Introduction to QA4SM

QA4SM Users Workshop
6th Satellite Soil Moisture Validation and Application Workshop, Perugia

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QA4SM: qa4sm.eu

Overview

Scientific background

- Use of in situ data for satellite SM validation and “fiducial” reference measurements (FRM4SM)
- Best practices and recent evolutions in satellite SM validation

Introduction to QA4SM

- What is QA4SM
- Technical overview and current status of the platform
- Philosophy of the platform: What it should and should NOT be
- Programme goals and future developments: QA4SM in the FRM4SM framework

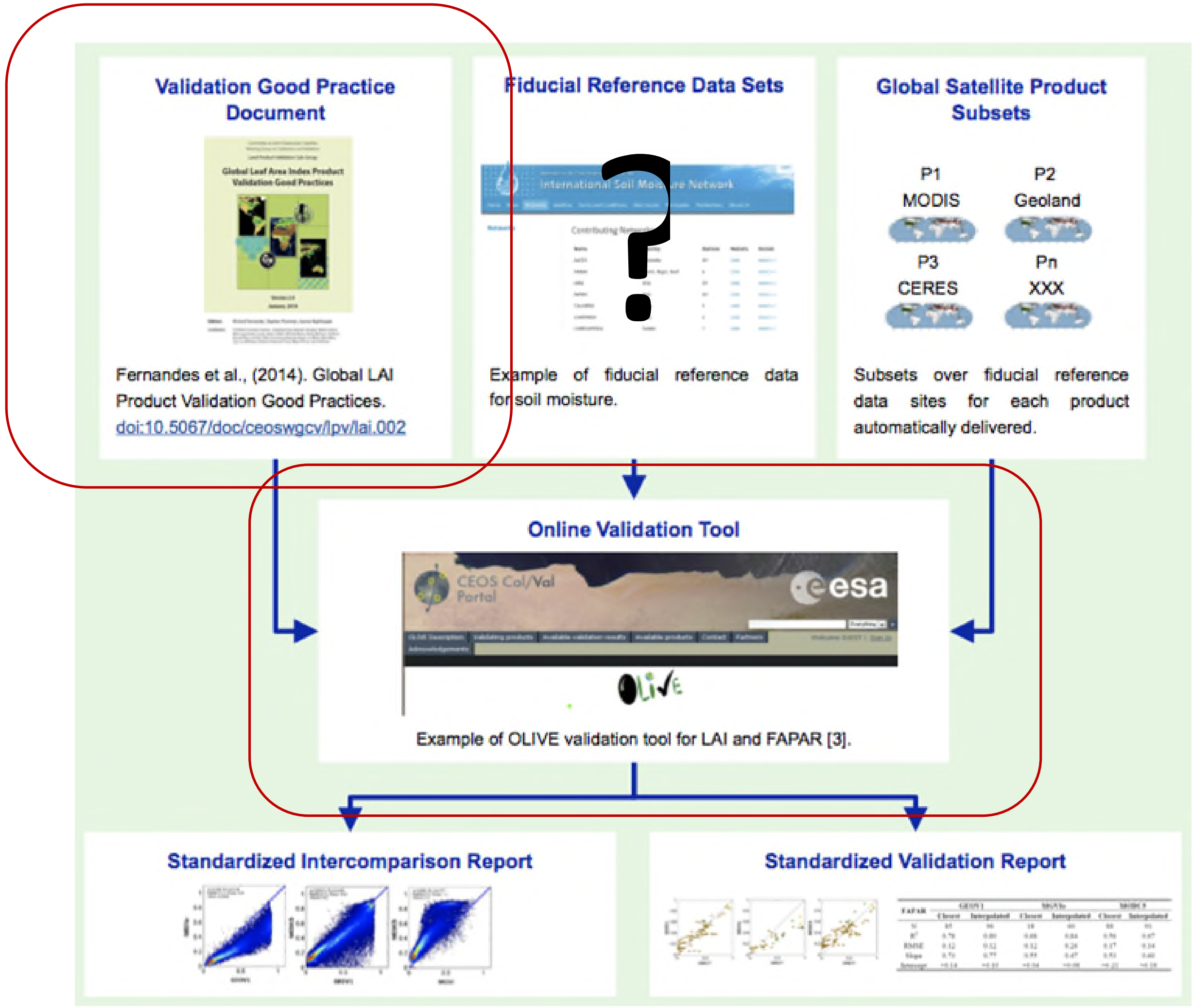
Scientific background

FRMs in satellite SM validation

*The suite of independent **ground measurements** that provide the maximum return on investment for a satellite mission by delivering, to users, the required confidence in data products, in the form of independent validation results and satellite measurement uncertainty estimation, over the entire end-to-end duration of a satellite mission (QA4VEG)*

- In practical terms, in situ measurements are characterized by:
  - Representativeness errors at the pixel level that depend on the scene heterogeneity
  - Mismatch with the scale of the SM (satellite) data to validate
  - Measurement errors that depend on calibration parameters, instrumental accuracy and its deterioration
  - Low representativeness of diverse environmental conditions (climates, land covers, ...)

Best practices in satellite SM validation



Framework for product intercomparison and validation as defined by LPV (https://lpvs.gsfc.nasa.gov/)

Best practices in satellite SM validation

Inherent issues with error characterization of satellite SM data sets:

- Uncertainties can be propagated to the L1 measurements in controlled conditions
- Retrieval models introduce complex errors which are difficult to account for
- Absence (at present) of fully characterized FRMs

How to cope with these issues?

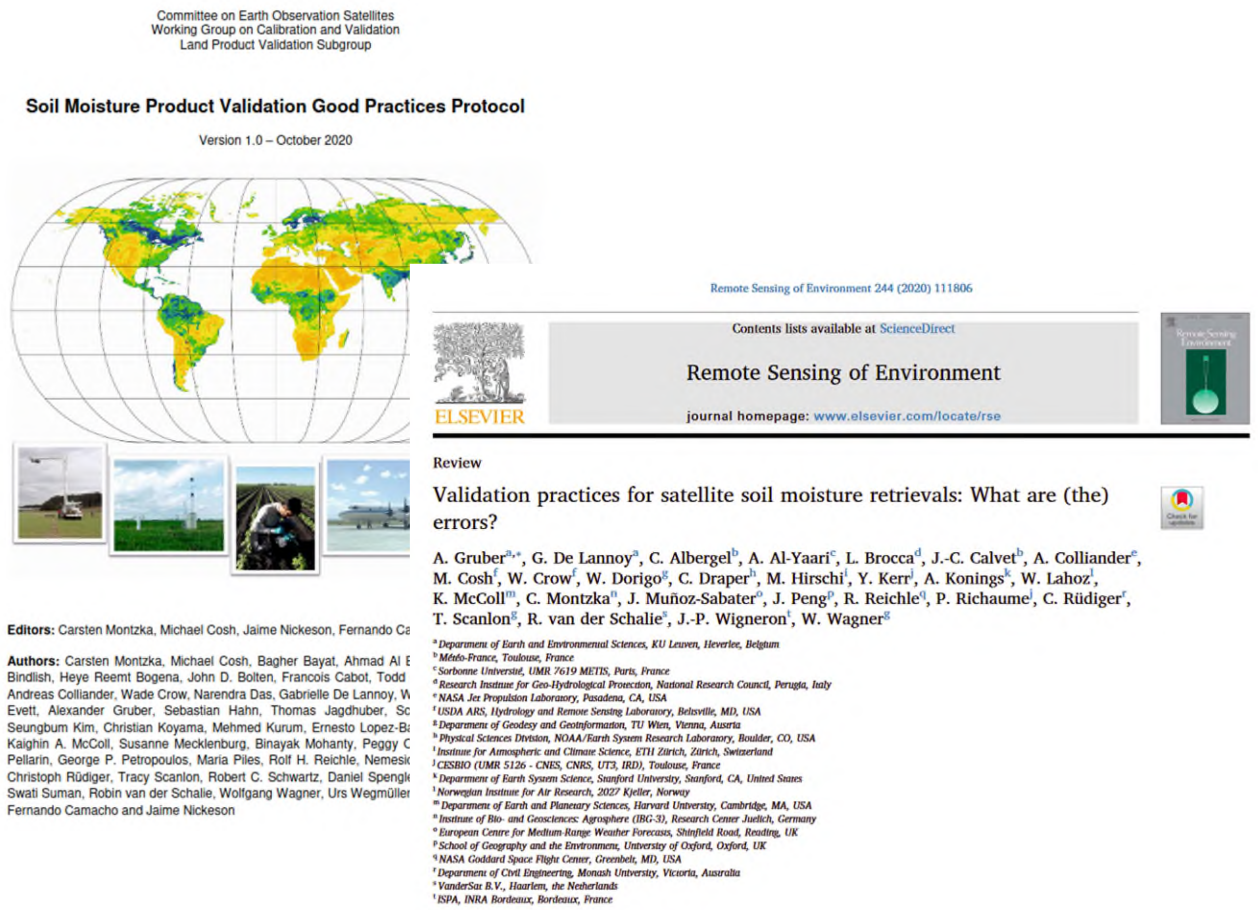
Best practices guidelines

- Validation strategies are designed to evaluate against reference data
- Land Surface Models (LSMs) simulations used to overcome coverage and scale mismatch
- Relative and independent (TCA) error metrics are used
- Confidence intervals are attached to the calculated scores

Best practices in satellite SM validation

Best practices are derived from:

- Authorities in the SM validation field
  - o WMO
  - o CEOS, working group on Calibration and Validation
- Guidelines provided for ECVs
  - o Land Product Validation Subgroup



Committee on Earth Observation Satellites
Working Group on Calibration and Validation
Land Product Validation Subgroup

Soil Moisture Product Validation Good Practices Protocol

Version 1.0 – October 2020

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Remote Sensing of Environment 244 (2020) 111806

Contents lists available at ScienceDirect

Remote Sensing of Environment

journal homepage: www.elsevier.com/locate/rse

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Review

Validation practices for satellite soil moisture retrievals: What are (the) errors?

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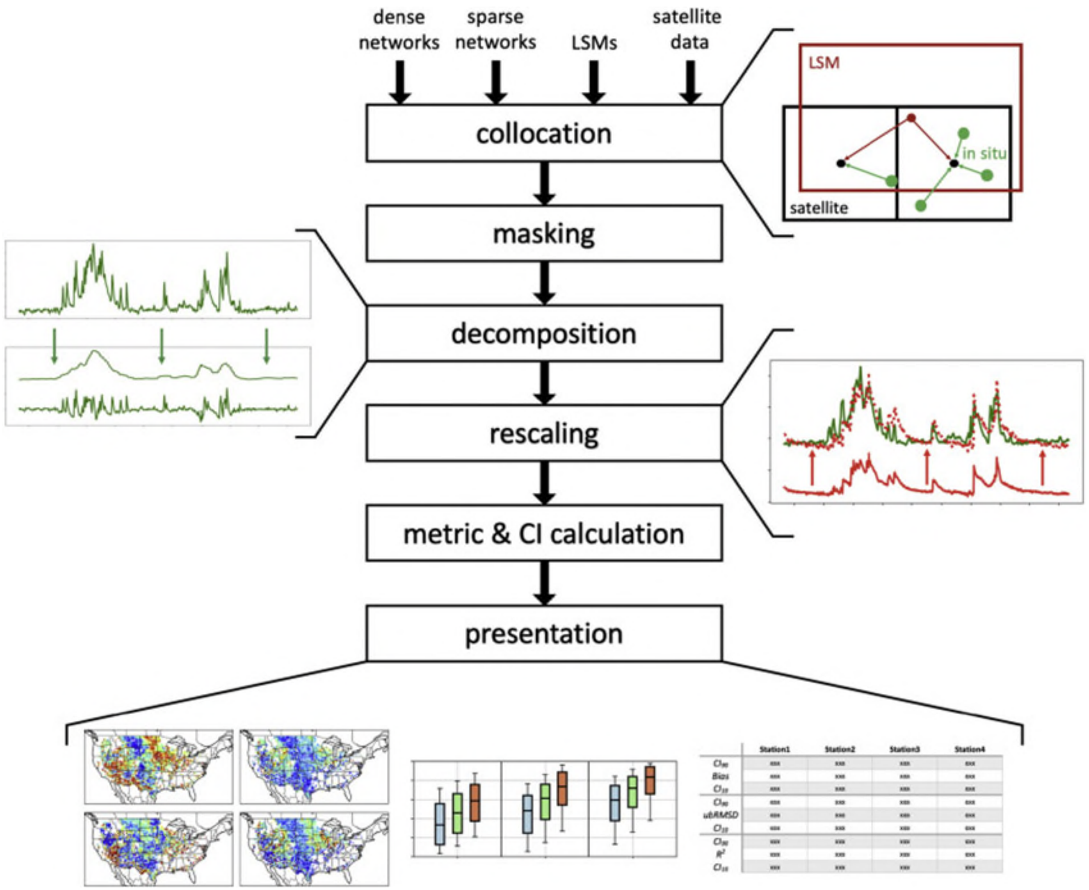
Best practices in satellite SM validation

Collocation of the measurements with the reference to minimize observational mismatches

Decomposition to separate error components of different magnitude



Statistical scaling to remove static biases and bring the data in the same units space

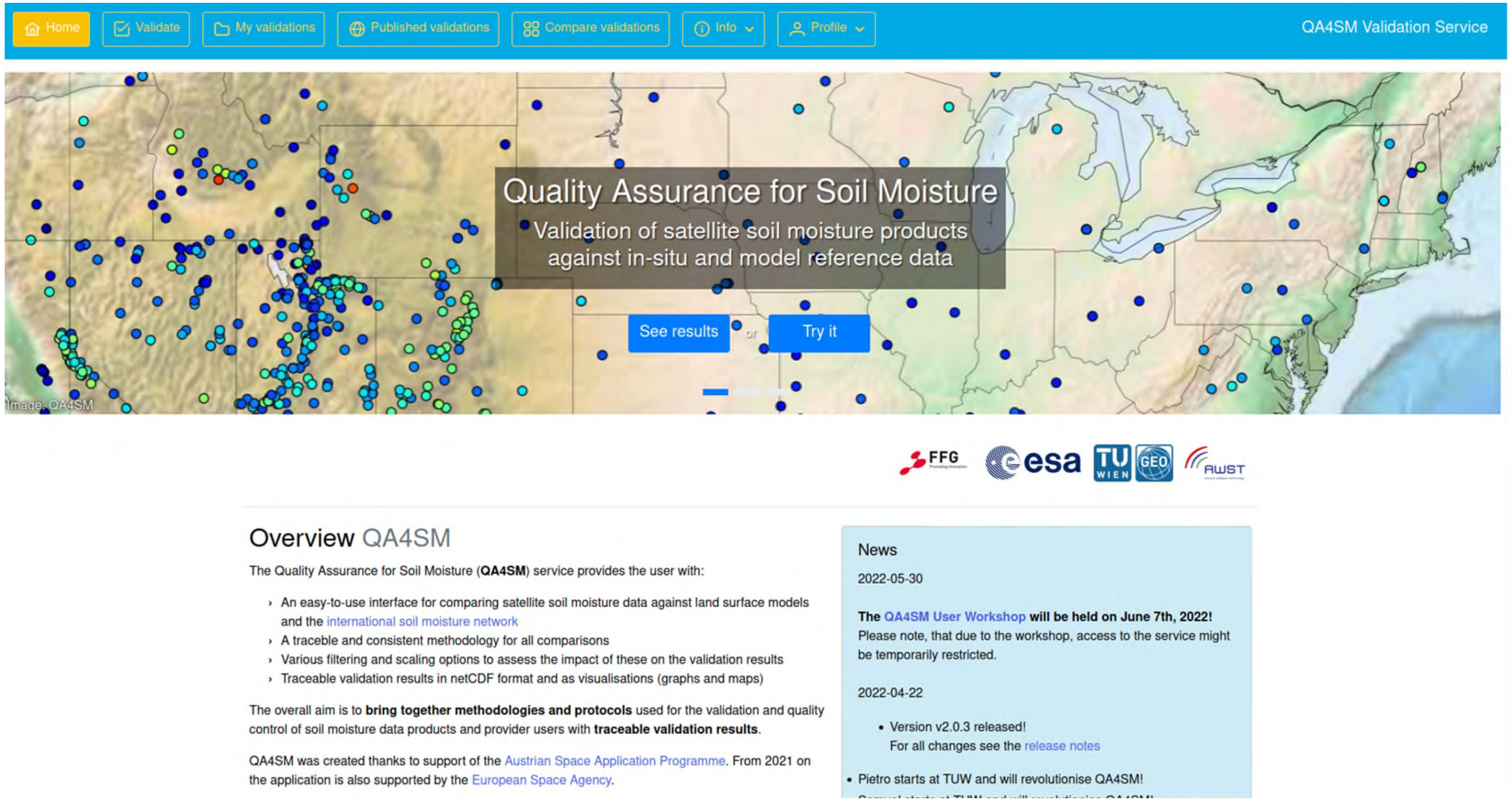
Calculation of the metrics and presentation of the results based on standard methods and facilitating inter-comparison

Validation good practice protocol illustration, reproduced from Gruber et al. (2020)

Introduction to QA4SM

What is QA4SM

1. A recipient of SM validation best practices
2. An easy-to-use GUI with flexible functionalities
3. A powerful computing environment
4. A direct access to validation of tens of data sets and versions

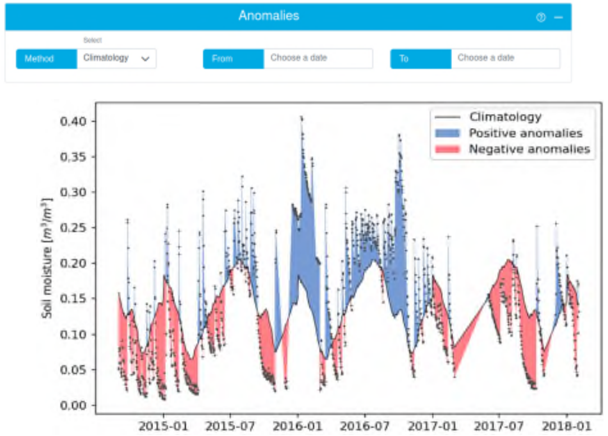


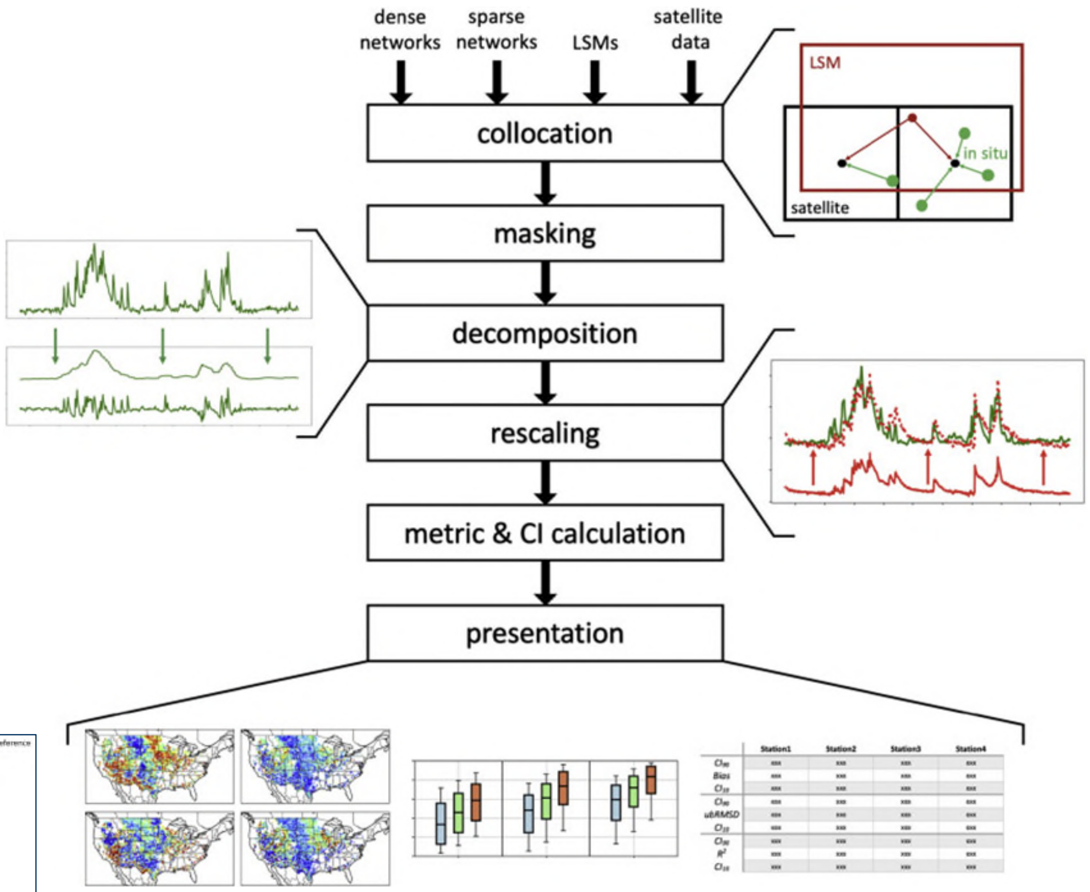
...and what will it be?

What is QA4SM

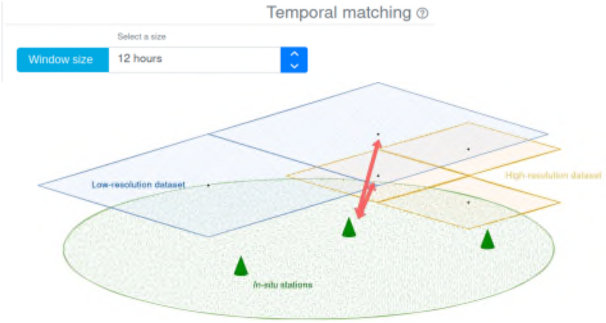
Selection of up to 5 data sets to be validated against a reference

Validation of daily anomalies

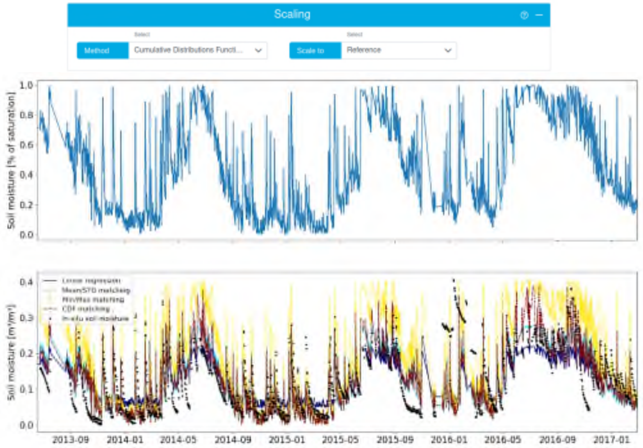




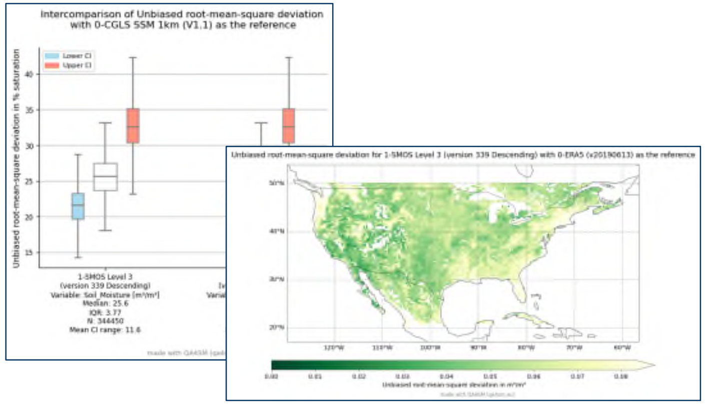
Validation good practice protocol illustration, reproduced from Gruber et al. (2020)



Selection of scaling techniques



Presentation of results



Technical overview and current status of the platform

- QA4SM is maintained and developed through open source packages
  - o Release 1 has been deployed early this week!
- 13 Satellite/ Modeled /In situ data sets are ingested in the service, including:
  - o The ISMN data set
  - o ERA5/-Land reanalysis
- Data sets are updated on a regular basis or at the release of new versions
- Scores are calculated on a large range of metrics:
  - o 'Difference' scores (RMSD, Bias, ubRMSD, ...)
  - o Correlation scores (including significance)
  - o Triple Collocation Analysis (SNR, error variance, scaling coeff.)


QA4SM

Source code repository for the QA4SM web validation service.

https://qa4sm.eu

The developers' guide for setting up your development environment is in [docs/developers_guide.md].

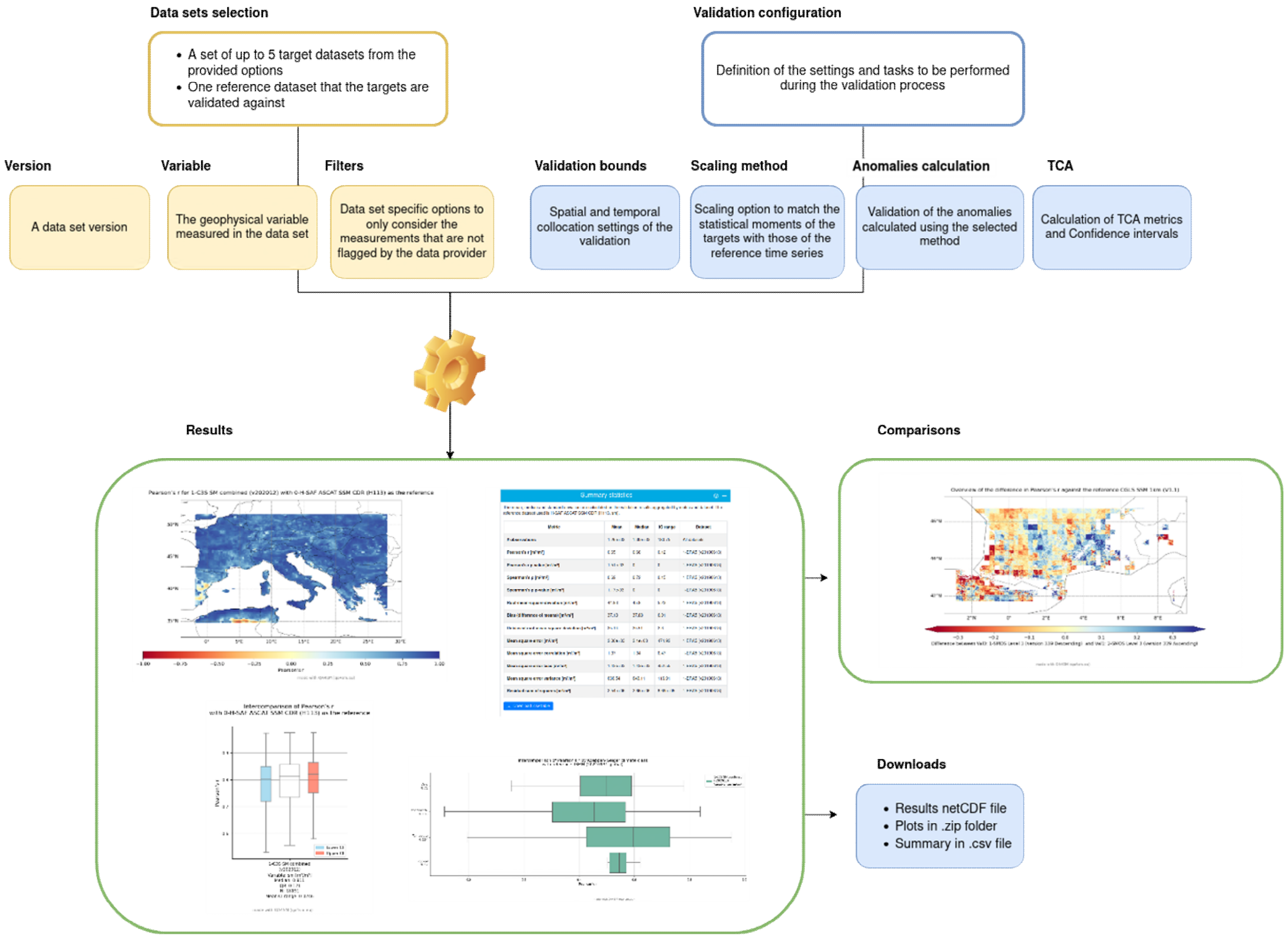
tests passing

pytesmo - a Python Toolbox for the Evaluation of Soil Moisture Observations

Automated Tests passing | coverage 86% | pypi package 0.14.0 | docs passing

pytesmo, the Python Toolbox for the Evaluation of Soil Moisture Observations, is a package/python toolbox which aims to provide a library that can be used for the comparison and validation of geospatial time series datasets with a (initial) focus on soil moisture.

Technical overview and current status of the platform



- Outputs are provided as:
  - o Reports (runtime, number of errors encountered)
  - o netCDF file with results for further analysis
  - o Plots (downloadable)
- Results can be shared and published through DOI's
- Results can be compared with one another through the dedicated module in the platform

"***QA4SM is perhaps the most advanced online validation platform*** *compared to the other ECVs investigated in this study. However, there is certainly room for improvement in QA4SM. Particularly, there is a* ***need to include more satellite SM products****, especially those with global coverage and longer time-series [...]. It* ***should also have the ability to implement user-generated SM products*** *in the near future. This can provide end-users with an opportunity to compare a local or regional product of their own [...]. Of course, it should be noted that* ***all new additions to the platform, either from satellites or in situ, should pass the CEOS LPV SM protocol requirements.***" Bayat et al. (2021)

Philosophy of the platform: What it should and should NOT be

*The "current mandate" of QA4SM is to provide 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***

What fits in this mandate? Should users be able to..

..define their own validation metric and pass it through the interface?

..validate their own data? How should the traceability of the data be ensured in this case?

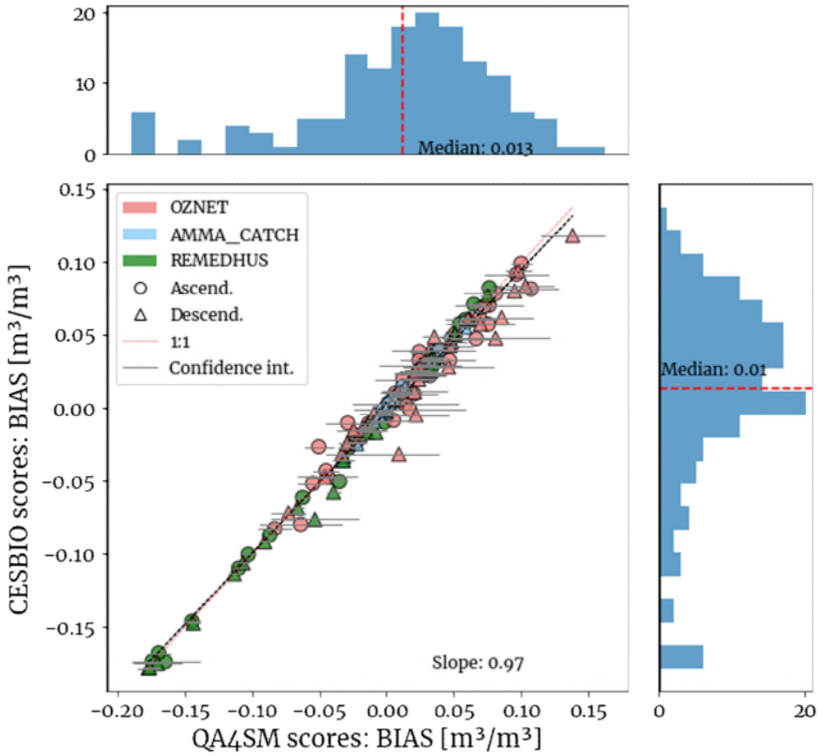
..define different temporal and spatial match up methods and functions?

..use more flexibly the selection of temporal and spatial reference data sets?

Philosophy of the platform: What it should and should NOT be

- Ultimately, QA4SM should be a service for the SM community
  - However, user uptake can be limited by the level of flexibility of the service
  - Is flexibility compatible with best practices?
- Feedback from users and the community at large is essential
- Future approach will give space for both, while drawing a line to distinguish “inside” and “outside” of best practices

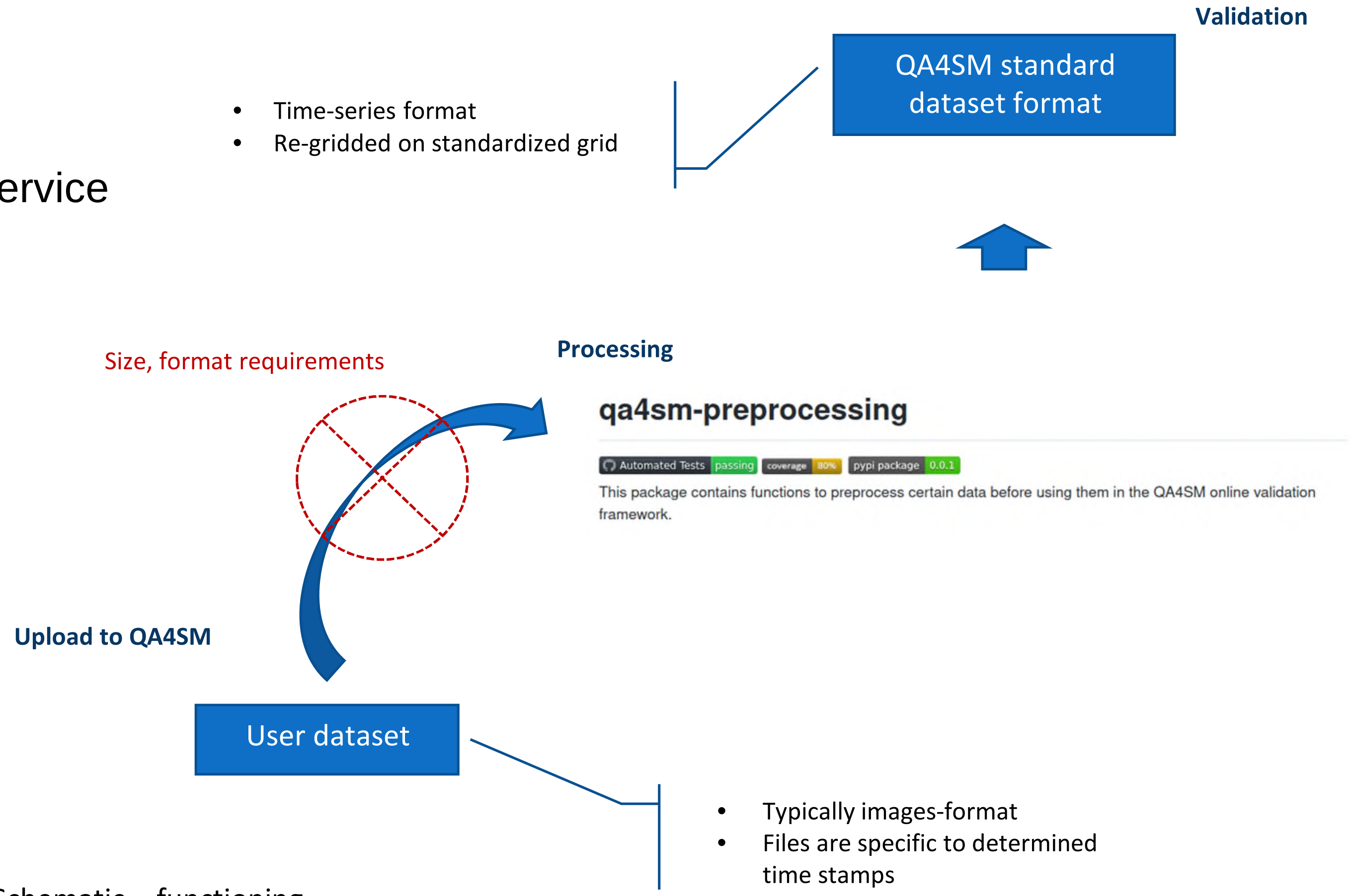
- Comprehensive documentation and verification of the service



Example output of the comparison of QA4SM with independent results (for the bias of SMOS L3 against ISMN)

Programme goals and future developments: QA4SM in the FRM4SM framework

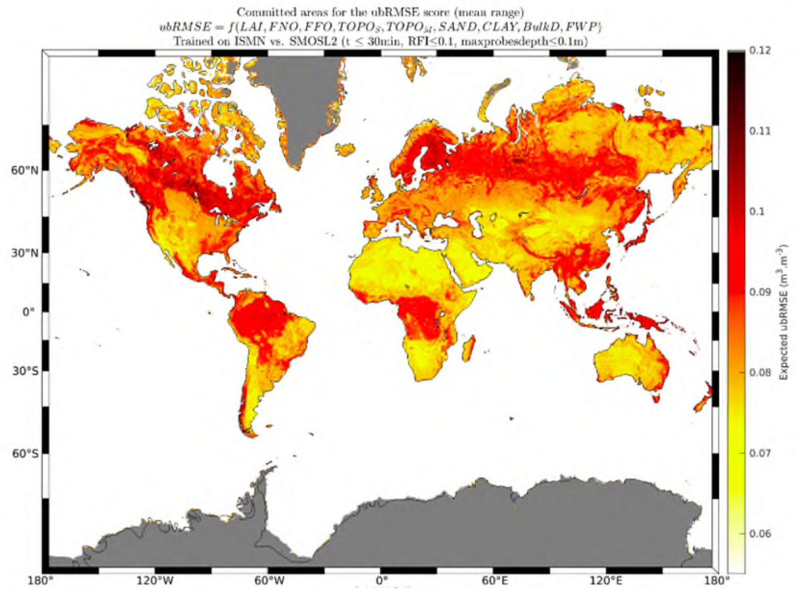
- Comprehensive documentation and verification of the service
- Technical developments
  - o Validation of user data sets



Schematic functioning of the universal reader

Programme goals and future developments: QA4SM in the FRM4SM framework

- Comprehensive documentation and verification of the service
- Technical developments
    - o Validation of user data sets
- Application target for the FRM4SM methods:
    - o Interaction with FRM sites definition
    - o Use of “committed area” in relation to satellite mission requirements



Committed areas defined based on the expected ubRMSE of SMOS. Reproduced from Gibon et al. (in prep.)

Programme goals and future developments: QA4SM in the FRM4SM framework

- Comprehensive documentation and verification of the service
- Technical developments
  - Validation of user data sets
- Application target for the FRM4SM methods:
  - Interaction with FRM sites definition
  - Use of “committed area” in relation to satellite mission requirements
- Towards and operational QA4SM service

To sum up..

- QA4SM implements the best practices in satellite SM validation
- Computational and programming resources are freely at the disposal of the community
- Many developments are foreseen in FRM4SM
- Looking for the “sweet spot” between flexibility and standards

How can I take advantage of QA4SM in my own research?

Thank you!

Workshop agenda

Session 1 (10:00 - 10:30 AM CEST)

QA4SM platform and project overview

- Introduction to FRM4SM (by ESA, Raffaele Crapolicchio)
- Presentation: Technical background / philosophy of QA4SM (by QA4SM team)
- Q&A

BREAK (10 mins)

Session 2 (10:40 - 11:50 AM CEST)

Hands-on session

- Participants are guided through running a validation
- Presentation: Currently planned changes and future directions (by QA4SM team)
- Feedback collection from all participants

BREAK (10 mins)

Session 3 (12:00 - 1:00 PM CEST)

Internal Session

Only project team and SAG members

Feedback discussion and development plan

References

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Appendix

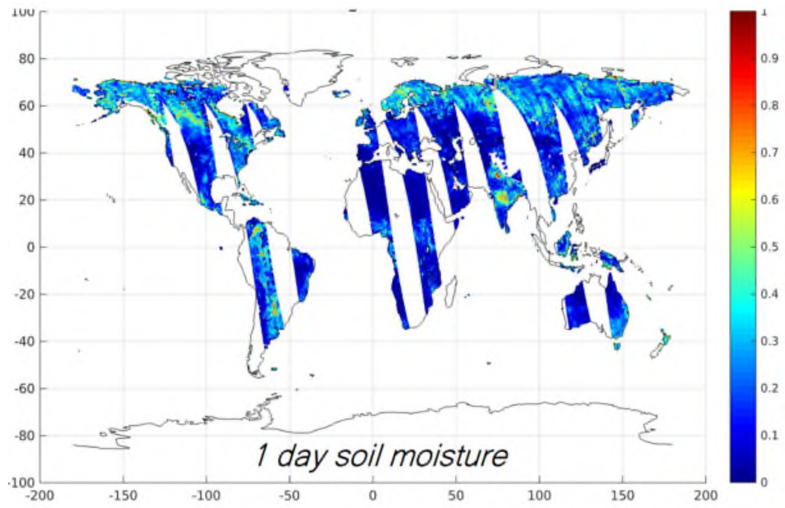
Appendix: Validation levels for ECVs

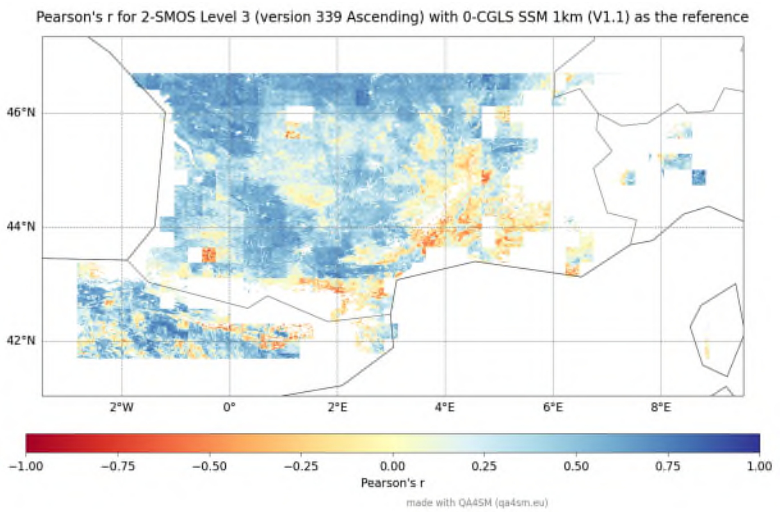
CEOS defined validation hierarchy (https://lpvs.gsfc.nasa.gov/)

Level	Validation Stage - Definition and Current State
0	No validation. Product accuracy has not been assessed. Product considered beta.
1	Product accuracy is assessed from a **small (typically < 30) set of locations** and time periods by comparison with in-situ or other suitable reference data.
2	Product accuracy is estimated over a **significant (typically > 30) set of locations** and time periods by comparison with reference in situ or other suitable reference data. **Spatial and temporal consistency of the product**, and its consistency with similar products, has been evaluated over globally representative locations and time periods. Results are **published** in the peer-reviewed literature.
3	**Uncertainties in the product and its associated structure are well quantified** over a significant (typically > 30) set of locations and time periods representing global conditions by comparison with reference in situ or other suitable reference data. Validation **procedures follow community-agreed-upon good practices**. Spatial and temporal consistency of the product, and its consistency with similar products, has been evaluated over globally representative locations and time periods. Results are published in the peer-reviewed literature.
4	Validation results for stage 3 are **systematically updated when new product versions are released or as the interannual time series expands**. When appropriate for the product, uncertainties in the product are quantified using fiducial reference measurements over a global network of sites and time periods (if available).

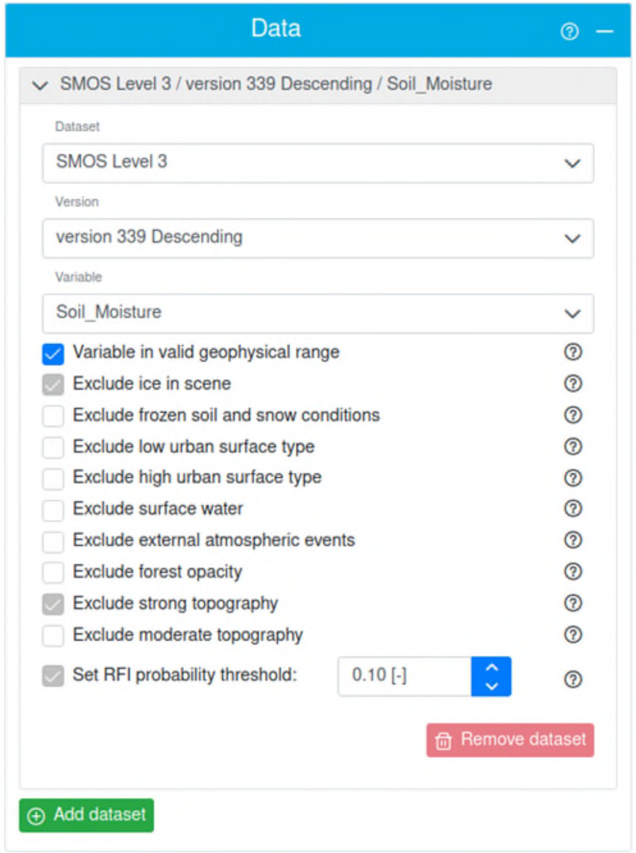
Appendix: SMOS L3 ingestion

- Availability of SMOS dataset (2010-2021) for validation in QA4SM
  - o Initially L3 daily product (v. 300, reprocessed and operative)
  - o For second release: L2 product (v. 700)





(**left**) L3 daily-aggregated SMOS soil moisture data (**right**) correlation of SMOS L3 Ascending with high-resolution CGLS SSM data



SMOS L3 selection interface in QA4SM