



FRM4SM – Fiducial Reference Measurements for Soil Moisture



QA4SM Software User Manual

Version 3.1

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Prepared by

Angewandte Wissenschaft, Software und Technologie GmbH



in cooperation with

Vienna University of Technology

CESBIO



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For any clarifications, please contact support@qa4sm.eu.

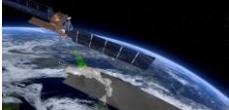
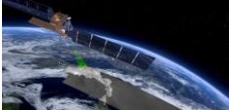
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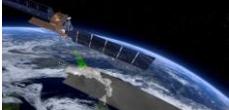
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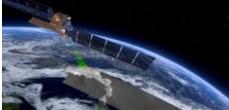
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Acronyms

AWST	Angewandte Wissenschaft Software und Technologie GmbH
C3S	Copernicus Climate Change Service
CCI	Climate Change Initiative
CDRs	Climate Data Records
CEOS	Committee on Earth Observation Satellites
CESBIO	Centre d'Etudes Spatiales de la Biosphère
CMUG	Climate Modelling User Group
DOI	Digital Object Identifier
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EODC	Earth Observation Data Centre
ESA	European Space Agency
FAQ	Frequently Asked Questions
FRM	Fiducial Reference Measurements
FRM4SM	Fiducial Reference Measurements for Soil Moisture
GCOS	Global Climate Observing System
GEO	Group on Earth Observation
GEWEX	Global Energy and Water Cycle Experiment
CGLS	Copernicus Global Land Service
GUI	Graphical user interface
GTOS	Global Terrestrial Observing System
ISMN	International Soil Moisture Network
NASA	National Aeronautics and Space Administration
NRT	Near Real Time
QA	Quality Assurance
QA4SM	Quality Assurance for Soil Moisture
RFI	Radio Frequency Interference
SAR	Synthetic Aperture Radar
SM	Soil Moisture
SMAP	Soil Moisture Active Passive
SMOS	Soil Moisture and Ocean Salinity
TC	Triple Collocation
TOPC	Terrestrial Observation Panel on Climate
TUW	TU Wien

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1 Introduction

1.1 Purpose and scope of document

The QA4SM Software User Manual describes how to use the QA4SM service qa4sm.eu to perform automatic validations of selected soil moisture datasets, how to interact with the QA4SM user interface and how to troubleshoot problems and get support. It also provides a high-level technical overview of the QA4SM service and an overview of the implemented validation methods and metrics. An example validation is used to describe the supported types of validations, the inputs and user options and the generated outputs together with their interpretation.

This document describes features of QA4SM release 3 for the FRM4SM project, which was deployed in December 2024.

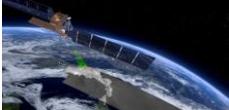
The current QA4SM Software User Manual is deliverable DT3-1 of the FRM4SM project under contract number 4000135204/21//I-BG. FRM4SM is an ESA project to establish best practice for validation of soil moisture derived from satellite measurements based on a metrological approach to define fiducial reference data.

1.2 Document overview

Following the general introduction in section 1, section 2 provides an introduction to the QA4SM service and its intended purpose. Section 3 describes the currently supported datasets, which are planned to get further extended during the FRM4SM project. Section 4 provides an overview of the validation methods and metrics which are implemented in QA4SM and contribute to the generated validation results. Section 5 describes the complete QA4SM user interface and is organised by the relevant QA4SM web pages which can be accessed. The subsequent section 6 outlines which types of validations are supported, which inputs and options user can select before starting a validation and which outputs and reports are generated for QA4SM validations. Section 7 illustrates this with a specific example validation and demonstrates the end-to-end user workflow from data selection to result interpretation. Section 8 contains a high-level technical overview of QA4SM and its IT environment. Section 9 describes how user can obtain support and contains a comprehensive list of frequently asked questions (FAQ). Finally, section 10 contains scientific references and a full list of references to all in-situ station networks which are integrated into ISMN.

1.3 Target audience

This document is addressed to the users of the QA4SM online validation service, focusing on EO scientists who need to validate soil moisture datasets or compare results between different data validations. It may also be of interest for scientists who work on general QA

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aspects of satellite-based soil moisture data or other EO variables and are interested in automated data validation methods. Beyond that, the user manual and the QA4SM service are available and freely accessible for all users who are interested in soil moisture data validation.

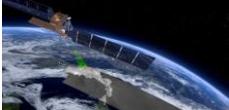
2 QA4SM introduction and overview

QA4SM is an online validation tool for soil moisture data products implementing best practice validation methods and providing full traceability and repeatability of validations performed by its users. It is geared towards facilitating scientific data validation studies and their mutual comparability.

Different factors contribute to errors in satellite derived climate data records. Their quality depends on the measurement principle, characteristics of the used sensor and the model respectively the algorithm to derive climate variables from raw observations. The aim of quality assurance (QA) in this context is not only to find processing errors in the data, but also to evaluate their representativeness of actual (environmental) conditions and to detect (local) artefacts in observations (Loew et al., 2017). The goal is to understand strengths and weaknesses of different data products and to answer the question which dataset is most suitable for a specific purpose.

Quality assurance of satellite derived climate data records has therefore been the topic of numerous studies in the past. It can be very specific - e.g., to analyse certain features in a specific dataset such as for example Radio Frequency Interference (RFI) in L-band observations (Olivia at al., 2016) - or general, to compare the overall (global) performance of different products (e.g., Al-Yaari et al., 2019; Beck et al., 2021). The satellite soil moisture community has, over time, adapted QA methods based on other climate variables, but also developed their own approaches to evaluate the performance of SM products. Guidelines which describe some of those best practices exist in works of e.g., Gruber et al., 2020 and Montzka et al., 2020. While there is a general agreement on best practices for SM validation, until recently there was no open platform that integrated them. QA4SM does this as a free-to-use web validation tool for (satellite) SM data. Best practices for satellite SM validation can change over time, due to the availability of new data products (e.g., Synthetic Aperture Radar (SAR) derived high resolution SM products (Bauer-Marschallinger et al., 2019)) or demands on how the data is used (e.g. applicability for long-term analyses) or further evolution on validation protocols (e.g. FRM4SM project). QA4SM aims to adapt to these new requirements while maintaining a general, not too specific and therefore easy to use interface with according options for users to choose from.

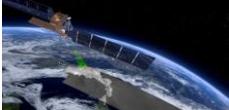
“Validation” in the context of QA4SM therefore refers to a process of inter-comparing two or more SM data products. One dataset is declared as the “reference”. While this “reference”

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does not represent the “true” SM state (which is impossible to know exactly) it is the benchmark that other datasets are compared to in terms of bias, correlation coefficients and other metrics. It is also the reference for temporal and spatial matching for datasets with different temporal/spatial sampling (the process of finding corresponding observation points and time stamps between multiple datasets), and the scaling reference (the process of removing biases between observations series caused by differences in data sampling). A more detailed description on this is given in sections 4.2 and 4.3.

With the constantly increasing number of available satellite sensors, data products / versions and processing libraries, and with the availability of Near Real Time (NRT) data products, it becomes more and more difficult to retrace the origin of data used in an application or independently repeat certain analyses. Therefore, in the Earth observation community, more and more effort is put into making data and software traceable and providing interfaces for using data in a consistent way. In QA4SM, a collection of versioned datasets is integrated, the platform and validation algorithm versions are tracked and an automated release procedure allows to maintain a reproducible history of changes made to the software. In addition, QA4SM allows users to publish results of validation runs and archive them on an independent platform (<https://zenodo.org/>) from where they can be downloaded using the assigned Digital Object Identifier (DOI). QA4SM also allows users to restore settings from previous validation runs (including from other users), to easily repeat certain analyses.

QA4SM is an open-source project, all code is publicly available on GitHub (<https://github.com/awst-austria/qa4sm>). The same applies to all dependencies, i.e. software libraries that are implemented in QA4SM, which includes all data pre-processing and validation results post-processing libraries. While all developed and integrated software is open source, the data used in the service may not be. This depends on restrictions set by the data provider. Therefore, it is not possible to download any data directly through the service. However, detailed instructions on the data origin, version and citation when using it in a publication are given on the service website as well as in the next section of this document.

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3 Available datasets

QA4SM implements a time-series based data model for all datasets available in the service. At the moment, most datasets in QA4SM are updated on an occasional basis. However, for some dataset versions, QA4SM is connected to operational datastreams, allowing automatic temporal extensions. More details about the affected versions are given in the following chapters.

It is up to the user to decide which dataset is used as the reference for a specific validation. The selected reference will affect the spatial sampling of validation results, the unit of some validation metrics and the scaling step (if selected). An up-to-date list of available datasets can be found at <https://qa4sm.eu/ui/datasets/>. This provides information on data sources, citations and availability/temporal coverage amongst others. Below, a short description of datasets currently available in the service is provided.

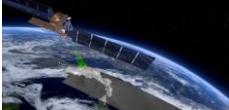
3.1 ESA CCI Soil Moisture (COMBINED)

The COMBINED product of ESA CCI SM (Dorigo et al., 2017; Gruber et al., 2019) merges satellite SM data from active (scatterometer) and passive (radiometer) sensors (compare sections 3.4 and 3.5) into one single, daily, harmonised record with 0.25° resolution and quasi global coverage (from 180°W 60°S to 180°E 90°) over land. Triple Collocation Analysis (TCA) is used to rate the performance of each sensor via its Signal-to-Noise ratio (SNR). Accordingly, merging weights are assigned to each sensor. At each location, all sensors are brought into the dynamic range of GLDAS Noah (0-10 cm Soil Moisture) using (trend-preserving) CDF scaling (Dorigo et al., 2012; Liu et al., 2011). The variable ‘sm’ in COMBINED is given in volumetric units (m³/m³) - same as for the PASSIVE product - but has a slightly different absolute value range due to the scaling to GLDAS. Quality flags and satellite overpass indicators are amongst the meta data for each observation and are used for (optional) filtering before using the data in a validation run. Mandatory quality flags (for dense vegetation, frozen soils and other conditions which make the merging process unreliable) are already applied to the SM variable. Therefore, generally no data is available at soil temperatures <0° C, in rainforest areas (compare Figure 1) and areas with high topographic complexity. It is recommended to use un-flagged (0=“good”) values for validation purpose. The original data are available at:

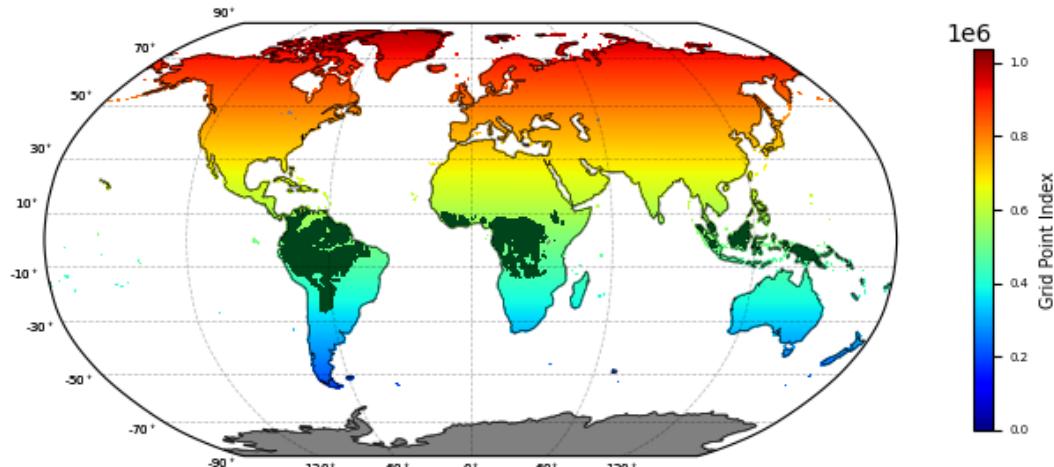
<https://www.esa-soilmoisture-cci.org/> and <https://catalogue.ceda.ac.uk/>.

The following versions of ESA CCI SM COMBINED are available in the service:

- **v4.4 / v4.5 resp. v4.7** were released in 2019 resp. in March 2020. For the first time, the COMBINED product was not generated from the merged ACTIVE and PASSIVE products directly, but - in the same way as the ACTIVE/PASSIVE products - from the original L2 input data. The temporal coverage is from 1978-11-01 to 2018-12-31 (v4.4 and v4.5), resp. 2019-12-31 (v4.7).

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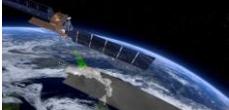
- **v5.2** was released in September 2020 and for the first time included SMAP in an official release of the product. The temporal coverage is from 1978-11-01 to 2019-12-31.
- **v6.1** was released in April 2021 and includes two new passive sensor products (GPM and FengYun-3B; in addition, TMI was extended until 2015) as well as various improvements on data flagging. The temporal coverage is from 1978-11-01 to 2020-12-31.
- **v7.1** was released in Spring 2022. Daytime observations were included for the first time for all sensors, using a new version of the retrieval model for passive sensor products. 3 additional sensors (ASCAT-C, FY-3C, FY-3D) were included as well as a temporal break correction algorithm (Preimesberger et al., 2021) and a seasonal CDF scaling approach.
- **v8.1** was released in Spring 2023 and came with intra-annual uncertainty estimates (Stradiotti et al., 2024) as well as a refined flagging strategy for frozen soils and barren grounds.
- **v9.1** was released in Summer 2024 and includes an update to the seasonal CDF matching from v7, where in some areas irrigation signals were lost. In addition, the temporal coverage was extended to the end of 2023.



*Figure 1: Spatial coverage of the ESA CCI SM and C3S SM products.
Rainforest areas (dark green) are masked out in the product.*

3.2 C3S Soil Moisture (COMBINED)

The COMBINED product of C3S SM implements the ESA CCI SM merging algorithm to generate long-term Climate Data Records (CDRs) from active and passive satellite sensor products in near-real-time (NRT). The data is available globally (from 180°W 60°S to 180°E 90°N, same as in Figure 1) in quarter degree (0.25°) resolution. The variable “sm” contains SM observations derived from both radiometer and scatterometer measurements. Same as ESA CCI SM, C3S SM contains a quality flag variable and a satellite overpass indicator variable that can be used to filter the input data for validation. Mandatory flags are already applied to the SM variable,

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meaning that no data is available for rainforest areas and under frozen soil conditions. We recommend using only values that are flagged as “good” (flag=0) for validation purpose. The original data are available at: <https://cds.climate.copernicus.eu>.

Currently the following versions of C3S SM that are available in the service.

- **v201706** was generated in June 2017 and is based on the ESA CCI SM v3 algorithm. The temporal coverage is 1978-11-01 to 2017-06-30.
- **v201812** was generated in January 2019 and is based on the ESA CCI SM v4 algorithm. The temporal coverage is 1978-11-01 to 2018-21-31.
- **v201912** was generated in January 2020 and is also (same as v201812) based on the ESA CCI SM v4 algorithm. Updates to the passive L2 input data were applied.
- **v202012** was generated in January 2021 and is based on the ESA CCI SM v5 algorithm, which introduced SMAP as an additional (passive) sensor product.
- **v202212** was generated in Spring 2022 and is based on the ESA CCI SM v7 algorithm. The data of this version of the C3S product is currently updated one per week in the QA4SM service.
- **v202312** was generated in Spring 2024 and is based on the ESA CCI SM v8 algorithm. The data of this version of the C3S product is currently updated one per week in the QA4SM service.

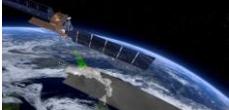
v202212 and v202312 are currently automatically extended on a weekly basis, meaning that the temporal coverage of the data in the service should generally be in line with the data available through CDS. C3S SM data on CDS shows a delay of ~20 days from present day.

3.3 CGLS SSM / SWI

The Copernicus Global Land Service Surface Soil Moisture (SSM) data (Bauer-Marschallinger et al., 2018) is derived from measurements of the Sentinel-1 C-Band Synthetic Aperture Radar (SAR) instrument. The retrieval algorithm applies a change detection model on the geo-corrected and radiometrically calibrated backscatter values to derive SSM on a ~1 km (1/112 degree) resolution over Europe. SSM is given in % saturation by linearly scaling the angle-normalized backscatter between the lowest/highest values at each location.

The original SSM data are available at <https://land.copernicus.eu/global/products/ssm>.

The CGLS Soil Water Index (SWI) (Bauer-Marschallinger et al., 2019) product is created from a fusion of Sentinel-1 C-Band SAR SSM and Metop ASCAT scatterometer measurements. It uses a two-layer water balance model which describes the relationship between surface and profile soil moisture as a function of time. It is an exponential filter that has one parameter (T) which is related to infiltration time. T-values 5 and 40 (corresponding to a top and one root-zone layer) are available in QA4SM as separate variables. Same as SSM, SWI available with a ~1 km resolution over Europe.

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The original SWI data are available at <https://land.copernicus.eu/global/products/swi>.

For both products QA4SM provides a filter to exclude values above/below the geophysical min/max (0-100 %).

CGLS and SSM product are produced in near-real-time, however the data in QA4SM are currently not regularly updated:

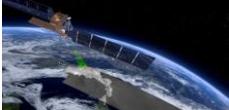
- CGLS SSM V1.1 is available from 2014-10-03 to 2020-08-31.
- CGLS SWI V1.0 is available from 2014-10-03 to 2020-08-31.

3.4 ESA CCI Soil Moisture (ACTIVE)

The ACTIVE product of ESA CCI SM merges spatially (0.25°) and temporally (daily) resampled scatterometer based SM products from ERS and MetOp ASCAT into one product. ERS SM is based on observations from ERS 1 and ERS 2; ASCAT Surface Soil Moisture (SSM) (compare section 3.6) uses MetOp ASCAT-A and ASCAT-B observations and is produced by H SAF (Hahn et al., 2018). Data coverage after 2007 is significantly higher than for earlier periods due to the availability of ASCAT from that year onwards. ERS observations are inter-calibrated to those from ASCAT to generate a harmonised long-term record. No observations are available in the period from 2003-02 to 2003-08 as no ERS data is available in that time. The TU Wien method is used to retrieve SM from backscatter measurements for all sensors (compare section 3.6). The variable ‘sm’ is used in QA4SM and describes the level of saturation of soil in percent. Values therefore range from 0-100 %. As for the other CCI SM products, no data is available over rainforest areas, areas with high topographic complexity and when soils are frozen. Similar as for other products, it is recommended to filter SM for “good” values based on the variable ‘flag’ and to use only values where flag=0. The original data are available at: <https://www.esa-soilmoisture-cci.org/> and <https://catalogue.ceda.ac.uk/>.

The following versions of ESA CCI SM Active are available in QA4SM:

- **v4.5** uses WARP 5.8.0 H113 & H114 ASCAT MetOp-A and MetOp-B data as input. The temporal coverage is from 1991-08-05 to 2018-12-31.
- **v5.2** uses H115: Metop ASCAT SSM CDR v5 12.5 km sampling, DOI: 10.15770/EUM_SAF_H_0006 and H116: Metop ASCAT Surface Soil Moisture Climate Data Record v5 Extension 12.5 km sampling; The temporal coverage is from 1991-08-05 to 2019-12-31.
- **v6.1** uses H-SAF H119 Metop ASCAT SSM 12.5 km CDR v5. The temporal coverage is from 1991-08-05 to 2020-12-31.
- **v7.1** uses H-SAF H120 12.5 km ASCAT SSM, and includes data from ASCAT C. The temporal coverage is from 1991-08-05 to 2021-12-31.
- **v8.1** uses H-SAF H120 12.5 km ASCAT SSM and covers the period from 1991-08-05 to 2023-12-31.

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- **v9.1** uses H-SAF H120 12.5 km ASCAT SSM and covers the period from 1991-08-05 to 2024-12-31.

3.5 ESA CCI Soil Moisture (PASSIVE)

The PASSIVE product of ESA CCI SM exclusively merges SM products derived from radiometer observations into one harmonised long-term product (1978-present). Observations from the following satellite sensors/platforms are used in this data: SMMR, SSM/I, TMI, Windsat, AMSR-E, AMSR-2, SMOS, SMAP¹, FengYun-3B² and GPM³. For most sensors (except SMOS, GPM and TMI) only data from the descending overpass is used. The Land Parameter Retrieval Model (LPRM) is used to derive SM from brightness temperature measurements (Owe et al., 2008; van der Schalie et al., 2016). All sensor products are spatially and temporally resampled (daily, 0.25°), scaled to AMSR-E and merged based on their SNR from TCA (compare section 3.1). The variable ‘sm’ is used for validations and describes the volumetric soil moisture in the top few centimetres of soil and is given in m³/m³ (the exact depth depends on the observations frequencies of merged sensors). No data is available in areas flagged as rainforests, as extremely mountainous or for frozen soils. It is recommended to filter SM for “good” values based on the variable ‘flag’ and to use only values where flag=0. The original data are available at:

<https://www.esa-soilmoisture-cci.org/> and <https://catalogue.ceda.ac.uk/>.

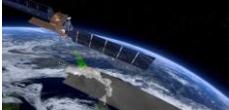
The following versions are available in QA4SM:

- **v04.5** uses LPRM v6 for SMOS, AMSR-E and AMSR2 and LPRM v5 for all other passive sensors. Available from 1978-11-01 to 2018-12-31.
- **v05.2** uses LPRM v6 for passive sensors products (incl. SMAP), available from 1978-11-01 to 2019-12-31.
- **v06.1** uses LPRM v6.1 for all passive sensor products (incl. GPM and FengYun-3B), available from 1978-11-01 to 2020-12-31.
- **v07.1** uses LPRM v7 for all passive sensors except SMAP and SMOS. Includes the following new sensors: FengYun-3C and -3D). Available from 1978-11-01 to 2021-12-31.
- **v08.1** uses LPRM v7 for all passive sensors except SMAP and SMOS. Uncertainty estimates were updated. Available from 1978-11-01 to 2022-12-31.
- **v09.1** uses LPRM v7 for all passive sensors except SMAP and SMOS, available from 1978-11-01 to 2023-12-31.

¹ From v5 onwards

² From v6 onwards

³ From v6 onwards

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3.6 HSAF ASCAT SSM

The EUMETSAT H-SAF ASCAT SSM provides global sub-daily soil moisture observations on a discrete global grid (DGG) with a 12.5 km sampling. Observations are provided from the ASCAT instruments on-board both Metop-A and Metop-B. SM is retrieved using the TU Wien change detection approach (Wagner et al., 1999) implemented in the Water Retrieval Package (WARP). HSAF ASCAT SSM provides SM in units of % saturation as well as multiple quality indicator fields (confidence flags, processing flags, surface state flag, correction flag). We recommend using only unflagged (good) observations. Data are available spatially from 180° W 90° S to 180° E 90° N. The original data are available at:

https://hsaf.meteoam.it/Products/ProductsList?type=soil_moisture.

The version available in the service is:

- **H113** was released in 2018 and contains data from 2007-01-02 to 2017-12-31 (Hahn et al., 2018).
- **H119⁴** was released in 2021 and contains data from 2007-01-02 to 2020-12-31

3.7 ERA5

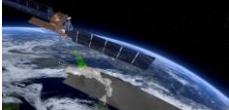
ERA5 is a global reanalysis product generated by ECMWF (Hersbach et al., 2018). It provides global, sub-daily simulations of variables for land, atmosphere and ocean waves. Values from the downloaded original 6-hourly (starting at 0:00 UTC) images of ERA5 Volumetric Soil Moisture and Soil Temperature with a spatial resolution of 0.25° are used in QA4SM. The ERA5 dataset starts in 1979 and is produced in NRT. Static snapshots of the data are used in QA4SM at the moment. The version number used in QA4SM indicates the date when the original data was downloaded. The volumetric soil water content of layer 1 variable (“swvl1”, in m³/m³) is used for validation. A filter to exclude values for frozen soil conditions can be activated. In that case for each time stamp it is checked if the soil temperature for layer 1 (“stl1”) is above 0° C. If not, frozen soil conditions (under which satellite SM cannot be retrieved) are likely, and swvl1 values are masked in the validation run. The data is available globally from 180°W 90°S to 180°E 90° N. The original data are available at:

<https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-single-levels>.

The version available in the service is:

- **v20190613** is a snapshot of the reanalysis from 2019-06-13, data ranges from 1979-01-01 to 2019-03-31. This version is **deprecated**, please use the “latest” version instead.
- **latest** is the generic version name for ERA5 data in QA4SM introduced after 2019. This includes is automatically updated on a weekly basis with new data from CDS. ERA5T

⁴ <https://hsaf.meteoam.it/Products/Detail?prod=H119> - DOI: [10.15770/EUM_SAF_H_0009](https://doi.org/10.15770/EUM_SAF_H_0009)

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(preliminary) data, which usually comprises the latest ~2 months of the record are **not** used, which means that on a given day the time series in the service should reach until about two months before that day. The latest version of ERA5 data used in the QA4SM service is currently updated once per week.

3.8 ERA5-Land

ERA5-Land (Muñoz Sabater, 2019; Muñoz Sabater et al., 2021) has been produced by replaying the land component of the ECMWF ERA5 climate reanalysis. The downloaded original 6-hourly (starting at 0:00 UTC) images of ERA5-Land Volumetric Soil Moisture (in m³/m³) and Soil Temperature have a spatial resolution of 0.1 degrees (~9 km). ERA5-Land is available from January 1981 onward with a delay of 3-4 months. The Soil Temperature variable (“stl1”) is used to mask Soil Moisture (“swvl1”) under frozen conditions if selected, as described in section 3.7. The version number used in QA4SM indicates the date when the original data was downloaded. The data is available globally from 180°W 90°S to 180°E 90°. The original data are available at: <https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-land>.

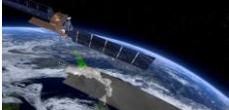
The version available in the service is:

- **v20190904** is a snapshot of the reanalysis data from 2019-09-04; time coverage from 2001-01-01 to 2019-04-30. This version is **deprecated**, please use the “latest” version instead.
- **latest** is the generic version name for ERA5-Land data in QA4SM introduced after 2019. This includes is automatically updated on a weekly basis with new data from CDS. ERA5-Land T (preliminary) data, which usually comprises the latest ~2 months of the record are **not** used, which means that on a given day the time series in the service should reach until about two months before that day. The latest version of ERA5-Land data used in the QA4SM service is currently updated once per week.

3.9 GLDAS Noah

The Global Land Data Assimilation System (GLDAS) models several land surface parameters using ground based and space based observations (Rodell et al. 2004). It was developed by the National Aeronautics and Space Administration (NASA) Goddard Space Flight Center (GSFC) and the National Oceanic and Atmospheric Administration (NOAA) National Centers for Environmental Prediction (NCEP). GLDAS drives multiple land surface models. In QA4SM simulations from the Noah model using GLDAS v2.1 are available globally between 180°W 60°S to 180°E 90°N with a resolution of 0.25°. Four SM layers are available in the service: 0-10 cm, 10-40 cm, 40-100 cm and 100-200 cm. SM in GLDAS Noah is given in kg/m². For each SM layer the according soil temperature fields can be used to exclude values where GLDAS Noah Soil Temperature is below 0° C upon selection. The original data are available at:

https://disc.gsfc.nasa.gov/datasets/GLDAS_NOAH025_3H_2.1/summary.

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The version in the service is:

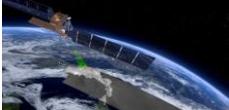
- **v2.1** is forced with a combination of model and observation data from 2000 onward. In the service, values from 2000-01-01 to 2017-12-31 are available.

3.10 International Soil Moisture Network (ISMN)

The ISMN (Dorigo et al., 2011; Dorigo et al., 2013; Dorigo et al.; 2021) has been established as a centralised data-hosting facility where globally available in-situ soil moisture measurements from operational networks and validation campaigns are collected, harmonised, and made available to users. It exists as a means for the geo-scientific community to validate and improve global satellite observations and modelled products. The measurements contributing to the ISMN are heterogeneous in that the measurement technique/device, depth represented, and other factors, may vary within the network. The temporal resolution of the datasets is very diverse depending on the site: 20 min, 30 min, hourly, 6-hourly, 12-hourly, daily and weekly. The temporal coverage also depends on the station. Measurements for different depth layers and depth ranges are available (between 0 to 2.6 m). Within the QA4SM service users can select specific networks and sensors in specific depths to use for validation. All ISMN networks are available in the service (references for all networks are given in section 10.1) from which a pre-selection of default networks in the user interface has been made upon recommendation of the ISMN data providers. The ISMN assigns standardised data flags to all their networks which indicated potential erroneous observations, e.g., due to the frozen soils or sensor malfunction. It is recommended to only use “G”-flagged values for validation. In addition to the flags distributed by the producer, there is an option in QA4SM to apply the “Representative sensors” flag, which uses the Fiducial Reference Measurement concept developed in FRM4SM project deliverable DT2-1, FRM Protocols and Procedures for Soil Moisture (FPP_SM), to distinguish between ‘representative’, ‘not representative’ and ‘undeducible’ (i.e., not classifiable) sensors for satellite SM validation. Multiple snapshots of the ISMN database are available in QA4SM. The version number indicates when the data was downloaded and what state of the database it therefore represents. Differences between versions can include additional networks, reprocessed flags and updated (meta) data. The original data are available at: <https://ismn.earth>.

Versions in the service are:

- **20191211 global**: This is a snapshot of the ISMN archive from from 2019-12-11.
- **20210131 global**: Contains additional networks and data until the end of January 2021 for NRT networks.
- **20230110 global**: Contains additional networks and data until the end of December 2022 for NRT networks.
- **20240314 global**: Contains all available networks and data as of March 2024.

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3.11 SMAP SPL3SMP

Soil Moisture Active Passive (SMAP) is a satellite launched by NASA that operates in the L-band range and is therefore specialized in measuring SM. While SMAP carries both a radiometer and radar, the radar stopped operating shortly after launch. Therefore, only radiometer measurements are widely used for SM retrieval. NASA provides their own L3 soil moisture products from SMAP. The official SPL3SMP product is integrated into QA4SM. It contains SM fields on a cylindrical 36 km Equal-Area Scalable Earth grid (EASE-Grid v2.0). SPL3SMP data is available for 2 satellite overpasses (AM/descending, resp. PM/ascending). At the moment, only data for the PM overpass are available in QA4SM. The spatial coverage is from -180° W, -85.044 °S to 180° E, 85.044° N. The original data are available at: <https://nsidc.org/data/spl3smp>.

- **v5 PM/ascending** contains data downloaded in December 2018 from the ascending overpass. The time range of this version is from 2015-03-31 to 2018-12-04.
- **v5 AM/descending** contains data downloaded in December 2018 from the descending overpass. The time range of this version is from 2015-03-31 to 2018-12-04.
- **v6 PM/ascending** contains data downloaded in May 2020 from the ascending overpass. The time range of this version is from: 2015-03-31 to: 2020-05-23.
- **v6 AM/descending** contains data downloaded in May 2020 from the descending overpass. The time range of this version is from: 2015-03-31 to: 2020-05-23.
- **v8 PM/ascending** contains data downloaded in July 2022 from the ascending overpass. The time range of this version is from: 2015-03-31 to: 2022-07-26.
- **v8 AM/descending** contains data downloaded in July 2022 from the descending overpass. The time range of this version is from: 2015-03-31 to: 2022-07-26.

3.12 SMAP SPL2SMP

This data set contains the Level 2 SMAP product, consisting of half-orbits with observations at 6.00 AM and 6.00 PM times. Sensor specifics, resolution and coverage are the same as for SMAP SPL3SM (§ 3.11).

- **v8** contains data downloaded in August 2022 with time range from: 2015-03-31 to: 2022-08-06.

3.13 SMOS-IC

Prior to SMAP, SMOS was launched by ESA in November 2009 as the first satellite mission specialized on retrieving SM over land. SMOS-IC is a data set produced by INRA / CESBIO (Fernandez-Moran et al., 2017). It uses brightness temperature observations from L-band together with a land cover class based algorithm from multi-angular observations to derive daily, global SM and VOD. Parameter retrieval is based on the inversion of the L-band

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Microwave Emission of the Biosphere (L-MEB) forward model (Wigneron et al., 2007). The processor is designed to be as independent as possible from any ancillary data. Assumptions, such as on the heterogeneity of pixels, simplify parts of the retrieval process by reducing the number of unknown model parameters, and allow performant generation of the product. SMOS-IC SM represents the water content in the top soil layer (~ 0-3 cm).

Multiple quality flags are provided for SMOS-IC to filter the data before using it in an application. Scene flags contain information on the surface state, and can be used to filter out locations where SM retrieval is unreliable due to various environmental conditions (frozen soils, strong topography etc.). Processing flags indicate cases where the SM retrieval failed or where it is suspected that the retrieval algorithm returned dubious results. For validation purpose we suggest using the un-flagged observations. The original data are available at:

<https://www.catds.fr/Products/Available-products-from-CEC-SM/SMOS-IC>.

Currently the following versions of SMOS-IC are available in QA4SM:

- **V.105_Ascending** contains SM derived from the ascending overpass of SMOS, released in version 1 of SMOS-IC. The data is available from -180° W, -83.5 °S to 180° E, 83.5° N. The temporal coverage of data in the service is from 2010-01-12 to 2018-12-31.

3.14 SMOS L3

SMOS Soil Moisture from another retrieval algorithm is included in QA4SM as “SMOS Level3 (L3)” (Al Bitar et al., 2017). This retrieval applies a qualitative filtering and binning to the L2 swath data to enhance and improve the robustness and quality of SM (and VOD) retrievals from multi-orbit, dual-polarisation brightness temperature measurements. The L3 data comes with a large number of quality flags to filter out SM measurements when the following factors are significantly present in the observed scene (1) ice surfaces; (2) frozen soils or snow cover; (3/4) low/high urban surface types;(5) surface water; (6) strong precipitation; (7) dense forest cover; (8) Radio Frequency Interference (RFI); (9/10) strong/moderate topography. Filters 1, 8 and 9 are always applied in QA4SM. Users can change the RFI probability threshold (between 0 and 1, where 1 would deactivate the filter). The data are stored on the 25 km Equal-Area Scalable Earth Grid version 2.0 (EASE-Grid 2.0). The original data are available at <https://www.catds.fr/Products/Available-products-from-CPDC>.

Currently the following versions of SMOS L3 are included in QA4SM

- **Version 339 Ascending** contains SM derived from brightness temperature measurements taken during the ascending (AM) overpasses of SMOS. Data is available from 2010-07-01 to 2022-05-07.
- **Version 339 Descending** contains SM derived from brightness temperature measurements taken during the descending (PM) overpasses of SMOS. Data is available from 2010-07-01 to 2022-05-07.

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3.15 SMOS L2

The Level 2 SMOS Soil Moisture product is geo-located in an equal-area grid system ISEA 4H9, which introduces less spatial distortions in the L1 measurements compared to the regular gridded L3 product. The pixels are stored in pole-to-pole files (one per half-orbit), with 29 half orbits per day. The product is accompanied with the following flags: (1) High confidence filtering of RFI ($RFI > 0.1\%$); (2) Good confidence filtering of RFI ($RFI > 0.2\%$); (3) Strong topography in scene; (4) Frozen ground in scene; (5) Ice in scene; (6) Open water in scene; (7) Snow in scene; (8) Retrieval quality threshold ($X^2 > 5\%$ by default). The original data is distributed at: <https://earth.esa.int/eogateway/catalog/smox-science-products>.

Currently the following versions of SMOS L2 are included in QA4SM:

- **Version 700:** contains SM derived from brightness temperature measurements taken during the ascending (AM) and descending (PM) overpasses of SMOS. The operational data stream is implemented in QA4SM. New data from FTP is downloaded on a weekly basis to extend the time series in the service. Data is available from 2010-07-01 to present day minus ~1 week. The version 700 data used in the QA4SM service is currently updated once per week.

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4 Implemented validation methods and metrics

The aim of the implemented validation routine is to provide a set of scores that describe the performance of a SM product with respect to a selected reference, according to well-defined accuracy metrics. Detailed descriptions of the available metrics can be found in section 4.1. An individual score represents the value obtained by applying a metric formula to the input time series extracted from the candidate and reference datasets⁵ (and additionally a third dataset in case of Triple Collocation (TC) metrics, see section 4.1.2). These time series are temporally and geographically collocated within the selected validation bounds and characterize SM for a certain location, according to their respective SM product. As each product consists of spatially distributed measurements, often supported by variable grids (e.g., for resolution or geometry, see section 3), a method is implemented to match the respective time series on discrete validation points. Section 4.2 describes how the candidate and reference dataset are spatially and temporally collocated and matched to one another. The accuracy of the candidate with respect to the reference is hence characterized at each validation point. In accordance with the guidelines on best practices in SM validation (Gruber et al., 2020; Montzka et al., 2020), several methods are implemented to perform statistical rescaling of the matched time series, as detailed in section 4.3. Finally, an additional processing option consists of anomalies- and climatology-based validation, using the method explained in section 4.4.

4.1 Validation Metrics

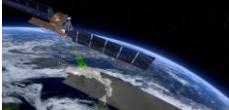
The available validation metrics belong to the categories of Common and Triple Collocation, taking respectively two (candidate and reference) or three input time series (two candidates and one reference). All the metric (and confidence intervals) calculation algorithms are implemented in the Python Toolbox for the Evaluation of Soil Moisture Observations⁶ (pytesmo). This package is routinely maintained and developed and contains the core validation processing routine of QA4SM.

4.1.1 Common Metrics

Considering two time series X and Y (corresponding to the candidate and reference, respectively), the following common metrics are calculated and can be defined as:

⁵ Please note that the term dataset is used here and in the following documentation to indicate a collection of temporal estimates of SM at distinct points or at a single point, or a specific SM product from the ones described in section 3.

⁶ Full documentation at: <https://pytesmo.readthedocs.io/en/v0.6.10/api/pytesmo.html>

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Pearson's r and p -value

The correlation of the two time series as expressed by covariance normalized over the two respective standard deviations:

$$r = \frac{\sigma_{XY}}{\sigma_X \sigma_Y} = \sum_{i=1}^N \frac{(X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^N (X_i - \bar{X})^2} \sqrt{\sum_{i=1}^N (Y_i - \bar{Y})^2}},$$

where the bar accent indicates the sample mean:

$$\bar{X} = \frac{1}{N} \sum_{i=1}^N X_i$$

and σ indicates the standard deviation, defined for X as:

$$\sigma_X = \sqrt{\frac{1}{N} \sum_{i=1}^N (X_i - \bar{X})^2}$$

The statistical significance of the correlation value, defined by a Student's t test with a threshold of 95% and dependent on the number of points in the two samples, is defined with the p-value.

Spearman's ρ

Defines the correlation between the ranks of the two time series, where a rank is given by the time series sorted by increasing value. Provides an improved characterization of the correlation of non-linearly dependent time series with respect to Pearson's r .

The p-value on Spearman's ρ is defined as for Pearson's r p-value.

Bias

The difference between the means of the two time series:

$$bias = \bar{X} - \bar{Y}.$$

Residual sum of squares (RSS)

Squared difference between the two time series:

$$RSS = \sum_{i=1}^N (X_i - Y_i)^2.$$

Mean squared error (MSE)

Average squared difference between the two time series:

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$$MSE = \frac{1}{N} \sum_{i=1}^N (X_i - Y_i)^2.$$

Mean squared error bias (MSE_{bias})

Squared bias:

$$MSE_{bias} = (\bar{X} - \bar{Y})^2.$$

Mean squared error variance (MSE_{var})

Squared difference of the standard deviations of the two time series:

$$MSE_{var} = (\sigma_X - \sigma_Y)^2.$$

Mean squared error correlation (MSE_{corr})

Decorrelation between the two time series, where r indicates the correlation as expressed by Pearson's r :

$$MSE_{corr} = 2\sigma_X\sigma_Y(1 - r).$$

Root mean squared difference (RMSD)

The root square of the mean quadratic differences:

$$RMSD = \sqrt{MSE} = \sqrt{MSE_{bias} + MSE_{corr} + MSE_{var}}.$$

Unbiased root mean squared difference (ubRMSD)

Bias-removed RMSD, calculated with:

$$ubRMSD = \sqrt{\frac{1}{N} \sum_{i=1}^N [(X_i - \bar{X})(Y_i - \bar{Y})]^2}.$$

In case rescaling is applied to the datasets prior to the metrics calculation, the bias component will be ~ 0 , and the above will be *de facto* analogous to:

$$ubRMSD = \sqrt{\frac{1}{N} \sum_{i=1}^N (X_i - Y_i^X)^2},$$

with Y_i^X indicating the *unbiased quantity* of Y_i .

4.1.2 Triple Collocation metrics

TC metrics stem from the homonymous theory, which characterizes the random error of a dataset measuring a geophysical variable given two ancillary statistically independent time series that estimate the same variable. TC has been consistently applied in the validation of

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satellite-retrieved SM; the interested reader is referred to Gruber et al. (2016) for an extensive overview of the state-of-the-art of TC for SM validation.

Considering three time series X , Y and Z , the error structure of each time series I can be expressed by:

$$I = \alpha_I + \beta_I \theta + \varepsilon_I,$$

where α_I , β_I and ε_I represent an additive and multiplicative bias and the random error of I with respect to the truth, θ . If the time series are rescaled against the arbitrarily defined X (in this case, the validation reference), considering $\alpha_X \equiv 0$ and $\beta_X \equiv 0$, the remaining two time series can be described as:

$$Y^X = \hat{\theta}^X + \varepsilon_Y^X,$$

$$Z^X = \hat{\theta}^X + \varepsilon_Z^X,$$

with the superscript indicating that a rescaling has been applied to match the statistical moments of X , and $\hat{\theta}$ representing the truth as observed by all datasets and affected by the systematic errors on X . The following metrics can be then defined for the non-reference datasets:

Scaling coefficient (β)

The scaling coefficient used to rescale the time series to the reference, β_Y^X and β_Z^X .

Signal-to-noise ratio (SNR)

Ratio of the signal variance on the random error variance, linearised to dB units:

$$SNR[dB] = 10 \log_{10} \left(\frac{\beta_I^2 \sigma_\theta^2}{\sigma_\varepsilon^2} \right),$$

where σ_θ^2 represents the signal variance and σ_ε^2 the error variance.

Standard deviation of the error (STD_{err})

Standard deviation of the estimated random error:

$$STD_{err} = StdDev(\varepsilon_I^X).$$

Values returned by QA4SM are scaled error variances, i.e. the scaling coefficient is applied to the estimated standard deviation of the random error of a dataset:

$$STD_{err,scaled} = \beta * STD_{err}.$$

4.1.3 Confidence intervals

Confidence intervals (CI) are calculated for the given metrics. An extensive overview of the statistical background, definitions and formulations is given in Gruber et al. (2020). Here, only

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a general outline of the equations and methods used for the CI calculation is given; the estimated CI always refer to a confidence level of 95%.

Analytical CI

Common metrics allow for an analytical estimation of the CI, i.e., these can be estimated directly from assumptions on the underlying distribution of the estimates, using their statistical moments (Gilleland, 2010). The generic expression for CI, if a normal distribution is assumed, is given by:

$$\hat{\theta} \pm z_{\alpha/2} * \widehat{se}(\theta),$$

where $\hat{\theta}$ is the central estimate, $z_{\alpha/2}$ is the $\alpha/2^{\text{th}}$ quantile in the cumulative distribution of the estimates, $1 - \alpha$ is the confidence level (i.e., 0.95) and \widehat{se} is the estimated standard error. For the CI around a mean estimate, the expression above takes the form:

$$\hat{\mu} \pm \frac{z_{\alpha/2} * \hat{\sigma}}{\sqrt{n}},$$

where μ is the mean, n is the sample size and the standard deviation is used as estimator of the standard error. In practice, given that the true variance is not known due to the finite (small) sample size, a Student's t distribution with $n - 1$ degrees of freedom is replaced to $z_{\alpha/2}$:

$$\hat{\mu} \pm \frac{t_{\alpha/2, n-1} * \hat{\sigma}}{\sqrt{n}}.$$

This expression is used in the calculation of the CI for the *bias*.

Variance-based CI

For *ubRMSD*, a central χ distribution is assumed, and the CI are given by:

$$\frac{\sqrt{n-1}ubRMSD^2}{\chi_{\rho, n-1}},$$

where $\rho = \alpha/2, 1 - \alpha/2$.

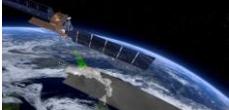
CI of the correlations

For the linear correlation estimates, the lower and upper CI are calculated using (Bonett et al., 2000):

$$\left(\frac{e^{2c_l} - 1}{e^{2c_l} + 1}, \frac{e^{2c_u} - 1}{e^{2c_u} + 1} \right),$$

where for linear (Pearson's) correlations, c_l and c_u are:

$$c_l = v - \frac{z_{\alpha/2}}{\sqrt{n-3}}$$

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$$c_u = \nu + \frac{z_{\alpha/2}}{\sqrt{n-3}}$$

and for Spearman's rank correlation:

$$c_l = \nu - \frac{z_{\alpha/2} * \sqrt{1 + \frac{r^2}{2}}}{\sqrt{n-3}},$$

$$c_u = \nu + \frac{z_{\alpha/2} * \sqrt{1 + \frac{r^2}{2}}}{\sqrt{n-3}},$$

with $\nu = 1/2 \ln \frac{1+r}{1-r}$ and r the Pearson's correlation value of the sample.

Bootstrapped CI

For some metrics, the analytical formulation of the CI is not straightforward (e.g., TC metrics, Gruber et al., 2020). However, the CI can be estimated from a synthetic reconstruction of the metric distribution, obtained through bootstrapping. QA4SM uses the percentile bootstrapping procedure described in Gilleland (2010), where for each estimate 1000 bootstrap samples are used, if a condition of minimum 100 points is met.

4.2 Spatial and temporal collocation of the time series

The datasets described in section 3 are represented in space through a grid that assigns for each measurement a grid point indicator (GPI), which is a different numerical value assigned to each point, and two geographic coordinates, longitude and latitude. For spatially distributed measurements (i.e., satellite- or model-derived datasets), the coordinates (and associated GPI) represent the centre of a sampling pixel, while for in-situ point measurements they represent the exact location of sampling (i.e., the ISMN station position). In the latter case, several GPIs might be associated with the same coordinates, indicating different sampling depths⁷. Provided that all SM products are defined by a grid, the spatial and temporal collocation takes the form of a resampling exercise in the following steps:

- The validation points for a run are provided by all the reference GPIs included in the initially selected (temporal and spatial) validation bounds.
- At each validation point (GPI), the nearest neighbouring (NN) GPI in the candidate grid is found and associated with that validation point. In case of multiple reference GPIs sharing the same NN, the candidate measurement will be validated against each of the

⁷ Detailed description of the ISMN characteristics and reader package at: <https://github.com/TUW-GEO/ismn/blob/master/docs/examples/interface.ipynb>

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reference GPIs measurements. The latter situation often occurs when the in-situ measurements are used as reference, due to several sampling depths or multiple stations falling under the same satellite pixel, or in case the reference grid has a higher resolution than that of the candidate dataset.

- In case the NN GPI found is further from the validation point than the resolution specific of the reference data set, the point is disregarded. For data sets that have no resolution specification (i.e., point measurement data sets like ISMN or user-uploaded data sets), a threshold of 30 km is applied.
- Having identified a candidate-to-reference association at each validation point, the time series between the specified start and end of the validation period are extracted from the datasets. If the candidate or reference GPI is not associated with any measurements for the period of interest, the validation point will not produce any effect on the overall validation result. This also applies when multiple candidate datasets are compared to the same reference; in case not all datasets can be associated with a measurement, the point will not weight on the validation outcome.
- If the time stamps of the candidate and reference time series differ (i.e., there is a time lag between the two closest measurements in time), the temporal sampling interval of the candidate(s) time series is/are mapped to that of the chosen temporal reference (see Figure 15). The nearest neighbour for each time stamp in the reference is found for each candidate time series within the chosen two-sided temporal window (Figure 2). The default window size is 12 hours (i.e. 6 hours before/after each reference time stamp). If the time lag is greater, the measurement is disregarded. Only measurements available for all datasets after temporal matching are used to calculate validation metrics. The optimal size the temporal window depends on the temporal sampling of all datasets and the chosen temporal reference dataset. If the chosen window is smaller than the temporal sampling of the some candidate, temporal matching will not find any quasi-collocated observations. If the chosen window is too large, oversampling will take place, and some observations will be matched multiple times, meaning that some of the matchups are not ideal and that a dataset is overrepresented after temporal matching. The concept is also described in Figure 3. Generally it is suggested to use a larger window, hence the default selection of 12 hours.

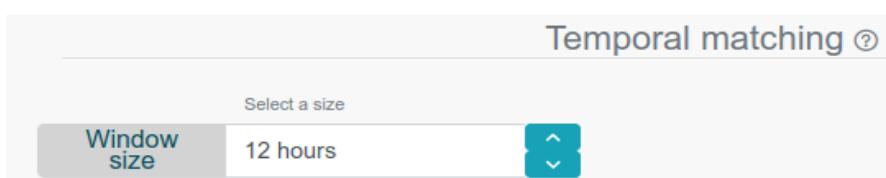


Figure 2: Selection of the temporal matching window in QA4SM.

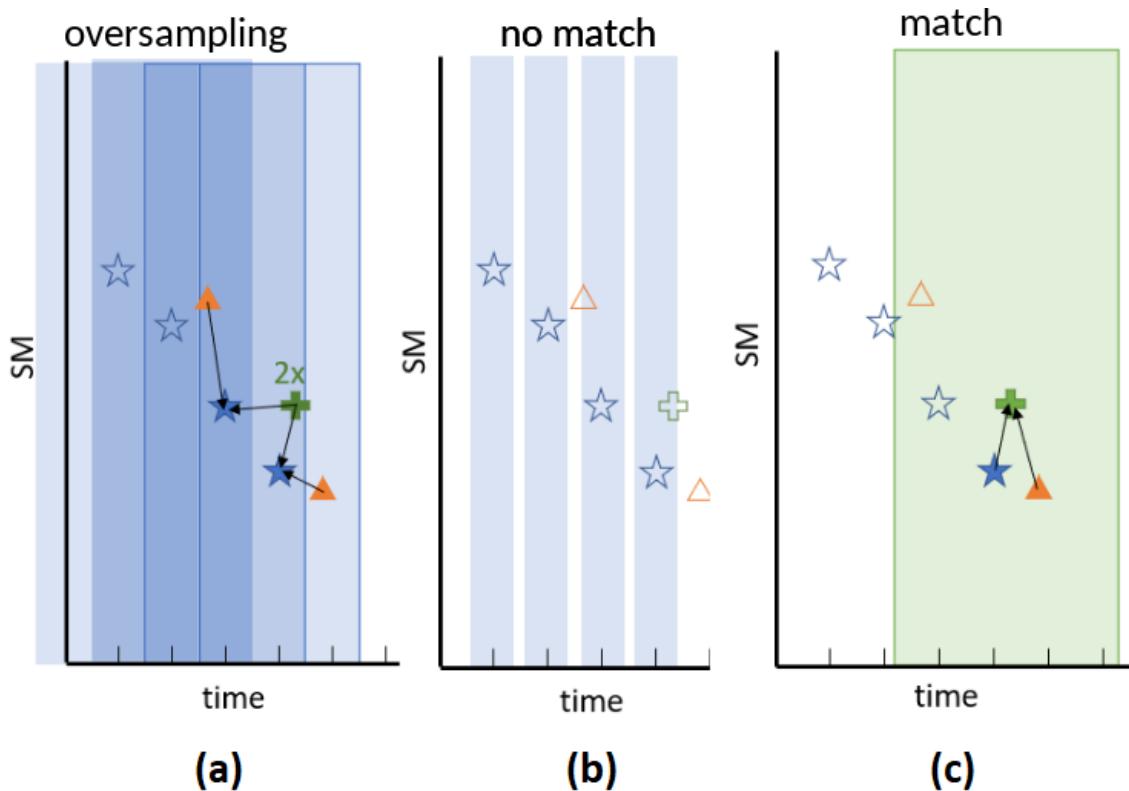
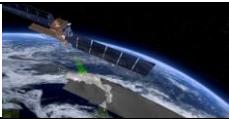


Figure 3 – Temporal matching cases with 3 datasets (symbols), different temporal window size (bars) and temporal reference (bar colours). In case (a) a too large temporal window around each reference time stamp (stars) is chosen leading to oversampling of one (cross) dataset. In case (b) a too small window around the reference time stamps (stars) is chosen, leading to no matches between all 3 datasets. In case (c), a different temporal reference (cross) with a large enough window is chosen, to find at least one observation of each dataset within the window.

Through this procedure, two (or three, in case of TC analysis) temporally and spatially collocated and matched time series are obtained. The spatial resampling procedure is illustrated below (Figure 4).

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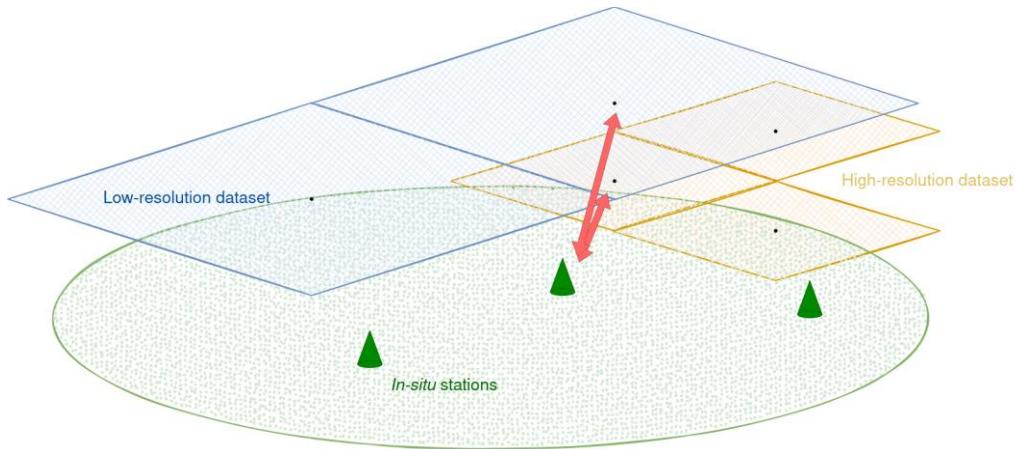


Figure 4: Representation of the resampling procedure. For each provided candidate dataset (blue and orange grids), a NN relationship (red arrows) between the reference (in this case, in-situ stations) and candidate GPIs is established. The time series extracted from this triplet will provide the metric scores associated to the reference GPI

4.3 Statistical rescaling

A set of rescaling options are provided to match the statistical moments of the candidate and reference datasets before calculating the metric-related scores, with the aim of removing the representativeness error. The latter is defined as a theoretical systematic error stemming from the inherent difference of spatial scale at which the same geophysical variable is measured, due to the difference in spatial support of the measuring sensors (Gruber et al., 2020). The systematic differences between two time series can be expressed with a linear dependency:

$$Y = a + bX,$$

where a and b are the additive and multiplicative bias; the statistical rescaling of Y to X , Y^X , can be achieved through the following methods, provided in QA4SM:

Linear regression

The two bias terms a and b are found through linear least-squares regression with the objective of minimizing the squared differences between Y and X , after which the rescaling is obtained through:

$$Y^X = \frac{Y - a}{b};$$

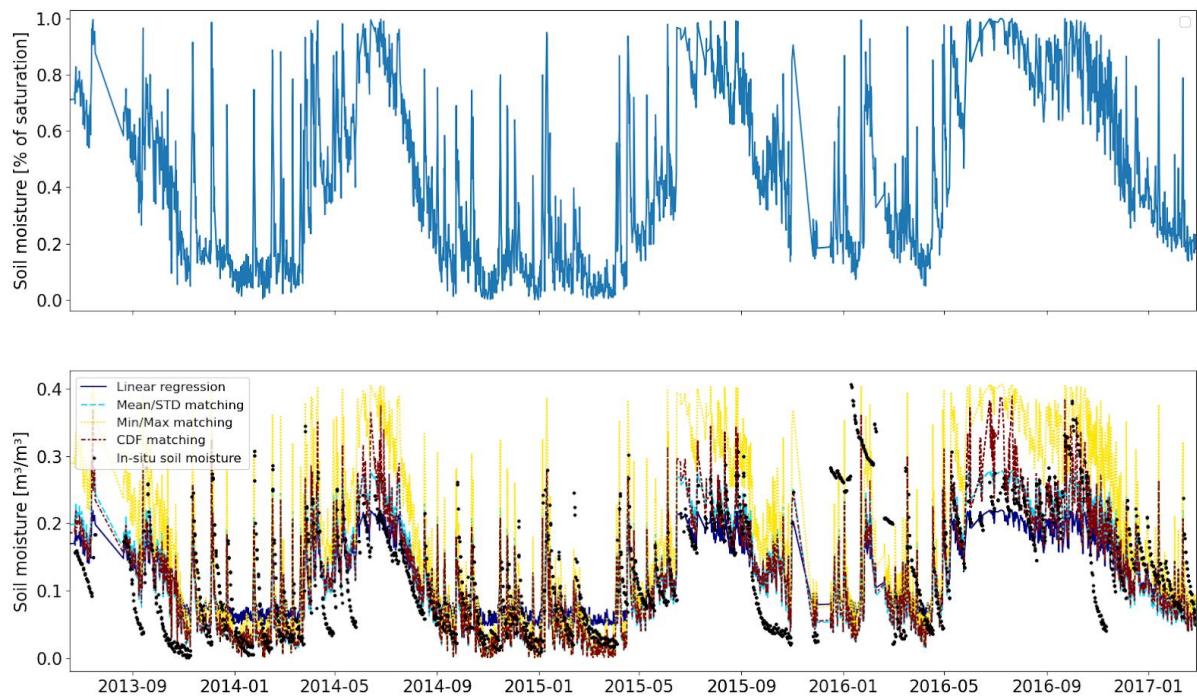


Figure 5: Satellite-retrieved soil moisture in units of saturation percentage (above) and the same time series after rescaling using the described methods (below)

Minimum and maximum matching

All values of Y are linearly rescaled to the range between the minimum and maximum of X:

$$Y^X = \frac{Y - Y_{\min}}{Y_{\max} - Y_{\min}} (X_{\max} - X_{\min}) + X_{\min};$$

Mean and standard deviation matching

All values of Y are linearly rescaled to match the mean and standard deviation of X:

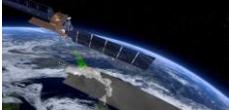
$$Y^X = \frac{Y - \bar{Y}}{\sigma_Y} \sigma_X + \bar{X};$$

Cumulative distribution function (CDF) matching

CDF matching is performed with the method described in Moesinger et al. (2020). The CDFs of the two time-series are divided in equally-sized quantile bins and dynamically adjusted to include a minimum of 20 observations, after which each bin of Y is matched to X by linear regression.

4.4 Anomalies and climatology calculation

In order to separate the long-term SM signal from short-term fluctuations, a climatology can be calculated from a provided time series, representing the average soil moisture by day of the year for the considered period. From this cyclic annual signal, individual events can be

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determined by taking the difference of the SM for a day of the year and the calculated climatology for the same day. To calculate the climatology, a time series is first smoothed by replacing each value with the average of a 5-days moving window; the aim of this operation is to gap-fill the data (missing points are replaced by the window average) and to dampen the effect of short-term precipitation events. Then, the climatology can be calculated with two methods⁸ (depending on the chosen configuration):

- by calculating the average SM state by day of the year over a defined period (Figure 6);
- by calculating the average SM state of a 35-days rolling window centred on the 18th day.

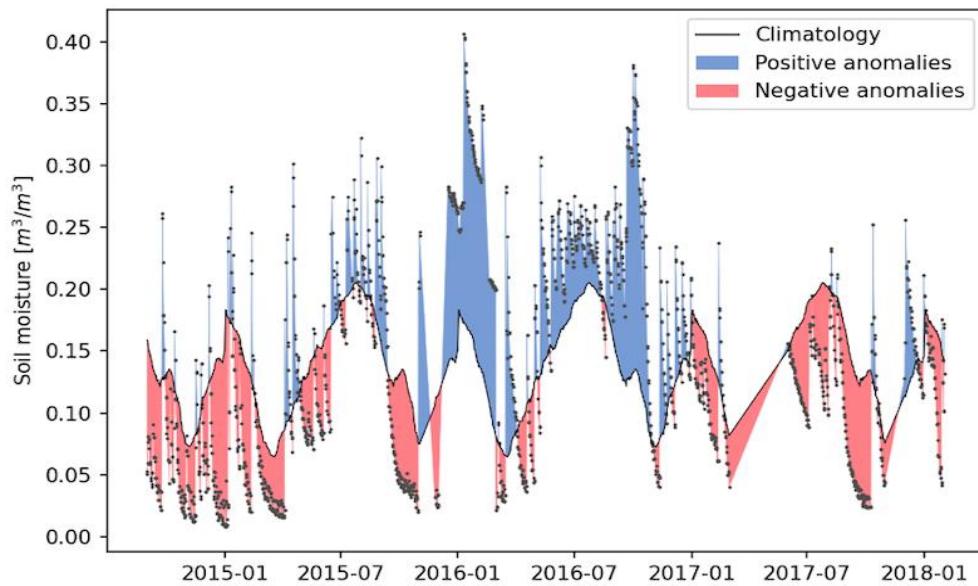


Figure 6: Time series with the climatology and anomalies calculated and plotted using the designated pytesmo functions

4.5 Intra-Annual Validation Metrics

Frequency

To enable the calculation of intra-annual variations in skill metrics, temporal sub-windows are introduced. This functionality allows to select from pre-defined temporal sub-windows, all of which are defined without a specific year (e.g., seasonally, S1: "1 December to 28 February"). The GUI offers seasonal (meteorological) and monthly sub-windows⁹. Their respective definitions are provided in [Tab. 1](#) below.

⁸ The pytesmo documentation on the methods used in climatology and anomalies calculation is available at:

<https://pytesmo.readthedocs.io/en/latest/examples/anomalies.html>

⁹ In principle, the source code of pytesmo allows to define an arbitrary number of sub-windows with arbitrary extent. Defined are temporal sub-windows in the source code of the [ga4sm-reader package](#). The user is invited to explore the option of injecting custom temporal sub-windows via [.json-files](#) when running the QA4SM service on a local server.

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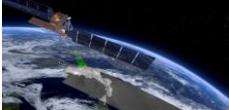
Frequency	Window Name	Start [MM-DD]	End [MM-DD]
Seasonal	S1	12-01	02-28
	S2	03-01	05-31
	S3	06-01	08-31
	S4	09-01	11-30
Monthly	Jan	01-01	01-31
	Feb	02-01	02-28
	Mar	03-01	03-31
	Apr	04-01	04-30
	May	05-01	05-31
	Jun	06-01	06-30
	Jul	07-01	07-31
	Aug	08-01	08-31
	Sep	09-01	09-30
	Oct	10-01	10-31
	Nov	11-01	11-30
	Dec	12-01	12-31

Table 1: Definition of temporal sub-windows implemented in the GUI

All metrics are then calculated for each temporal sub-window in addition to the entire validation period (bulk case). If the validation period covers more than one year, data of the same sub-windows in different years are stacked together. That is, metrics are calculated, for example, for data from all S1, all S2, and so on (in case seasonal sub-windows were provided).

Overlap

Calculating validation metrics over temporal sub-windows can substantially reduce the available sample size. This, in turn, can lead to increased sampling uncertainty and low confidence in the resulting estimates. To mitigate this issue, an 'overlap' parameter is introduced into QA4SM. This parameter is in units of days and extends all temporal sub-windows on both sides symmetrically by the defined amount. Note, however, that this overlap leads to correlations between estimates of neighboring sub-windows. One, therefore, needs to find a balance between sample size and temporal autocorrelation of the skill metrics. By

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default, monthly and seasonal skill estimates do not use any overlap. Table 2 below lists the allowed ranges of overlap.

Frequency	Minimum [days]	Maximum [days]
Seasonal	0	45
Monthly	0	15

Table 2: Range of allowed values for the overlap parameter

4.6 Stability Metrics

To assess the temporal stability of skill metrics, the stability metrics feature uses annual temporal sub-windows (e.g., 2010: "1 January 2010 to 31 December 2010") for each year within the specified time range in the GUI. This allows for the calculation of annual metrics for common statistical measures such as BIAS, MSE, MSE_BIAS, MSE_CORR, MSE_VAR, R, ρ (rho), RMSD, RSS, and uRMSD. For example, the annual BIAS metric is calculated as the mean of all BIAS values from temporal matches between two datasets at a grid point. Additionally, for R, BIAS, and ubRMSD, a decadal Theil-Sen slope (Sen, 1968) is calculated using `scipy.stats` at each grid point to assess trends over time.

Theil-Sen slopes:

For each pair of distinct points (x_i, y_i) and (x_j, y_j) , where $i < j$, the slope s_{ij} is computed using the formula:

$$s_{ij} = \frac{(y_j - y_i)}{(x_j - x_i)}, \quad x_j \neq x_i$$

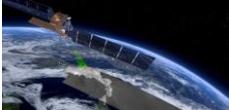
This gives a set of slopes for all combinations of points. To estimate the overall slope, take the median of the set of slopes:

$$\text{slope} = \text{median}(\{s_{ij} \mid 1 \leq i < j \leq n\})$$

The Theil-Sen estimator, which primarily consists of a slope and an intercept, is less sensitive to outliers compared to ordinary least squares regression. This makes it a reliable measure of temporal changes in the selected metrics, as it robustly captures the trend over time.

4.7 Handling of validation errors

Errors can occur in the validation processing chain at several points, due to particular properties of the data, statistical methods applied or selected settings which lead to impossibility to compute metric scores. To provide means for understanding the sources of such errors, a 'status' code is provided in the validation outputs, referring to the exact issue

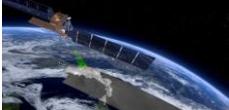
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encountered in the processing. The various errors largely reflect the structure of the source code and the various modules where they originate from in the Pytesmo package¹⁰.

The following status codes are generated:

- **0 - OK:** Validation run successfully and returned valid results.
- **1 - INSUFFICIENT_DATA:** Data for all data sets exists, but not enough to calculate metrics (by default >10 data points are required).
- **2 - METRICS_CALCULATION_FAILED:** Data for all data sets is available, but due to unforeseen reasons the calculation failed.
- **3 - TEMPORAL_MATCHING_FAILED:** Temporal matching failed due to other reasons
- **4 - NO_TEMP_MATCHED_DATA:** At least one of the datasets doesn't have data, or no temporal overlap with other datasets.
- **5 - SCALING_FAILED:** The scaling procedure failed, e.g., due to insufficient data.
- **6 - VALIDATION_FAILED:** as 'UNCAUGHT', but occurring at a different point in the processing chain.
- **7 - NO_GPI_DATA:** One dataset does not have any data at the given grid point index.
- **8 - DATA_MANAGER_FAILED:** For some unforeseen reason, the calls to get data from the data manager fail.
- **-1 - UNCAUGHT:** refers to behaviour that is not foreseen in any way.

¹⁰ https://github.com/TUW-GEO/pytesmo/blob/master/src/pytesmo/validation_framework/error_handling.py

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5 QA4SM user interface

The QA4SM user interface consists of several views and a navigation bar (Figure 8) enabling easy navigation between all the views. Under the main address qa4sm.eu, the home view is available, which contains a short overview of the service, navigation buttons and a news section. The news section provides the user with the current version number, date of the last release and a link to the list of updates (Figure 7). The navigation buttons navigate a non-logged in user to the list of published validations and to the sign-up. For a logged in user, the buttons provide navigation to the validation form and custom validation list, comparison module and custom



Figure 7: News section on the home page, containing the current version number, date of the last release and link to the list of updates.

data sets section. The sign-up form is available from the home page only. The log-in form is additionally shown every time a non-logged in user tries to access restricted sections. Without logging into the service, it is possible to visit all the sections available under the Info tab of the navigation bar, study results that have been published, study user data upload help section, and get familiar with the validation form, without a possibility of starting computations



Figure 8: Menu for navigation through the user interface

5.1 Publicly available sections

Using the Info tab in the navigation bar, a non-logged in user can navigate to the Help, Datasets and Terms sections (Figure 9). They can also download the User Manual. The **Help** section provides the user with a concise manual on how to run a validation, how to access and manage obtained results, how to compare validations as well as how to publish the results using the Zenodo¹¹ service. The **Datasets** section contains information on datasets (including versions, time span, filters, etc.) available for validation in the QA4SM application. The **Terms** section contains terms and conditions and privacy policy that the user has to accept, as well as citation rules that applies whenever QA4SM results are used in publications.

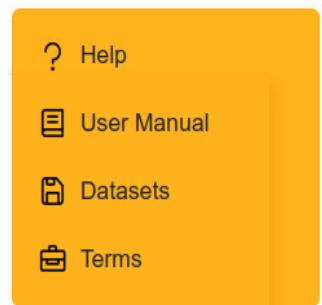


Figure 9: Menu tab expanded - a non-logged in user view

¹¹ <https://zenodo.org/>

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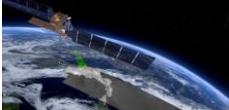
The **Upload Data Help** section, available under the **Dataset upload/Data Preparation** tab and provides users with comprehensive guidelines on preparing a custom data file.

The Published Validations section is also publicly available. It is accessible from the navigation bar **Results/Published validations** (Figure 8) or under the “See results” button on the home page. The page contains a list of validations that have been published with Zenodo by their authors. Each validation on the list is described by its name, DOI, used datasets and the creation date. The list can be sorted according to validation name, date, status and the reference dataset, in descending or ascending order. On the right side of each validation summary, there are three buttons, if the user is logged in, or only one if they are not. The folder button (always visible) navigates the user to a more detailed description of the particular validation (for more details see in section 5.6). The round-arrow button reloads settings of the particular validation, redirecting the user to the validation form. Please note that in order to use this functionality, the user must be logged in. Logged in users can also see ‘+’ or ‘x’ buttons, enabling adding or removing the particular validation to or from the list of pinned validations. Published validations results can be downloaded by a non-logged in user. Downloading buttons are available in a single validation view, accessible by clicking the folder button and described in section 5.6.

Without logging in, it is also possible to explore the validate (Validate menu button) form to see which datasets and settings can be selected for computations. Users can choose different settings and verify the available options; however, running computations is not possible. The validate form is further described in section 5.6.

5.2 Sign-up form

QA4SM is entirely free of charge. However, running own validations is possible only after registration. The sign-up form consists of nine fields and help text provided when hovering over the question mark icon on the right side of each field. To register a new user, it is necessary to provide a unique username, a password and its confirmation and an email address. Additionally, it is possible to provide the first and the last name, a name of the organisation the user works for or represents, the country where the organisation or the user resides and user’s ORCID number. Please note, that if the team suspects that the request has been made by a bot or the provided email address is considered to be a spam address, the account will not be activated. In order to use QA4SM it is required to accept the QA4SM terms, conditions and privacy policy. After providing the required user data, the form can be submitted using the “Sign up” button. If the data has been correctly submitted, the user is redirected to the after-registration page and a new account is created automatically. The account will be activated as soon as possible by the support team. In case of errors, notifications will show up indicating the specific problems. Typical problems occurring while registering a new user refer to:

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- already existing username,
- non-matching password entries (between password and password confirmation fields),
- password too short or too similar to the username,
- wrong format of the ORCID number.

In case of problems not related to the incorrect user data, please contact the support team. After the account activation, the user receives a notification on the email address provided while registering. From this point on, the user has access to all the functionalities of the service.

5.3 Log-in form and user profile view

The log in form can be accessed via Log in button in the menu or when trying to access restricted sections. To log in it is necessary to provide the username and password. In case of forgotten password, there is a link provided that navigates to the password reset form. To reset the password, it is necessary to enter the email address that was provided while registering and follow given instructions.

After logging in, under the My account tab, the user gains access to their account and to logging out (Figure 10). The user profile view contains the same fields as the sign-up form. It is possible to change user data anytime, apart from the username. Please note, that the rules for changing data, are the same as for registering (e.g., the password cannot be too short, or too similar to the username). Changed data needs to be approved with the “Save” button. User can also deactivate the account using the red “Deactivate my account” button. The account will be automatically deactivated and removed by the service provider. The deletion of the user account will remove access to the service and all non-published validations. Once deleted, the account cannot be restored, neither by the user nor the QA4SM team.

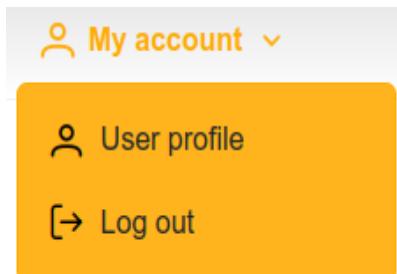


Figure 10: Menu tab expanded - a non-logged in user view

5.4 Validate form

The main functionality of the service, i.e., data validation, is available in the Validate section, accessible from the navigation bar or using ‘Try it’ button (for logged in users) on the main page. The view consists of a few components referring to the various validation parameters. In the header of each component there are a question mark icon and (for most of the components) a collapse +/- button. The first one, when hovering over it, provides the user with information on the particular component. The second one enables folding up (-) and folding down (+) the particular area.

Data

> ISMN / 20240314 global / soil_moisture (spatial reference)

▽ C3S SM combined / v202312 / sm (temporal reference)

Dataset: C3S SM combined

Version: v202312

Variable [units]: sm [m^3/m^3]

Variable in valid geophysical range
 Ascending mode only
 Descending mode only

Remove dataset

+ Add dataset

Reference

② Spatial reference
Select dataset (version)
ISMN (20240314 global)

② Temporal reference
Select dataset (version)
C3S SM combined (v202312)

Scaling

Method:
Select scaling method
No scaling

Figure 11: Components for selecting datasets for validation, available on the validation page

The first two components refer to datasets used for validation and enable adding datasets and choosing the reference ones (Figure 11). In the component entitled Data, users can choose the data to be validated - including the data set name, the version of the data set, and one of the soil moisture variables provided in the data set. Users can also set filters on the input data (see section 3). Under a black question mark icon next to each option additional information on the particular filter is provided. In some cases (e.g., for SMOS Level 2 data set), there are filters that cannot be unchecked. It means that the provided data set has been filtered according to the given rule and it cannot be reverted. For SMOS and ISMN data, there are available so called parameterized filters.

For SMOS (both Level 2 and Level 3) data sets, there is a filter called 'Set retrieval quality threshold' with an input field provided. The provided value has to be in the range from 0 to 1, and can be introduced manually, or using arrows

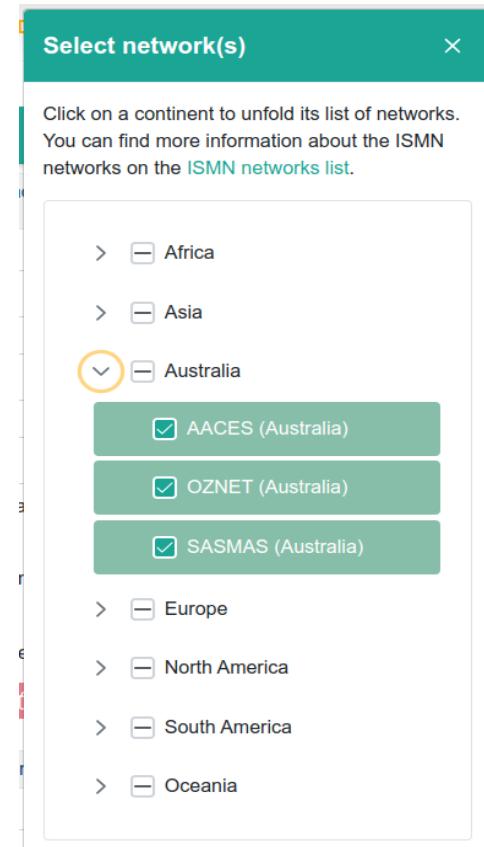


Figure 12: ISMN networks selection dialogue window

next to the field. For the ISMN data set two filters are available, where choosing parameters is possible. They cannot be switched off, and there is a ‘select...’ link which opens a dialogue window. The first filter refers to the network selection (Figure 12), where networks are sorted according to the continent they are mostly placed on. Clicking on the arrow next to the continent name folds down a list of networks and countries the networks belong to. To toggle the particular network, it is enough to click on its name. To toggle all networks on a continent, it is enough to click the name of the continent. The choice does not have to be approved, it is enough to close the dialogue window and the choice will be saved. The second filter refers to the depth at which the measurements were done (Figure 13). It is possible to insert minimum and maximum depths and approve them with the “OK” button or just close the dialogue window.

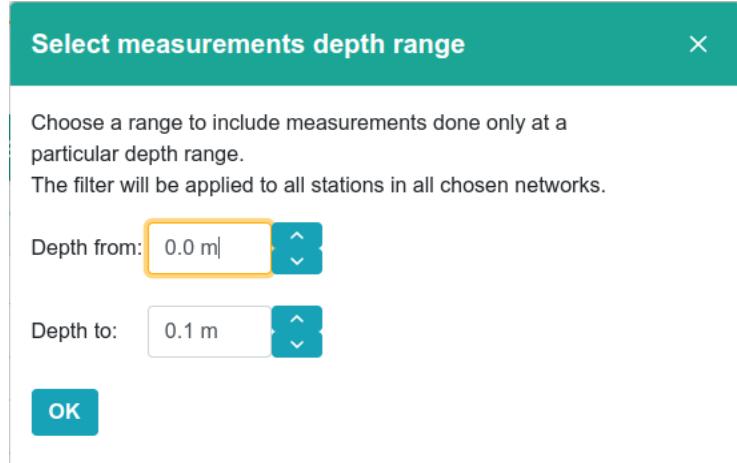


Figure 13: Measurement’s depth selection dialogue window

It is possible to choose up to six datasets, using the “Add dataset” button in the left lower corner. When six datasets are chosen, the button gets disabled. Each dataset can be removed using the “Remove dataset” button placed on the chosen dataset tab.

The Reference component enables selecting, separately, spatial and temporal reference data set. If the ISMN dataset belongs to the data set pool, it is automatically set as the spatial reference, and there is no option to change it (Figure 14).

Temporal reference, on the other hand, can be defined by any dataset added to validation (see Figure 15). Please note that we do not recommend using ISMN as the temporal reference,

Data	Reference
<ul style="list-style-type: none"> > ISMN / 20240314 global / soil_moisture (spatial reference) > C3S SM combined / v202312 / sm (temporal reference) > SMOS Level 3 / version 339 Descending / Soil_Moisture 	<ul style="list-style-type: none"> ② Spatial reference Select dataset (version) ISMN (20240314 global) <li style="background-color: #009640; color: white;">ISMN (20240314 global) Select dataset (version) C3S SM combined (v202312)

Figure 14: Spatial reference choice list, when ISMN dataset belongs to the dataset pool

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as it is sampled hourly and would result in oversampling compared to the 1-3 daily satellite observations. The data set selected as the reference (both spatial and temporal) is

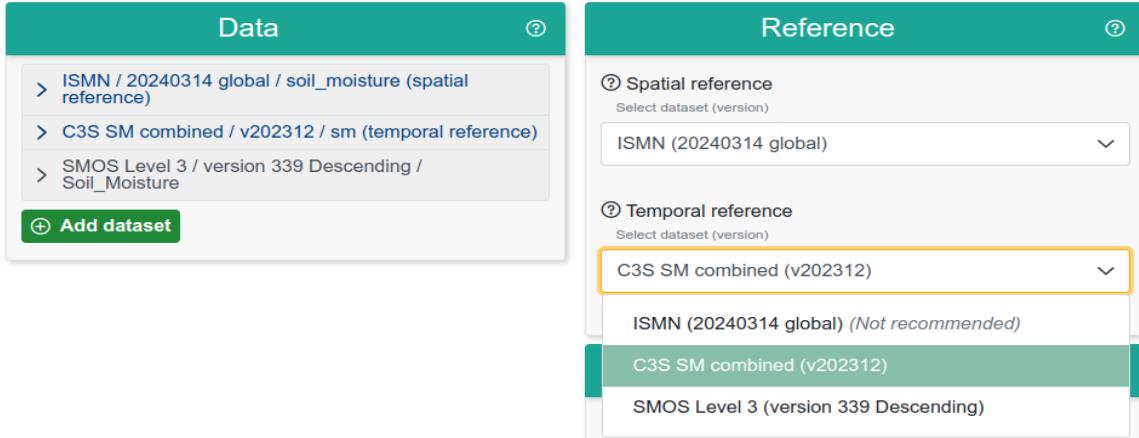


Figure 15: Temporal reference choice list

automatically marked as such in the header of the proper tab. Additionally, when expanding any of the reference lists and hovering over options, proper data set gets highlighted (in the Data component), so there is no doubt which entry refers to which data set.

Below the “Reference” component, the “Scaling” section can be found. This section enables choosing how the data will be scaled before metrics calculation. The data can be scaled to any dataset selected for validation (see Figure 16). The scaling method determines how values of one dataset are mapped onto the value range of the other dataset for better comparability. By default, ‘No scaling’ is set, and none of the dataset is marked as the scaling reference, however when expanding the method list, possible options are:

- No scaling,
- Min/max,
- Linear regression,
- Mean/standard deviation,
- Cumulative Distribution Functions (CDF) matching.

Choosing any other method than ‘No scaling’ causes the ‘Scale to’ list to show up. By default, the first data set on the list is set as the scaling reference. However, it can be easily changed using the scaling reference list. Similar to the ‘Reference’ component, when expanding ‘Scale to’ list and hovering over each option, a proper data set in the ‘Data’ component will get highlighted, and when selecting data set, the proper one will get marked as ‘scaling reference’. Details about each scaling method can be found in section 4.3.

Next two components are strongly combined with each other. The “Spatial subsetting” component, enables choosing the geographic area over which the validation should be

performed (Figure 19). It is possible to provide latitude and longitude of the lower left and upper right corners of the bounding box, or choose the box from a map. The map is available in the map component above the “Spatial subsetting” component. The trash bin button can be used to erase introduced coordinates. With no coordinates provided, a global validation will be run. The map for selecting the spatial subsetting is shown in Figure 17. If the ISMN data set is one of the selected data sets, the approximate location of the stations will be displayed on the map. As you zoom in, the locations will become more accurate, and hovering over the icon will reveal additional information about the stations. To create a bounding box, choose the pencil button, click on the map and drag. There is no possibility to edit a bounding box, if a correction is needed a new box needs to be drawn. To remove the box, use the trash bin button placed in the “Spatial subsetting” component. Zooming in and out is possible with a mouse scroll wheel. There is no need to confirm the area choice.

In the next component, called “Temporal subsetting”, users can choose the date range over which the validation should be performed and temporal matching window size (Figure 19). The only accepted date format for the validation period is: YYYY-MM-DD. It is also possible to choose a date from a calendar, available when clicking the date input field. By default, the date range is determined through temporal matching of the data and reference selected. If the validation period fields are left empty, the validation will not be started. For temporal matching window size, the default (and recommended) value is 12 hours and possible choices are integer numbers between 1 and 24 hours.

If there are at least three datasets chosen for validation (including the reference dataset), it is possible to select, in the component

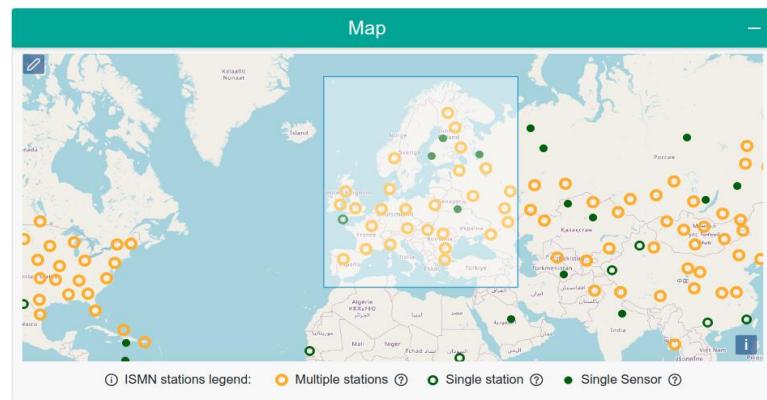
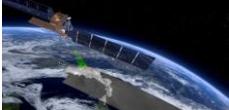


Figure 17: Map for choosing the spatial subsetting for validation



Figure 16: Scaling component with ‘No scaling’ (left picture) and ‘Min/Max’ (right picture) methods set.

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entitled Metrics, if triple collocation (TC) analysis shall be performed. If the TC metric is chosen it is also possible to choose “Bootstrap Triple Collocation metric confidence interval” option. When it is chosen confidence intervals are calculated via bootstrapping with 1000 repetitions, however the validation time might be up to 5 times longer.

Stability and Intra-Annual Metrics can be included in computations regardless of the number of selected datasets. Please note that Stability and Intra-Annual metrics are mutually exclusive, which means that it is not possible to select both of them for the same validation. When the Intra-Annual Metrics checkbox is selected (Figure 18), additional settings become available. The 'Frequency' dropdown allows you to choose the temporal sub-windows over which all metrics are calculated. The 'Overlap' value symmetrically extends each temporal sub-window by the specified number of days.

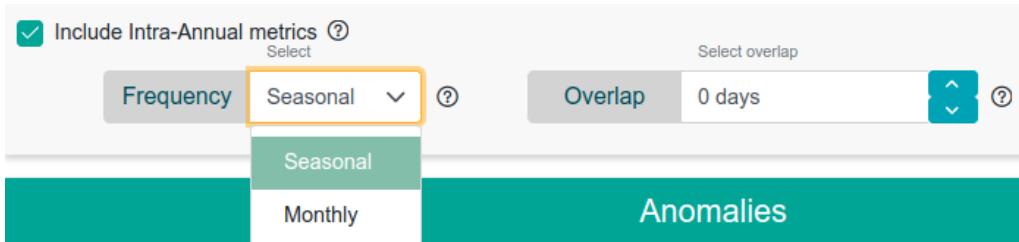


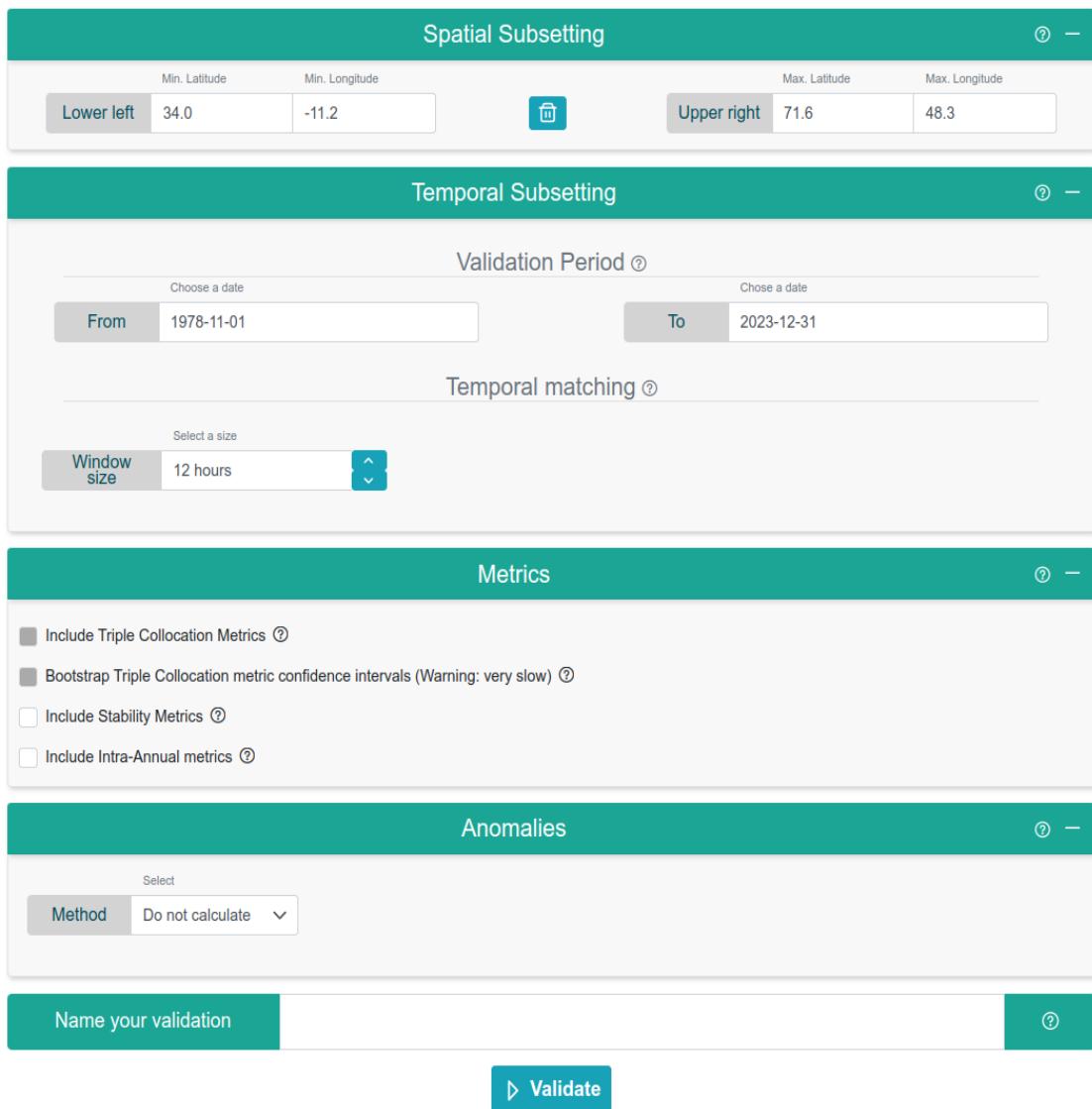
Figure 18:
Intra-Annual
Metrics
settings.

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The “Anomalies” section can be used to calculate the validation metrics from anomalies instead of absolute values of the time series. To do that, select the desired method in the “Method” drop-down menu. The options are:

- Do not calculate,
- 35 day moving average,
- Climatology – if climatology is selected the years to be used for climatology calculation need to be specified.

Details about each method can be found in section 4.4.



The screenshot shows the validation configuration interface with four main sections:

- Spatial Subsetting:** Allows defining a geographic area by specifying coordinates for the lower-left and upper-right corners. The current values are Lower left (34.0, -11.2) and Upper right (71.6, 48.3).
- Temporal Subsetting:** Contains two sub-sections: "Validation Period" (From: 1978-11-01, To: 2023-12-31) and "Temporal matching" (Window size: 12 hours). The "Window size" is currently set to 12 hours.
- Metrics:** A list of validation metrics with checkboxes:
 - Include Triple Collocation Metrics
 - Bootstrap Triple Collocation metric confidence intervals (Warning: very slow)
 - Include Stability Metrics
 - Include Intra-Annual metrics
- Anomalies:** A dropdown menu for selecting the method to calculate validation metrics. The current selection is "Do not calculate".

At the bottom, there is a "Name your validation" input field and a large blue "Validate" button.

Figure 19: Optional validation settings and the start validation button, available on the Validate page

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The last component enables naming the validation. Naming the validation is optional, and the name can be changed later.

The “Validate” button starts the validation and the user is redirected to a single validation view, where the information about the validation being still running is displayed. Once the validation is finished, the results will be displayed instead of the notification.

In some cases, the user may get a notification that there exists a validation with the same settings like the validation which is about to be run (Figure 20). If it is the case the user can choose whether to run a new validation or to see the existing one. Regardless if the existing

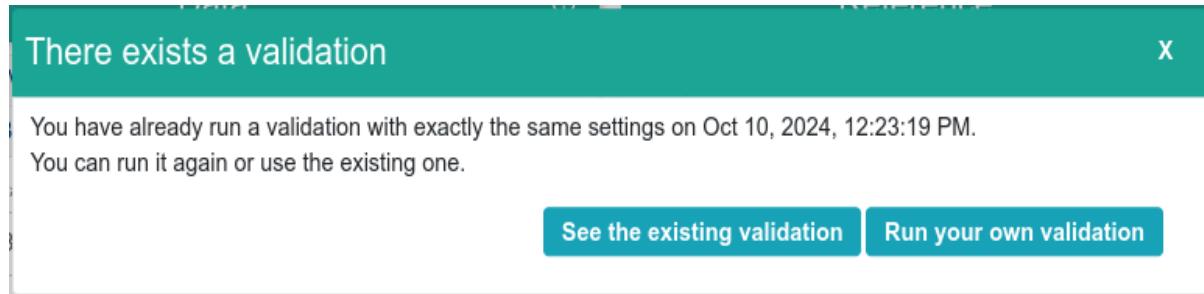


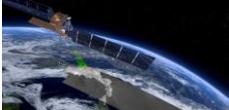
Figure 20: Notification on the existing validation

validation belongs to the current user or not, or it is a published one, the “See the existing one” button will navigate the user to this validation. If the user is redirected to a validation that does not belong to them and has not been published, there is a possibility of copying such a validation. More details about copying a validation can be found in section 5.6.

5.5 My validations

All the validations run by the currently logged in user are available in “My validations” section, accessible from the navigation bar (Figure 8). Similar to the published validations, each custom validation on the list is described by its name, the creation date and used datasets. Additionally, a status is provided along with an icon in the title bars. The icons indicate the following:

- The validation was cancelled.
- The validation is still running and has no results yet.
- The validation has completed. It will be removed by the auto-cleanup process 60 days after completion, unless you extend or archive it. You can see the expiration date by hovering your mouse over the icon.
- The validation has been archived and will not be automatically removed by the cleanup process.
- The validation will expire within the next 7 days and will then be removed by the auto-cleanup process, unless you extend or archive it. You can see the expiration date by hovering your mouse over the icon.

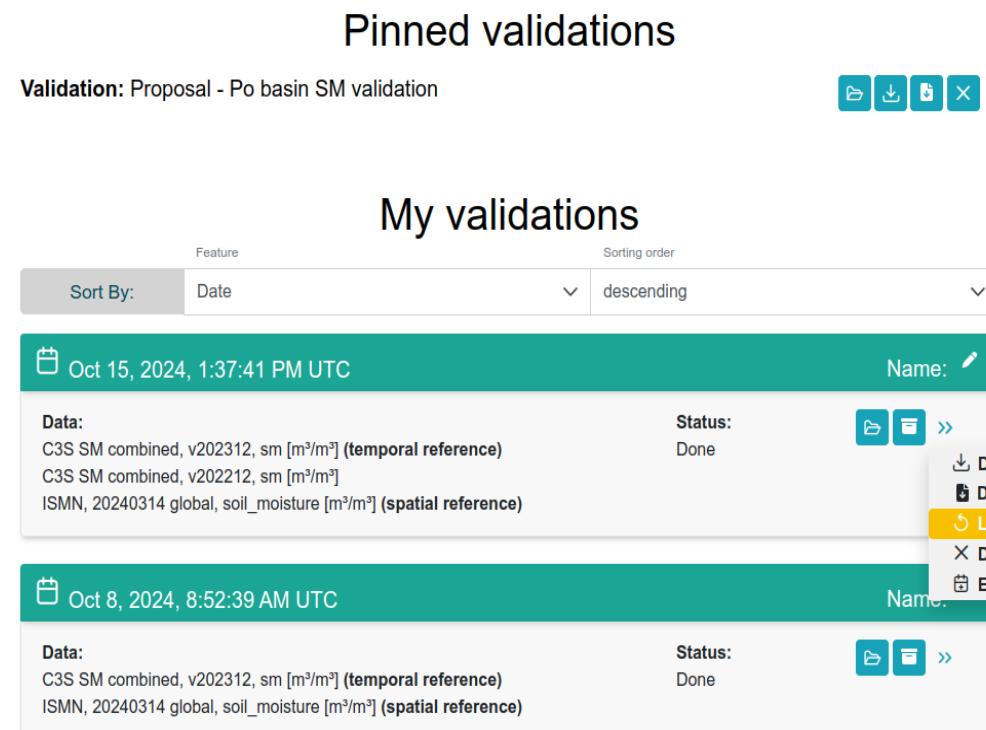
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-  This result has been published with Zenodo. It will NOT be automatically removed during cleanup.

The list can be sorted according to validation name, date, status and the reference dataset, in descending or ascending order. On the right side of each validation summary, there are two buttons and a drop down list, folding down when hovering over the double arrow icon (Figure 21). The buttons on the right-hand side of each validation have the following effects:

Pinned validations

Validation: Proposal - Po basin SM validation



My validations

Feature	Sorting order
Sort By: Date	descending

Oct 15, 2024, 1:37:41 PM UTC Name: 

Data: C3S SM combined, v202312, sm [m^3/m^3] (temporal reference)
C3S SM combined, v202212, sm [m^3/m^3]
ISMN, 20240314 global, soil_moisture [m^3/m^3] (spatial reference)

Status: Done   

Oct 8, 2024, 8:52:39 AM UTC Name: 

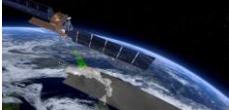
Data: C3S SM combined, v202312, sm [m^3/m^3] (temporal reference)
ISMN, 20240314 global, soil_moisture [m^3/m^3] (spatial reference)

Status: Done   

Download Graphs
Download NetCDF File
Load Validation Settings
Delete Validation Run
Extend Life Span

Figure 21: My validations view

-  Accessing the results details page of a validation;
-  Cancelling validation; visible only while the validation is still running;
-  Removing validation permanently; visible once the validation has finished or was aborted; for tracked or published validations it unpins the validation from the list of tracked validations;
-  Downloading graphs - allows downloading all the graphs produced for the validation (in .png and .svg formats) in a zip archive; not available when the validation has been cancelled or produced an error;
-  Downloading NetCDF file - allows downloading the validation result; not available when the validation has been cancelled or produced an error;
-  Extending lifespan - enables resetting the auto-cleanup period of a result and thus postpone its automatic removal; available for non-archived results only;

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- ⚠ Archiving - enables excluding a validation from auto-cleanup and thus keep it indefinitely; available for non-archived results only;
- 🕒 Jn-archiving - makes a validation eligible for auto-cleanup again. It will be automatically extended, so the user will have another 60 days before deletion and will be notified again; available for archived results only;
- ⟳ Reloading - reloads settings of the particular validation, redirecting the user to the validation form; not available when the validation has been cancelled or produced an error;
- ✚ Adding a validation to the list of tracked validations; available only for published validations.

Additionally, there is a pencil button next to the validation name, enabling its change. The change must be confirmed with the floppy disc button, which shows up along with a text input field.

Apart from the validations run by the logged in user, there is a list of pinned validations available in the “My validations” section. Published validations of particular interest to the user can be added to the list of tracked validations using the plus button. This way, the validation is quickly accessible, without the need to look it up in the list of all published validations. Note that the “x” button on the list of tracked validations only removes the validation from the tracking list, while the published validation is not deleted.

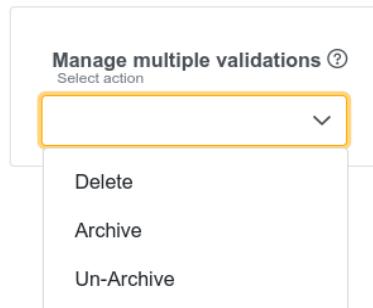


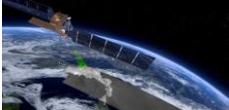
Figure 22: Drop down for managing multiple validation actions.

It is possible to modify multiple validations at once. On the left side, there is a dropdown menu where you can select an action (Delete, Archive, Un-Archive, Figure 22). Choosing an action will enable the selection of the validations to which the action will be applied (Figure 23). The action is confirmed by pressing the appropriate button, or canceled by pressing 'Cancel'. If the checkbox next to a validation is disabled, it means the action cannot be applied to that validation. You can select all validations (All, for which the action can be applied) or clear the current selection (Clear selection).

5.6 Single validation view

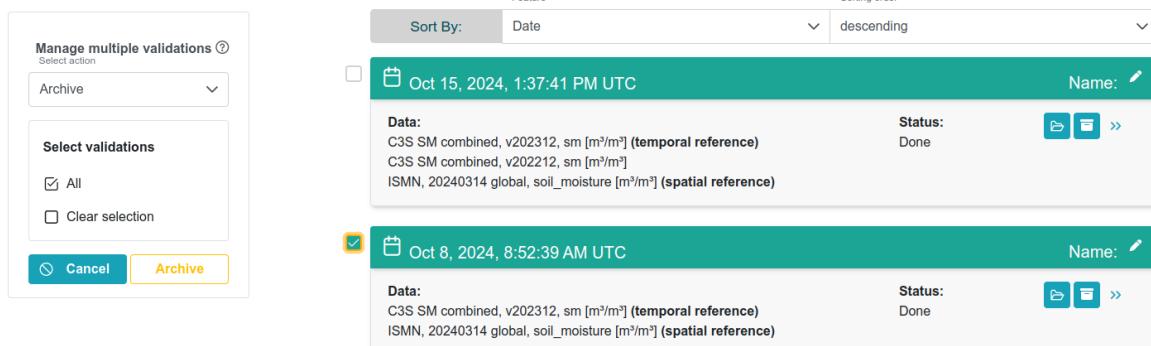
Each validation has assigned its own view in the service, which can be accessed by using the folder button, as described above. The view contains three components: Summary, Summary statistics and Results files.

The Summary (Figure 47 in section 7.2) contains the validation process output, i.e., all the validation settings, processing time, percentage and number of points for which validation metrics could not be calculated as well as information if the validation has been published,

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archived or it is going to be removed soon. The summary contains buttons with the same functionalities as the summary on the validation list (see section 5.5 for custom validations and section 5.1 for published ones). Additionally, in case of custom validations, there is a “Publish” button, which enables publishing results (see section 5.7). The “Publish” button is not displayed, if the validation contains data uploaded by the user (read more in section 5.9). If a user has an access to another user’s non-published validation, there will be only two action buttons available, ‘Load settings’ (see section 5.5) and ‘Copy validation’. Clicking the ‘Copy validation’ button enables copying the existing validation and adding it as a new one to “My validations” lists. There will be information added that the validation has been copied, but the user will have a full control over it, including name change, archiving, deleting or publishing. Similar to publishing, copying and reloading settings of another user’s validation that contains custom data, is not possible.

The summary statistics component contains a table with the mean, median and standard deviation calculated on the validation results aggregated by metric and dataset (for more details check sections 6.3.7 and 7.3.1). The table can be downloaded by clicking on the ‘Download .csv table’ button, at the bottom of this component.

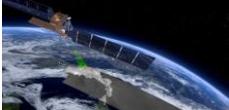


The screenshot shows a modal window titled 'Manage multiple validations'. On the left, a sidebar allows selecting actions like 'Archive'. Below it, a 'Select validations' section has a checked 'All' option. At the bottom are 'Cancel' and 'Archive' buttons. To the right, a main area displays two validation runs in a table format:

		Sort By: Date	descending
<input type="checkbox"/>	Oct 15, 2024, 1:37:41 PM UTC	Name: <input type="text"/>	<input type="button"/> <input type="button"/> <input type="button"/>
Data: C3S SM combined, v202312, sm [m³/m³] (temporal reference) C3S SM combined, v202212, sm [m³/m³] ISMN, 20240314 global, soil_moisture [m³/m³] (spatial reference)		Status: Done	<input type="button"/> <input type="button"/> <input type="button"/>
<input checked="" type="checkbox"/>	Oct 8, 2024, 8:52:39 AM UTC	Name: <input type="text"/>	<input type="button"/> <input type="button"/> <input type="button"/>
Data: C3S SM combined, v202312, sm [m³/m³] (temporal reference) ISMN, 20240314 global, soil_moisture [m³/m³] (spatial reference)		Status: Done	<input type="button"/> <input type="button"/> <input type="button"/>

Figure 23: Archiving multiple validation runs.

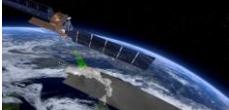
The Result files component contains the results presented in graphical form. On the left side there is a boxplot of the distribution of a particular metric for all evaluated locations presented. On the right side there are plots depicting maps with the distribution of the same metric for all dataset combinations. Above you can find a dropdown list to switch between metrics see Figure 24. If the ISMN dataset is used as the reference, there is an additional dropdown list present, to switch between boxplot classification (see options in Table 3).

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Metrics	Additional Classifications
Observations	Unclassified
Status	Land cover classification
Bias (difference of means)	Climate classification
Mean square error	Soil type classification
Mean square error bias	FRM classification
Mean square error correlation	Network
Mean square error variance	
Pearson's r	
Pearson's r p-value	
Residual sum of squares	
Root-mean-square deviation	
Signal-to-noise ratio	
Error standard deviation	
TC scaling coefficient	
Spearman's rho	
Spearman's rho p-value	
Theil-Sen slope of BIAS	
Theil-Sen slope of R	
Theil-Sen slope of urmsd	
Unbiased root-mean-square-deviation	

Table 3: Dropdown Menu Options

There are also two buttons for downloading results. The ‘Download graphs’ button enables downloading all graphs produced for the validation (in .png and .svg formats) in a zip archive. The ‘Download NetCDF’ button allows downloading the validation result. If Intra-Annual metrics are included in the computations, an additional plot section will be available upon selecting a metric. This section contains results based on the assessment of either intra-annual product performance. However, only graphs highlighting the key findings are displayed here, while further results can be downloaded. If stability metrics are included in the computations, an additional plot section will become available, similar to the intra-annual case. This section displays an annual boxplot for the selected metric.

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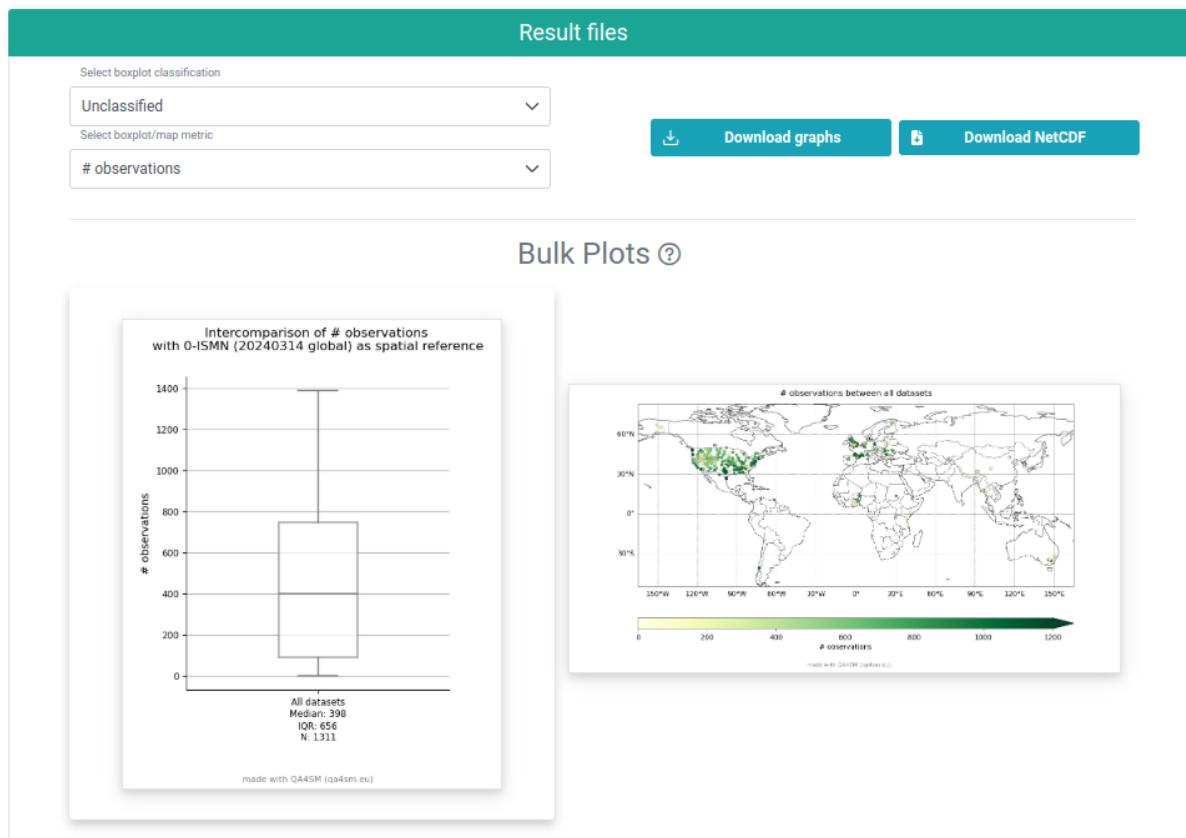


Figure 24 - Plot results section

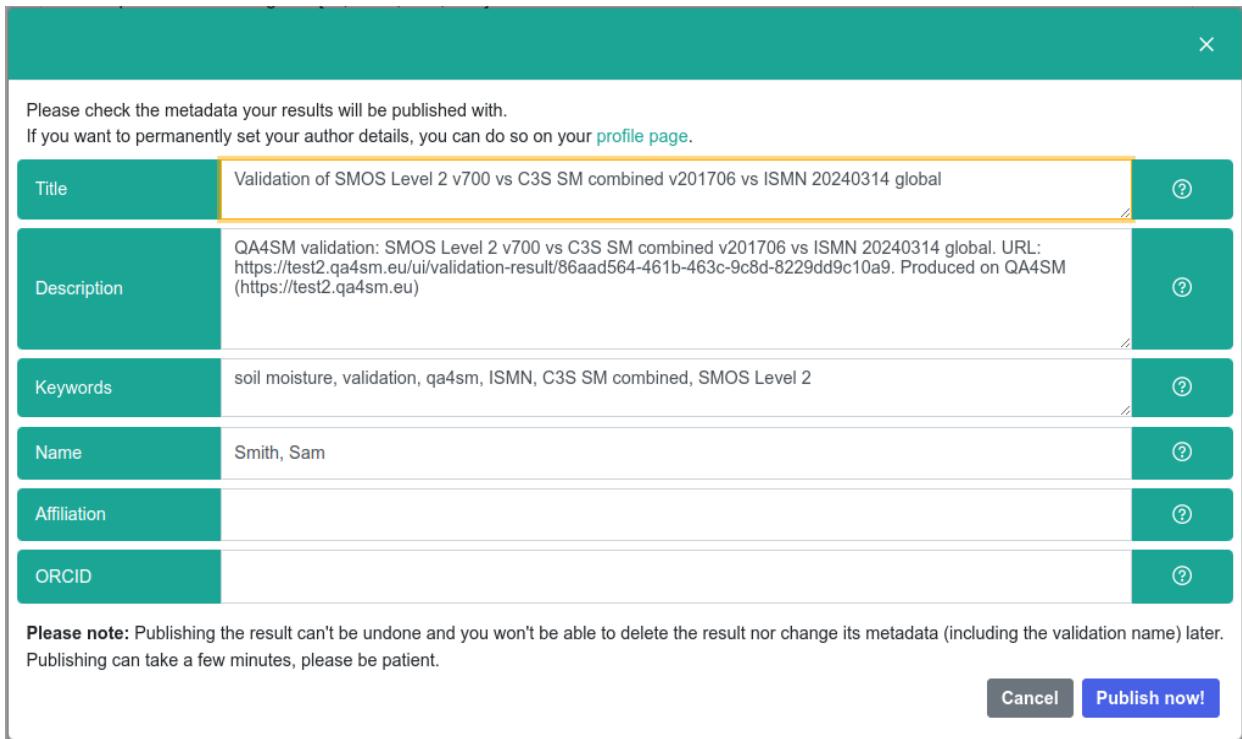
5.7 Publishing form

The QA4SM service provides the user with the possibility of publishing their results. This feature allows publishing the result NetCDF file of the particular validation to Zenodo under the user's own name but without creating a Zenodo account. This gives the user a DOI for the published validation results, which can be cited in publications and provides the readers with open access to the published result data.

Publishing results is available under the 'Publish' button on the single validation view. After clicking on the button, the publishing form shows up (Figure 25). All the fields of the form are filled with the default values. The default title contains names and versions of all the datasets used in the validation. The description contains additionally a link to the results and information that they were produced using the QA4SM service. Default key words contain soil moisture, validation, qa4sm and used datasets names. These fields can be changed to the user liking within some limits. It should be noted that we require 'qa4sm' to be one of the keywords, and that they are mandatory fields. Name, affiliation and ORCID fields, by default, contain information provided within the user profile. If the information is not provided, the Name field will be filled with the word "Anonymous" (as the field is also mandatory) while the two other fields will remain empty. Note, that any user data provided in this publishing form

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is not stored in the QA4SM user profile. Once all required data has been inserted it is possible to start the file upload to Zenodo by clicking the ‘Publish now!’ button.



Please check the metadata your results will be published with.
If you want to permanently set your author details, you can do so on your [profile page](#).

Title	Validation of SMOS Level 2 v700 vs C3S SM combined v201706 vs ISMN 20240314 global	?
Description	QA4SM validation: SMOS Level 2 v700 vs C3S SM combined v201706 vs ISMN 20240314 global. URL: https://test2.qa4sm.eu/ui/validation-result/86aad564-461b-463c-9c8d-8229dd9c10a9 . Produced on QA4SM (https://test2.qa4sm.eu)	?
Keywords	soil moisture, validation, qa4sm, ISMN, C3S SM combined, SMOS Level 2	?
Name	Smith, Sam	?
Affiliation		?
ORCID		?

Please note: Publishing the result can't be undone and you won't be able to delete the result nor change its metadata (including the validation name) later. Publishing can take a few minutes, please be patient.

[Cancel](#) [Publish now!](#)

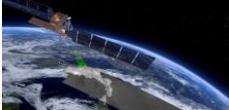
Figure 25: Result publishing form

The upload can take a few minutes. In case of failure, please try again a few hours later. If it still does not work, please email us at support@qa4sm.eu and include the error message you received.

Please be aware, that the NetCDF file and the metadata will be stored at Zenodo under the account of the QA4SM project but with the name provided by the author. Zenodo is a separate website run at CERN over which the QA4SM team has no control. More details about the service can be found at <https://about.zenodo.org>.

Assigning a DOI to a result also means that it cannot easily be unpublished or deleted - see also Zenodo's FAQ.

It is also possible to use the user's own Zenodo account - the QA4SM publication feature is just for convenience. In this case the user has to download the NetCDF result file and upload the file through Zenodo's submission process with the user's own account. We request to include “qa4sm” and “frm4sm” in the keyword list, so that all published QA4SM results and the FRM4SM project can easily be found on Zenodo with a keyword search.

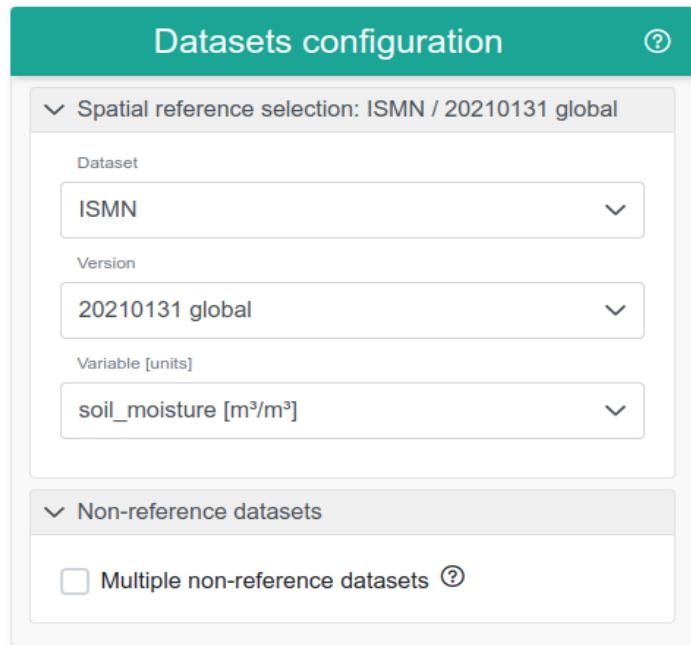
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5.8 Validation comparison

With the QA4SM version 2.1 (and later) it is possible to compare existing validations that belong to the currently logged-in user or have been published. The comparison module is available for a logged-in user under the “Compare validations” button in the navigation bar (Figure 8). It enables two comparison modes - a comparison of two validations with the same reference data set and one non-reference dataset or a comparison between two non-reference datasets used in one validation. The module consists of three main components: Dataset Configuration (Figure 26), Validations selection (Figure 27) and Spatial extent (Figure 28).

The Datasets configuration component enables choosing the dataset that was used as the reference one (including its version and the variable name) and selecting the comparison mode. Checking ‘Multiple non-reference datasets’ switches on the ‘one validation’ comparison mode.

The Validations selection component gets updated with every change of the reference dataset and shows validations available for comparison. A selected validation has to be added by clicking the ‘Add validation’ button. If the maximum number of validations has been added, the ‘Add validation’ button gets disabled. Added validations are listed below the selection box as red



Datasets configuration

Spatial reference selection: ISMN / 20210131 global

Dataset: ISMN

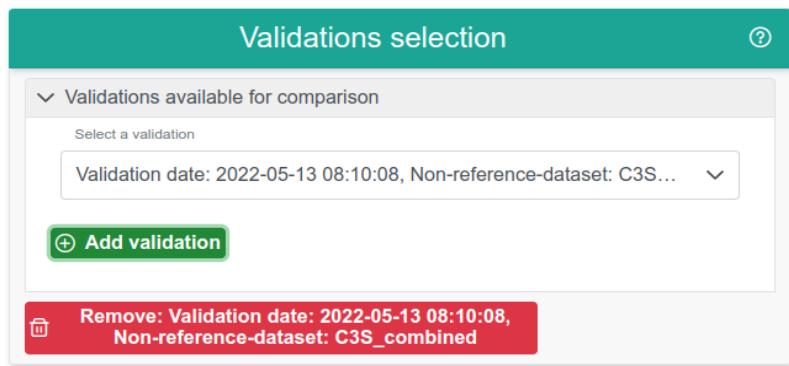
Version: 20210131 global

Variable [units]: soil_moisture [m³/m³]

Non-reference datasets

Multiple non-reference datasets

Figure 26: Datasets configuration component on the validation comparison page



Validations selection

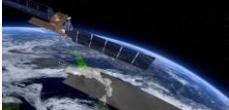
Validations available for comparison

Select a validation: Validation date: 2022-05-13 08:10:08, Non-reference-dataset: C3S...

+ Add validation

Remove: Validation date: 2022-05-13 08:10:08, Non-reference-dataset: C3S_combined

Figure 27: Validations selection on the validation comparison page

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‘Remove validation’ buttons. Clicking a remove button will remove the appropriate validation from the list.

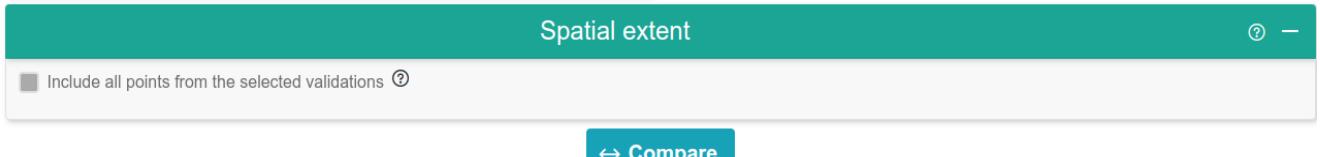


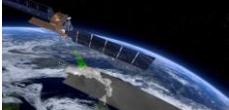
Figure 28: Spatial extent selection and ‘Compare’ button on the validation comparison page

In general, it is possible to compare any two validations that have the same reference dataset. If additionally, the two validations have a common spatial extent, a user can choose if the comparison should be performed on all points or only on the common ones. If validations have no common points, the option ‘Include all points...’ is disabled (Figure 28).

The comparison is started by clicking the ‘Compare’ button. As a result, users get four components:

- A. Comparison summary containing summaries, as described in Section 5.6, of chosen validations or validation (if ‘one validation’ mode was used);
- B. Selected comparison extent containing:
 - a. a plot with marked area for which comparison was performed,
 - b. a button for downloading the plot;
- C. Comparison statistics containing:
 - a. a table of validation statistics calculated for both validations and differences between them,
 - b. a button for downloading the table in .csv format;
- D. Comparison plots containing:
 - a. a drop-down list for metric selection,
 - b. a box plot depicting particular metric for each validation and a button for downloading it (if there is no common spatial extent between compared validations or if ‘Include all points from the selected validations’ option was chosen),
 - c. or a box plot depicting particular metric for each validation and the difference between them, a map depicting differences between the chosen metric on all points for which the comparison was performed and buttons for downloading both plots (if there was a common spatial extent between validations).

Please note, that since the comparison module is still being developed and the comparison is done on the fly, there is a risk that a particular comparison may not be performed due to too big validation results file. If that is the case the user is advised to run smaller (in terms of spatial subsetting) validations and compare them one more time.

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5.9 User data sets

Since version 2.2.0 of the QA4SM platform, it is possible to upload and validate own user data. A description of supported file formats is available at <https://qa4sm.eu/ui/user-data-guidelines>. Additional formats may be supported in the future.

After log in, the data upload form can be found under “Dataset upload/My datasets” in the navigation bar (Figure 8). If no files have been uploaded yet, only the upload file form is displayed (Figure 29).

To upload your own data, click the “Select file” button to open the upload data form for providing a proper file and the required metadata. Click the button “Add file” (Figure 30) and

select the file you want to upload. Note, that only netCDF and zip files are supported. When you select a file, a form to provide metadata will show up (Figure 31). You

Upload your data

You can use up to 5 GB space for your data. You still have 5 GB available.

No file chosen yet.

Select file

Upload file

Note: To validate your data with in situ observations, consider uploading time series at ISMN locations

Figure 29: Upload file page

need to provide data set and version names. Additionally, you can introduce display names for both the data set and its version, which will be used in the list of available data sets. If no display name is provided, the basic name is going to be used. At this stage it is still possible to change the file, you can do so by clicking the 'Change file' button. To save the provided information, click the “Save” button, which will close the

metadata form but will not start the file upload yet. To start the upload, click the “Upload file” button. Please note, that by default each user has 5 GB space assigned. If the file is too large it will not be uploaded. In such a

case you can remove already uploaded files which are not needed anymore, or contact the user support (see section 9) to discuss the specific situation.

Depending on the file size and your internet connection, the upload may take from a few seconds up to tens of minutes. You will see a blue spinner and information about the progress of the uploading process. When the file gets uploaded and preprocessed, a row with basic information about the uploaded file will show up. You will be able to change the data set and version names and to choose a different variable, if the default variable is improper or there are several variables in the file. By clicking the 'Remove data set' button, you can remove the

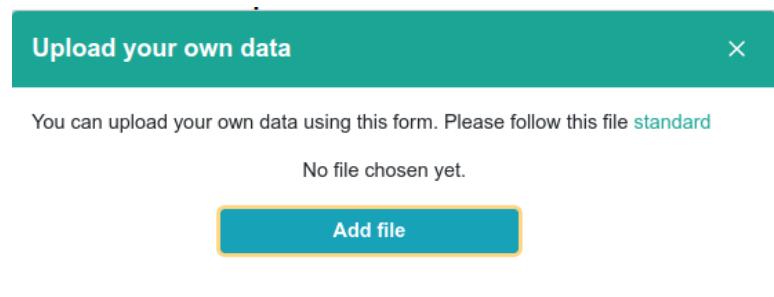
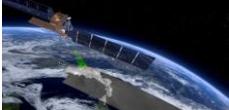


Figure 30: Upload data form

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Upload your own data X

You can upload your own data using this form. Please follow this file [standard](#)

sampleFile.sm.nc

[Change file](#)

Dataset name
 [?](#)

Dataset display name (optional)
 [?](#)

Version name
 [?](#)

Version display name (optional)
 [?](#)

[Save](#)

Figure 31: File metadata form

uploaded file. Note that, for traceability reasons, removing data files is only possible if the uploaded data have not yet been used in any validation.

Once the file with your data has uploaded and the metadata you provided is stored in the QA4SM database, you can use the file in validations by going to the “Validate” page and selecting your data set in the list of available data sets.

QA4SM users can only access their own uploaded data. The data cannot be downloaded or used in validations by any other user. A validation utilizing the uploaded data can be still shared with other users, but other users cannot reload settings or copy the results for their own validation activities in QA4SM. At the current stage, validations involving your own data cannot be published (section 5.7).

6 Supported validation types and outputs

At the core of the QA4SM functionality is the validation of one or more candidate datasets against a reference dataset and the production of pertinent metric-based scores. The service includes several options to provide a more insightful analysis and to accommodate for the user's needs.

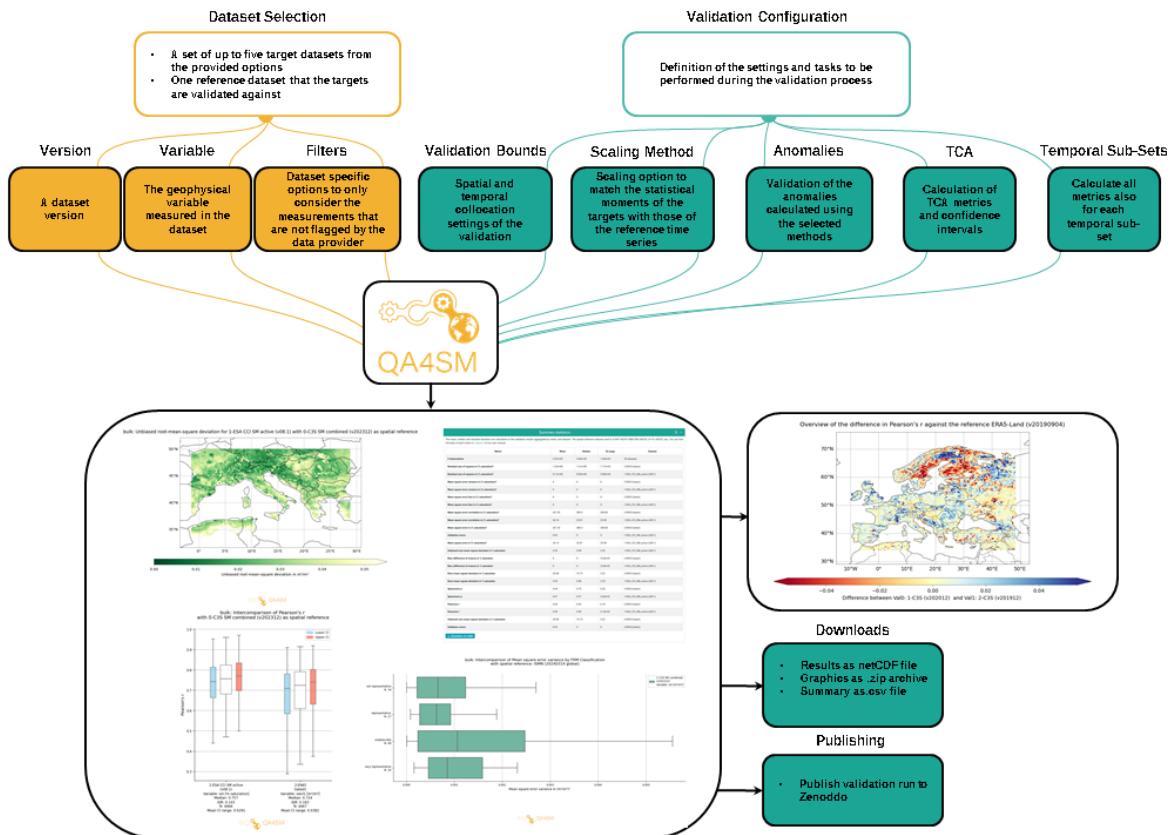
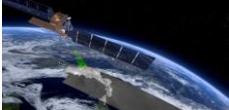


Figure 32: Conceptual scheme of the service with the available options

All accessible configurations and potential workflows are described in this section, including all the features that have been implemented in the QA4SM web service at the time of writing of this document¹². Several validation types are supported by the service as detailed in section 6.2. The optional steps taken in the validation process according to the user-defined options are outlined in section 6.1. Figure 32 provides an overview of the general validation workflow.

¹² As there is usually a time lag between the development of a feature in the source packages and its GUI implementation, the user might find that additional options are available in the source scripts (e.g., the post processing analysis, section 7.3). The interested user is also encouraged to explore the packages without the GUI support.

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6.1 Processing options

The selection of a validation configuration starts by defining the spatial and temporal bounds for which the validation metrics will be calculated. Restrictions might be applied on the spatial bounds of the validation, depending on the selected data sets; in the most up-to-date version of the service, CGLS SSM 1km and CGLS SWI 1km are the only data sets with spatial limitations (resp. over Europe only, due to the size of the data sets). In addition, necessary limitations on the temporal bounds are the first and last available date that are common to all selected datasets (the bounds are applied automatically and do not require prior knowledge of the user). Spatial and temporal re-sampling and collocation procedures are applied based on this initial selection and as described in section 4.2. The additional processing steps taken in the validation are subject to the choice of the user and can be summarized as follows:

Time series rescaling

By choosing a rescaling option, the statistical moments of a time series are matched to those of a different time series using one of the options described in section 4.3. When only a reference and candidate datasets are selected, the rescaling can be performed on the reference or on the candidate dataset, i.e., $Target^{Ref}$ or Ref^{Target} respectively, using the notation defined in section 4.3. However, when more than one candidate dataset is selected (i.e., more than two total datasets), the rescaling can only occur from the candidates onto the reference. This is avoid introducing erroneous rescaling factors in the metric score calculations of the individual candidates.

Validation of anomalies

By choosing to calculate the anomalies of the given time series using one of the methods described in section 4.4, the metric scores are calculated from the anomalies of the candidate validated against the anomalies of the reference time series. With this option active, the number of output files remains unchanged.

6.2 Validation types

The service allows for three distinct types of validation, of which an overview is given Table 4. These are not strict categories, but represent sensible workflows that can be achieved through QA4SM; however, the user is given flexibility in deciding what configuration best fits their purpose.

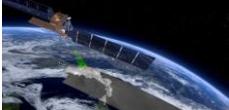
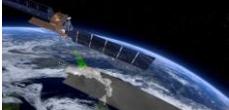
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Table 4: Validation types and the respective options.

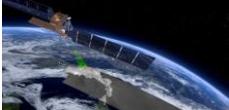
Processing options	Individual validation	Inter-comparison validation	Triple Collocation analysis	Intra-Annual Metrics	Stability Metrics
Number of non-reference datasets	1	2 +	2	1-5	1-5
TC metrics calculation	Never active	Optional. If selected, TCA will be applied to all datasets triplets combinations containing one reference	Always active	Optional.	Optional.
Anomalies calculation	Optional	Optional	Optional	Optional.	Optional.
Bootstrapping of TCA Confidence Intervals	Never active	Can be activated if TCA is selected	Can be activated	Optional. (May take long time)	Optional. (May take long time)
Rescaling	Optional. The candidate or the validation reference can be chosen as scaling reference	Optional. If selected, the validation reference is always used as scaling reference	Optional. Independently of the selection, TC metrics are always calculated on the candidates rescaled against the validation reference	Optional. The candidate or the validation reference can be chosen as scaling reference	Optional. The candidate or the validation reference can be chosen as scaling reference
Outputs					
Metric box plots	Always produced	Always produced. Each metric box plot compares the scores of all the selected datasets	Always produced. Box plots of the TC metrics are additionally calculated, each referring to a single combination of candidate and reference datasets	Always produced for all temporal sub-windows and bulk case	Always produced for bulk case

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Metric map plots	Always produced	Always produced. Each map plot corresponds to a single candidate-reference combination	Always produced. Each map plot corresponds to a single candidate-reference combination	Always produced for bulk case, not for temporal sub-windows	Always produced for bulk case
Metric box plots with metadata classification	Always produced when ISMN is selected as reference	Always produced when ISMN is selected as reference	Always produced when ISMN is selected as reference	Always produced for bulk case and temporal sub-windows when ISMN is selected as reference	Always produced when ISMN is selected as reference
Additional Options					
Validations comparison	The output can be compared with another individual validation (having the same reference data set) through the “Validation Comparison” module and the relative page	If only 2 data sets are considered in the validation, they can be compared to one another through the “Validation Comparison” module and the relative page	The two non-reference data sets can be compared to one another through the “Validation Comparison” module and the relative page	Not yet implemented	Not yet implemented
Additionally Produced Output					
Special Plots	None	None	None	Clustered Boxplots for all (TCA) metrics for temporal sub-windows	Clustered Boxplots for all (TCA) metrics and stability metrics plots

1. Individual validations

The basic functionality offered by the service is the validation of a single dataset against the reference. Any of the datasets listed in section 3 can be chosen as candidate; the ISMN makes an exception, in that it can only be used as validation reference. This design reflects the fact that ISMN measurements represent an approximation of the ‘ground truth’ against which

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developed products can be assessed. Moreover, without any method to aggregate the point measurements, using ISMN as non-reference would exclude the majority of the in-situ data from the validation, with the current spatial collocation procedure (section 4.2).

2. Inter-comparison validations

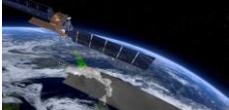
The current configuration of the service supports the selection of up to 5 candidate datasets that can be validated against a common reference. In an inter-comparison validation, the scores achieved by all the datasets against the reference are compared in the output plots. This validation type is useful in evaluating the performance of different products in the exact same validation conditions.

3. Validations with Triple Collocation Analysis

As detailed in section 4.1.2 TC metrics can be calculated from a triplet of measurements, hence requiring that at least two candidate datasets are included in the validation. If this condition is met, the option to calculate TC metrics is available. A validation with TC analysis will provide the output scores (and plots) of TC metrics in addition to the *common metrics* scores. In addition, the confidence intervals on the TCA scores can be calculated by selecting the option for ‘Bootstrapping of confidence intervals’ in the validation interface. This will have an impact on the effective validation run time.

No restrictions are applied in terms of which datasets can be used for TC analysis, and it is the user’s responsibility to ensure that the necessary assumptions of TC are met. One of the fundamental assumptions of TC is error orthogonality, meaning that the sources of errors of the datasets composing the triplet should be distinct and uncorrelated (Gruber et al., 2016). The following datasets combinations violate this condition:

Dataset	Non-error orthogonal datasets	Source of error correlation
ESA CCI SM combined	<ul style="list-style-type: none"> • SMAP SPL3SMP • SMAP SPL2SMP • SMAP SPL2SMP • SMOS IC • SMOS L2 • SMOS L3 • H-SAF ASCAT SSM CDR • ESA CCI SM passive • ESA CCI SM active • GLDAS • C3S SM combined 	The ESA CCI combined product merges data from different active and passive SM satellite missions. GLDAS is used as TC reference in the merging process of the ESA CCI combined product
C3S SM combined	<ul style="list-style-type: none"> • ESA CCI SM combined 	The dataset is based on the ESA CCI products

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	<ul style="list-style-type: none"> • SMAP SPL3SMP • SMAP SPL2SMP • SMOS L2 • SMOS L3 • SMOS IC • H-SAF ASCAT SSM CDR • ESA CCI SM passive • ESA CCI SM active • GLDAS 	
ERA5	<ul style="list-style-type: none"> • ERA5-Land 	ERA5-Land is based on a re-processing of the ERA5 product
ERA5-Land	<ul style="list-style-type: none"> • H-SAF ASCAT SSM CDR 	ERA5-Land assimilates data from ASCAT
CGLS SSM 1km	<ul style="list-style-type: none"> • CGLS SWI 1km • ESA CCI SM active • H-SAF ASCAT SSM CDR • ESA CCI SM combined • C3S SM combined 	The active observation system onboard Sentinel 1 has similar error sources to the other active products in the service.
CGLS SWI 1km	<ul style="list-style-type: none"> • CGLS SWI 1km • ESA CCI SM active • H-SAF ASCAT SSM CDR • ESA CCI SM combined • C3S SM combined • CGLS SSM 1km 	The active observation system onboard Sentinel 1 has similar error sources to the other active products in the service.
ESA CCI SM passive	<ul style="list-style-type: none"> • SMAP SPL3SMP • SMOS L2 • SMOS L3 • SMAP SPL2SMP • SMOS IC 	The passive product combines several passive sensors, including SMOS and SMAP
ESA CCI SM active	<ul style="list-style-type: none"> • H-SAF ASCAT SSM CDR 	The active product combines several active sensors, including ASCAT-A and B
SMOS L3	<ul style="list-style-type: none"> • SMAP SPL3SMP • SMAP SPL2SMP • SMOS L2 • SMOS IC • ESA CCI SM passive 	Passive sensors are characterised by similar error sources

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4. Validation with Intra-Annual Metrics

As detailed in section 4.5, all validation metrics can be calculated for temporal sub-windows in addition to the bulk case. The validation configuration follows the steps and limitations pointed out above in points [1. Individual validations](#) and [3. Validations with Triple Collocation Analysis](#).¹³

5. Validation with Stability Metrics

As detailed in section 0, all common validation metrics can be calculated for annual temporal sub-windows in addition to the bulk case. Currently, stability metrics cannot be calculated together with intra-annual metrics at the same time.

6.3 Output files and reports

As output of the validation, the service provides information on the status of the process, along with graphical results that can be interpreted immediately and a condensed summary in the form of a table. Moreover, the raw data on the validation metric scores are also made available and can be accessed directly.

6.3.1 Validation process output

In case the validation has been cancelled during the process, or it has encountered an unexpected error, the only process output is a report with information on the status of the validation. In case no error has been encountered during the validation, or all encountered errors could be handled correctly (e.g., absence of data for a specific validation point), the process output will be summarized in a report along with the results files. The information contained in the report can be summarized as:

- Outline of the validation configuration: complete information on the selected configuration settings, including the selected datasets, versions and filtering options, scaling, anomalies and TC metrics options, spatial and temporal settings of the validation.
- Process diagnostics: start and end time of the validation run, total run time, number of validation points with percentage of points producing errors during the validation, information on the storage of the results and their automatic clean-up.

6.3.2 Image files

Two types of graphic results are automatically generated, consisting of a box plot and a map plot of the scores achieved for the validation metrics. For each *common* metric, the scores of all datasets are plotted in the same box plot image (Figure 33; for TC metrics, a separate box

¹³ It should be noted however, that the calculation of intra-annual metrics can take considerably longer. If TCA and possibly even bootstrapping are activated, the time required might increase dramatically once again.



plot is produced for each metric and dataset, allowing a comparison of the scores achieved by all the possible triplet combinations. Box plots are aimed at providing concise and fully informative graphics on the distribution of the values and its main statistical moments. Map plots, on the other hand, necessarily only represent a single validation metric and a candidate to reference combination (Figure 34). Their purpose is to allow for the interpretation of the spatial trends in the dataset's performance.

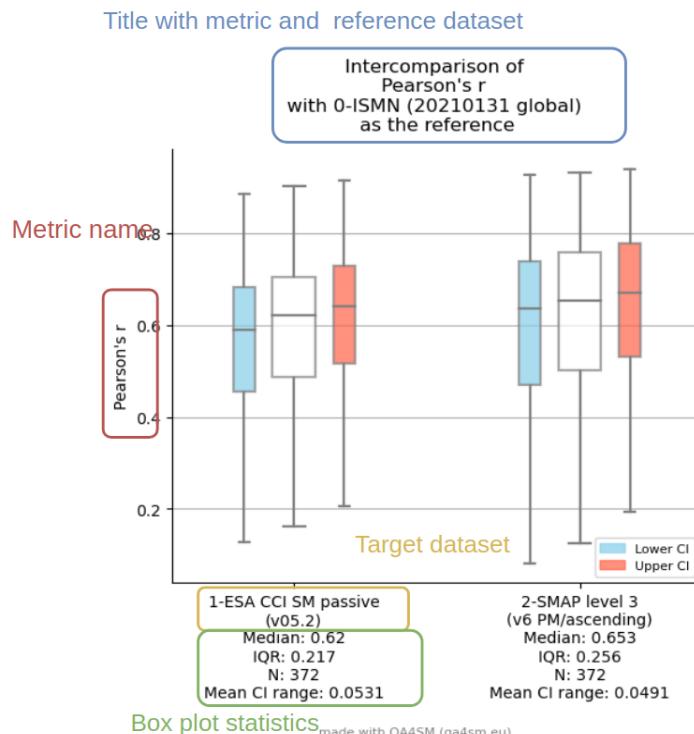


Figure 33: Example of a box plot where two datasets are validated against the same reference and compared. The box plot statistics provide information on the estimate median (Median), the interquartile range (IQR, between 1st and 3rd quartile) and the number of points (N)

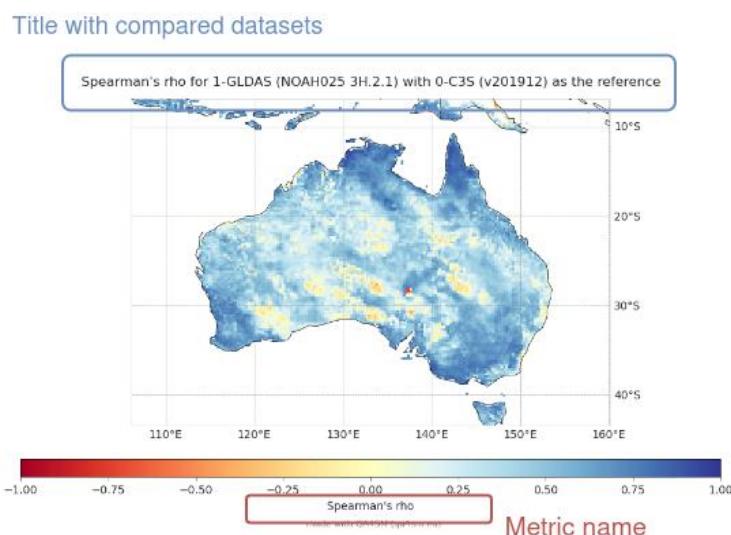


Figure 34: Example of a map plot

In addition to the metric scores, the output plots provide an overview of the ‘statuses’ of each validation point (see Section 4.7), showing the relative abundance and spatial patterns in the errors encountered in the validation process (Figure 35). Note that a unique ‘status’ plot is produced, representing all the metrics.

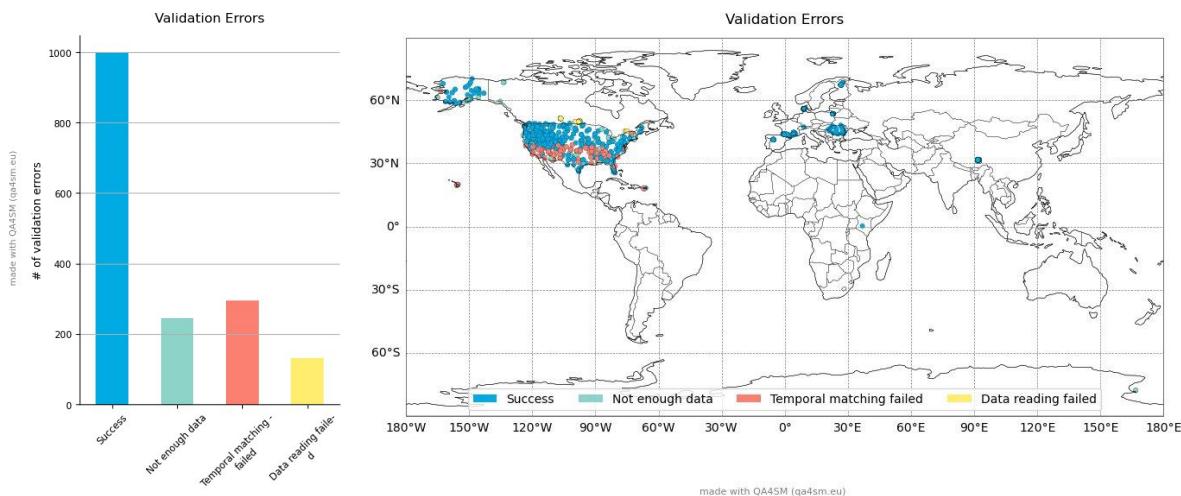


Figure 35: ‘Status’ output box plot and map for an example validation.

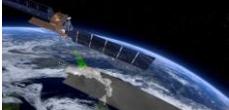
6.3.3 Metadata-classified outputs

When a validation is run with ISMN as reference data set, the environmental and sampling information provided with the ISMN database¹⁴ can be used to enhance the analysis of the validation results. The metadata information used in QA4SM and the respective variable collected from the ISMN database are presented in Table 5.

Table 5: Metadata types used in QA4SM and the corresponding ISMN variable.

Classification as presented in QA4SM	Variables used from ISMN database	Source	Description
Land Cover	<i>lc_2010</i>	ESA CCI Landcover Classes 2010-v1.6.1:	<p>A static land cover map from 2010 is used as a proxy for land cover. This does not account for changes taking place in the land cover over the different validation periods.</p> <p>The classes are grouped in the following:</p> <ul style="list-style-type: none"> • Grassland • Tree cover

¹⁴ For more information, visit: <https://ismn.earth/en/data/additional-datasets>

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			<ul style="list-style-type: none"> • Urban areas • Cropland • Other 															
Climate	<i>climate_KG</i>	Köppen-Geiger database (Peel et al., 2007)	<p>The acknowledged Koeppen-Geiger climate classification is used, where the original classes are grouped in the following:</p> <ul style="list-style-type: none"> • Arid • Tropical • Temperate • Continental • Not provided 															
Soil type	<i>sand_fraction</i> <i>clay_fraction</i> <i>silt_fraction</i> <i>instrument_depthfrom</i> <i>instrument_depthto</i>	Harmonized World Soil Database (HWSD)	<p>The soil type classification is based on the soil type diagram, which is used to distinguish between medium, coarse and fine granulometry as shown in Figure 36. The measurements are also binned by measurement depth, as specified by the sensor dept information of ISMN.</p>															
Fiducial Reference Measurements classification	<i>frm_class</i> <i>frm_snr</i>	<p>Processing of ISMN according to the FRM Protocols and Procedures for Soil Moisture (FPP_SM), FRM4SM deliverable DT2.1</p>	<p>The FRM classification based on the representativeness measure calculated from the Signal-to-Noise ratio value with ERA5 and the ESA CCI Soil Moisture data sets. A more comprehensive description of the FRM flagging procedure is provided in FRM4SM project deliverable DT2-1, FRM Protocols and Procedures for Soil Moisture (FPP_SM).</p> <p>The thresholds used for classification are given in the following table. The sensor counts refer to ISMN time series between 0.10 cm depth and for which triple collocation was possible.</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="background-color: #0070C0; color: white;">Estimated SNR⁽¹⁾</th> <th style="background-color: #0070C0; color: white;">QI class</th> <th style="background-color: #0070C0; color: white;"># sensors</th> </tr> </thead> <tbody> <tr> <td>NaN</td> <td>undeducible⁽²⁾</td> <td>1066</td> </tr> <tr> <td>< 0 dB</td> <td>not representative</td> <td>720</td> </tr> <tr> <td>0 – 3 dB</td> <td>representative</td> <td>556</td> </tr> <tr> <td>> 3 dB</td> <td>very representative</td> <td>604</td> </tr> </tbody> </table> <p style="text-align: center;">⁽¹⁾ based on TCA with ERA5-Land and CCI Passive (0.25 deg) ⁽²⁾ when # samples < 100 or CI (80%) < 3 dB</p>	Estimated SNR ⁽¹⁾	QI class	# sensors	NaN	undeducible ⁽²⁾	1066	< 0 dB	not representative	720	0 – 3 dB	representative	556	> 3 dB	very representative	604
Estimated SNR ⁽¹⁾	QI class	# sensors																
NaN	undeducible ⁽²⁾	1066																
< 0 dB	not representative	720																
0 – 3 dB	representative	556																
> 3 dB	very representative	604																

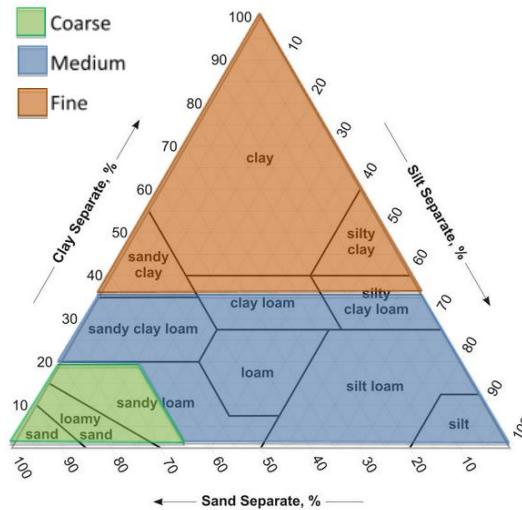


Figure 36: Soil type triangle and classification by soil granulometry, used for the metadata classification.

In practice, the validation scores can be binned according to the selected metadata type, and classified in the resulting box plots (Figure 37).

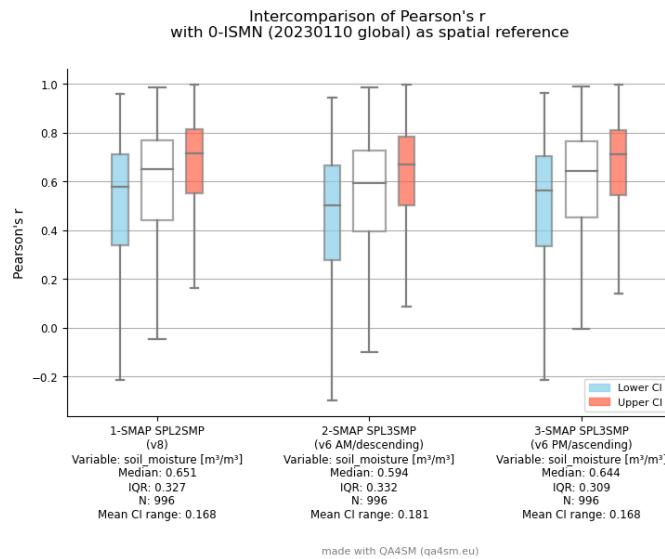
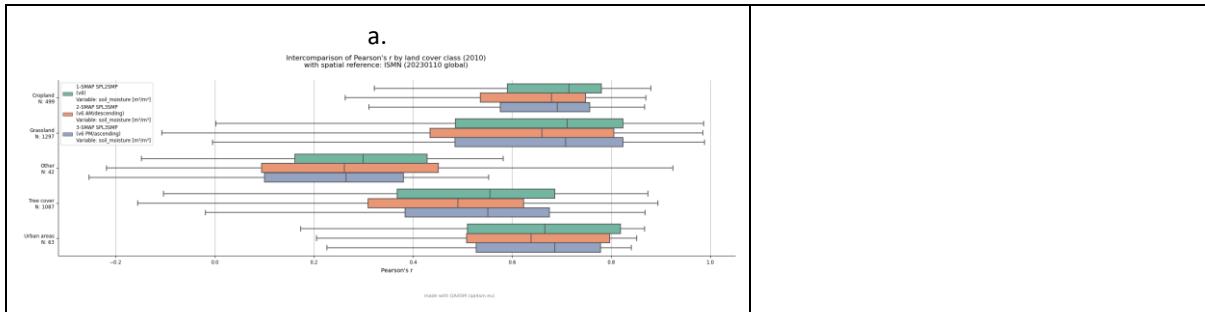


Figure 37: Example output showing box plots of the correlation for three data sets against ISMN as a reference.



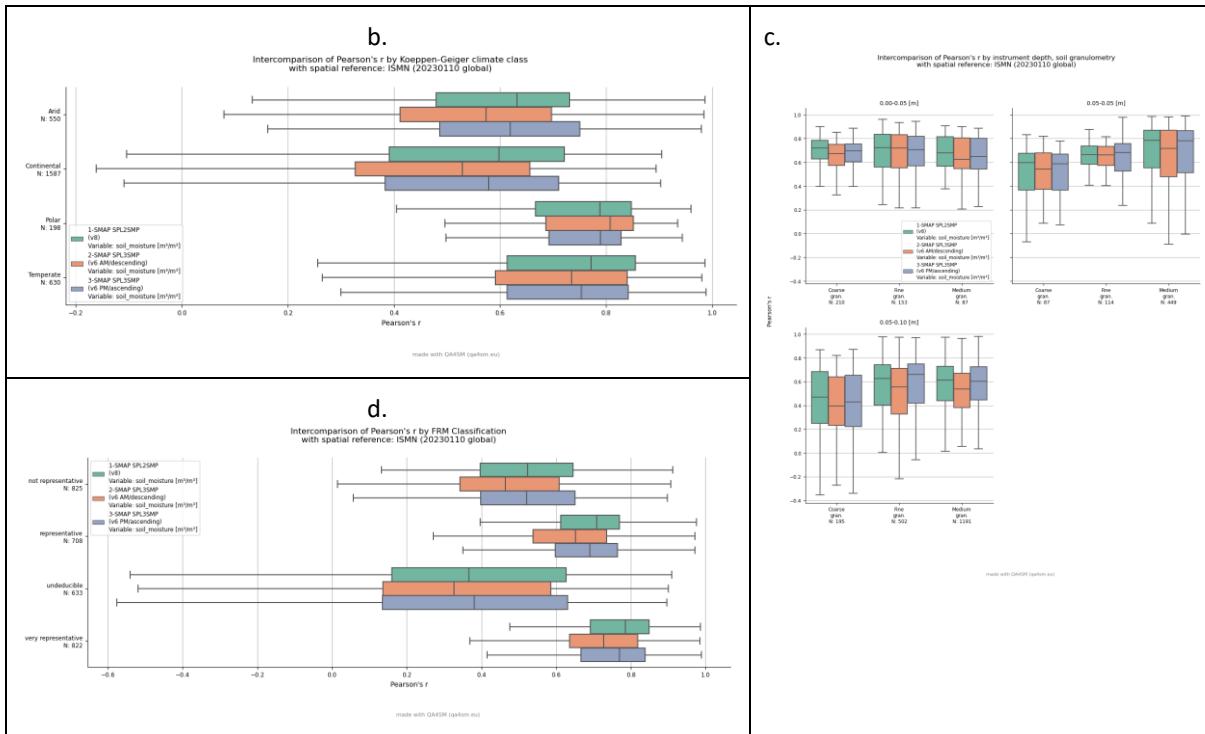


Figure 38: Same output as Figure 37, but classified according to (a.) land cover type (b.) Koeppen-Geiger climate class and (c.) sampling depth and soil granulometry (d) FRM classification.

6.3.4 Validations comparison

The validation scores of two data sets can be compared directly using the “Validation Comparison” module and the respective page (Section 0). The only prerequisite for this is to have access to the validation scores of two separate data sets, validated against the same reference data set. These can either come from the same validation run, if two non-reference (candidate) data sets were included, or from two separate runs with only one candidate data set each. The selection procedure is described more extensively in Section 0.

The outputs of the comparison are:

- a map showing the spatial extent of both validations and the points used in the calculation of the difference scores Figure 39
- a table providing a comparison summary through the difference in the median scores of both validations
- Graphic results (in all similar to the output plots of a normal validation) of the difference by validation score (Figure 40)

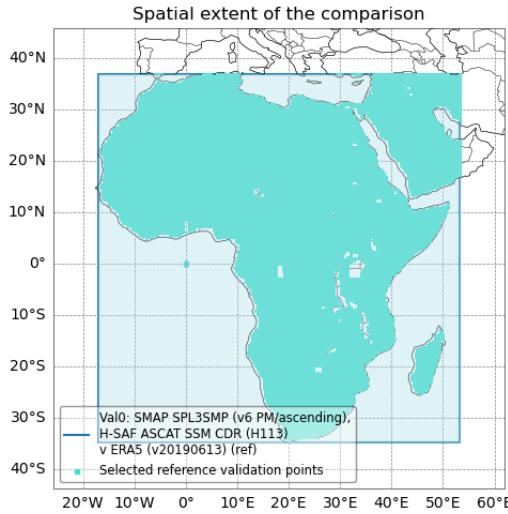


Figure 39: Example output of the comparison module. The spatial extent of the comparison and the GPIs considered for the calculation of the scores difference are shown in the plot.

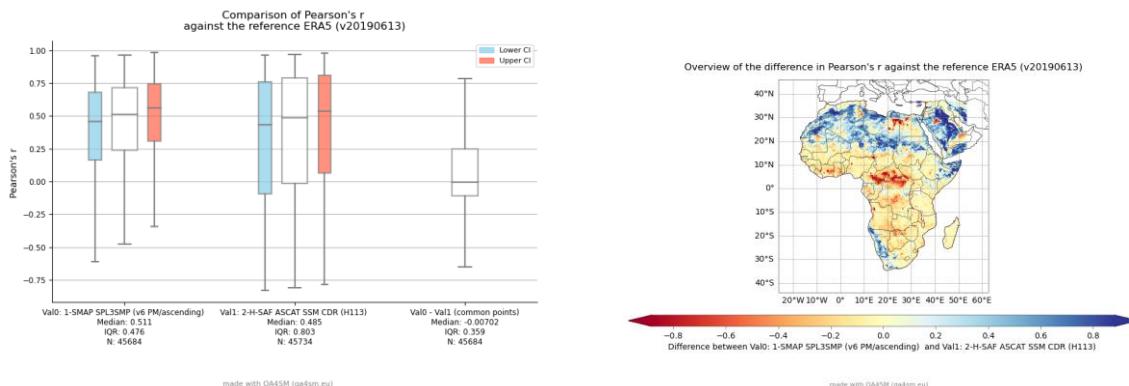


Figure 40: Example output of the comparison module. The box plots and map plot show a difference of the correlation of two data sets (SMAP SPL3SMP, H-SAF ASCAT SSM CDR) validated against ERA5.

When two individual validations are compared, their spatial extent can differ (Figure 41). Therefore, a choice can be made to compare only the GPIs that are common between the two validations or to simply compare all validation points of the two validations (this is also the only option available when the two validations have non-overlapping extents; for instance, when the performance of a SM product is to be assessed between different geographical locations). This generally results in different comparison outcomes (Figure 42).

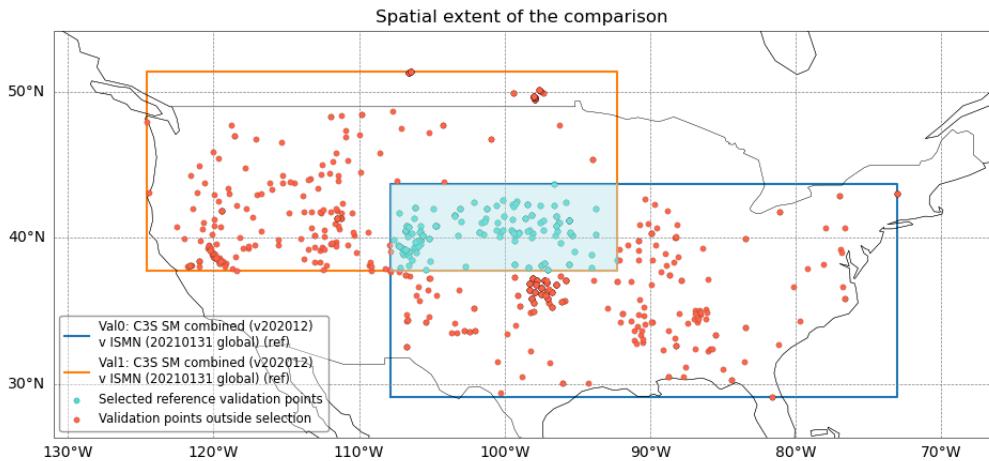


Figure 41: Example of validations with partially overlapping geographic extents.

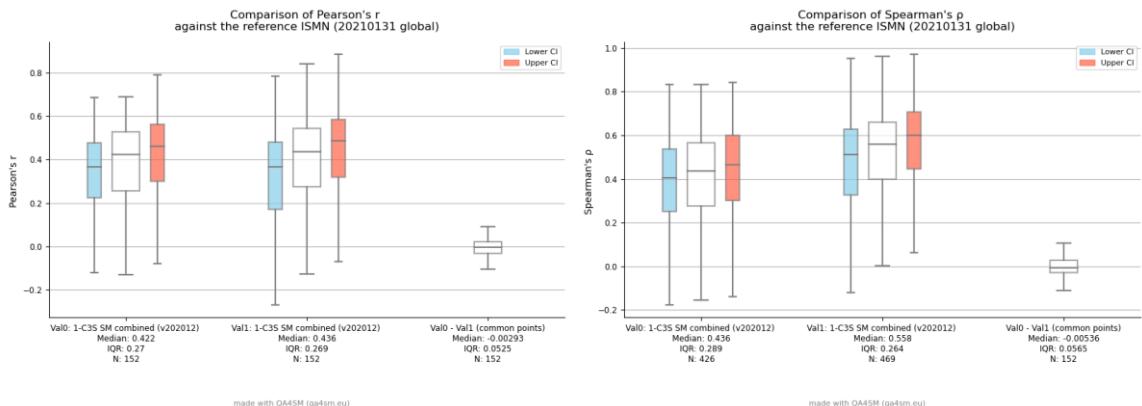


Figure 42: Output of the comparison shown in Figure 41, where only the common points (left) and all validation points (right) are taken into account.

6.3.5 Intra-Annual Metric Results

As introduced in sections 4.5 and 6.2, activation of the intra-annual metric feature effectively computes all desired metrics for the bulk case and each temporal sub-window. Map plots, # status plots, # observation plots and metadata plots are exclusively provided for the bulk case. All other metric boxplots, common and TCA, are provided for each of the temporal sub-windows, too. Additionally, each a clustered boxplot (or metric intercomparison plot) is provided for each common and TCA metric. Figure 43 below depicts such a clustered boxplot. To facilitate a direct comparison of a given metric of each temporal sub-window, these

clustered boxplots only take into account GPIs, that have valid data for all temporal sub-windows.

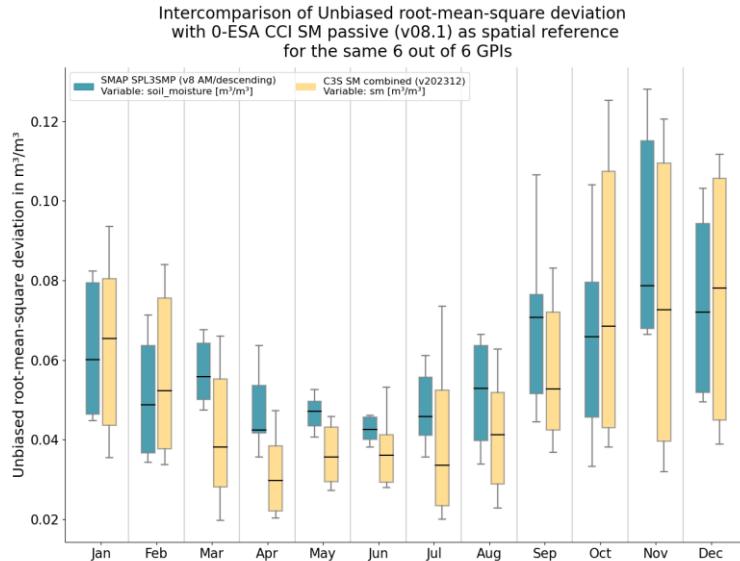


Figure 43: Clustered boxplot of ubRMSD for the same 6 out of 6 GPIs for a monthly frequency of temporal sub-windows.

As the overall amount of produced graphics is large, the GUI only shows all bulk case plots as well as the clustered boxplots. The entirety of plots, including a statistics table for each temporal sub-window, is available upon download of the .zip archive (see section 6.3.8 below).

6.3.6 Stability Metrics Results

As introduced in sections 0 and 6.2, activation of the stability metric feature computes all metrics for the bulk case and each temporal sub-window (i.e., annual windows for each year in the selected date range). All general plots, as well as stability metric plots (e.g., map plots for the Theil-Sen slope of BIAS; see Figure 44), are generated exclusively for the bulk case. Additionally, a clustered boxplot is provided for each common metric.

bulk: Theil-Sen slope of BIAS for 1-SMOS Level 3 (version 339 Descending) with 0-ERA5-Land (v20190904) as spatial reference

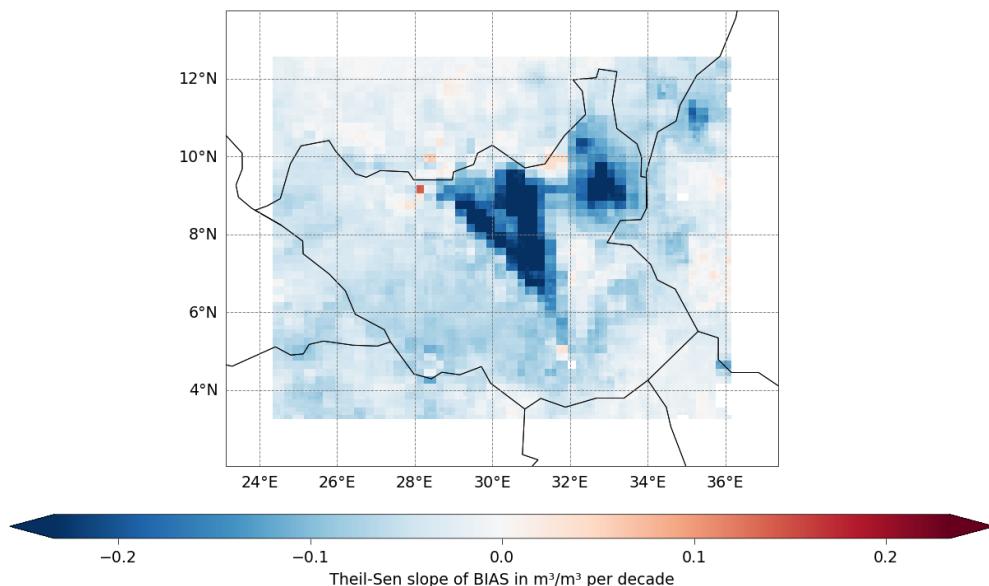


Figure 44: Mapplot of Theil-Sen Slopes of BIAS in South Sudan.

In the GUI, the Theil-Sen slopes of BIAS, R, and uRMSD are displayed alongside all bulk case plots.

6.3.7 Results summary

The metric scores are summarized in a table for an easy, quick inspection of the results. Here, the statistical moments of mean, median and inter-quartile range for each metric distribution and dataset are given (Figure 45). Note that for non-additive scores, such as Pearson's and Spearman's correlation, the averaging method proposed in Alexander (1990) is used to compute the mean value. The significance scores are not included in the summary.

6.3.8 Download files

The following files can be downloaded from the validation results:

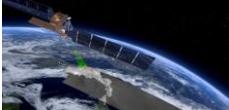
Summary statistics

The summary statistics table can be downloaded in the comma-separated values (.csv) format.

netCDF File

A Network Common Data Form¹⁵ (netCDF) file which provides the raw metric scores data. This is organized in variables containing as many values as the number of points used in the

¹⁵Documentation at: unidata.ucar.edu/software/netcdf/

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validation. Each variable either provide geographical information on the validation point (e.g., longitude, latitude or GPI) or metric scores for a specific candidate to reference pair (or triplet, for TC metrics). Additional variables are included when the ISMN dataset is used in the validation, containing metadata on the environmental and measurement characteristic of the in-situ stations. In addition to this, global attributes provide information on the datasets and configuration options of the validation.

Summary: ERA5 v. ASCAT - ref ISMN anomalies 	
<ul style="list-style-type: none"> Started validation on Oct 18, 2024, 7:01:48 AM UTC, finished on Oct 18, 2024, 7:08:12 AM UTC. Compared 3 datasets: <ul style="list-style-type: none"> 1-ERA5 (v20190613, swvl1 [m³/m³]) (temporal reference) Filters: <ul style="list-style-type: none"> Soil not frozen; Variable in valid geophysical range; 2-H-SAF ASCAT SSM CDR (H113, sm [% sat.]) Filters: <ul style="list-style-type: none"> Soil not frozen (or state not known); No confidence flags raised; No processing flags raised; Variable in valid geophysical range; 0-ISMN (20210131 global, soil_moisture [m³/m³]) (spatial, scaling reference) Filters: <ul style="list-style-type: none"> Quality flag is "good" (G); Variable in valid geophysical range; Use ISMN networks: ARM, SCAN, SNOTEL, USCRN; Use measurements at given depth: 0.00, 0.10; Spatial filter bounding box: [23.779, -134.328, 49.785, -63.936]. Validation period / temporal filter: Jan 2, 2007, 12:00:00 AM UTC to Dec 31, 2017, 12:00:00 AM UTC. Temporal matching window size set to 3 hours. Validation metrics calculated from anomalies against climatology computed on years 2007 through 2018. Triple collocation analysis was activated. Bootstrapping of confidence intervals for Triple Collocation Analysis was deactivated. Intra annual metrics were deactivated. Scaling reference: ISMN (20210131 global, soil_moisture) [Filters: Quality flag is "good" (G); Variable in valid geophysical range; Use ISMN networks ARM,SCAN,SNOTEL,USCRN Use measurements at given depth 0.00,0.10] Scaling method: CDF matching with beta distribution fitting. Processing took 6 minutes (wall time). for 61.725% (458 of 742) of the processed locations (grid points) the validation metrics could not be calculated. For an overview of potential causes select '# status' (available from version 2.2) in the 'Result files' section. <input checked="" type="checkbox"/> This validation will be automatically removed during cleanup on Dec 17, 2024, 7:08:12 AM UTC. 	

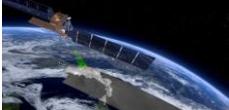
Figure 45: Quick inspection table with the main statistical moments for each metric, providing a summary of the validation result

Plot files

A compressed (.zip) folder contains all box plots and map plots from the validation. The files follow the naming conventions specified in Table 6.

Variable components change based on specific plot characteristics:

- Range:** Time Range / Temporal Window (bulk, season (S1) or month name (Jan)).
- Metric:** Statistical measure as introduced in section 4.4

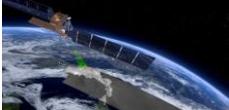
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- Common (for all metrics types): n_obs
- Pairwise (between reference dataset and other datasets): R, p_R, rho, RMSD, BIAS, urmsd, mse, mse_corr, mse_bias, mse_var, RSS, tau, p_tau, status
- Triple Collocation: snr, err_std and beta
- Stability Metrics: slopeURMSD slopeR and slopeBIAS
- **Dataset:** Dataset identifier (one of the available datasets in chapter 3 or user uploaded dataset).
- **Type:** Metadata Type, only for ISMN validations. (frm_class, lc_2010, climate_KG, instrument_depth_and_soil_type, or network) see metadata-classified outputs in section 6.3.3.
- **Extension:** File format (.png or .svg).

Plot Type	Naming Pattern	Example	Description
Barplot	Range_*barplot*_status*	bulk_barplot_status.png	Only used for the status metric
Boxplot (Standard)	Range_*boxplot*_metric	bulk_boxplot_BIAS.png	Standard boxplots for various metrics
Boxplot (Triple Collocation)	Range_*boxplot*_metric_for_dataset	bulk_boxplot_beta_for_2-GLDAS.svg	Generated when triple collocation is selected
Boxplot (Metadata)	Range_*boxplot*_metric_metadata_type	bulk_boxplot_urmsd_metadata_climate_KG.png	Only generated when ISMN is included
Mapplot (Standard)	Range_*overview*_dataset1_and_dataset2_metric	bulk_overview_0-ISMN_and_1-C3S_combined_RMSD.png	Spatial distribution maps
Mapplot (Triple Collocation)	Range_*overview*_dataset1_and_dataset2_and_dataset3_metric_for_dataset	bulk_overview_0-ERA5_and_1-C3S_combined_and_2-SMOS_L3_snr_for_1-C3S_combined.png	Spatial distribution maps
Comparison	*comparison*_boxplot*_metric	comparison_boxplot_BIAS.png	Generated for intra-annual or stability metrics

Table 6: Plot files naming convention

Fixed keywords (appearing exactly as shown in all filenames) are marked with asterisks: for, metadata, overview, and, comparison, boxplot.

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7 Sample data validation

This section provides an overview of a sample validation, including the initial configuration set up, report analysis and results interpretation.

7.1 Validation set-up

A set of two satellite datasets are validated against in-situ measurements from the ISMN dataset, using the configuration in the table below.

Dataset	Version	Applied filters
ISMN (Reference)	20210131global	<ul style="list-style-type: none"> • Variable in valid geophysical range • Quality flag is "good" (G) • Use measurements at given depth: 0-0.1 m • Chosen ISMN networks: ARM, SCAN, SNOTEL, USCNR
ERA5 (Data)	v20190613	<ul style="list-style-type: none"> • Variable in valid geophysical range • Soil not frozen
H-SAF ASCAT SSM CDR (Data)	H113	<ul style="list-style-type: none"> • Variable in valid geophysical range • Soil frozen (or state not known) • No confidence flags raised • No processing flags raised

The datasets configuration options are selected in the dedicated section of the ‘Validate’ page (Figure 46). In order to filter out points where the physical conditions hamper the SM retrieval in the satellite time series, measurements with frozen soil conditions or unknown state are masked in the H-SAF ASCAT SSM CDR (ASCAT) dataset, together with flags raised by the data providers regarding the reliability of the measurements. Frozen soil is masked in the ERA5 dataset as well, for consistency. For the in-situ data, only measurements flagged as ‘good’ by the ISMN standards are considered (information on the flagging algorithms used for the available datasets in section 3), from a total of 4 selected networks. Furthermore, for all datasets only SM measurements with a value in a realistic geophysical SM range are considered.

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Data

> H-SAF ASCAT SSM CDR / H113 / sm (temporal reference)

> ERA5 / v20190613 / swvl1

✓ ISMN / 20210131 global / soil_moisture (spatial, scaling reference)

Dataset: ISMN

Version: 20210131 global

Variable [units]: soil_moisture [m³/m³]

Variable in valid geophysical range

Quality flag is "good" (G)

Include only representative sensors (FRMs)

Use ISMN networks: select...

Use measurements at given depth: select...

Remove dataset

Add dataset

Reference

② Spatial reference
Select dataset (version)
ISMN (20210131 global)

② Temporal reference
Select dataset (version)
H-SAF ASCAT SSM CDR (H113)

Scaling

Method:
Select scaling method
CDF matching with beta distribution fitting

Scale to:
Select scaling reference
ISMN (20210131 global)

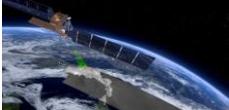
Figure 46: Datasets selection for the sample validation

The maximum available period for the datasets, between 2007.01.02 and 2017.12.31, is chosen for a subset over the US:

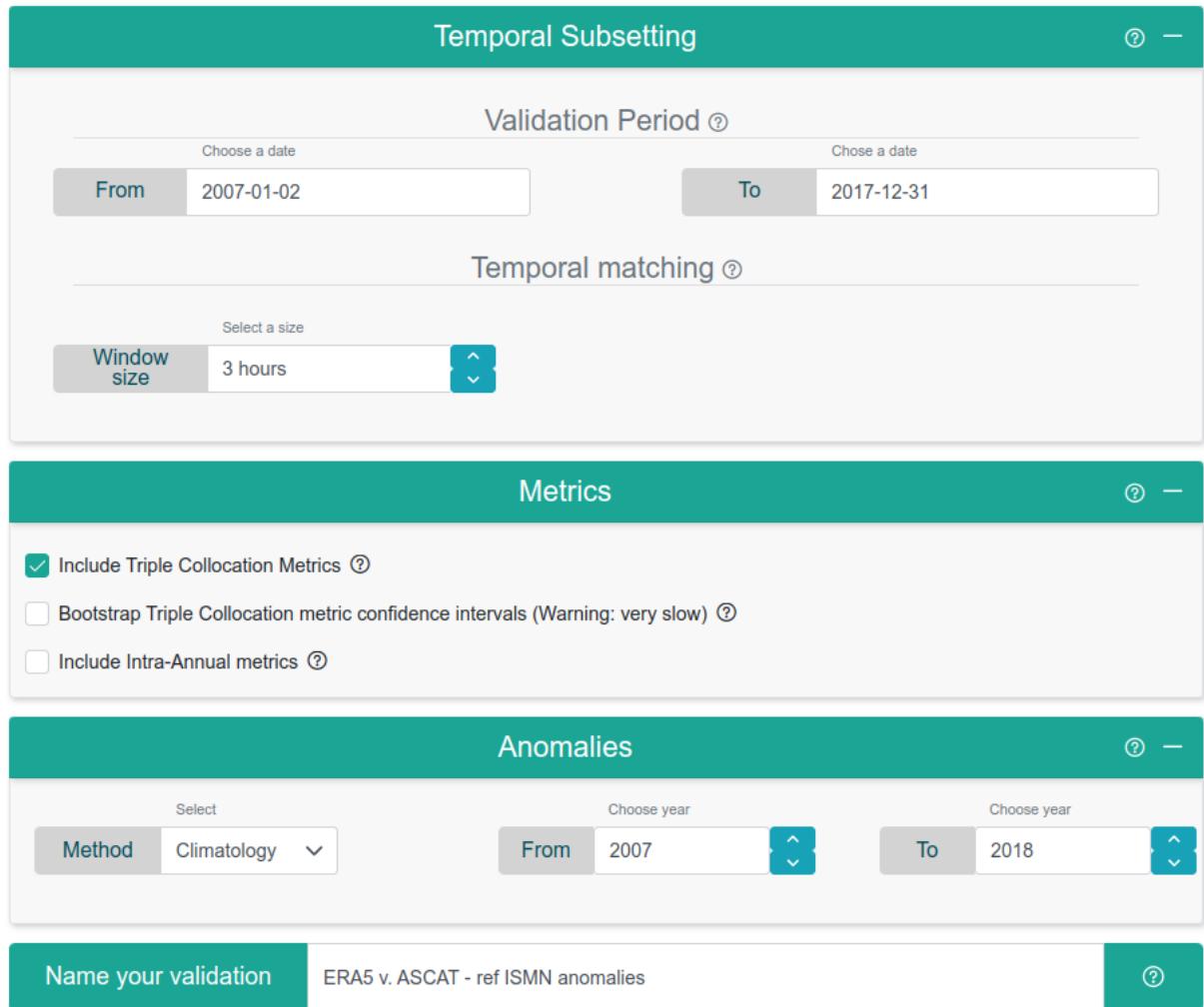


Figure 47: Selected geographical validation subset

A matching window of 3 hours is selected as a stricter temporal collocation than the default (12 hours) is preferred here. As three datasets are available, the TC metric calculation is toggled in the validation configuration options (Figure 48). Furthermore, the anomalies calculation is selected using the climatology of the considered period. To account for climatic

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trends, for instance when a multi-decadal validation is performed, using a rolling average could be a preferable option (section 4.4). To eliminate the biases between the two candidate datasets and the reference, a CDF matching rescaling procedure is applied; with respect to the other rescaling options, this could better account for non-linear relationships in the extremes ranges of SM.



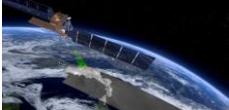
The screenshot shows three stacked configuration panels:

- Temporal Subsetting:** Set validation period from 2007-01-02 to 2017-12-31. Temporal matching window size is set to 3 hours.
- Metrics:** Includes checked options for Triple Collocation Metrics and Intra-Annual metrics, and an unchecked option for Bootstrap confidence intervals.
- Anomalies:** Set method to Climatology, validation period from 2007 to 2018, and validation name to "ERA5 v. ASCAT - ref ISMN anomalies".

Figure 48: Validation configuration

7.2 Validation report analysis

After the validation has run, and having received the automatic e-mail message, the result can be accessed from the overview page with all the user validations (Figure 49).

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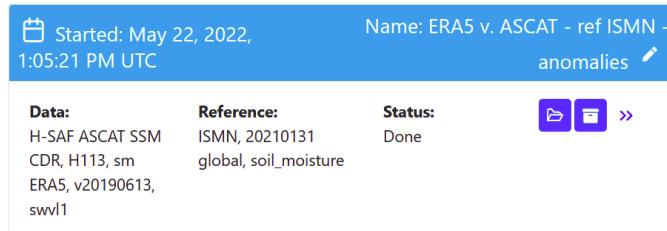


Figure 49: Result access in the ‘My validations’ page with status of the validation ‘Done’. The results can be accessed through the open folder icon.

In the results page, the ‘Results summary’ section, containing an overview of the validation configuration and run results, is used to inform the user of the overall validation status (Figure 50). As can be inferred from the summary, no errors have been produced during the run (“0% of the metrics could not be calculated”), meaning that at all validation points the complete metrics set has been calculated. In addition, for the sample validation a total of 9 minutes runtime has elapsed¹⁶.

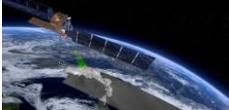
Summary: ERA5 v. ASCAT - ref ISMN anomalies ↗

- Started validation on Oct 18, 2024, 7:01:48 AM UTC, finished on Oct 18, 2024, 7:08:12 AM UTC.
- Compared 3 datasets:
 - 1-ERA5 (v20190613, swvl1 [m³/m³]) (temporal reference)**
 - Filters:
 - Soil not frozen;
 - Variable in valid geophysical range;
 - 2-H-SAF ASCAT SSM CDR (H113, sm [% sat.])**
 - Filters:
 - Soil not frozen (or state not known);
 - No confidence flags raised;
 - No processing flags raised;
 - Variable in valid geophysical range;
 - 0-ISMN (20210131 global, soil_moisture [m³/m³]) (spatial, scaling reference)**
 - Filters:
 - Quality flag is "good" (G);
 - Variable in valid geophysical range;
 - Use ISMN networks: ARM, SCAN, SNOTEL, USCRN;
 - Use measurements at given depth: 0.00, 0.10;
- Spatial filter bounding box: [23.779, -134.328, 49.785, -63.936].
- Validation period / temporal filter: Jan 2, 2007, 12:00:00 AM UTC to Dec 31, 2017, 12:00:00 AM UTC.
- Temporal matching window size set to 3 hours.
- Validation metrics calculated from anomalies against climatology computed on years 2007 through 2018.
- Triple collocation analysis was activated.
- Bootstrapping of confidence intervals for Triple Collocation Analysis was deactivated.
- Intra annual metrics were deactivated.
- Scaling reference: ISMN (20210131 global, soil_moisture) [Filters: Quality flag is "good" (G); Variable in valid geophysical range; Use ISMN networks ARM, SCAN, SNOTEL, USCRN Use measurements at given depth 0.00, 0.10]
- Scaling method: CDF matching with beta distribution fitting.
- Processing took 6 minutes (wall time).
- for 61.725% (458 of 742) of the processed locations (grid points) the validation metrics could not be calculated. For an overview of potential causes select '# status' (available from version 2.2) in the 'Result files' section.
- This validation will be automatically removed during cleanup on Dec 17, 2024, 7:08:12 AM UTC.

X Delete ↗ Renew 📁 Archive 📄 Publish ⚙ Load settings

Figure 50: ‘Results summary’ with the overview of the validation run configuration and status.

¹⁶ Note: this validation was run on the production server.

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7.3 Results interpretation

A series of plots and statistics are generated as output of each validation run, providing the scores achieved by the candidate datasets against the reference dataset, on the basis of the validation metrics.

7.3.1 Results summary table

The most immediate way to interpret the validation results is by looking at the ‘Summary Statistics’ table in the results page (Figure 51). Here, metric-wise scores are displayed to compare the validation outcome of the candidate datasets between one another, with the exception of the ‘# of observations’, which indicates the number of reference measurements per validation points on which the score is based. For the validation configuration, a mean of 10300 points were present in the time series, taking all validation points into account (Figure 51). This number can be greatly affected by the strictness of the filtering options and the temporal window used in the matching of the observations (here, 3 hours). Looser filtering options will provide more observations, although the quality on the individual measurements could be impacted. From a quick glance at the table, it can be noticed that the ERA5 dataset is characterized by a higher median and mean Spearman’s and Pearson’s r with respect to ASCAT. This indicates that the dataset is overall better correlated with the in-situ measurements; furthermore, since the interquartile ranges are similar, it can be deduced that the distribution of values is similar for the two products. Looking at the difference metrics, a similar conclusion is drawn in that ERA5 is in better agreement to the in-situ measurements than ASCAT (e.g., median RMSD 0.056 and 0.065 [$(m^3/m^3)^2$], respectively), for this particular validation configuration.

Metric	Mean	Median	IQ range	Dataset
# observations	1.03e+04	1.02e+04	9.58e+03	All datasets

Figure 51: Section of the summary table

7.3.2 Output plots and figures

In the bottom section of the result page, each metric can be analysed separately by means of a box plot, showing the distribution of the result by dataset, and a map plot, which shows for each dataset and metric the distribution of the validation values across the validation points.

For *common metrics* (see section 4.1.1), the scores achieved by the two datasets can be directly compared in the same plot. In Figure 52, the correlation and RMSD for the sample validation can be interpreted. ERA5 shows a moderately good positive correlation with the in-

situ data, with a median r close to $\sim 0.55 [-]$ ¹⁷. ASCAT has an overall (lower) median correlation of $\sim 0.4 [-]$, with a few outlying points in stronger disagreement with the ground data, as indicated by the lower quartile value (Figure 52). The RMSD similarly characterizes the ERA5 product as performing better than ASCAT, for the given configuration. Although the former attains only a slightly lower median value, the overall distribution has a smaller spread around the median, with a noticeably lower upper quartile value.

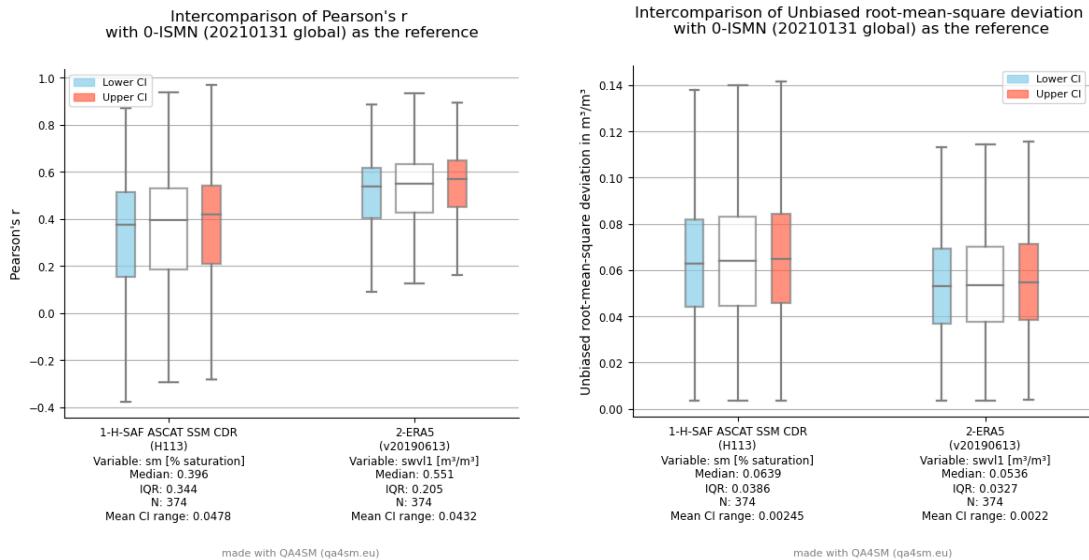
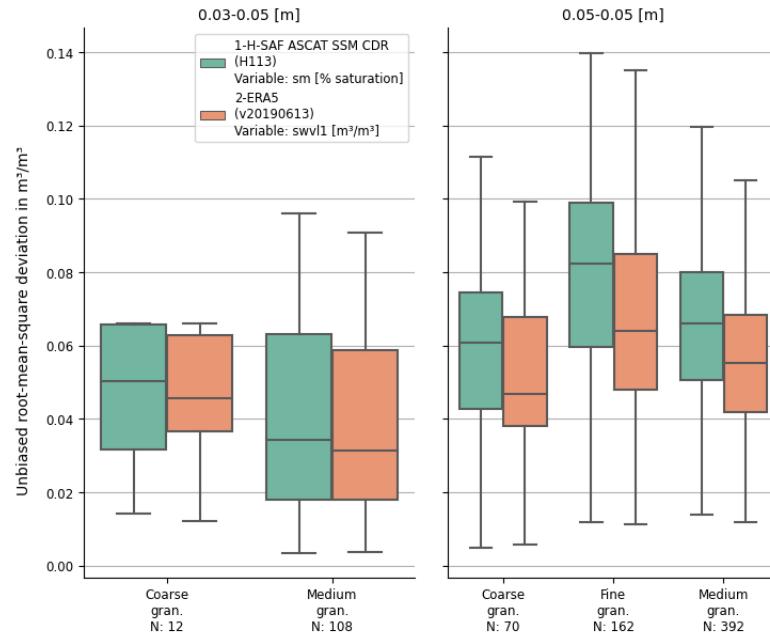


Figure 52: Box plots of Pearson's r (left) and unbiased RMSD (right) between the datasets and the reference, for the selected validation configuration

As can be noticed by looking at the distribution of the correlation values for ASCAT (Figure 54, below), the highest values are in the central-eastern part of the US, while the correlation tends to decrease along the western coastline. This could be attributed to the effect of topographic features on the retrieval of SM from the satellite measurements. On the contrary, ERA5 shows a homogeneous spatial behaviour (Figure 54). Looking at the “soil type” metadata classification (Figure 53), it can be observed that ERA5 outperforms ASCAT at all sampling depths and for the different soil compositions. Moreover, the unbiased RMSD is deteriorating with depth more noticeably for ASCAT, due to the penetration limit of microwave observations. Similarly, the soil granulometry has a larger impact on the satellite product compared to the reanalysis data set.

¹⁷ We use the notation $[-]$ for dimensionless values, i.e., values without units.

Intercomparison of Unbiased root-mean-square deviation by instrument depth, soil granulometry
with reference: ISMN (20210131 global)

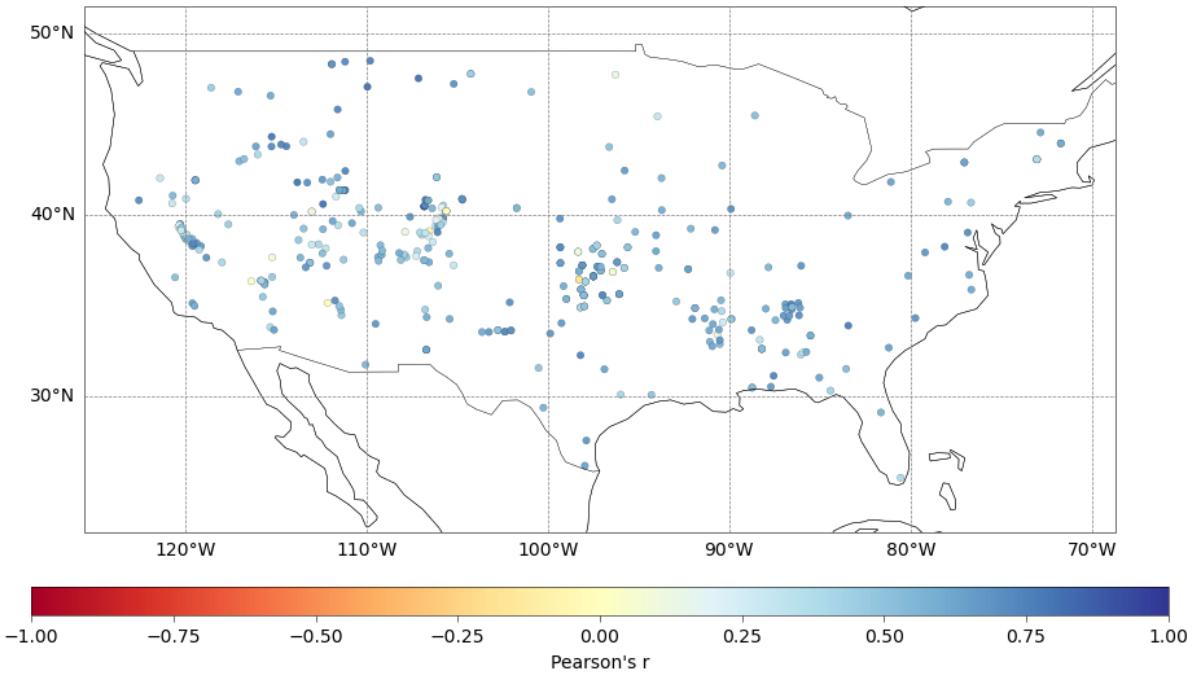


made with QA4SM (qa4sm.eu)

Figure 53: Classification of the unbiased RMSD for based on the soil granulometry and depth.

Overall, ERA5 performs better than ASCAT and agrees reasonably well with the in-situ data, especially considering the difficulty of characterising anomalies from satellite measurements, compared to the general climatology or the bulk signal.

Pearson's r for 2-ERA5 (v20190613) with 0-ISMN (20210131 global) as the reference



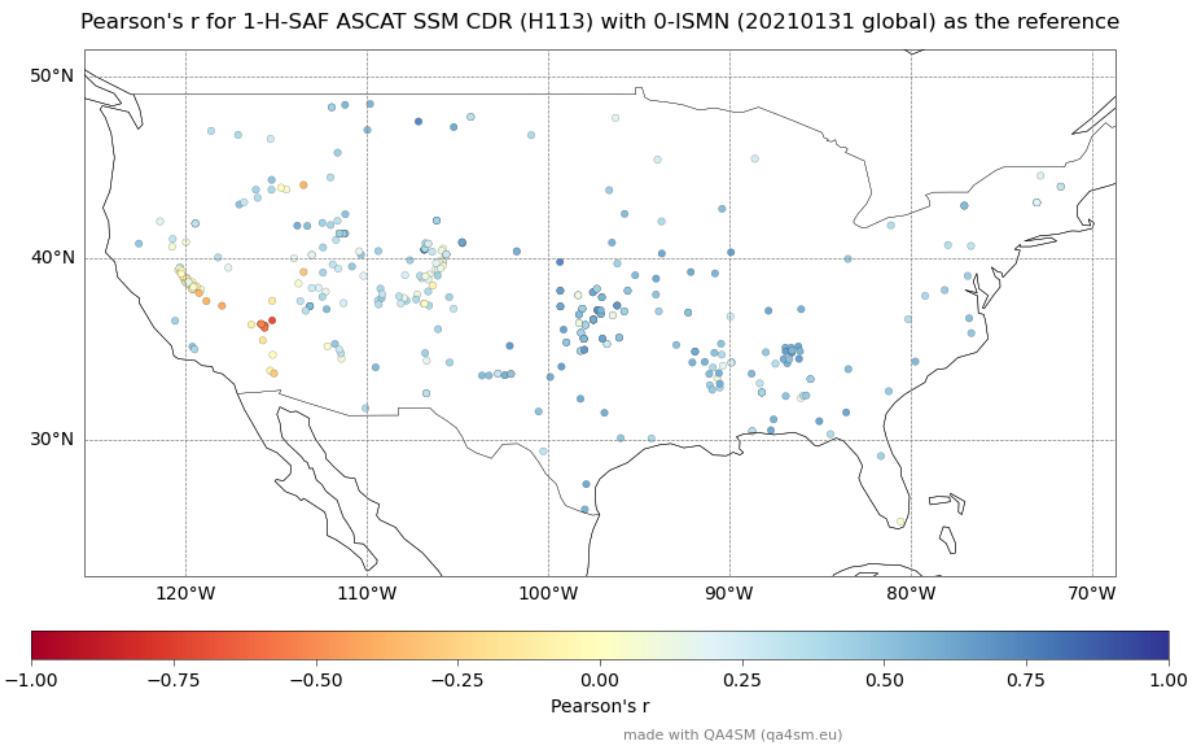


Figure 54: QA4SM plot showing the spatial distribution of Pearson's r for the validation configuration for ERA5 (above) and H-SAF ASCAT SSM CDR (below)

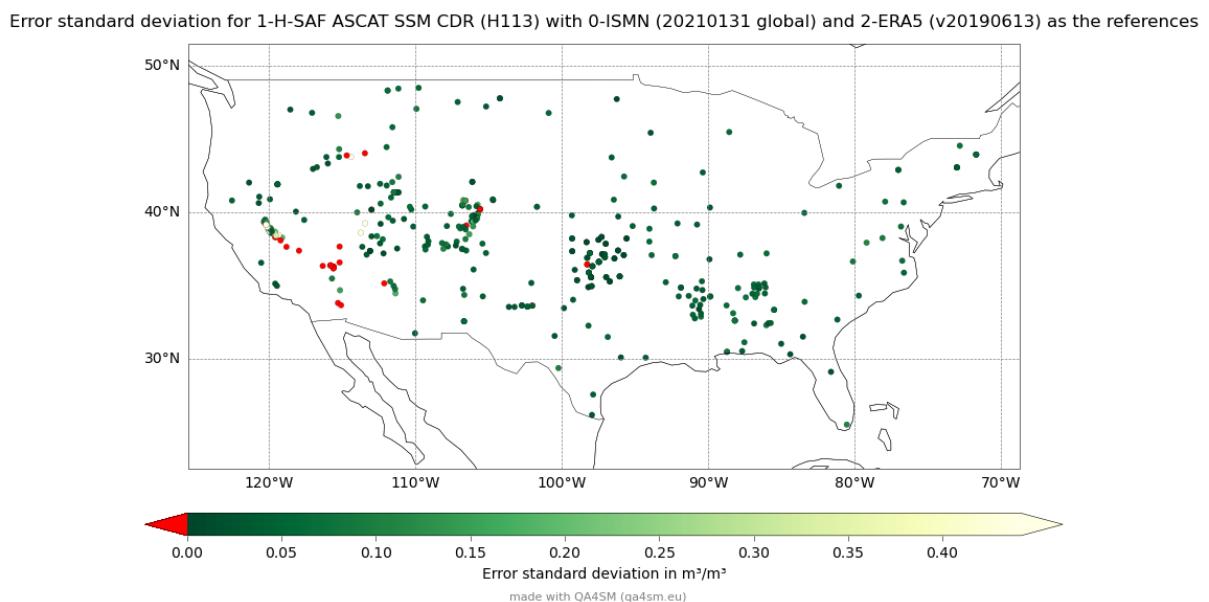


Figure 55: QA4SM plot showing the spatial distribution the STD_{err} that characterizes ASCAT¹⁸

¹⁸ Negative STD_{err} values can occur as statistical artifacts and should be interpreted as the STD_{err} value cannot be estimated at that point (see for instance González-Gambau et al., 2020).

Additional information on the quality of the datasets, independently of the reference, can be gathered from the scores achieved on the TC metrics. The datasets are affected by a substantially different noise level, with median SNR of 3.14 and -1.34 [dB] for ERA5 and ASCAT, respectively. Remarkably, the STD_{err} in the ASCAT dataset shows a similar pattern to the correlation, where a localised performance decrease can be observed in the western US (Figure 55).

The two data sets can also be compared directly using the “Validation comparison” module. This allows to visualize the spatial difference in the validation scores, as well as quantitatively through the difference box plot (Figure 56).

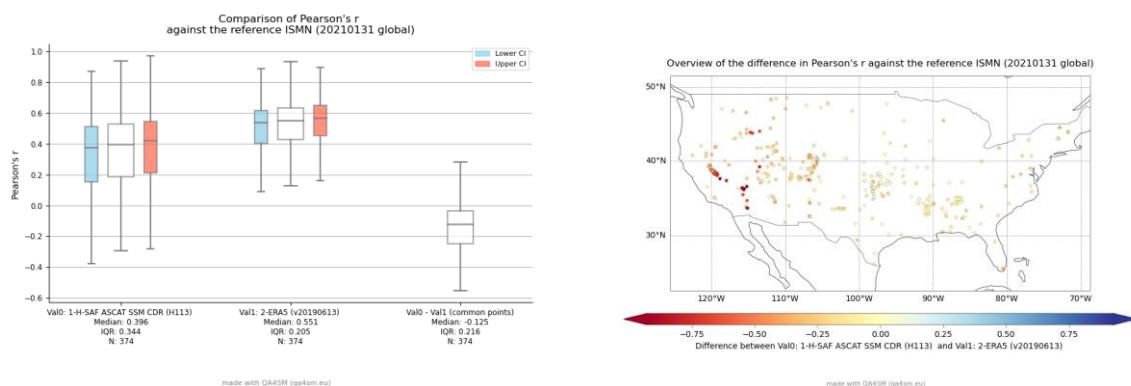
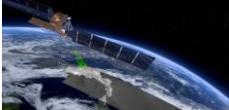


Figure 56: Outputs of the validation comparison module for the Pearson's correlation scores in the box plot (above) and map plot (below) form.

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8 Description of the QA4SM platform

QA4SM is an online, open-source service with all source code available in the qa4sm GitHub repository <https://github.com/awst-austria/qa4sm>. The metric calculation and ISMN data reading functionality is provided with the `pytesmo` and `ismn` open-source python packages developed by TU Wien's Department of Geodesy and Geoinformation and supported by other necessary modules and packages. The full list of packages used in QA4SM service is available in the GitHub repository. New dependencies are added as needed during development of new functionalities, and currently used packages are updated to the latest versions with every QA4SM release. If necessary, restrictions are imposed on packages versions, so that there are no dependency conflicts.

8.1 High-level software architecture and components

Users can access the QA4SM service using the user interface, described in section 5. Application's back-end is handled using python's framework Django and the front-end is created using Angular. Information on datasets, versions, filters, settings, along with registered users and validations are stored in a database. Soil moisture input data is stored in

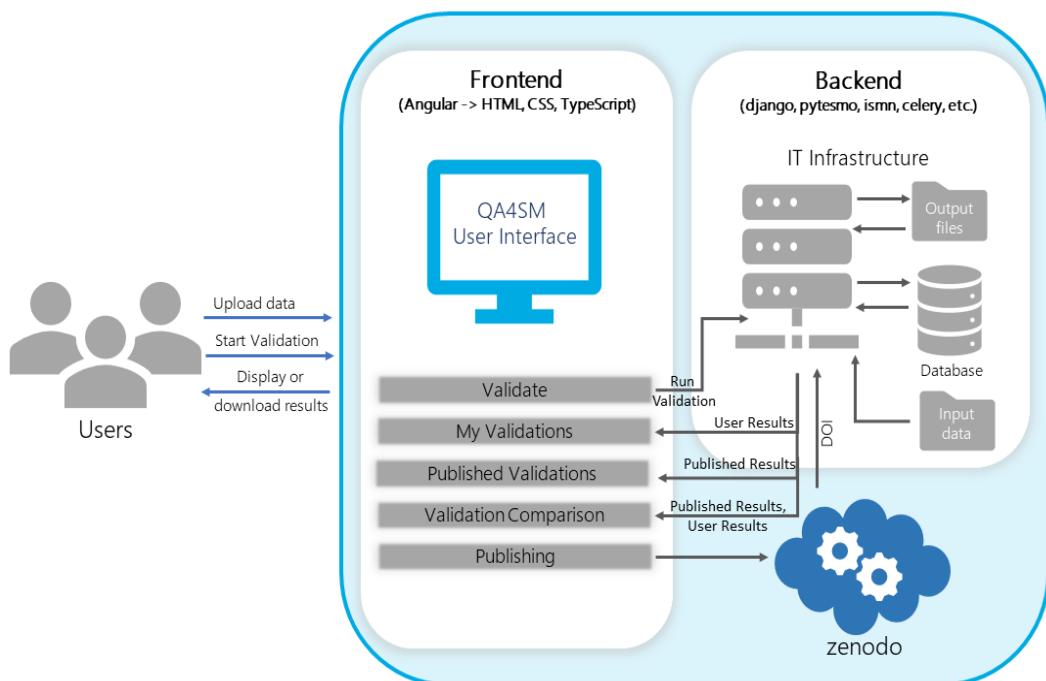


Figure 57: QA4SM platform architecture diagram

NetCDF or .csv formats, which speeds up reading. The data is not available for users to be downloaded. When a user runs a validation, the data is read using a reader appropriate for the particular data set, processed according to the chosen settings (using the `pytesmo` package for metrics calculation), and results are saved in the output directory. Settings are saved in the database and displayed on particular views, along with buttons for downloading

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results. The detailed interaction with the QA4SM user interface is described in section 5. QA4SM also provides access to the Zenodo service, which enables publishing a validation by creating and assigning a DOI identifier. The identifier is added to the appropriate validation in the QA4SM database and all validations with DOI are displayed on the Published validations page which is publicly accessible. A high-level operation diagram of the QA4SM application is shown in Figure 57.

Currently, one operational instance and two test instances of the QA4SM service are maintained. The test instances are used by the development team for testing new features, modifications and releases in a quasi-operational environment before deployment in the operational service instance.

8.2 Data access, storage, retention, deletion

8.2.1 Datasets and results

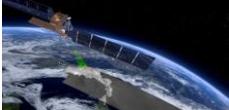
Datasets used for validations are not available for users in their raw form. Links to the actual dataset sources are provided on the Datasets page of the service and in section 3 of this user manual. Results of validations are available to users for downloading in the netCDF format, as graphic files and as a csv file, containing a statistics summary. The graphic files and summary statistics are also available directly on the website (see e.g., section 3 for details).

It is possible for users to download their own results, results of published validations and results of validations run by another user if they are provided with a direct link to the specific validation. Results management, however, is only possible for the user's own validations. Users can remove, archive or extend the retention period / life span of their results, unless the results have been already published. Published results cannot be removed, even by their owners. If the results have not been published, archived or their retention period has not been extended they are automatically removed 8 weeks after their creation.

Since QA4SM version 2.2.0 users can upload their own data. Such data can be used in a validation and removed by the owner, but it cannot be downloaded, neither by the owner nor other users. Moreover, users have no access to the data uploaded by different users, even for validation purposes. Platform administrators have access to the user files stored on the server but cannot interactively access these files in the QA4SM service, so they cannot run validations with data uploaded by other users.

8.2.2 User Profile Data

All personal user data are managed in agreement with the EU General Data Protection Regulation (GDPR). On registration, users are required to provide a username, password and a valid email address. Additionally, users can provide the given name, family name,

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organisation, country and ORCID number. Providing this information is optional and not required for creating an account.

Any data provided by the users are not conveyed to third parties, other than for the delivery of the specified emails, the provision of the QA4SM web service (e.g., mentioning a user's full name in emails sent to them) or as required by law. Aggregated user information, including the number of users per country and organisation, may be passed on to funding agencies or others to advertise the service or attract more funding. This is aimed at helping to cover the cost of the free QA4SM service.

The QA4SM web service writes logs about connections made to it, which include the users' IP addresses. This information is used to investigate errors, attempts to disrupt the service, etc. The logs are not conveyed to third parties unless legally required or needed for the prosecution of disruptions of the service or the investigation of malfunctions. Aggregated information about connections may be passed on together with aggregated user information. Logged information is deleted at regular intervals.

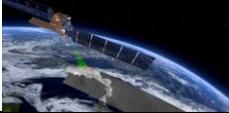
Apart from the username, all the data can be updated anytime. Users who want to delete their account should go to the user profile page (see section 5.3) and chose the 'Deactivate my account' button. The account will automatically be deactivated and removed by the service provider. The deletion of the user account will remove access to the service and all non-published validations. Restoring an account is not possible. Creating a new account with the same username will not restore access to validations previously run by the removed user.

The full QA4SM terms and conditions are available at <https://qa4sm.eu/terms>.

8.3 IT infrastructure resources and platform

All instances of the QA4SM service are maintained on the cloud computing infrastructure provided by TU Wien. They are isolated and technically independent from each other, but computing and storage resources of the underlying cloud infrastructure can be allocated and moved between instances to meet the operational demand and provide sufficient resources for critical verification tests. The following IT infrastructure resources are currently available to the QA4SM project:

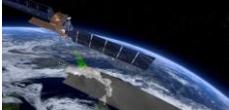
- 2 x CPUs (32 Cores each)
- 512 GB RAM
- 10 GBit Ethernet Adapter
- 2 x SSD, 6.4 TB each

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8.4 Known technical issues and limitations, planned improvements

Currently recognized technical issues and limitations include the following matters:

- It may happen that for some selected validations a comparison cannot be performed. The reason is that the comparison computations are done on the fly and validations may be too large to be processed and produce the desired output with the current hardware resources.

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9 User support

This manual provides users with detailed information on all aspects of the QA4SM service. Remember though, that the service is under continued development and features and functionalities will evolve over time. Therefore, when working with the QA4SM service, please regularly check the News section on the QA4SM main page and the online help page. Also, please always read notifications and popups that show up on the website. Some of them may indicate problems, e.g., when a user is trying to register but the chosen username is already in use, while others may warn users that the action they are about to undertake cannot be undone, e.g., removing a validation.

In case of problems, questions or doubts, please check the FAQ in section 9.1 and the known technical issues in section 8.4. If you cannot find an answer to your question or you have some suggestions, please do not hesitate to contact the QA4SM support help desk by email at support@qa4sm.eu. Note, that the help desk is currently only available via email, there is no chat or help desk contact form in the service itself. We will provide an initial response to email requests within three working days. When reporting a problem, please describe in detail what happened, what notification you received or what doubts you have. If it helps, you can attach a print screen.

If the problem concerns a validation, please send us your username, a validation ID and describe the issue you refer to. You can find the validation ID in the address bar, when you are in a validation view, as shown in Figure 58. The ID number in this case is 7673c97e-53fe-46df-a8f3-135fe8605bb8.

If you have problems finding or copying the number, you can

Figure 58: Address of a single validation view containing the validation ID

send us your username and details about the validation you refer to. In this case, please send us the start time of the validation and the names of the datasets used.

If you have doubts regarding the obtained results, you do not have to send us the resulting NetCDF file. It is sufficient to send us the validation ID. If you have doubts about particular plots, though, it will be useful to attach the files you are referring to.

Please avoid general descriptions like 'there is something wrong with my validation', but describe what is wrong in particular. For instance, 'I started my validation (with ID ...) 2 days ago, but it still has Scheduled status' or 'I started a validation with settings (listed settings) but it seems like the settings ... have not been saved'. Please remember that the more exact and unambiguous your issue description is, the quicker the issue can likely be identified and resolved.

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9.1 Frequently asked questions

User registration

What data do I need to provide while registering?

You need to provide a username, password and its confirmation and email. The rest of the fields are optional.

Do I need to provide my business email, or can I use my private address?

This is up to you. The email address will be used, for instance, to send you notifications about finished validations or to recover your password.

Should I provide my personal data while registering?

It is up to you. Please note though, that if the support team gets the impression that the new account request is created by a bot, the account will not be activated.

Why is there a field for the ORCID number in the registration form?

QA4SM is geared towards supporting the scientific community. The ORCID number allows direct identification of the particular scientist and is often required when publishing articles. Since the service enables publishing results, the ORCID number can be used during this process for unambiguous assignment of the scientist to the results.

Datasets

Which datasets and versions are available for validation in the service?

Various types of datasets, covering satellite-based data, in situ measurements and land surface models are available. The specific datasets with versions and filter options are described in section 3 of this manual. An up-to-date list of supported datasets is also available at <https://qa4sm.eu/ui/datasets>.

Do the available datasets cover the same time periods?

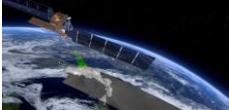
No. Different datasets and different versions may cover different time ranges. For available time spans please check section 3.

Can I upload my own data for validation?

Yes, this is supported in the QA4SM service. Please note, that the data has to conform to the data format specification available at <https://qa4sm.eu/ui/user-data-guidelines>. The uploading procedure is described in section 5.9.

How many files can I upload?

Only one file can be uploaded at a time, but there is no limit on the total number of files. However, there is a limit to the total file storage size per user, which is currently 5 GB. In

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justified cases, additional storage space can be provided upon request. In cases, where data sets are of general interest for the user community, users may request the integration of the data in the publicly available datasets supported by QA4SM.

How can I obtain more space for my data sets or propose the integration of additional public data sets?

To get more space for your uploaded data or propose the integration of publicly available data into QA4SM, please contact the support team at support@qa4sm.eu.

Validate

How many data sets can I compare within one validation?

You can compare up to six datasets.

How can I add and remove data sets in the Data component?

You can add data sets using the ‘Add dataset’ button on the bottom of the component. The button gets disabled if you reach six data sets. You can remove a data set using the ‘Remove dataset’ button on the tab of the currently selected data set. If there are only two data sets, the remove button gets disabled, as at least two data sets are needed for a validation.

Are all data sets available for selection in the Reference component?

Generally yes, except if ISMN data is selected. QA4SM allows users to separately set spatial and temporal references. For the temporal reference, any selected data set can be set. For the spatial reference this is only the case when no ISMN data set is selected. If ISMN data is selected it must be used as spatial reference.

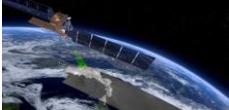
Why can some filters of the ISMN dataset not be switched off?

There are two groups of filters that cannot be switched off. The first group are filters that introduce parameters, for instance the network selection and selection of measurement depth for ISMN dataset. You can change these parameters to select different networks or measurement depths, but you cannot switch them off. If you do not change or select anything, the default values are used.

The second groups are mandatory filters that are by default applied during computations. They are listed below the particular dataset to inform users what kind of preselection has been done, but there is no possibility to switch them off.

Can I choose the same dataset multiple times in the same validation?

Yes, you can do so.

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Why does the default spatial sub-setting cover only Europe? Does this mean that the default datasets do not have measurements outside Europe?

The default settings are most often used by new users who want to test the service, so the default settings have been chosen such that the resulting validation does not take too much time and computing resources to be processed. There is no particular relationship to the geographic coverage of the default datasets which is in fact global.

If I leave spatial sub-setting fields empty, will the validation run?

Yes. If you leave them empty, the maximum available spatial coverage (of the reference data set) will be used. This means that a validation, limited by the combined geographic and temporal coverage of the selected datasets, will be run.

How is the default validation period set?

The default validation period is the widest time span covered by all selected datasets. However, this does not apply to the ISMN dataset. Each ISMN station may cover different time periods and this information is not always available in the metadata, therefore it is not included in the default validation period.

Can I leave the validation period empty?

No, you cannot. The validation will not start.

Why is the triple collocation switch disabled?

Triple collocation analysis is only available if at least three datasets are chosen (including the reference dataset).

Do I have to name my validation or does it get a default name? Can I change the name later?

You do not have to name your validation, but no default name is assigned. You can change the name later, unless you publish your validation. Published validations cannot be altered in any way.

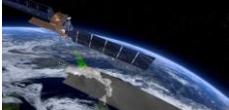
Can I name multiple validations with the same name?

Yes, you can do so.

I received a notification that a validation with the same settings exists. What should I do about that?

In this case, you can still run your validation if preferred, or you can go directly to the results of the existing validation. If you run a new validation, you will have to wait for the results, but they will include all up-to-date metrics and plots.

If you choose to use the existing validation, you will be redirected to the appropriate result page. If the existing validation was created by a different user and was not yet published, there

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will be a ‘Copy validation’ button available that enables you copying a validation and adding it to the list of your validations. You will have full control over the copy, i.e., you will be able to access the results, delete the validation from your list, extend it, etc. Please note that for copied validations the results may not contain plots or metrics that were added to the QA4SM service after the validation had been originally created. However, the results are directly available, so this solution may be useful if you do not want to wait. You can check for potentially relevant differences in the list of releases in the QA4SM [GitHub](#) repository.

You can of course also close the notification, introduce some changes to the settings and run a new validation.

Can I share my non-published validation with someone else?

Yes, you can share your validations by sending a link to your validation to any recipient. The link can be accessed without QA4SM account. You find the link in the address line of your browser after opening your validation with the ‘View results’ button on the ‘My validations’ page. Please note, that it is possible to share a validation that uses your own data, however, the user you are sharing with, will not be able to copy it nor reload settings.

How much time does it take to run a validation?

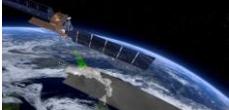
It may take from couple of minutes to couple of days depending on the chosen settings and the total number of QA4SM validations running at the same time. Using the default-settings a single validation currently takes about 3 minutes to process if there are no other concurrently running validations from other users. The number of selected datasets, the spatial resolution of the selected data and the selected spatial sub-setting do in particular have a relevant impact on the required execution time to complete the validation. Also, if there are other concurrently running validations, the resulting time to completion may be longer.

How many validations can I run?

Currently, there is no specific limitation, i.e., you can run as many validations as you need. This may be subject to change in the future if the user demand exceeds the available computing resources or if we determine that QA4SM resources are unreasonably used by specific users. Remember in any case that the results are available for two months and if you do not archive them, they will automatically be removed.

Can I stop a running validation?

Yes, you can use the square button in the result summary area, on the ‘My validations’ page. The button will cancel your running validation.

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Can I check if there are other currently running validations in QA4SM?

You have access only to the list of your own validations, so you can see only if your validations are running. If you are planning a large validation job and are unsure about the available computing resources, please contact support via support@qa4sm.eu.

My validations

What does the ‘Scheduled’ status mean?

Scheduled validations are in a preparatory state and the required data are being read before the actual validation computations are started. Depending on the validation settings and the number of currently running validations it may take some time to begin data processing. This will happen automatically and you do not need to intervene, unless you want to cancel the running validation.

My validation has an Error status. What should I do about it?

In most cases the Error status means that no data was available for comparison. For instance, if you chose a time span not covered by the chosen datasets. You can check if this is the case, by opening the validation and checking how many points could not be validated. If you get a red field notification ‘for ’100% (**0 of 0**) of the processed locations (grid points) the validation metrics were not calculated.’’, this means that there was no data to be validated. In this case you can change your settings and start a new validation. If this is not the case, please contact the support team. Please send us your username and the validation ID. The validation ID can be found in the browser’s address bar, after entering the validation view.

I started my validation a couple of hours/days ago but it still has the ‘Scheduled’ status. What can I do about it?

Please note, that starting a validation may take a while, but if it takes several hours or more, please contact the support team. Please send us your username and the validation ID. It can be found in the address bar, when entering the validation view.

I ran a validation, the status is ‘Done’, there are no errors produced, but I have no Summary statistics nor Results files available in the validation view. Also, it is not possible to download the result files. What should I do about it?

If you encounter such a problem, please contact the support team. Please send us your username and the validation ID. It can be found in the address bar, when enter the validation view.

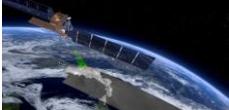
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Where can I find the validation ID?

When you enter a particular validation view using the ‘View results’ button on the ‘My validations’ page, the ID will be provided in the browser’s address bar like in the following example:

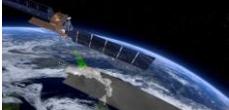
 qa4sm.eu/result/cf590fee-581f-4267-9999-f5c5e762a874/

The ID is the last part of the provided URL. In this example the validation ID is cf590fee-581f-4267-9999-f5c5e762a874.

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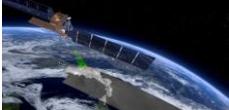
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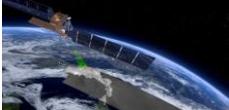
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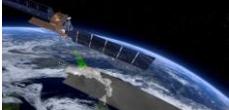
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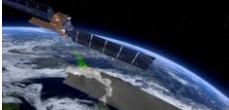
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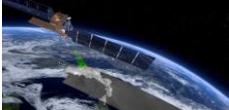
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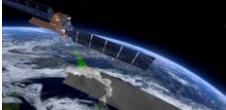
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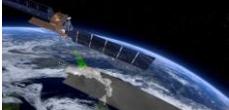
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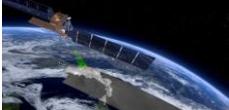
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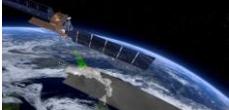
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