteristics such as temperature and moisture are provided in four layers (thickness: 0–10 m, 10–40 cm, 40–100 cm and 100–200 cm). In this validation study, model soil moisture of the first layer are converted into volumetric units by:

$$SM\left[m^3m^{-3}\right] = SM\left[kg\ m^{-2}\right] * 0.001 * 1/d \qquad \text{Eq. 3-1}$$

where d denotes the thickness of the soil layer in meter and the factor 0.001 is due to the assumption that 1 kg of water represents 1000 cm^3 which is 0.001 m^3.

3.2. Preprocessing

Masking

As described in Section 3.3, the committed product area is limited to specific climate, vegetation and land cover regimes, excluding (i.e., spatially masking) areas for which it is as yet not possible to compute meaningful soil moisture estimates. For the remaining regions, temporal masking has to be applied for certain time periods during which the soil moisture cannot be determined (in particular due to snow and frozen soil conditions). To this end, auxiliary information such as the surface state flag (SSF), included in the ERS ESCAT soil moisture products, and also the frozen land/snow cover probabilities available as static layers can be used. If available, reference data sets with good quality can also contribute to the masking procedure by providing valuable information such as soil temperature, snow depth etc.

Spatial matching

The spatial resolution and distribution of the data sets needs to be harmonised – i.e., they have to be mapped to a common spatial reference grid – before a validation can take place. There exist numerous methods which can be employed for this task: e.g. Optimal Interpolation, Inverse Distance Weighting, Kriging, Kernel estimation and so on. The most commonly used method is the nearest-neighbor (NN) interpolation, which is simple and computationally not too expensive.

[4] http://apps.ecmwf.int/datasets/data/interim-full-daily
[5] http://disc.sci.gsfc.nasa.gov/datacollection/GLDAS_NOAH025SUBP_3H_V001.shtml

Temporal matching

The temporal resolution and/or representation of the data sets might be different and needs to be collocated on a reference timeline. Several approaches, e.g. window functions, nearest-neighbor (NN), linear, polynomial interpolation etc., are possible, but commonly the nearest-neighbor method is used.

Scaling

Validation means the comparison to other satellite-based, model or in situ soil moisture products expressed in various measurement units. If a direct conversion between different measurement units is not possible, because conversion parameters are unknown, scaling techniques can be used to transform the data sets into the same data space [Albergel et al., 2012]. Several methods are commonly used, e.g. Min/Max, CDF matching, Mean/Std, linear regression.

3.3. Validation Benchmarks

With reference to the Algorithm Theoretical Baseline Document (ATBD) [RD-1], soil moisture retrievals of C-band scatterometers are limited to certain areas because of know limitations of the retrieval model. Accordingly, the validation activity focuses on a committed area, see Figure 3.1, representing a restricted geographical region with confidence in the successful retrieval of surface soil moisture information from ERS ESCAT. The committed area is restricted to following conditions:

- low to moderate vegetation regimes
- unfrozen and snow free soil
- low to moderate topographic variations
- no wetland and coastal areas

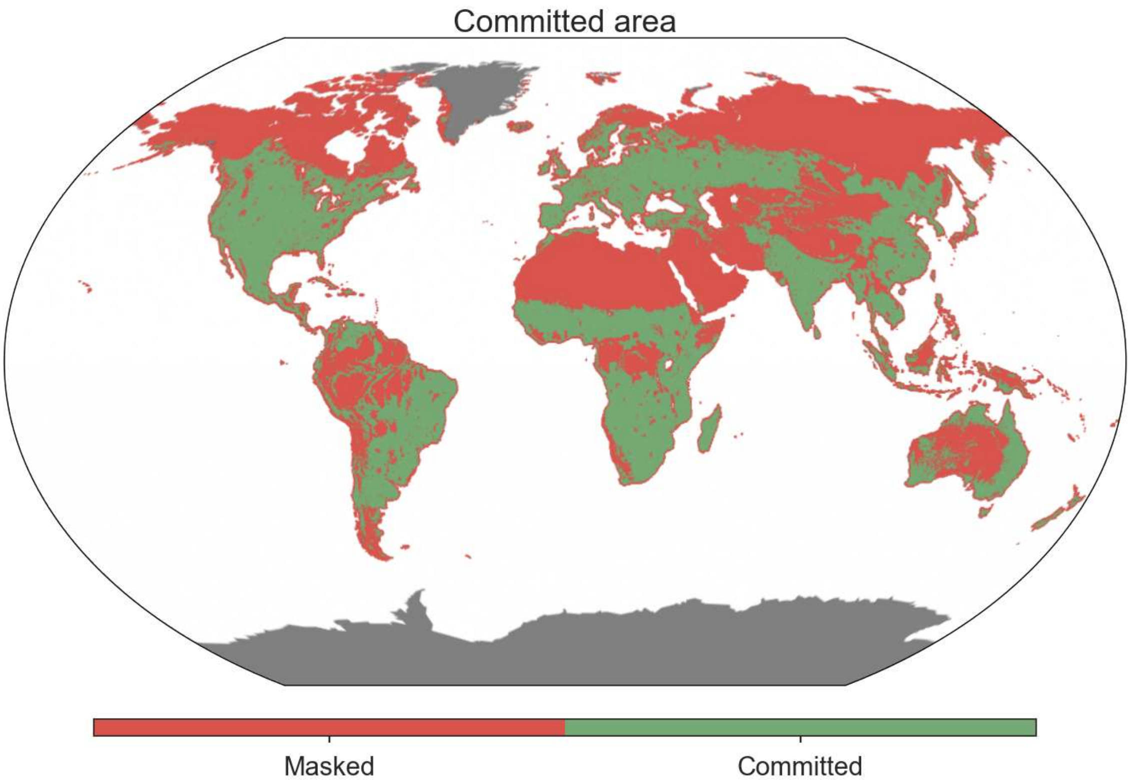

Figure 3.1: Committed area for ERS ESCAT soil moisture data records.

The validation is performed based on standard quality benchmarks anticipated to sufficiently reflect the error structure of individual soil moisture products. A standard quality benchmark for the soil moisture data records is the signal-to-noise ratio (SNR), which is one way to characterize errors in soil moisture products computed by Triple Collocation Analysis (TCA). The signal-to-noise ratio is supported by the Pearson correlation coefficient (R), which is commonly used in validation studies of remotely sensed data. They are the main criteria by which to the quality of the ERS ESCAT soil moisture products are evaluated; accuracy thresholds are shown in Table 3.1. SNR and R are complemented by additional statistics, such as bias, ubRMSD etc.

Benchmark	Threshold	Target	Optimal
SNR	0 dB	3 dB	6 dB
R	0.5	0.65	0.8

Table 3.1: Standard quality benchmark thresholds for validation.

Triple collocation analysis (TCA)

The triple collocation analysis (TCA) is a statistical tool used for error characterization, first introduced by Stoffelen [1998]. It simultaneously estimates the error structure of three spatially and temporally collocated data sets Θ_1, Θ_2 and Θ_3, which are linearly related to the hypothetical (unknown) truth Θ with uncorrelated errors [Scipal et al., 2010]:

$$i = \alpha_i + \beta_i \cdot \Theta + \epsilon_i \qquad \textbf{Eq. 3-2}$$

α_i and β_i are systematic additive and multiplicative biases of data set i with respect to the true state Θ, and ϵ_i represents zero-mean random noise. The underlying assumptions of the error model are: (i) linearity between the true signal and the observations, (ii) signal and error stationarity, (iii) independence between the errors and the signal, and (iv) independence between the errors of Θ_1, Θ_2 and Θ_3 (zero error cross-correlation). The mean squared random error of all three data sets (i.e. MSE $= \langle \epsilon_i^2 \rangle$, with $\langle . \rangle$ denoting the temporal average) is estimated individually by TCA. There are two common ways to solve for MSE_i, either by cross-multiplying differences between the three a-priori scaled data sets (difference notation) or using a combination of covariances (covariance notation). Both approaches are identical from a mathematical point of view [Gruber et al., 2016].

Difference notation

Two data sets have to be rescaled against an arbitrarily chosen reference data set and the error variances can be estimated by averaging cross-multiplied differences between the three data sets.

$$\begin{aligned} \sigma_{\epsilon_X}^2 &= \left\langle \left(X - Y^X\right)\left(X - Z^X\right) \right\rangle \\ \sigma_{\epsilon_Y}^2 &= \left\langle \left(Y^X - X\right)\left(Y^X - Z^X\right) \right\rangle \\ \sigma_{\epsilon_Z}^2 &= \left\langle \left(Z^X - X\right)\left(Z^X - Y^X\right) \right\rangle \end{aligned} \qquad \textbf{Eq. 3-3}$$

In this case the superscript X denotes the scaling reference, representing the data space of the estimated error variances $(\sigma_{\epsilon_X}^2, \sigma_{\epsilon_Y}^2, \sigma_{\epsilon_Z}^2)$. In order to avoid errors introduced by means of rescaling of the data, the scaling parameters have to be inferred using a consistent estimator, which is possible by using TCA. The rescaling coefficients β_X^* and β_Z^* can be estimated using:

$$\begin{aligned} \beta_Y^* &= \frac{\beta_X}{\beta_Y} = \frac{\left\langle \left(X - \bar{X}\right)\left(Z - \bar{Z}\right) \right\rangle}{\left\langle \left(Y - \bar{Y}\right)\left(Z - \bar{Z}\right) \right\rangle} = \frac{\sigma_{XZ}}{\sigma_{YZ}} \\ \beta_Z^* &= \frac{\beta_X}{\beta_Z} = \frac{\left\langle \left(X - \bar{X}\right)\left(Y - \bar{Y}\right) \right\rangle}{\left\langle \left(Z - \bar{Z}\right)\left(Y - \bar{Y}\right) \right\rangle} = \frac{\sigma_{XY}}{\sigma_{ZY}} \end{aligned} \qquad \textbf{Eq. 3-4}$$

and applied to the data sets with:

$$\begin{aligned} Y^X &= \beta_Y^* \left(Y - \bar{Y}\right) + \bar{X} \\ Z^X &= \beta_Z^* \left(Z - \bar{Z}\right) + \bar{X} \end{aligned} \qquad \textbf{Eq. 3-5}$$

The same scaling coefficients can be used to convert the error variances (**Eq. 3-3**) back into their original data space.

Covariance notation

The variances σ_i^2 and covariances σ_{ij} of data sets can be used to compute the (unscaled) error variances (σ_ϵ^2). The relationship between the true soil moisture variance σ_Θ^2 and the measured signal can be written as:

$$\begin{aligned} \sigma_i^2 &= \beta_i^2 \sigma_\Theta^2 + \sigma_\epsilon^2 \\ \sigma_{ij} &= \beta_i \beta_j \sigma_\Theta^2 \end{aligned} \qquad \textbf{Eq. 3-6}$$

with $i, j \in [X, Y, Z]$ and $i \neq j$. The term $\beta_i^2 \sigma_\Theta^2$ can be understood as the sensitivity of data set i to changes in the soil moisture signal. The individual unscaled error variances can be computed using the following formulation:

$$\begin{aligned} \sigma_{\epsilon_X}^2 &= \sigma_X^2 - \frac{\sigma_{XY}\sigma_{XZ}}{\sigma_{YZ}} \\ \sigma_{\epsilon_Y}^2 &= \sigma_Y^2 - \frac{\sigma_{YX}\sigma_{YZ}}{\sigma_{XZ}} \\ \sigma_{\epsilon_Z}^2 &= \sigma_Z^2 - \frac{\sigma_{ZX}\sigma_{ZY}}{\sigma_{XY}} \end{aligned} \quad \textbf{Eq. 3-7}$$

The soil moisture sensitivity estimates can be obtained through:

$$\begin{aligned} \beta_X^2 \sigma_\Theta^2 &= \frac{\sigma_{XY}\sigma_{XZ}}{\sigma_{YZ}} \\ \beta_Y^2 \sigma_\Theta^2 &= \frac{\sigma_{YX}\sigma_{YZ}}{\sigma_{XZ}} \\ \beta_Z^2 \sigma_\Theta^2 &= \frac{\sigma_{ZX}\sigma_{ZY}}{\sigma_{XY}} \end{aligned} \quad \textbf{Eq. 3-8}$$

Logarithmic signal-to-noise ratio (SNR)

The signal-to-noise ratio (SNR) can be used to represent the error variance in relation to the signal variance. The major advantage of using the SNR is that it overcomes the dependency of the chosen scaling reference and allows to sustain the possibility to compare error variances of various data sets. In the logarithmic domain a value of zero means that the signal variance is equal to the error variance, and every ± 3 dB the signal is doubling/halving compared to the error. The SNR can be computed using the following formulation:

$$\mathrm{SNR}_i\,[\mathrm{dB}] = 10 \log \left(\frac{\beta_i^2 \sigma_\Theta^2}{\sigma_{\epsilon_i}^2} \right) = -10 \log \left(\frac{\sigma_i^2 \sigma_{jk}}{\sigma_{ij}\sigma_{ik}} - 1 \right) \quad \textbf{Eq. 3-9}$$

with $i, j \in [X, Y, Z]$ and $i \neq j$.

Bias

Eq. 3-10 describes the mean difference between the validation data set and the reference data.

$$bias = \frac{1}{N} \cdot \sum_k^N x_k - y_k \quad \textbf{Eq. 3-10}$$

Root Mean Square Difference (RMSD)

The Root Mean Square Difference (RMSD) estimates differences between two data sets that may contain errors. This means that neither the validation or the reference data set are treated as “true” values.

$$RMSD = \sqrt{\frac{1}{N} \cdot \sum_k^N (x_k - y_k)^2} \quad \textbf{Eq. 3-11}$$

The RMSD is very sensitive to biases in either the mean or the amplitude of fluctuations in the retrieval [Entekhabi et al., 2010]. By computing the unbiased Root Mean Square Difference (ubRMSD) the bias effect will be removed. The relation between RMSD and ubRMSD is defined as:

$$RMSD^2 = ubRMSD^2 + bias^2 \qquad \textbf{Eq. 3-12}$$

Correlation coefficients

Correlation coefficients (CC) are used to reveal similarities between two data sets detecting monotonic correlations, either linear or nonlinear. The CC are dimensionless metrics, with values ranging between -1 and +1. When CC is equal to 0, there is no correlation between the data sets. Positive CC values indicate that both data sets increase/decrease simultaneously, whereas negative CC values show the opposite behavior of the considered data sets [Helsel and Hirsch, 2002]. Correlation coefficients are supported by hypothesis tests to evaluate the statistical significance of the coefficient ($p < 0.05$).

Pearson's correlation coefficient (R)

The Pearson's correlation coefficient (R) is the most commonly used measure of linear dependencies between two data sets. Pearson's R is very sensitive to outliers [Helsel and Hirsch, 2002], because its calculation is based on means and standard deviations (see **Eq. 3-13**). Consequently, the investigation of larger amounts of data does not necessarily ensure a better performance of Pearson's CC. Certain scenarios can generate misleading values of Pearson's R (e.g. see Anscombe's quartet[6]) or even cause a failure in the correlation detection [Wilcox, 2009].

$$R = \frac{\sum_k^N (x_k - \bar{x}) \cdot (y_k - \bar{y})}{\sqrt{\sum_k^N (x_k - \bar{x})^2} \cdot \sqrt{\sum_k^N (y_k - \bar{y})^2}} = \frac{\sigma_{xy}}{\sqrt{\sigma_x^2 \cdot \sigma_y^2}} \qquad \textbf{Eq. 3-13}$$

Spearman correlation coefficient (ρ)

The detection of linear and non-linear associations between two data sets can be performed by using the Spearman correlation coefficient. This rank-based CC provides evidence on the strength of the relationship between two data sets and it is robust with respect to outliers. Spearman's CC can be interpreted as Pearson's CC applied on ranked data sets [Wilcox, 2009]. The input data sets, x and y, are firstly ranked independently among themselves, then ρ is computed as:

$$\rho = \frac{\sum_{i=1}^n (Rx_i \cdot Ry_i) - n \cdot \left(\frac{n+1}{2}\right)^2}{n \cdot (n^2 - 1)/2} \qquad \textbf{Eq. 3-14}$$

where Rx and Ry represent the ranks of x and y, and $(n + 1)/2$ is the mean rank of the data sets [Helsel and Hirsch, 2002].

3.4. Validation Setup

The standard validation setup of soil moisture products derived from ERS ESCAT is based on the comparison with reference data sets, represented by soil moisture from land surface models (GLDAS NOAH, ERA-Interim), satellite data (Passive ESA CCI product) and in situ measurements. Depending on the temporal period under investigation, suitable reference data sets are chosen for the validation process. During

[6] https://en.wikipedia.org/wiki/Anscombe%27s_quartet

the preprocessing step, the involved data sets are spatially and temporally matched, as well as masked. The validation is performed by making use of the validation framework implemented in the Python Toolbox for the Evaluation of Soil Moisture Observations (pytesmo) [Christoph Paulik et al., 2016]. Eight validation scenarios have been set up to quantify the physical reliability of the ESCAT soil moisture products on global and local scales (see Table 3.2). Each validation scenario is set up with three independent soil moisture data sets to calculate the defined standard quality benchmarks (SNR, R, etc.).

Scenario	Dataset 1	Dataset 2	Dataset 3
Global Scale			
1	ESCAT high res.	GLDAS NOAH	Passive ESA CCI
2	ESCAT nominal res.	GLDAS NOAH	Passive ESA CCI
3	ESCAT high res.	ERA-interim	Passive ESA CCI
4	ESCAT nominal res.	ERA-interim	Passive ESA CCI
Local Scale			
5	ESCAT high res.	GLDAS NOAH	In situ
6	ESCAT nominal res.	GLDAS NOAH	In situ
7	ESCAT high res.	ERA-interim	In situ
8	ESCAT nominal res.	ERA-interim	In situ

Table 3.2: Soil moisture datasets used in the different validation scenarios.

Data Masking

Data records used in the validation are masked for frozen soil and snow either using information from land surface models (i.e. temperature and Snow Water Equivalent (SWE)) or advisory flags (i.e. snow and frozen soil probability). The following thresholds have been applied for masking with respect to the land surface model records of GLDAS NOAH and ERA-Interim: (i) SWE $==$ 0. (ii) surface temperature <3 °C. In addition, ERS ESCAT soil moisture products are masked by making use of the included surface state flag (SSF) to exclusively select observations with either 0 (unknown state) or 1 (unfrozen) surface states.

Scaling

ERS ESCAT soil moisture products are given in units of degree of saturation. Accordingly, a rescaling to volumetric units was done by utilizing GLDAS soil porosity information as outlined in the ATBD [RD-1]. GLDAS soil moisture estimates are rescaled from gravimetric to volumetric units by employing **Eq. 3-1**.

Spatial and temporal matching

The validation data sets are spatially and temporally matched using the nearest-neighbor (NN) approach. With respect to "Global Scale" validation scenarios, ERS ESCAT soil moisture was taken as the spatial and temporal reference data set to match the others (see Table 3.3). For "Local Scale" validation scenarios, in situ station data was taken as the spatial and temporal reference.

Dataset	Spatial	Temporal
Global Scale		
GLDAS	35 km	8 h

ERA-interim	80 km	8 h
Passive ESA CCI	35 km	8 h
Local Scale		
GLDAS	35 km	8 h
ERA-interim	80 km	8 h
ERS ESCAT	8 km	8 h

Table 3.3: Nearest-neighbor (NN) parameters used for spatial and temporal matching.

3.5. Global Scale Validation Results

Validation results obtained by "Global Scale" analysis for ERS ESCAT soil moisture products are discussed in following. The discussion focuses on validation result computed by means of the defined standard quality benchmarks; scores for supplementary quality criteria are given in Appendix B. Four scenarios were used in the global scale validation; these were selected to identify possible differences in the ESCAT soil moisture retrievals w.r.t. different spatial resolutions (nominal vs. high resolution) of the products. Hereafter, global maps and boxplots of the computed quality benchmarks are provided. Global maps are used to show the spatial distribution of the performance of the ESCAT soil moisture products. The overall performance of the products is summarized in boxplots. The whiskers of the boxplots indicate the 5th and 95th percentile, whereas the size of the box represents the Inter Quartile Range (IQR). In addition, a percentage indicating the number of locations exceeding the threshold/target/optimal requirements is given as well.

Signal-to-Noise-Ratio

In general, the SNR indicates a good performance of the ERS ESCAT soil moisture products over the entire mission lifetime. A reduced performance of the products is found for parts of North America, the Eastern parts of the Iberian Peninsula and Western Australia indicated by yellowish to reddish colors (see Figure 3.2). The reduced performance of the products in these regions may be related to the fact that these regions are featured with a rather low soil moisture dynamics in general. Spatial patterns of the SNR are consistent across the validation scenarios utilizing different land surface models (GLDAS/ERA-interim). Furthermore, the computed magnitudes of the SNR for the nominal and high resolution ESCAT soil moisture products are almost identical, confirming the consistency of the data sets. The good performance of the ERS ESCAT soil moisture products is summarized in Figure 3.3, revealing a slightly better performance of the nominal resolution product in comparison to the high resolution ESCAT soil moisture product. With respect to the nominal resolution soil moisture product, 76% (GLDAS) and 80% (ERA-interim) of the validated areas exceed the threshold value of 0 dB globally and values of 83% (GLDAS) and 88% were found for the committed area. The high resolution product shows a somewhat reduced performance with values of 81% (GLDAS) and 86% (ERA-interim) over the committed area. Only a small percentage of about 20% are below the threshold requirement. Overall, the ERS ESCAT soil moisture products show the best SNR performance in comparison to GLDAS and ERA-interim with about 60% of the committed area exceeding the target value of 3 dB and almost 40% exceeding the optimal value of 6 dB.

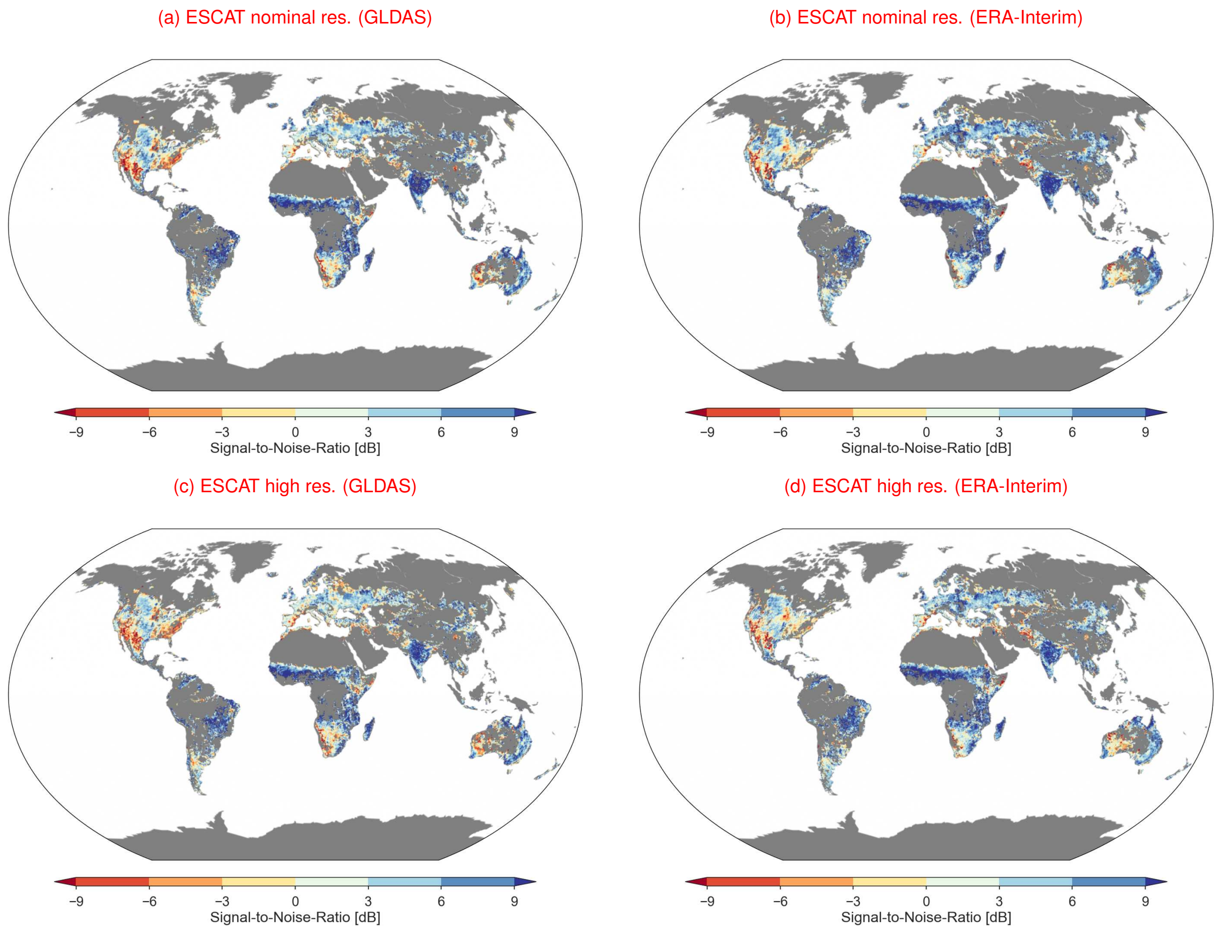

Figure 3.2: Signal-to-Noise Ratio maps of the Global Scale Validation.

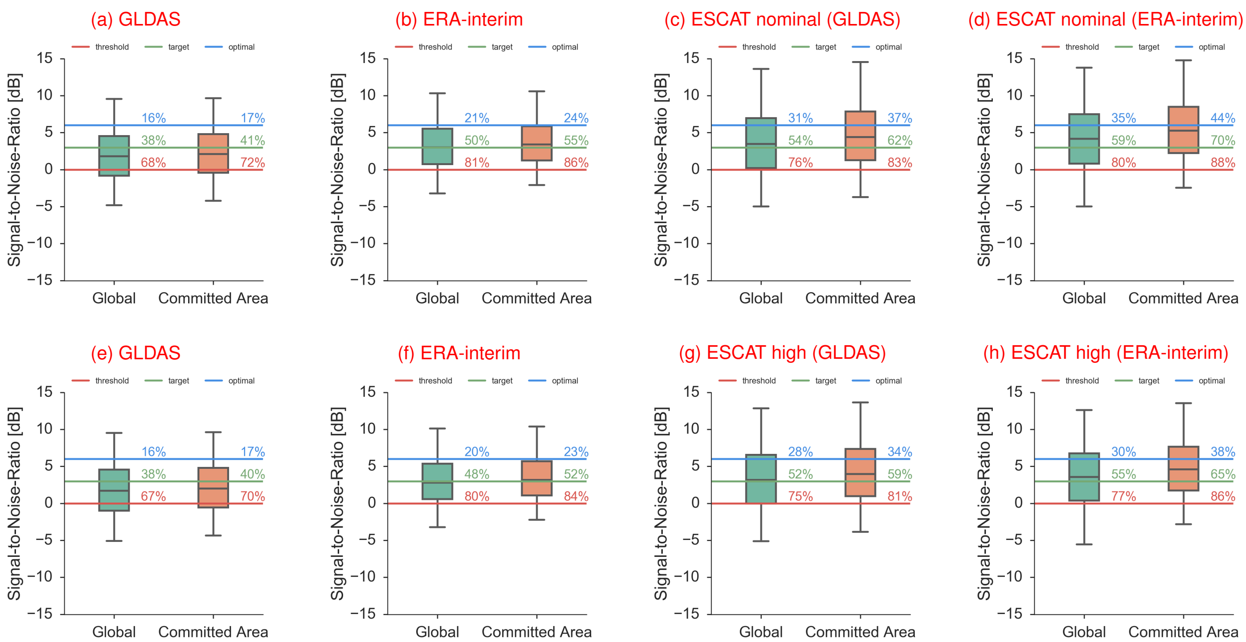

Figure 3.3: Signal-to-Noise Ratio boxplots of the Global Scale Validation.

Pearson Correlation Coefficient

Global scale validation results of the Pearson correlation coefficient indicate a good performance of the ESCAT soil moisture products in comparison to model derived estimates. Higher correlations were found in comparison to ERA-interim with 81% of the high resolution and 84% of the nominal resolution product data exceeding the threshold value of 0.5 in the committed area. In general, the nominal resolution product achieves higher scores of about 3% than the high resolution product. On a global scale, the majority of negative correlations were detected in very dry regions (e.g. deserts) or in densely vegetated areas. Spatial patterns of regions with a high correlation coefficient match those of Signal-to-Noise Ratio patterns with a good SNR metric.

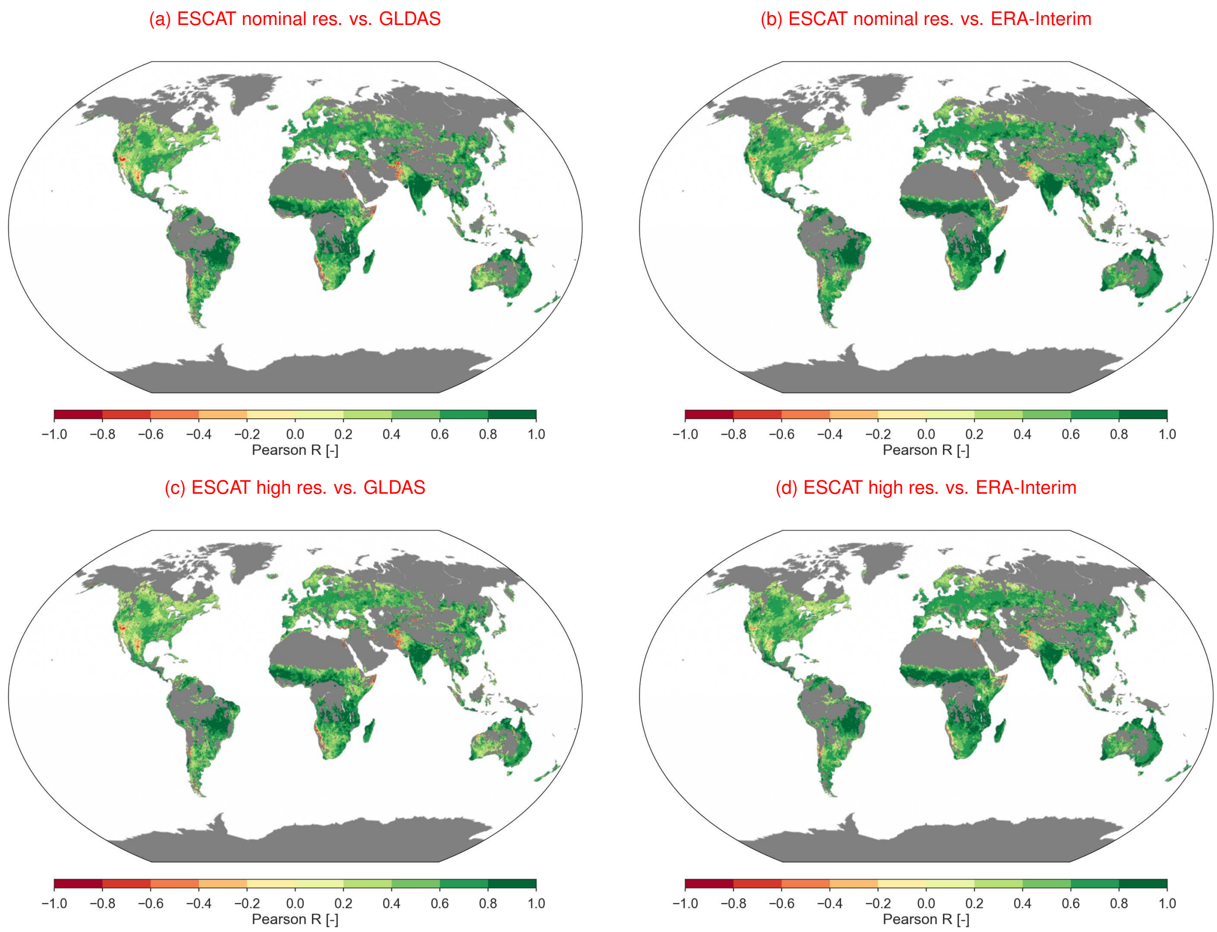

Figure 3.4: Pearson Correlation Coefficient maps of the Global Scale Validation.

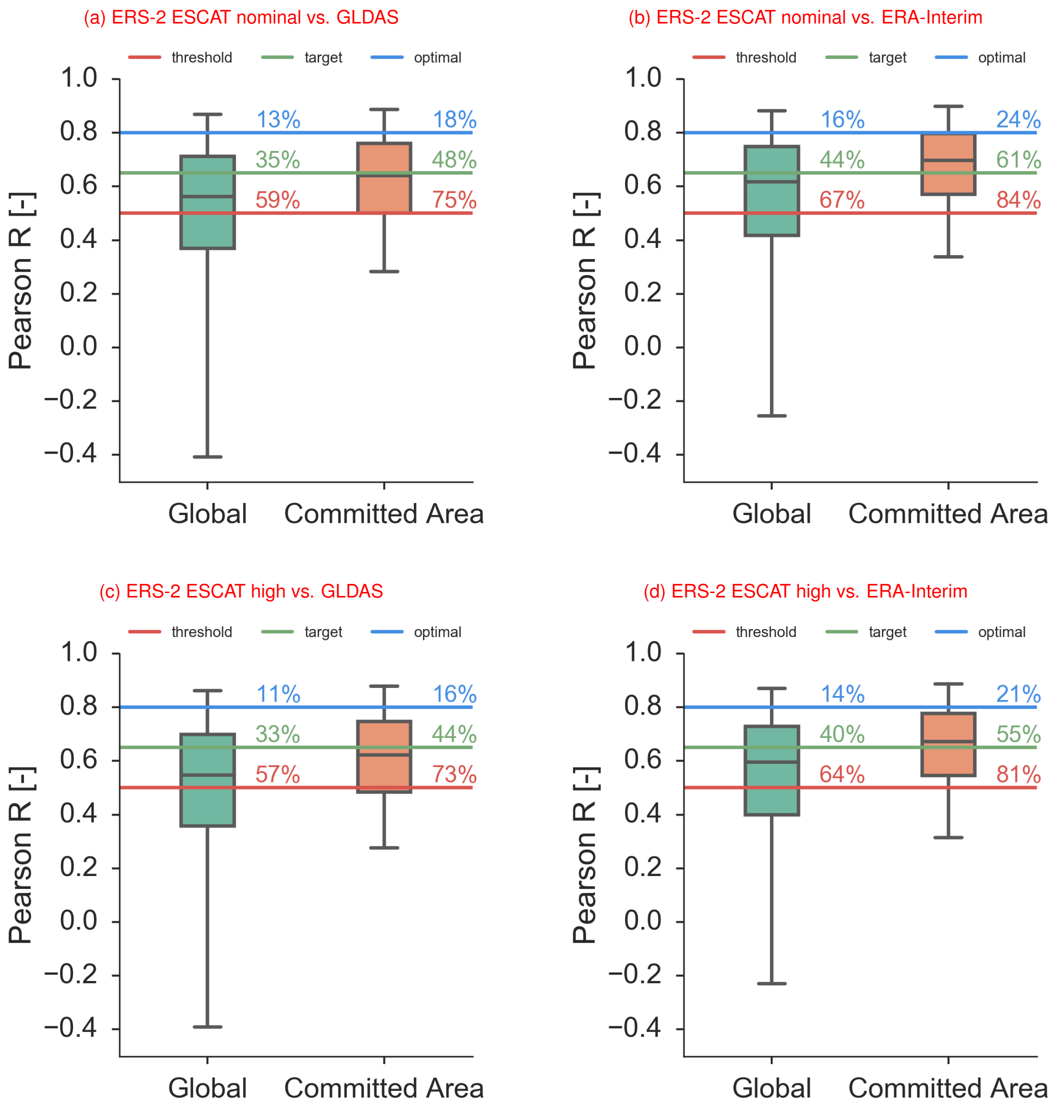

Figure 3.5: Pearson Correlation Coefficient boxplots of the Global Scale Validation.

3.6. Local Scale Validation Results

Local scale validation was performed with respect to in situ soil moisture observations. 42 networks with almost 1350 stations that were active during observation period of ERS-2 ESCAT ranging from May 1996 to July 2011 (see Figure 3.6) were selected. The majority of available stations for validation are located in North America. As before, the discussion focuses on the standard quality benchmarks, while supplementary quality scores are provided in the Appendix C. It should be noted that, the calculation of standard quality benchmarks was not possible for the complete set of stations and networks, because of the reduced amount of collocate observations restricted by spatial and temporal matching of the data. Four scenarios to validate the ERS ESCAT soil moisture products with respect to point-scale in situ observations have been selected as given in Table 3.2. This set up of local scale validation was chosen to quantify the performance of the ESCAT soil moisture products and to identify possible differences in the product related to the spatial resolutions. Local scale validation results are presented via boxplots of the benchmark results per network. The whiskers of the boxplots indicate the 5th and 95th percentile, whereas the size of the box represents the Inter Quartile Range (IQR).

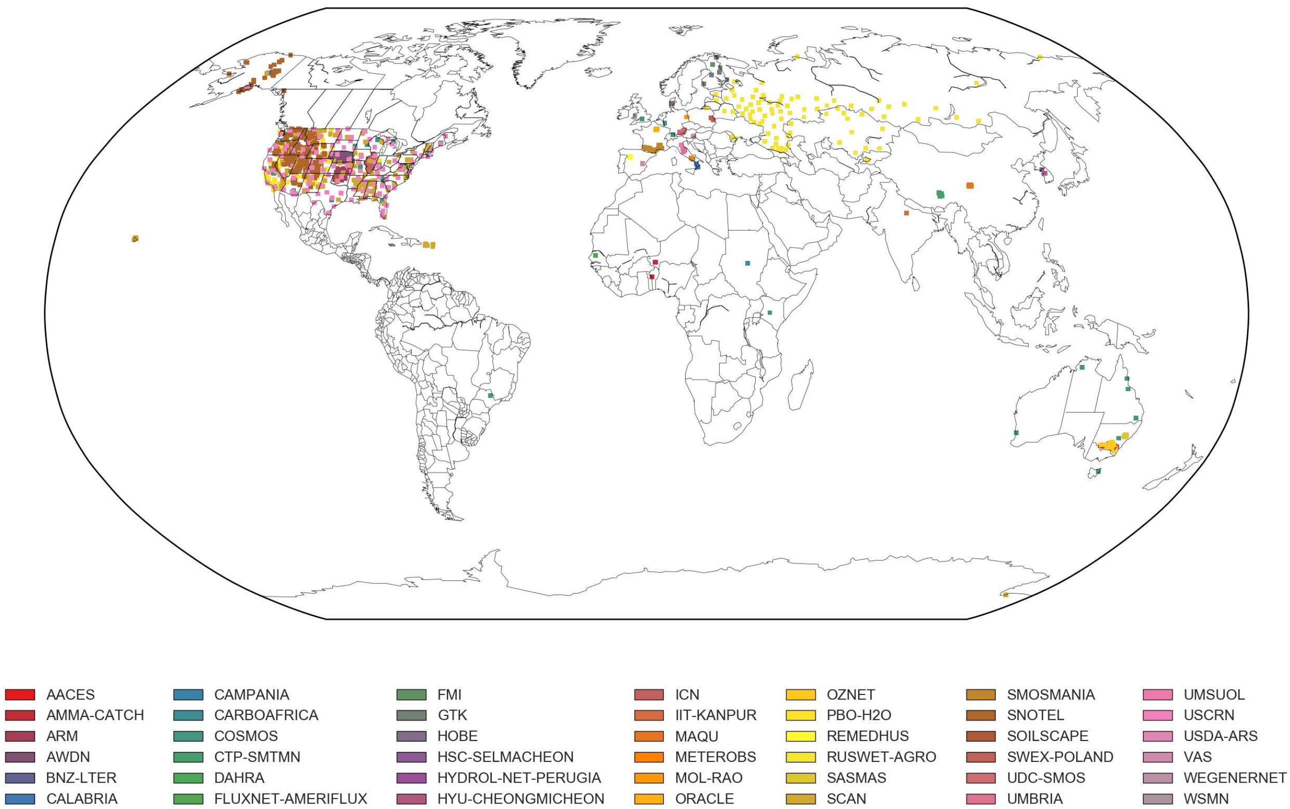

Figure 3.6: Overview of in situ stations per network used for local scale validation.

Signal-to-Noise-Ratio

The performance of ESCAT soil moisture observations expressed in the Signal-to-Noise Ration (SNR) strongly varies from network to network. Overall, a good performance of both ESCAT soil moisture products was found with respect to the SNR quality benchmark. Boxplots presented in Figure 3.7 show that hightest SNR values are achieved by modeled soil moisture, followed by ESCAT soil moisture products and in situ observations in general. On average, 6 out of 19 networks show a median SNR value less than the defined threshold of 0 dB. The remaining networks indicate a good performance of the ESCAT soil moisture products with values above the 0 dB SNR threshold. The SNR performance benchmarking reveal a better performance of the ESCAT soil moisture products for the validation scenarios using ERA-interim modeled data instead of GLDAS data. Highest SNR values of the ERS ESCAT soil moisture products are observed for the DAHRA network in Senegal, West Africa, with SNR values greater than 9 dB. In addition, high SNR values of the ERS ESCAT soil moisture products are observed for the OzNet network in south-east Australia, with an estimated median SNR value of about 9 dB with respect to the high resolution product and around 6 dB for the nominal resolution product. The poorest SNR performance of ESCAT soil moisture was found for the SNOTEL network with an average median value of about -3 dB. Nominal and high resolution ESCAT soil moisture products show almost the same performance with a minimal performance degradation with respect to the high resolution product.

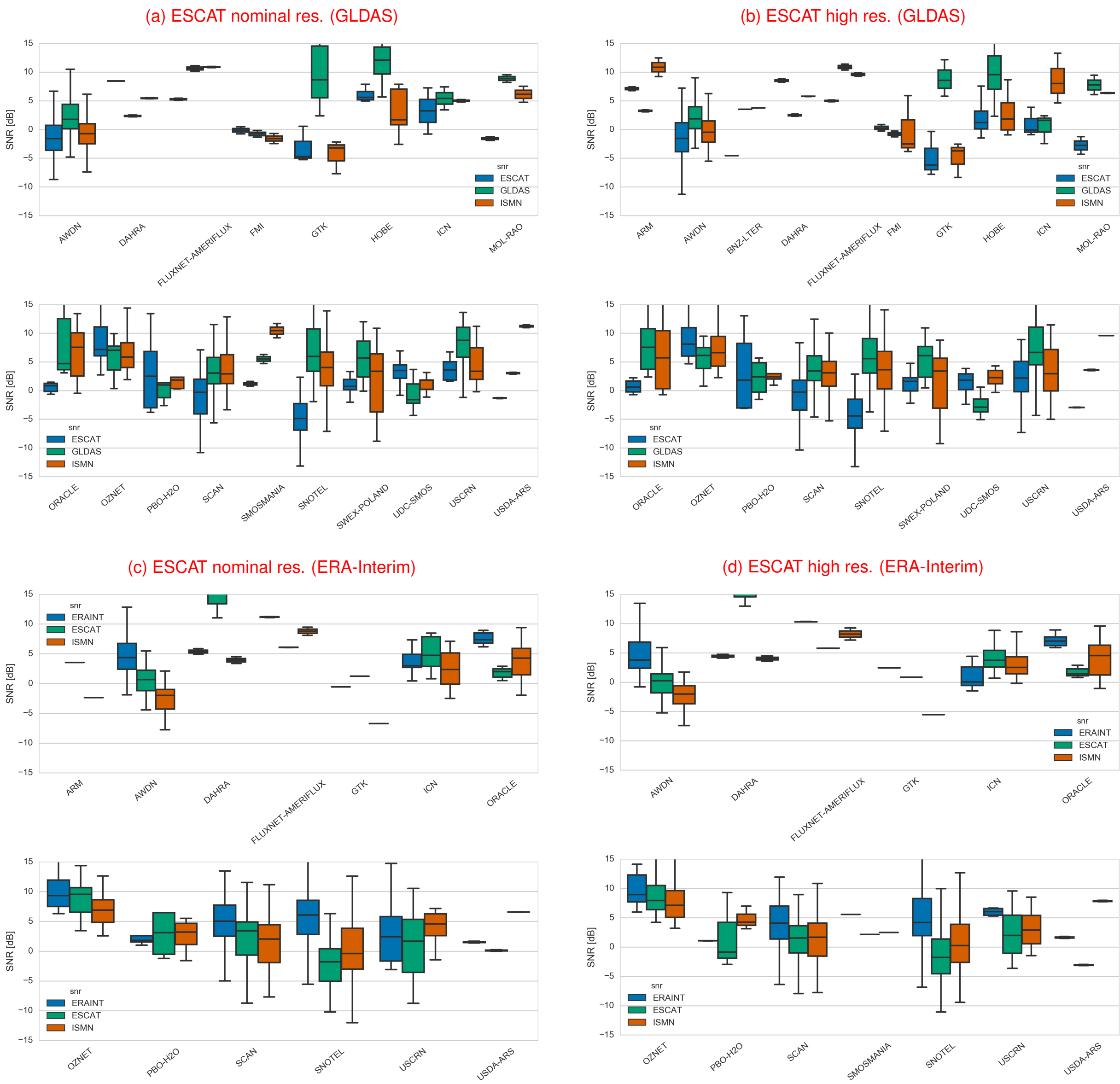

Figure 3.7: Signal-to-Noise Ratio boxplots per in situ network of the Local Scale Validation.

Pearson Correlation Coefficient

Pearson correlation coefficients computed with respect to in situ soil moisture observations show consistent results for nominal and high resolution ESCAT soil moisture products. The majority of networks indicate a slightly higher correlation to modeled soil moisture estimates than to ESCAT soil moisture observations, even by equivalently high correlations between the model and ESCAT soil moisture. A median correlation coefficient greater than 0.5 was found for approximately 50% of the networks.

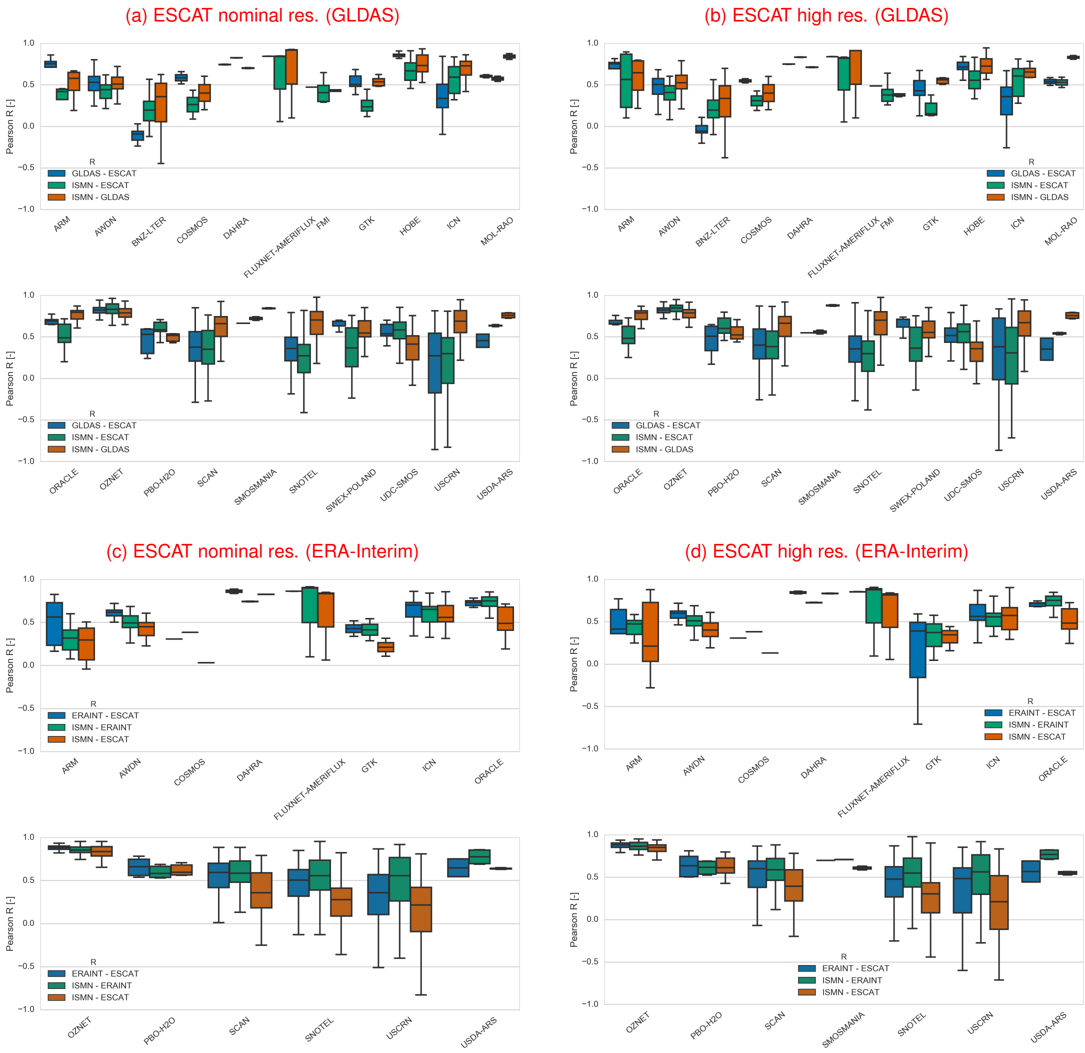

Figure 3.8: Pearson Correlation Coefficient boxplots per in situ network of the Local Scale Validation.

4. Conclusions

Results of the performed verification and validation activities undertaken within the SCIRoCCo project are summarized in this report to prove the completeness and quality of the ERS ESCAT soil moisture retrievals. Verifications performed with respect to the computed model parameters state a successful and complete estimation of these. All model parameters are in the expected ranges enabling a global retrieval of soil moisture from ERS ESCAT backscatter observations. Two soil moisture products types have been generated within the SCIRoCCo project. The ESCAT soil moisture orbit products are derived by making use of the WARP orbit processor and corresponding model parameters. Performed integration tests confirm the successful transfer of the TU Wien soil moisture retrieval model to the WARP orbit processor. Consequently, consistency of the two soil moisture retrieval processors is proven, so that both processor instances provide the same output by same input. With respect to that, the performed validation of the ESCAT soil moisture time series products are representative for the quality of the soil moisture orbit products of ESCAT. Validation results obtained by the global and local scale validation scenarios prove the physical correctness of the soil moisture retrievals. On a global scale, about 80% of the retrieved ESCAT soil moisture estimates are greater than the defined thresholds for each performance benchmark indicator (SNR, R). Local scale validation results underpin the good performance of the ESCAT soil moisture products, indicating similar values of the quality benchmarks as obtained by global scale validation analyses. In conclusion, ERS ESCAT soil moisture products, time series and orbit, have been successfully verified and validated confirming high quality retrievals of soil moisture.

5. References

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A. Model Parameter Verification Results

A.1. Azimuth Coefficients (Correction)

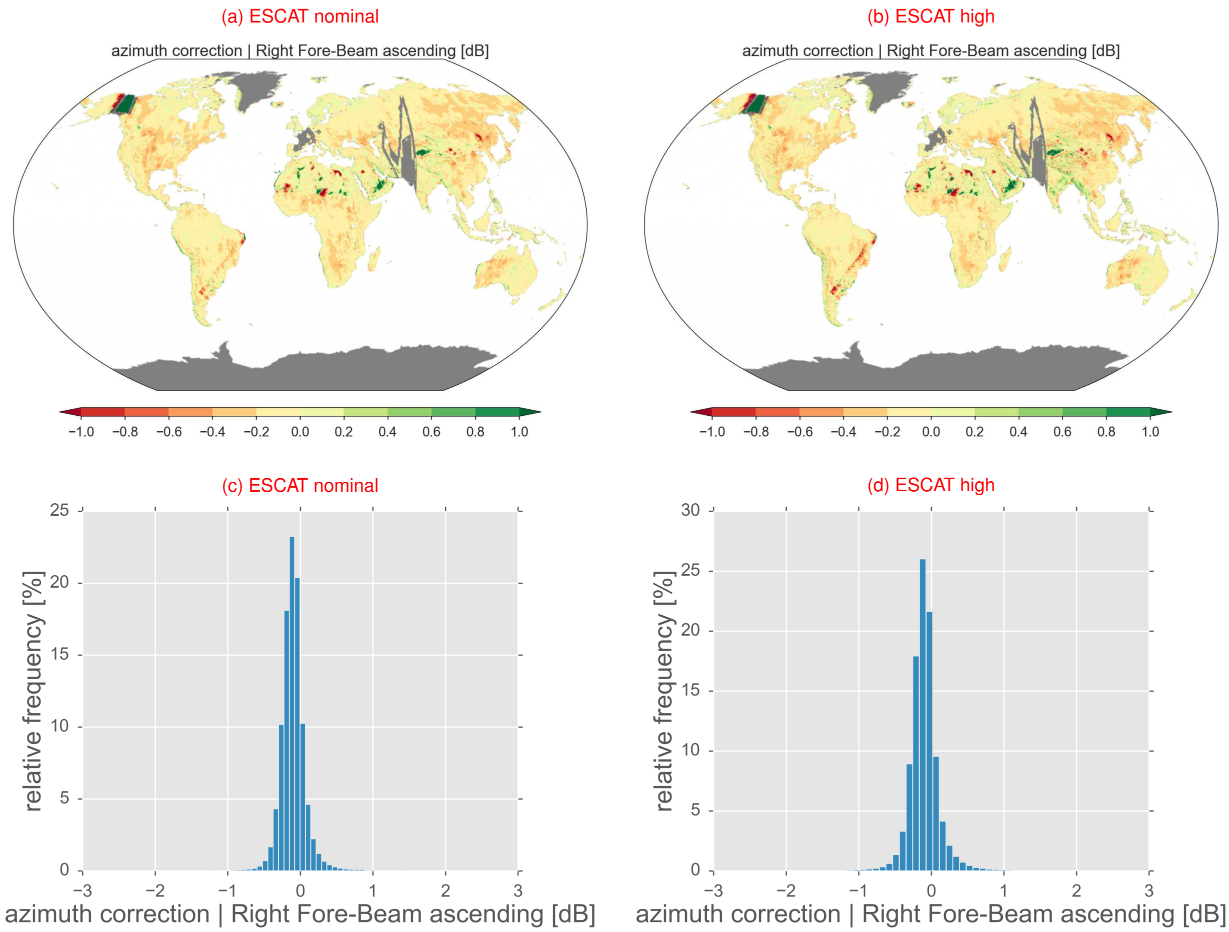


Figure A.1: Mean azimuth correction Fore-beam | ascending overpass

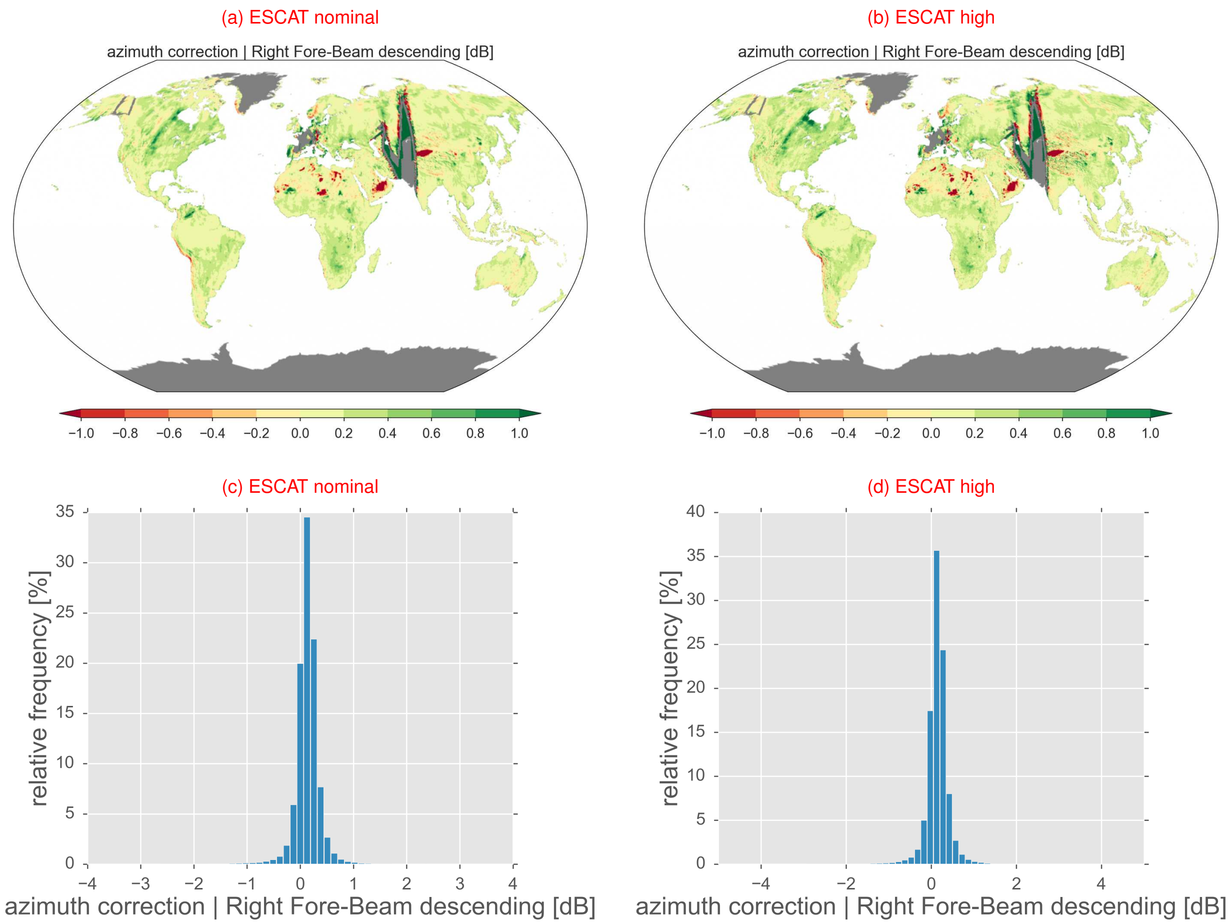


Figure A.2: Mean azimuth correction Fore-beam | descending overpass

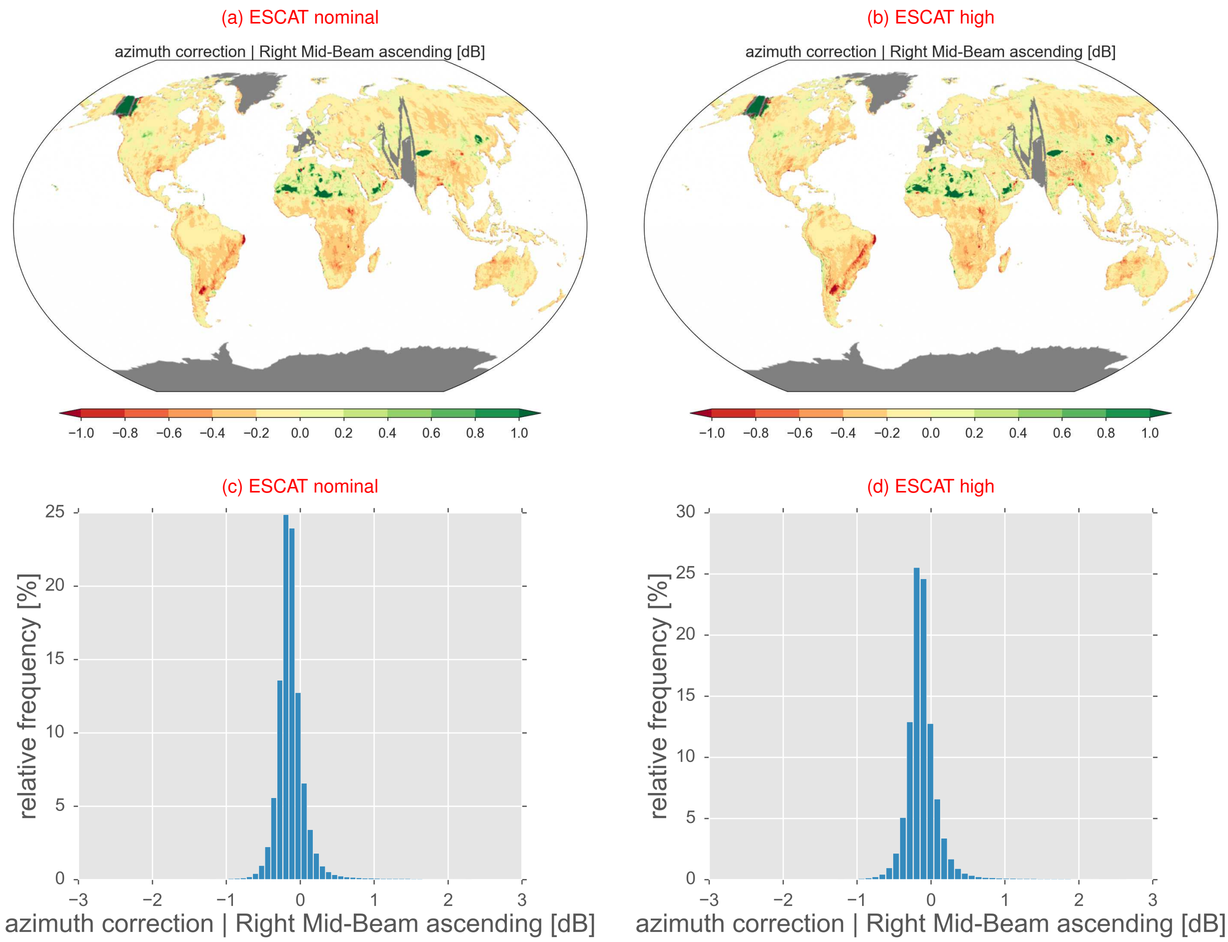


Figure A.3: Mean azimuth correction Mid-beam | ascending overpass

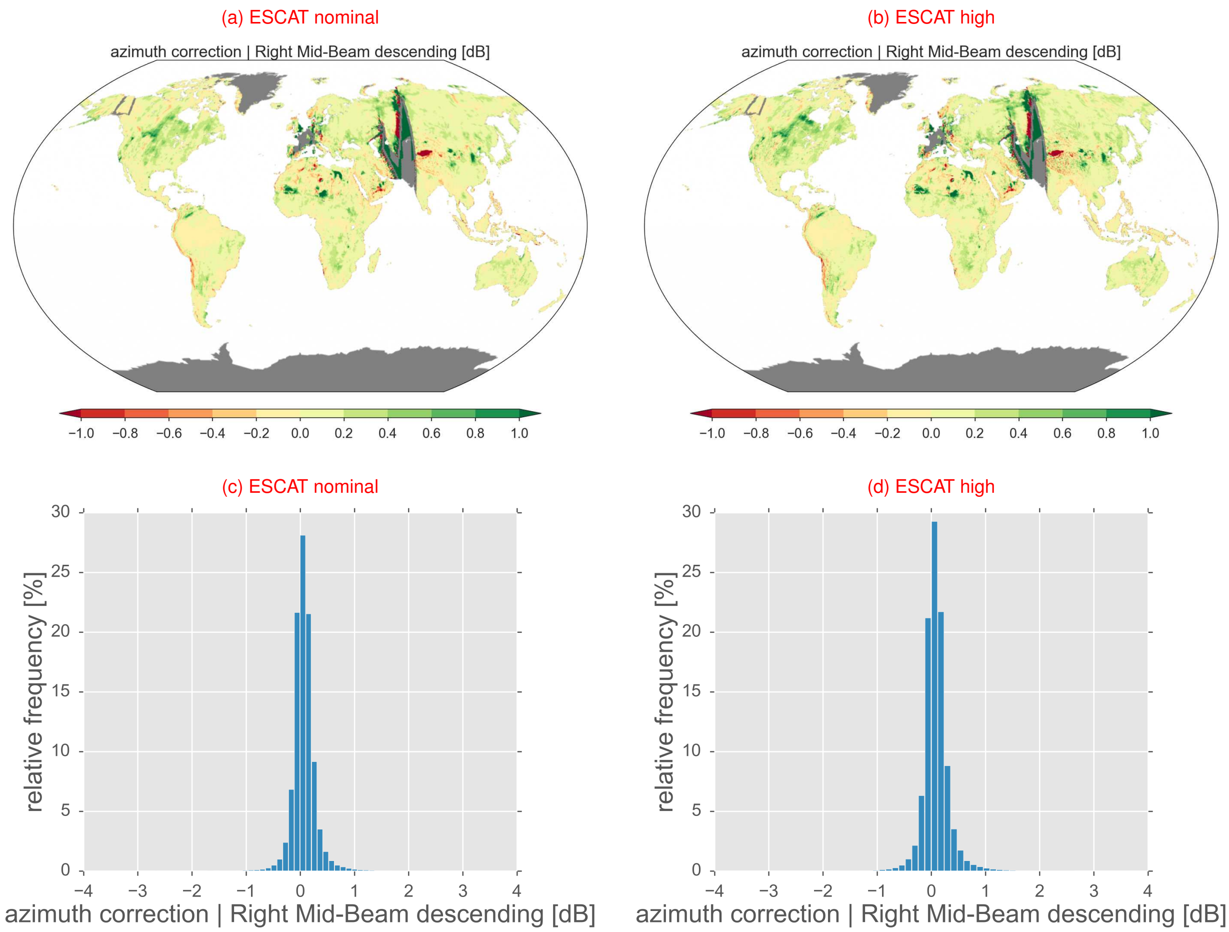


Figure A.4: Mean azimuth correction Mid-beam | descending overpass

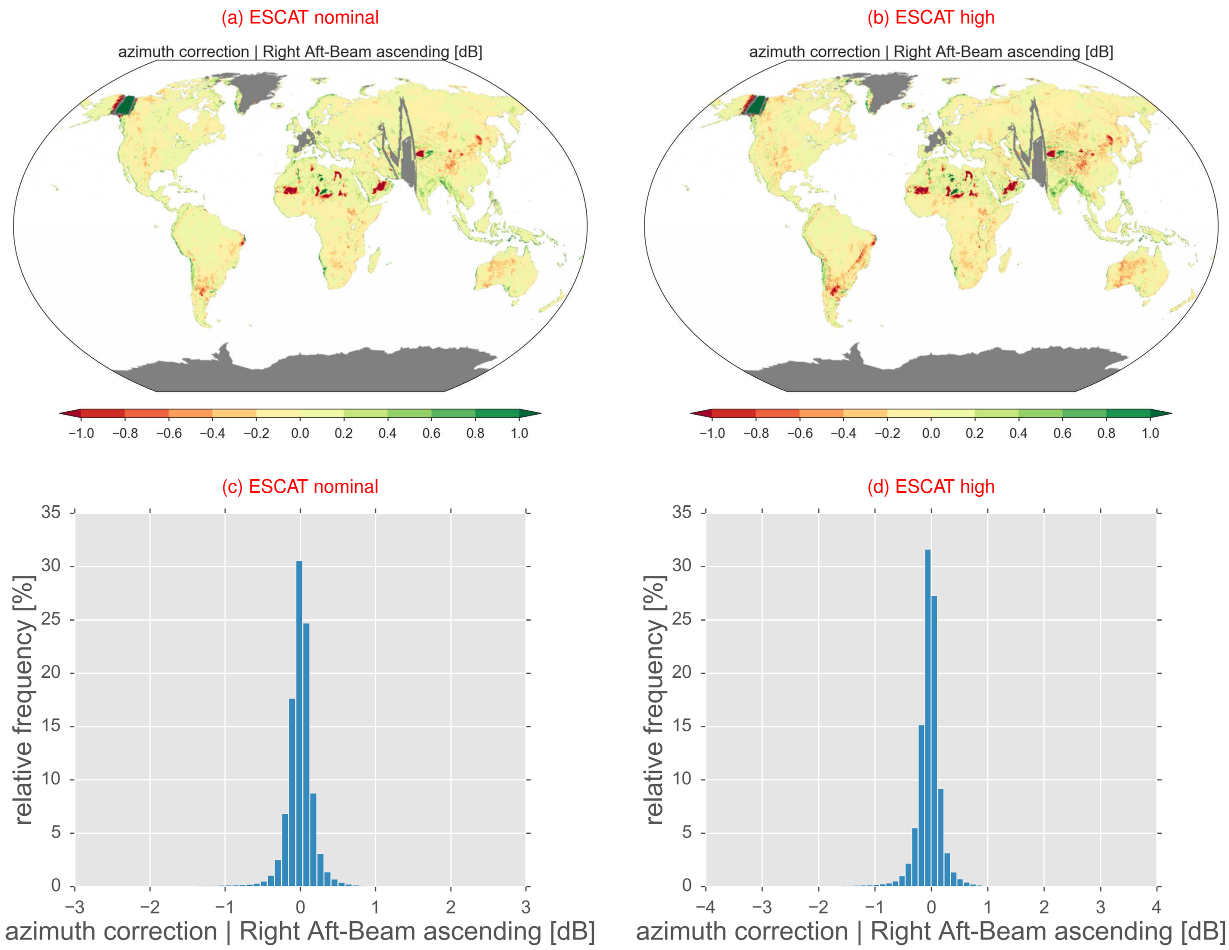


Figure A.5: Mean azimuth correction Aft-beam | ascending overpass

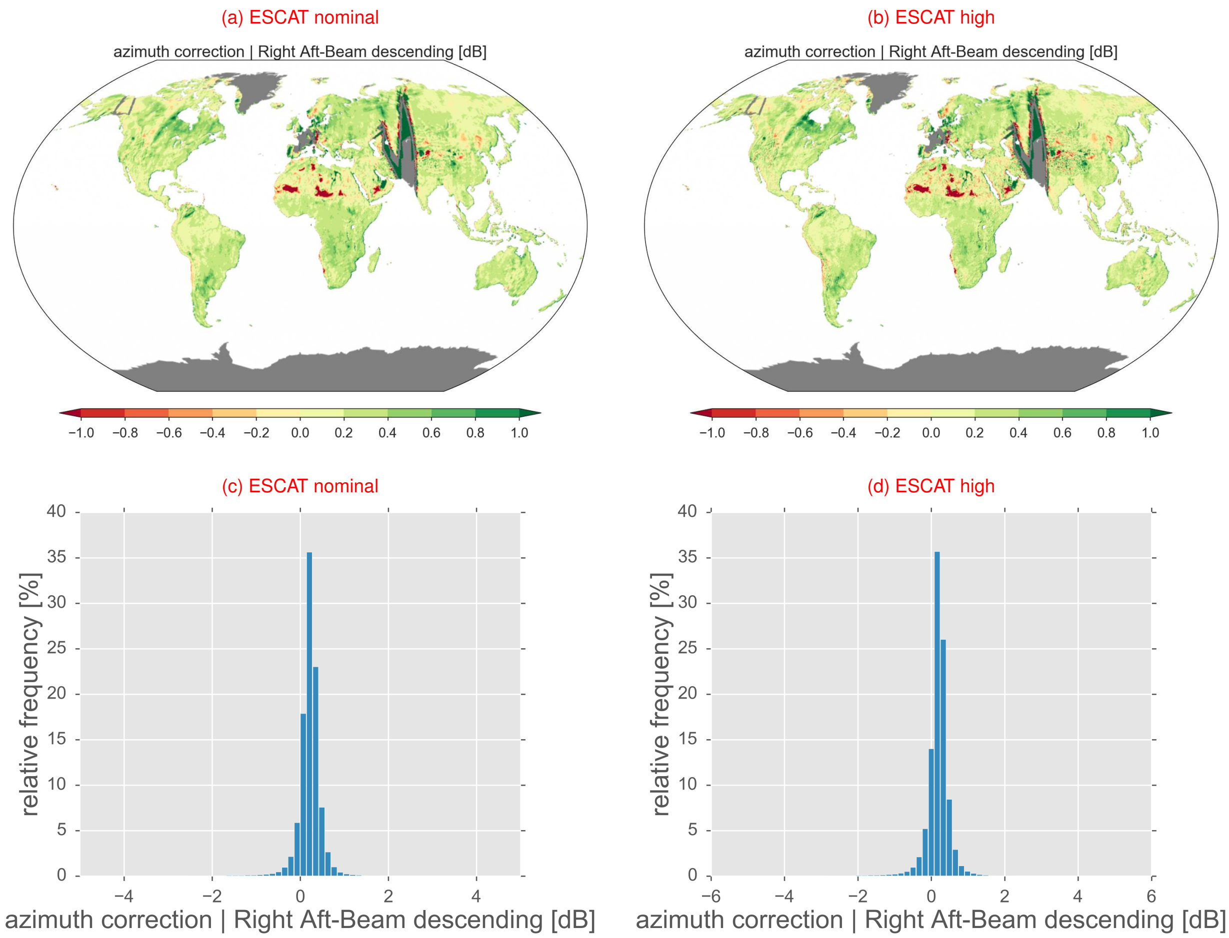


Figure A.6: Mean azimuth correction Aft-beam | descending overpass

A.2. ESD after Azimuth Correction

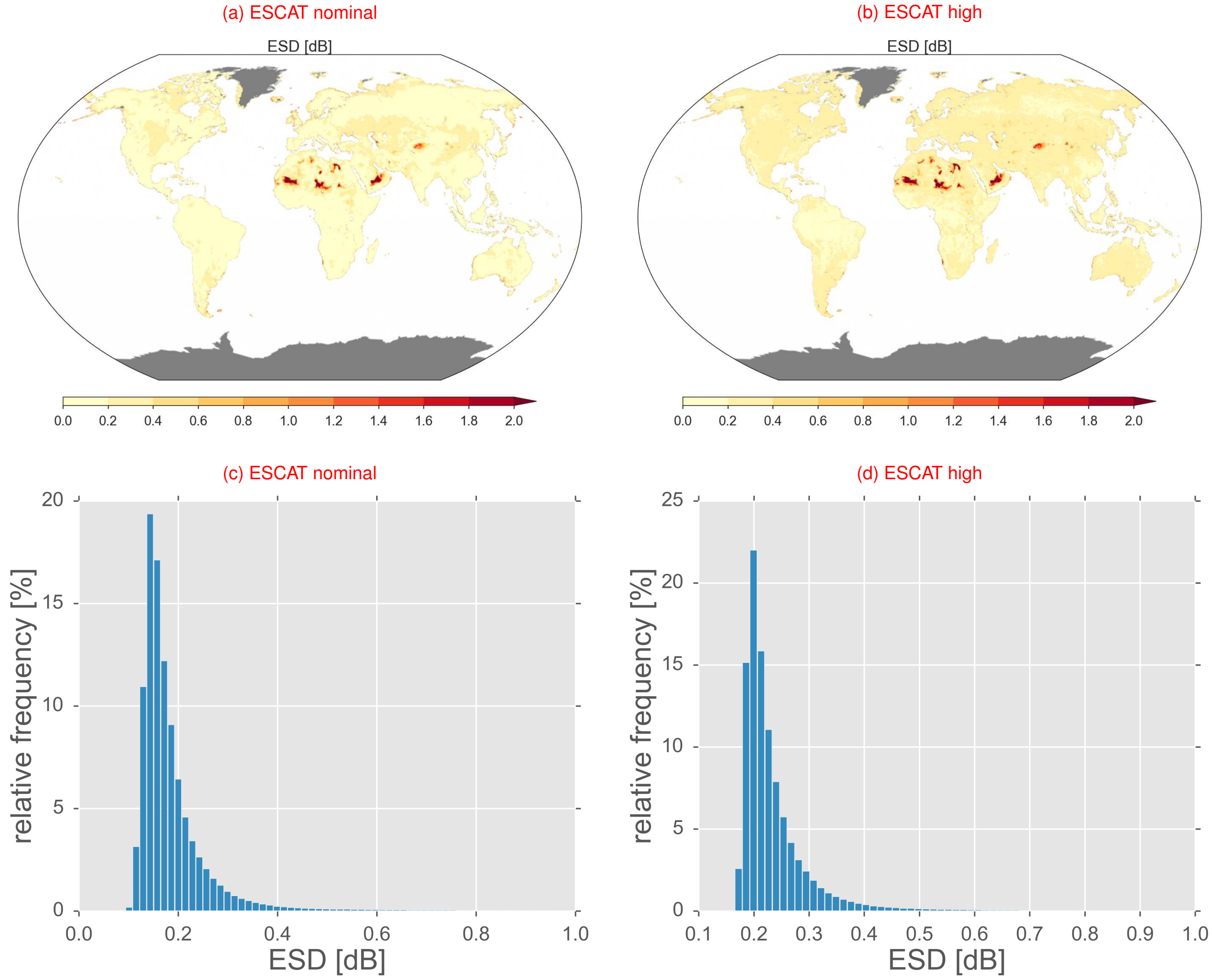


Figure A.7: Estimated Standard Deviation (ESD) after Azimuth Correction

A.3. Slope/Curvature

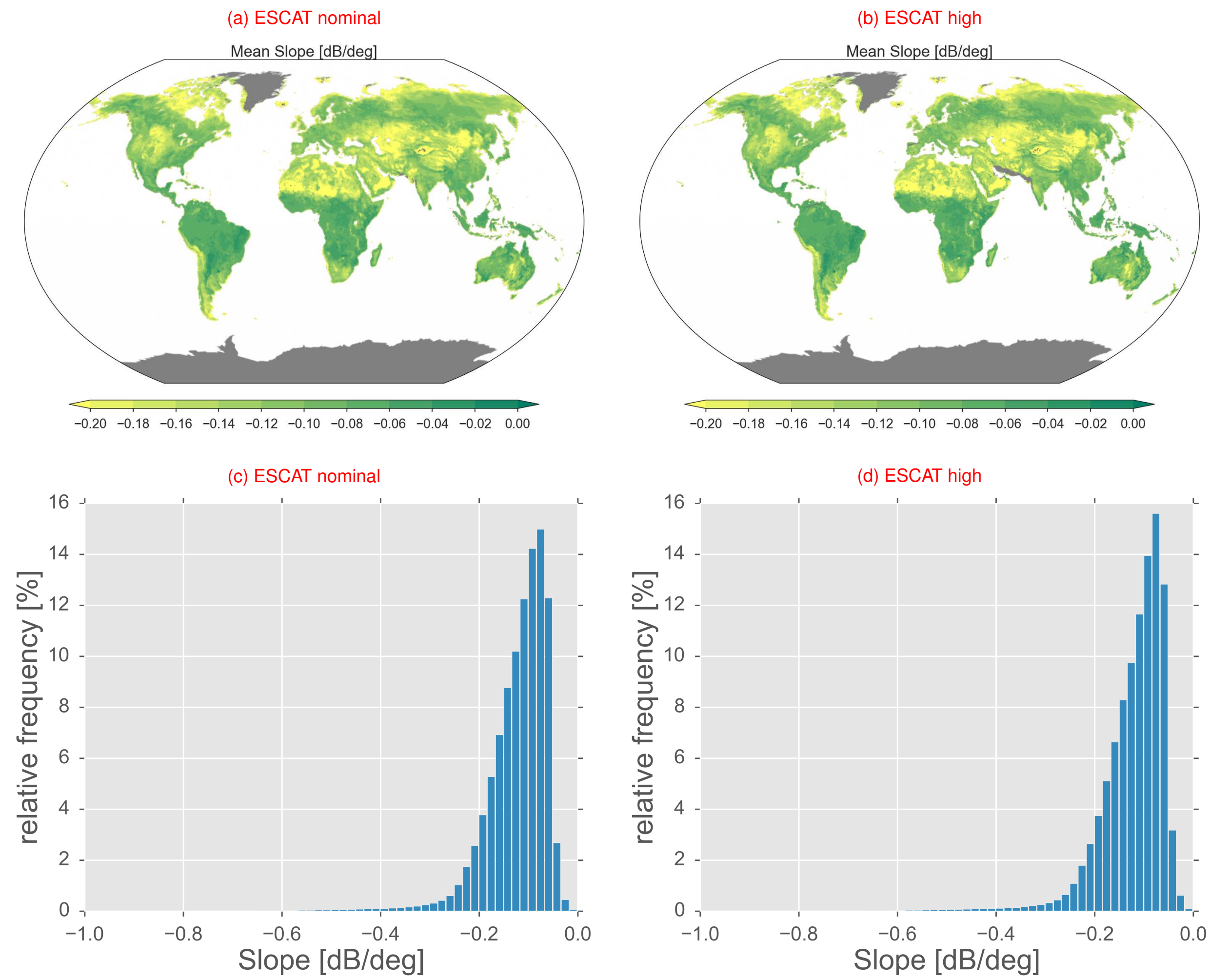


Figure A.8: Mean Slope Parameter

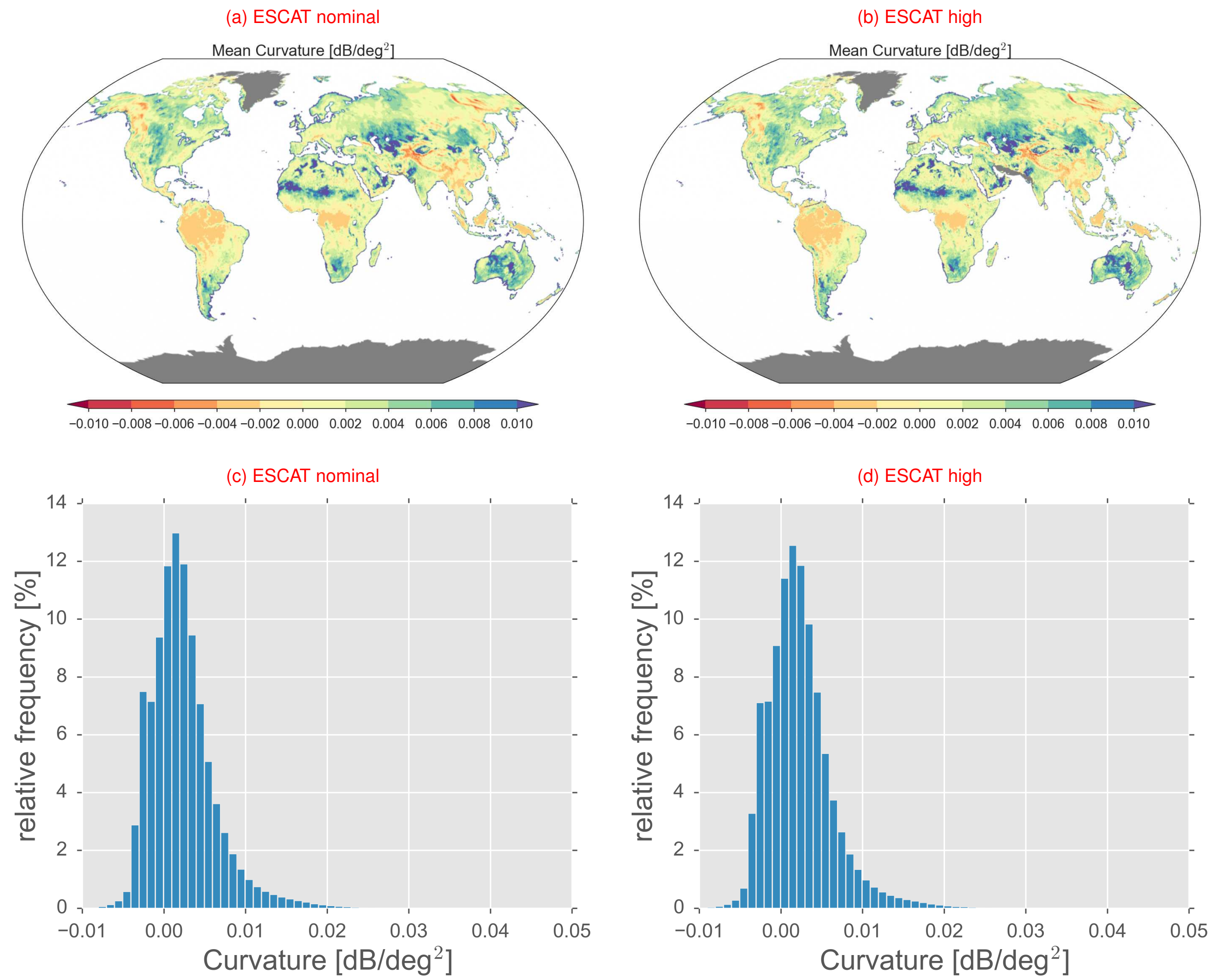


Figure A.9: Mean Curvature Parameter

A.4. Dry/Wet Reference

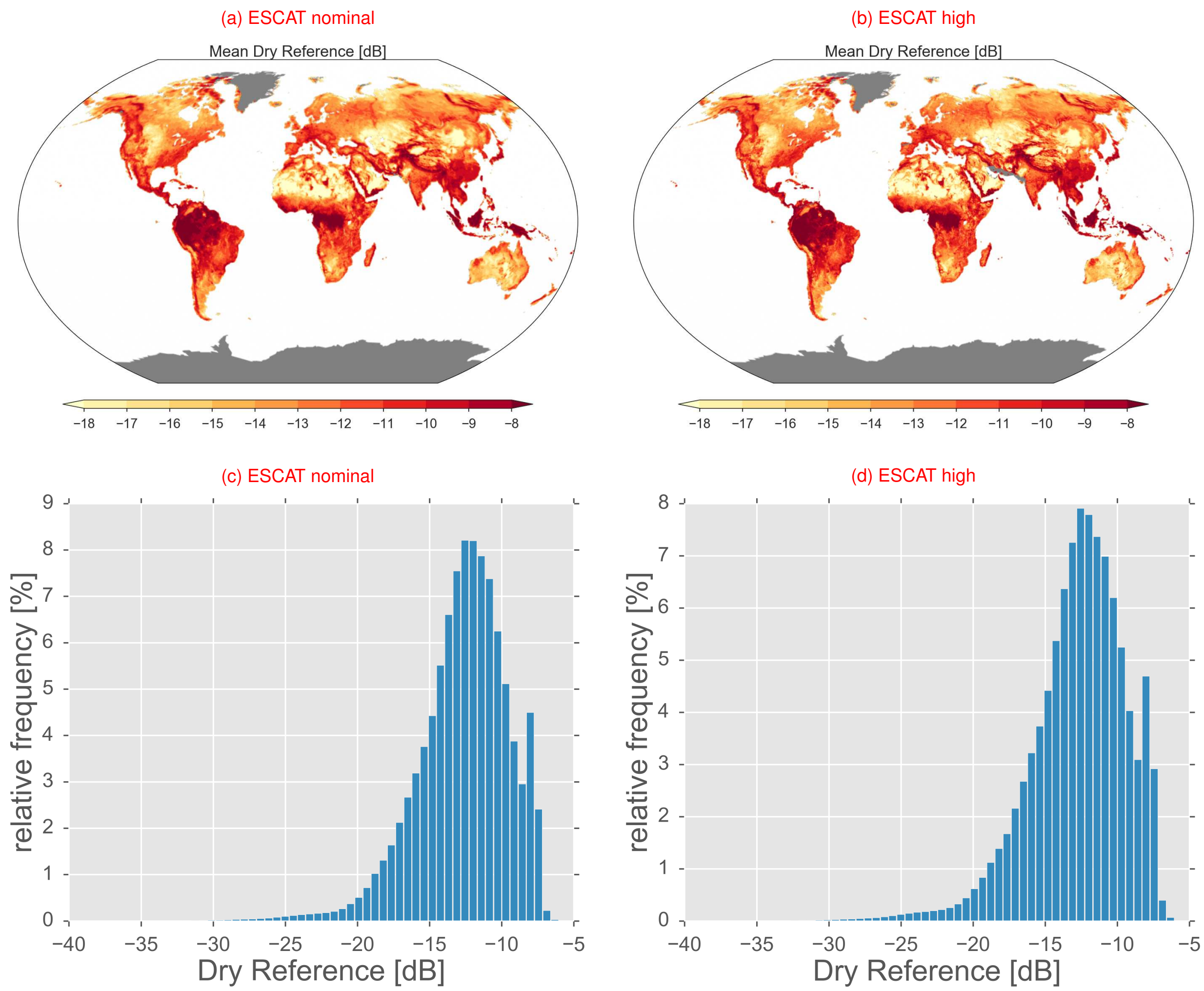


Figure A.10: Mean Dry Reference

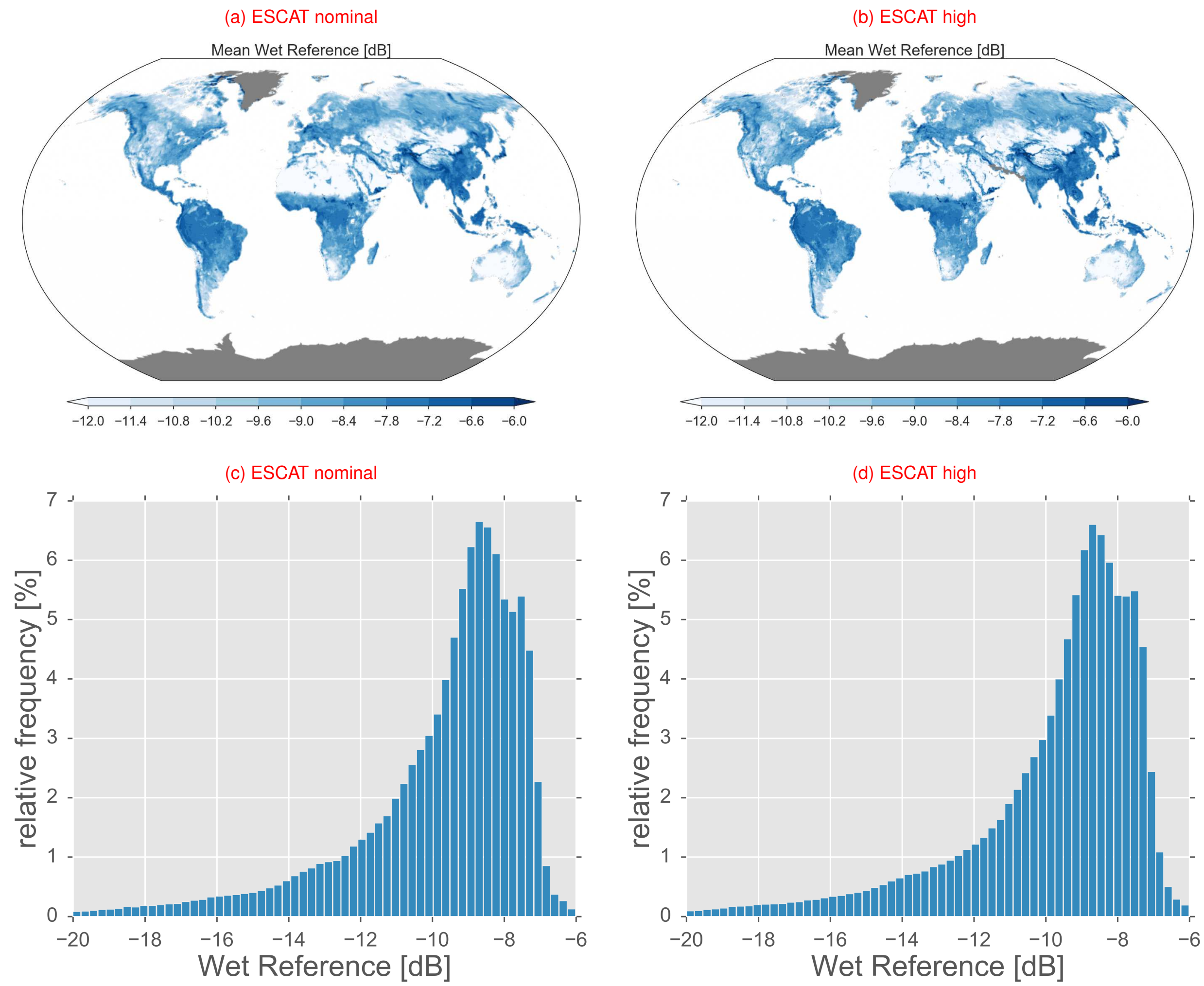


Figure A.11: Mean Wet Reference

A.5. Wet Correction

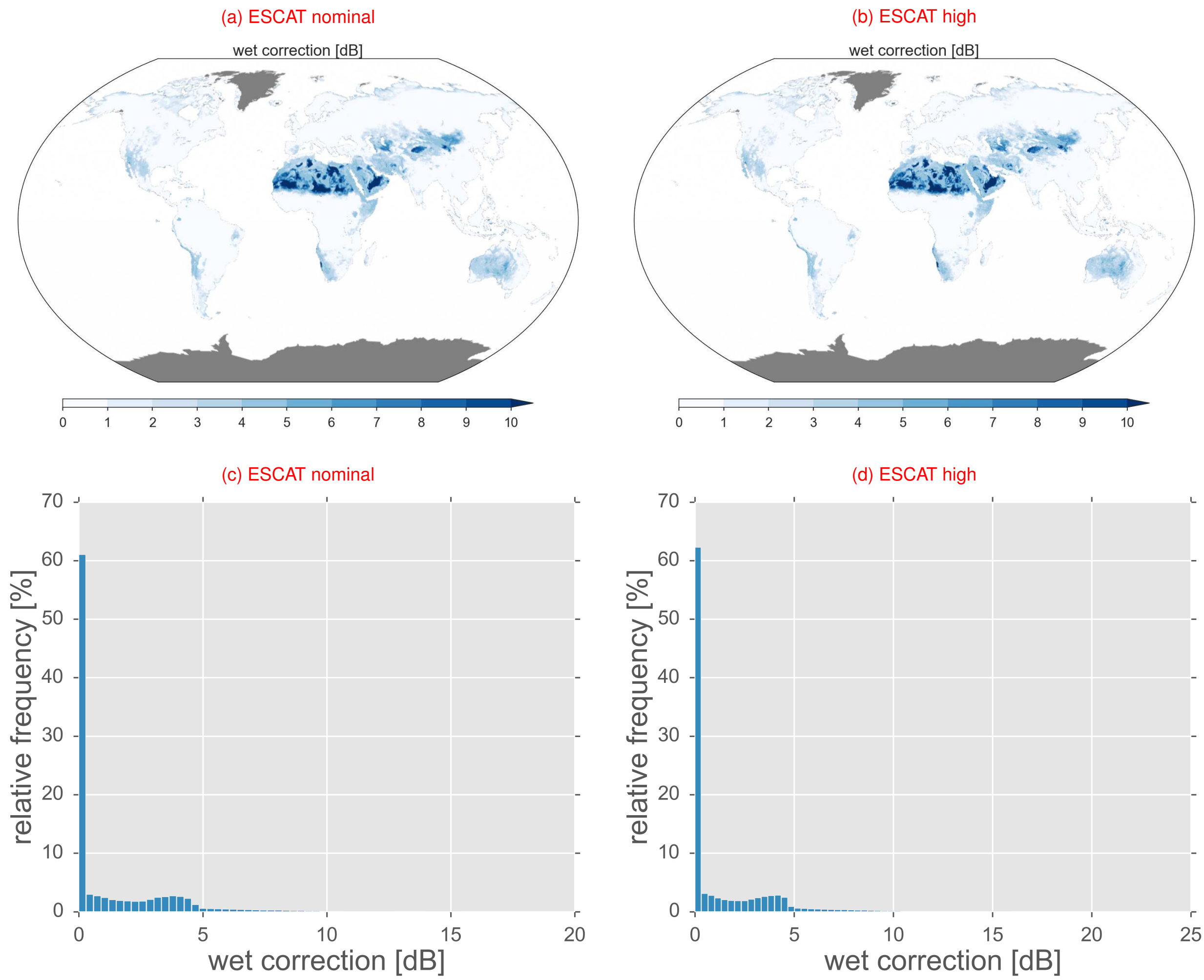


Figure A.12: Wet Correction

B. Global Scale Validation Results

B.1. Error Standard Deviation

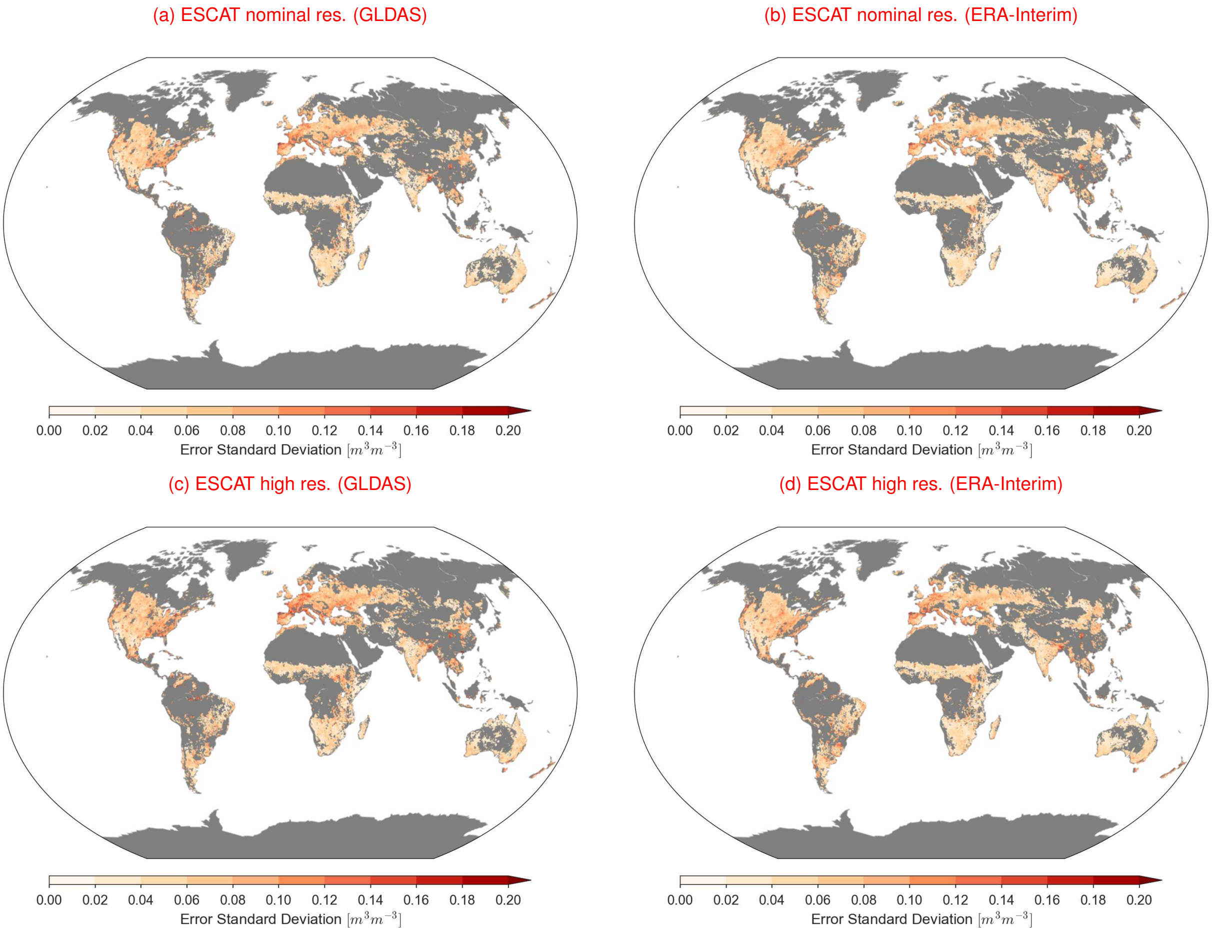


Figure B.1: Error Standard Deviation maps of the Global Scale Validation.

B.2. Spearman ρ

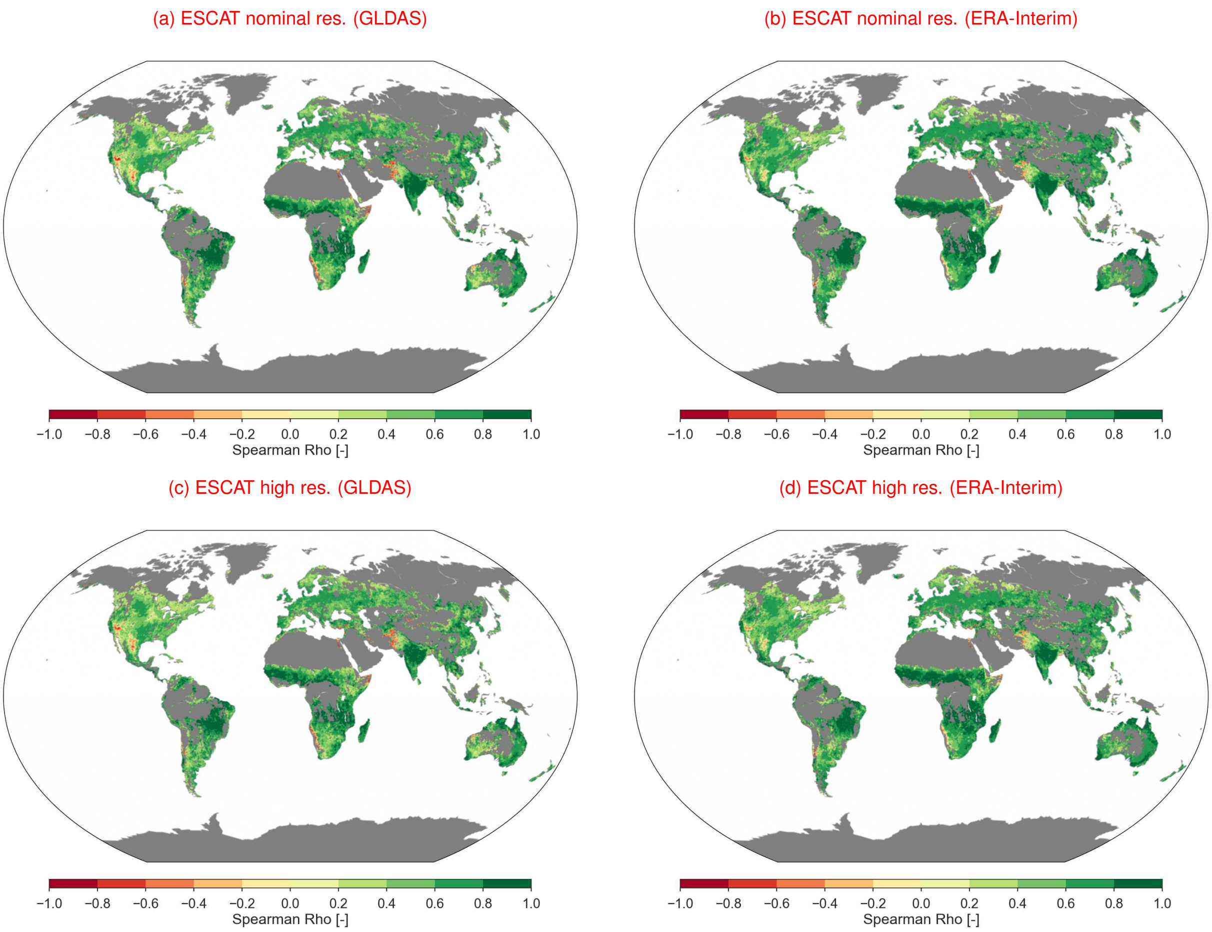


Figure B.2: Spearman Correlation Coefficient maps of the Global Scale Validation.

B.3. Bias

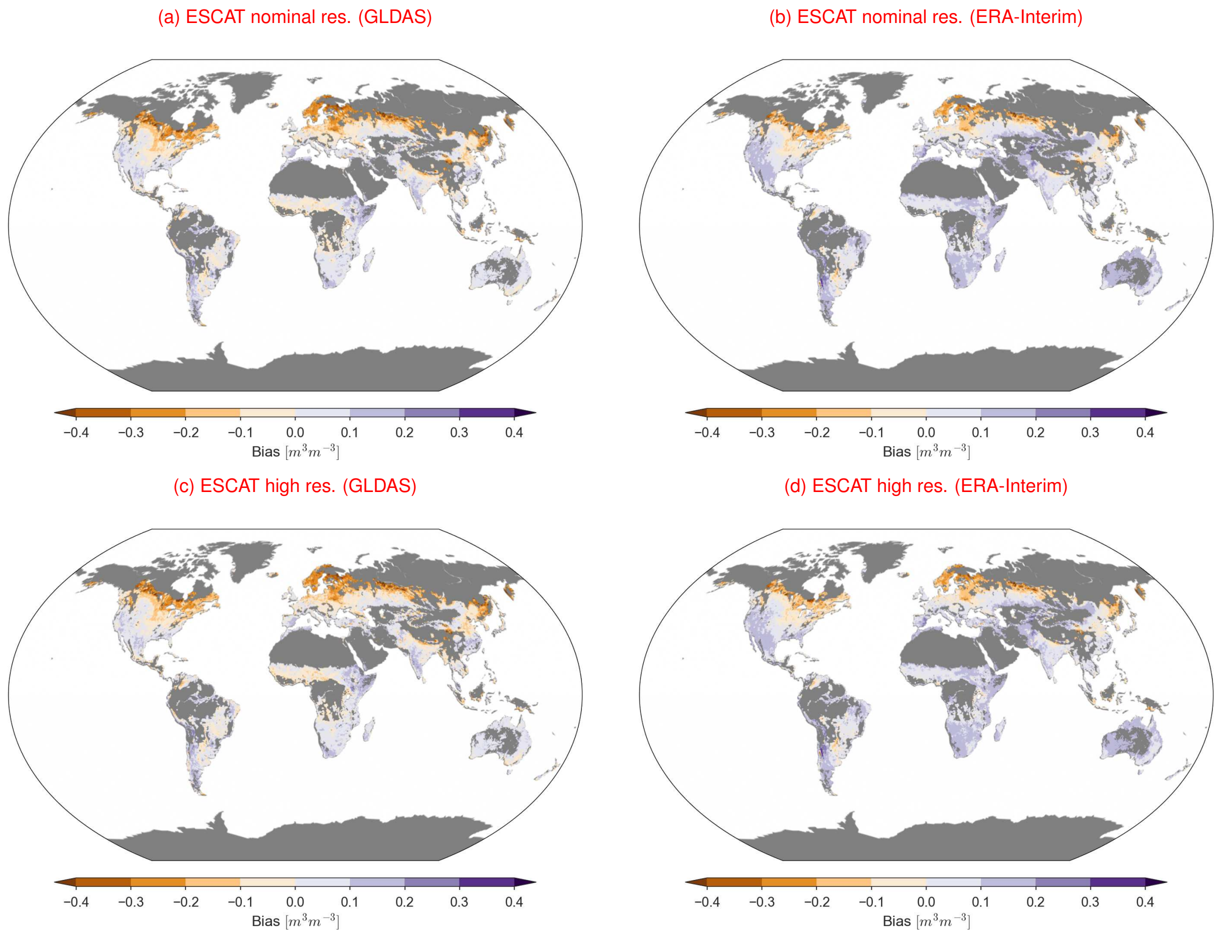


Figure B.3: Bias maps of the Global Scale Validation.

B.4. Unbiased Root Mean Square Difference

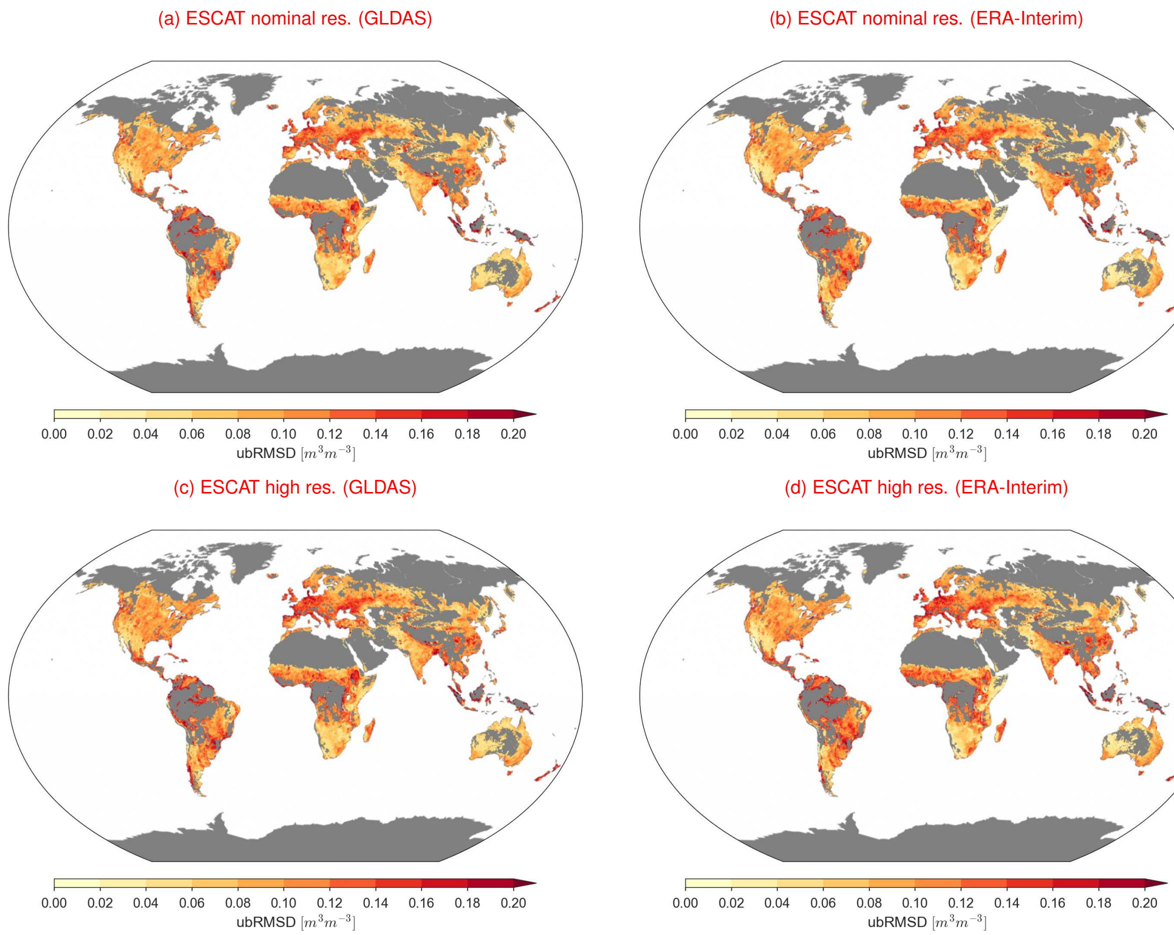
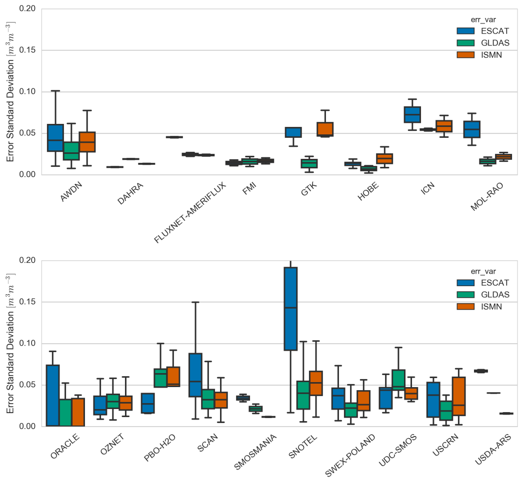


Figure B.4: Unbiased Root Mean Square Difference maps of the Global Scale Validation.

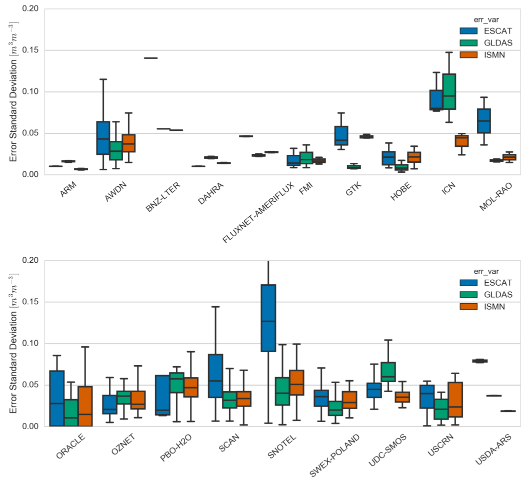
C. Local Scale Validation Results

C.1. Error Standard Deviation

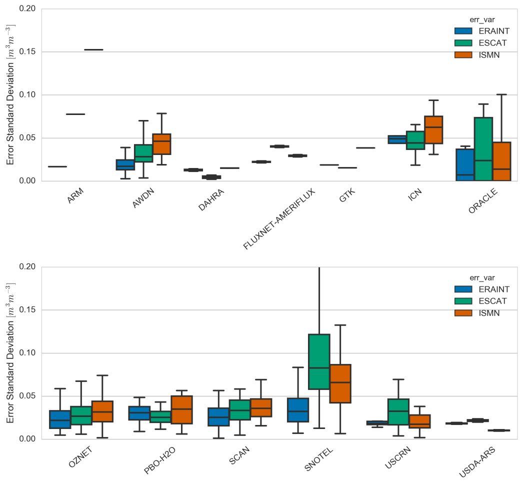
(a) ESCAT nominal res. (GLDAS)



(b) ESCAT high res. (GLDAS)



(c) ESCAT nominal res. (ERA-Interim)



(d) ESCAT high res. (ERA-Interim)

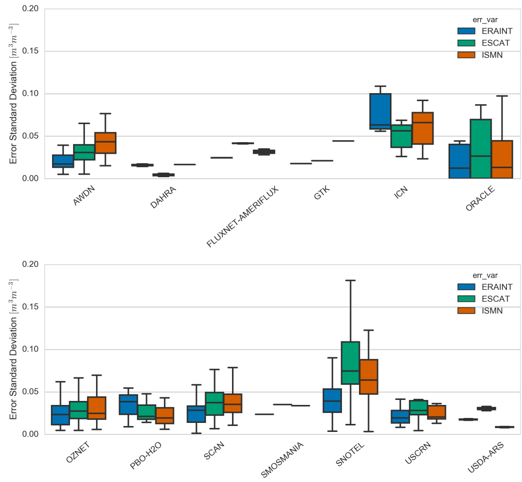


Figure C.1: Error Standard Deviation boxplots per in situ network of the Local Scale Validation.

C.2. Spearman ρ

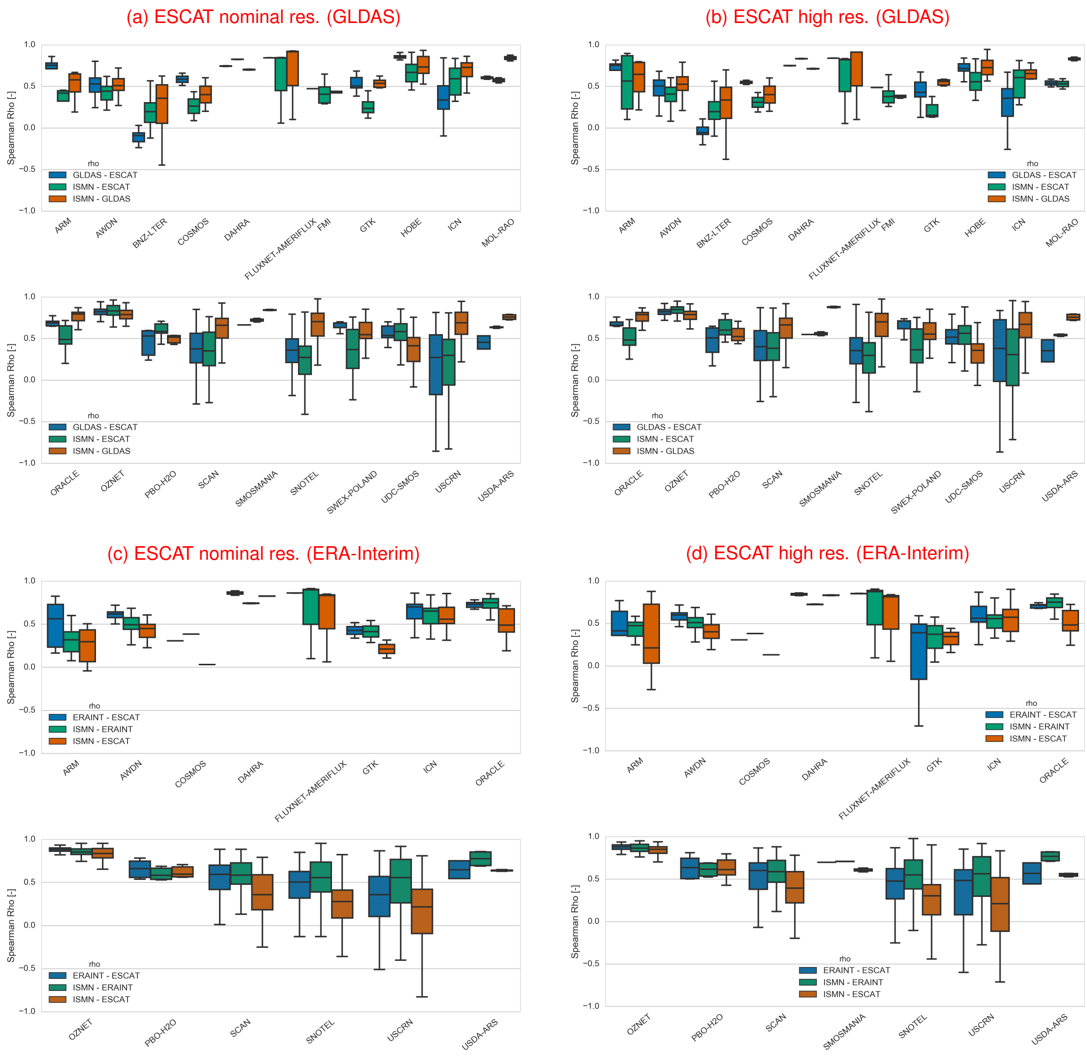


Figure C.2: Spearman Correlation Coefficient boxplots per in situ network of the Local Scale Validation.

C.3. Bias

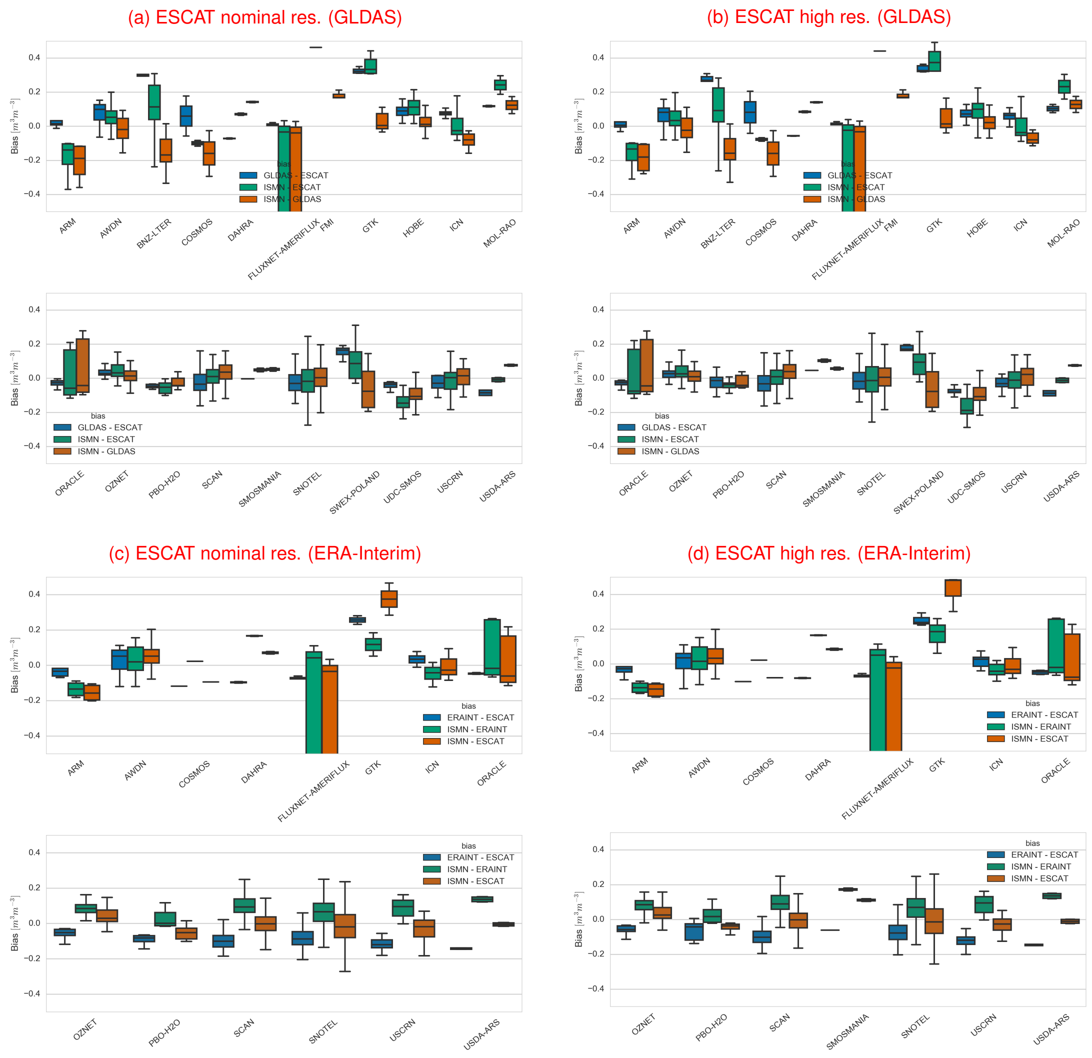


Figure C.3: Bias boxplots per in situ network of the Local Scale Validation.

C.4. Unbiased Root Mean Square Difference

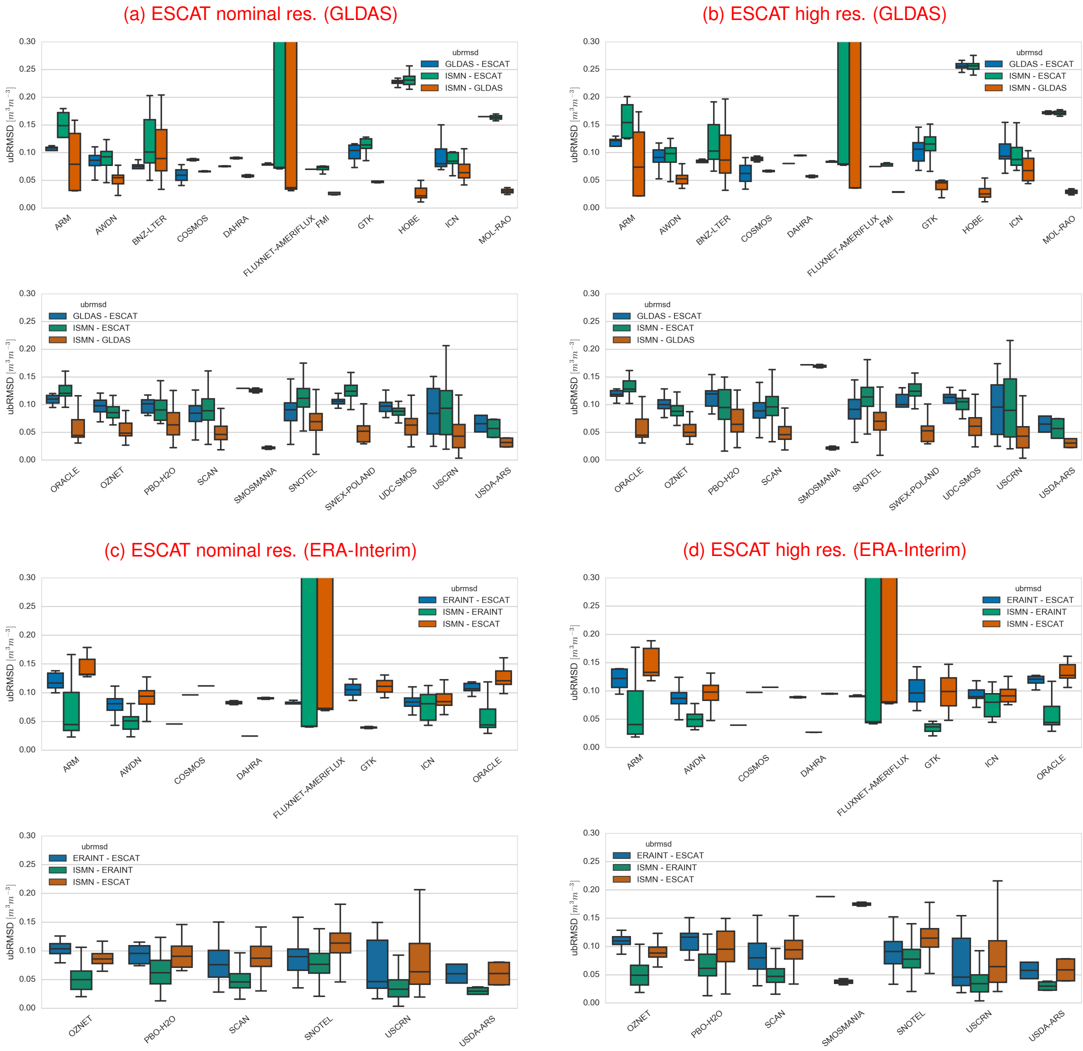


Figure C.4: Unbiased Root Mean Square Difference boxplots per in situ network of the Local Scale Validation.