Climate Change Initiative+ (CCI+) Phase 2

Sea Surface Salinity

Product User Guide (PUG)

Customer: ESA
Ref.: ESA-EOP-SC-AMT-2021-26
Version: v4.0

Ref. internal: 4000123663/18/I-NB
Revision Date: 21/01/2024
Filename: SSS_cci_PHASE#02_D4.3-PUG-v4.docx
Deliverable code: D4.3

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Amendment Record Sheet

	Document Change Record	
Date / Issue	Description	Section / Page
29/06/2019	Delivery to ESA	New document
29/11/2019	AR update	New document
05/03/2020	Comments from ESA before publication	New document
01/07/2020 / v2.1	AR2 update	New document
13/01/2021 / v2.2	MS#4	New document
28/07/2021 / v3.1	Phase 1 final version including final ESA revision	All
15/12/2023 / v4.0	Delivery to ESA for version 4 of the product, the first version in Phase 2	New Document
16/02/2024 / v4.1	ESA Review	

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1 Introduction

1.1 Executive Summary

The Product User Guide (PUG) serves to document the Sea Surface Salinity (SSS) Essential Climate Variable (ECV) time series production within the CRDP (Climate Research Data Package) as produced by the SSS processing system. The PUG is requested in the Statement of Work (Task 3 SOW ref. ESA-EOP-SC-AMT-2021-26) and it is aimed at providing key information to users of the CCI+SSS products. It is structured as an answer to the System Specification Document (SSD) aiming to specify the production chain operated in the frame of the project and accounting for the requirements expressed in the User Requirement Document (URD).

This document will also record relevant feedback provided by the Validation Team and it will be re-issued every cycle together with each CRDP release.

The SSS ECV products v4.4 consist of two Level-4 datasets:

- A monthly mean product centered on the 1st and 15th day of each month.
- A 7-day running mean product provided at one day time sampling

The L4 products are delivered in two grids, a regular ¼° grid for the global ocean and a cylindrical Equal Area (EASE-2) grid with 25 km grid resolution for polar regions (Northern Hemisphere for latitude > 45° and Southern Hemisphere for latitude <-45°).

Input data used to produce the datasets are (see ATBD):

SMOS Level 2

SMOS ESA Level 2 [06/2010-10/2022] reprocessed by ESA Data Processing Ground Segment (DPGS) (v700 L2OS products) except for the satellite commissioning period (SMOS CATDS L2P products [01/2010-05/2010]).

Aquarius Level 3

Aquarius Level 3 daily (ascending and descending separately) from v5.0 [08/2011-06/2015].

SMAP Level 2

SMAP RSS Level 2 v5.0 products [04/2015-10/2022].

We limit as much as possible external information other than the satellite signal to generate L4 products. The remaining external information used to build our L4 SSS, and to build L2 SSS entering in the L4 products, is as follows:

- <u>CCI L4 algorithm:</u>
    - Representativity error derived from Mercator model (monthly climatology)
    - Adjustment of absolute SSS value, in each pixel, using 8-year mean ISAS SSS

    - Latitudinal correction of seasonal biases using ISAS
- Individual sensor calibration:
    - SMOS – ***geographical dependency correction***: Ocean Target Transformation (OTT) - Mean SMOS Tb (Brightness Temperature) in a SE Pacific Ocean box (45S-5S) over ~10days adjusted to mean modelled Tb derived from ISAS-Argo Surface Salinity
    - Aquarius – ***geographical dependency correction***: Ocean Target Calibration (OTC) - Mean global Aquarius Ta (Antenna Temperature) adjusted every 7day to mean global Ta derived from Scripps-Argo (or HYCOM model, if Argo not available) surface salinity
    - SMAP – ***latitudinal dependency correction***: weekly latitudinal correction based on Scripps-Argo (or HYCOM model, if Argo not available)

In each grid point, based on the internal consistency of the temporal variability measured by each sensor, an adjustment of their systematic errors is estimated following a procedure similar to the one described in Boutin et al. (2018). It depends on SMOS and SMAP geometry and on monthly climatologies of SSS natural variability as inferred from Mercator ocean model (see Boutin et al., 2021). The CCI+ SSS is derived using a temporal optimal interpolation.

The product complies with the latest version of the CCI Data Standard requirements [DSTD].

1.2 Purpose and scope

This document is the Phase-2 Product User Guide (PUG) for the Sea Surface Salinity (SSS) ECV project of the Climate Change Initiative+ (CCI+) led by the European Space Agency (ESA). It provides a description of the products data format, filenames, metadata, and their contents.

In essence:

- It capitalizes on the multiple sources of data available at the time of processing and further acquired during the 3 years of Phase-1 cycles: this encompasses satellite, in situ and all other relevant data that may confer the best value to the computation of the SSS ECV time series.
- It aims at supporting the scientists involved in the Climate change assessment by providing the best quality long term sea surface salinity monitoring dataset with the corresponding uncertainties. The algorithms used to produce the dataset are described in ATBDs and tuned along the way by the project Science Team during the 3 years of Phase-1 in order to improve their reliability and adequacy with the CCI+ expectation; the validation of the product by the validation team is described in the [PVIR] and case studies making scientific use of the product are described in the [CAR].

The system used to produce the dataset is described in the [SSD]. The products are customized according to the Users feedback as reported in the project [URD]. It results from the requirements established in the [SRD].

This fourth version of the document corresponds to v4 products (namely v4.4, see section 3). This dataset constitutes the first version of the products generated in Phase-2 of the project.

The purpose of the Product User Guide (PUG) is to describe the ECV data product in a manner that is understood by the product user with specific focus on:

- the geophysical data product content
- the product flags and metadata
- the data format
- the product grid and geographic projection
- known limitations of the product.

1.3 Structure of the document

The document contains the following major Sections:

- ✓ Section 1: Introduction to the document (this Section)
- ✓ Section 2: Sea Surface Salinity
- ✓ Section 3: Specification of the products
- ✓ Section 4: Annex detailing Level 4 netCDF products structure

1.4 Applicable Document

DSTD	CCI Data Standards, CCI-PRGM-EOPS-TN-13-0009	V2.3, 26/07/2020
SRD	System Requirement Document	SSS_cci_-D3.1-SRD-i1r5
SSD	System Specification Document	SSS_cci_ PHASE#02-D3.2-SSD-v4.0
URD	User Requirement Document	SSS_cci_PHASE#02-D1.1-URD-v3.0
DARD	Data Access Requirement Document	SSS_cci-D1.3-DARD-v1r3
PSD	Product Specification Document	SSS_cci_PHASE#02-D1.2-PSD-v3.0
SoW	CCI+ Statement of Work	
E3UB	End-to-End ECV Uncertainty Budget	SSS_cci_PHASE#02-D2.3-E3UB-v4.0
ATBD	Algorithm Theoretical Baseline Document	SSS_cci_PHASE#02-D2.3-ATBD-v4.0
SMAP_L2C	NASA/RSS SMAP Salinity: Version 5.0 DOI:10.5067/SMP50-2SOCS	
ALGO_L2_SMOS	CATDS (2022). CATDS-PDC L3OS 2P Algorithm Theoretical Basis Document. Available at: https://archimer.ifremer.fr/doc/00811/92266/	ATBD_L30S_v5.0
ALGO_L2_SMAP	SMAP_NASA_RSS_Salinity_Release_V5.0	RSS Technical Report 033122
ALGO_L2_AQUA	Aquarius Official Release Level 2 Sea Surface Salinity v5.0 ATBD.	RSS Technical Report 120117
ALGO_L3_AQUA	Aquarius Official Release Level 3 Sea Surface Salinity v5.0. Aquarius L2 to L3 Processing Document.ATBD.	AQ-014-PS-0017_Aquarius_L2toL3ATBD_DatasetVersion5.0

Table 1 – Applicable documents

1.5 Reference Document

RD-1	Systematic Observation Requirements for Satellite-based Products for Climate: Supplemental Details to the satellite-based component of the "Implementation Plan for the Global Observing System for Climate in support of the UNFCCC (GCOS-92)", GCOS-107, September 2006 (WMO/TD No.1338). Available online at http://www.wmo.int/pages/prog/gcos/Publications/gcos-107.pdf
RD-2	2015 Update of Actions in The Response of the Committee on Earth Observation Satellites (CEOS) to the Global Climate Observing System Implementation Plan 2010 (GCOS IP-10). Available online at http://ceos.org/document_management/Working_Groups/WGClimate/WGClimate_The-CEOS-CGMS-Response-to-the-GCOS-2010-IP_Jun2015.pdf
RD-3	The Second Report on the Adequacy of the Global Observing Systems for Climate in Support of the UNFCCC, GCOS – 82, April 2003 (WMO/TD No.1143). Available online at http://www.wmo.int/pages/prog/gcos/Publications/gcos-82_2AR.pdf
RD-4	IPCC, 2007: Climate Change 2007: Synthesis Report. Contribution of Working Groups I, II and III to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change [Core Writing Team, Pachauri, R.K and Reisinger, A. (eds.)]. IPCC, Geneva, Switzerland, 104 pp. All four documents contributing to the Fourth Assessment Report are available online at http://www.ipcc.ch/publications_and_data/publications_and_data_reports.htm
RD-5	The ESA Climate Change Initiative – Description, issue 1 revision 0 - 30/09/09 EOP-SEP/TN/0030-09/SP Available online at: http://cci.esa.int/sites/default/files/ESA_CCI_Description.pdf
RD-6	Climate Change Initiative web site: http://climate.esa.int
RD-7	GCOS Climate Monitoring Implementation Principles, November 1999. Available online at: http://www.wmo.int/pages/prog/gcos/documents/GCOS_Climate_Monitoring_Principles.pdf
RD-8	Guideline for the Generation of Satellite-based Datasets and Products meeting GCOS Requirements, GCOS Secretariat, GCOS-128, March 2009 (WMO/TD No. 1488). Available online at: http://www.wmo.int/pages/prog/gcos/Publications/gcos-128.pdf
RD-9	Quality assurance framework for earth observation (QA4EO): http://qa4eo.org
RD-10	The ESA Data User Element: http://due.esrin.esa.int/
RD-11	IPCC, 2013: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, 1535 pp. Available online at: http://www.ipcc.ch/report/ar5/wg1/
RD-12	EU Research Programmes on Space and Climate: H2020 (http://ec.europa.eu/programmes/horizon2020/en/h2020-section/space, https://ec.europa.eu/programmes/horizon2020/en/h2020-section/climateaction-environment-resource-efficiency-and-raw-materials) and Copernicus (http://www.copernicus.eu/).
RD-13	Implementation Plan for the Global Observing System for Climate in support to UNFCCC (2010 Update), GCOS-138, August 2010. Available online at:

	http://www.wmo.int/pages/prog/gcos/Publications/gcos-138.pdf.
RD-14	Systematic Observation Requirements for Satellite-Based Data Products for Climate - 2011 Update, GCOS-154, December 2011. Available online at: http://www.wmo.int/pages/prog/gcos/Publications/gcos-154.pdf.
RD-15	The Global Observing System for Climate: Implementation Needs, GCOS-200, October 2016. Available online at: https://library.wmo.int/opac/doc_num.php?explnum_id=3417, http://www.wmo.int/pages/prog/gcos/index.php?name=News
RD-16	Status of the Global Observing System for Climate - Full Report, GCOS-195, October 2015. Available online at: http://www.wmo.int/pages/prog/gcos/Publications/GCOS-195_en.pdf
RD-17	ESA CCI: CCI Project Guidelines EOP-DTEX-EOPS-SW-10-0002, 2010. Available at: http://cci.esa.int/sites/default/files/ESA_CCI_Project_Guidlines_V1.pdf
RD-18	ESA CCI Status 2012 v1.1, CCI-MNGT-EOPS-TN-12-0045, September 2012. Available at: http://cci.esa.int/sites/default/files/CCI_StatusReport_2012_for_web_complete.pdf
RD-19	M. Dowell, P. Lecomte, R. Husband, J. Schulz, T. Mohr, Y. Tahara, R. Eckman, E. Lindstrom, C. Wooldridge, S. Hilding, J. Bates, B. Ryan, J. Lafeuille and S. Bojinski, 2013: Strategy Towards an Architecture for Climate Monitoring from Space. Pp. 39. This report is available from: http://ceos.org/document_management/Working_Groups/WGClimate/WGClimate_Strategy-Towards-An-%20Architecture-For-Climate-Monitoring-From-space_2013.pdf
RD-20	S. Bojinski, J-L. Fellous, June 2013: Response by ESA to GCOS - Results of the Climate Change Initiative Requirement Analysis, GCOS Secretariat, CCI-PRGMEOPS-TN-13-0008. Available online at: http://cci.esa.int/sites/default/files/ESA_Response_to_GCOS_v3_2a.pdf
RD-21	Hollmann, R.; Merchant, C.J.; Saunders, R.; Downy, C.; Buchwitz, M.; Cazenave, A.; Chuvieco, E.; Defourny, P.; De Leeuw, G.; Forsberg, René; Holzer-Popp, T.; Paul, F.; Sandven, S.; Sathyendranath, S.; Van Roozendael, M.; Wagner, W. The ESA climate change initiative: Satellite data records for essential climate variables. American Meteorological Society. Bulletin, Vol. 94, No. 10, 2013, p. 1541-1552. Available online at: http://journals.ametsoc.org/doi/abs/10.1175/BAMS-D-11-00254.1
RD-22	(Joint Committee for Guides in Metrology, 2008, Evaluation of measurement data — Guide to the expression of uncertainty in measurement (GUM), JGCM 100: 2008. Available online at: http://www.bipm.org/en/publications/guides/gum.html.
RD-23	Merchant, C., et al, 2017, Uncertainty information in climate data records from Earth observation, Earth Syst. Sci. Data Discuss., doi: 10.5194/essd-2017-16, 2017.
RD-24	Ohring, G., 2007: Achieving Satellite Instrument Calibration for Climate Change. National Oceanographic and Atmospheric Administration, 144 pp.
RD-25	Ohring, G., Tansock, J., Emery, W., Butler, J., Flynn, L., Weng, F., St. Germain, K., Wielicki, B., Cao, C., Goldberg, M., Xiong, J., Fraser, G., Kunkee, D., Winker, D., Miller, L., Ungar, S., Tobin, D., Anderson, J.G., Pollock, D., Shipley, S., Thurgood, A., Kopp, G., Ardanuy, P. And Stone, T., 2007, Achieving satellite instrument calibration for climate change. Eos, Transactions American Geophysical Union, 88, p. 136
RD-26	ESA Third Party Missions: www.esa.int/Our_Activities/Observing_the_Earth/Third_Party_Missions_overview

RD-27	Copernicus Space Component: www.esa.int/Our_Activities/Observing_the_Earth/Copernicus/Space_Component
RD-28	European Cooperation for Space Standardization: ecss.nl
RD-29	Data Standards Requirements for CCI Data Producers (v1.2, March 2015) cci.esa.int/sites/default/files/CCI_Data_Requirements_Iss1.2_Mar2015.pdf
RD-30	Supply, A., J. Boutin, G. Reverdin, J.-L. Vergely, and H. Bellenger, 2020: Variability of satellite sea surface salinity under rainfall. In: Satellite Precipitation Measurement, V. Levizzani, C. Kidd., D. B. Kirschbaum, C. D. Kummerow, K. Nakamura, F. J. Turk, Eds., Springer Nature, Cham, Advances in Global Change Research, 69, 1155-1176, https://doi.org/10.1007/978-3-030-35798-6_34.
RD-31	Boutin et al. (2016), Satellite and In Situ Salinity: Understanding Near-surface Stratification and Sub-footprint Variability, Bulletin of American Meteorological Society, 97(10), doi: 10.1175/BAMS-D-15-00032.1).
RD-32	A. Supply, Etude des dessalures à la surface d'un océan stratifié à partir d'observations satellitaires et de mesures in-situ, PhD thesis, Sorbonne Université, Paris, December 2020.
RD-33	Boutin, J., J.-L. Vergely, E. P. Dinnat, P. Waldteufel, F. D'Amico, N. Reul, A. Supply, and C. Thouvenin-Masson (2020), Correcting Sea Surface Temperature Spurious Effects in Salinity Retrieved From Spaceborne L-Band Radiometer Measurements, *IEEE Transactions on Geoscience and Remote Sensing*, 1-14, doi:10.1109/tgrs.2020.3030488.
RD-34	Klein, L., and C. Swift (1977), An improved model for the dielectric constant of sea water at microwave frequencies, *IEEE Transactions on Antennas and Propagation*, *25*(1), 104-111.
RD-35	Boutin, J., Reul, N., Koehler, J., Martin, A., Catany, R., Guimbard, S., et al. (2021). Satellite-based sea surface salinity designed for ocean and climate studies. *Journal of Geophysical Research: Oceans*, 126, e2021JC017676. https://doi.org/10.1029/2021JC017676

Table 2 – Reference documents

1.6 Acronyms

AD	Applicable Document
ADP	Algorithm Development Plan
ATBD	Algorithm Theoretical Basis Document
C3S	Copernicus Climate Change Service
CAR	Climate Assessment Report
CATDS	Centre Aval de Traitement des Données SMOS
CCI	The ESA Climate Change Initiative (CCI), formerly known as the Global Monitoring for Essential Climate Variables (GMECV) element of the European Earth Watch programme
CCI+	Climate Change Initiative Extension (CCI+), an extension of the CCI over the period 2017–2024
CDR	Climate Data Record
CMUG	Climate Modelling User Group
CPU	Central Processing Unit
CR	Cardinal Requirement
CRDP	Climate Research Data Package
CRG	Climate Research Group
CSCDA	Copernicus Space Component Data Access System
CSWG	Climate Science Working Group
DARD	Data Access Requirements Document
DEWG	Data Engineering Working Group
DOI	Digital Object Identifier
DPM	Detailed Processing Model
DPMC	Data and Processing Management Core system
DTBT3	Database for Task 3
DUE	Data User Element
E3UB	End-to-End ECV Uncertainty Budget
EC	European Commission
ECMWF	European Centre for Medium Range Weather Forecasts
ECSAT	European Centre for Space Applications and Telecommunications
ECSS	European Cooperation for Space Standardization
ECV	Essential Climate Variable
EO	Earth Observation
EOV	Essential Ocean Variable (of the OOPC)
ESA	European Space Agency
ESGF	Earth System Grid Federation
ESM	Earth System Model
EU	European Union
FCDR	Fundamental Climate Data Record
FIDUCEO	Fidelity and uncertainty in climate data records from Earth Observations
FP7	EU Framework Programme 7

FRM	Fiducial Reference Measurements
GAIA-CLIM	Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring
GEO	Group on Earth Observations
GCOS	Global Climate Observing System
GCW	Global Cryosphere Watch
GMECV	Global Monitoring of Essential Climate Variables – former element of the European Earth Watch programme.
GNSS	Global Navigation Satellite System
GOOS	Global Ocean Observing System
H2020	Horizon 2020 programme
Hs	Significant Wave Height (see also SWH)
H-SAF	EUMETSAT's Hydrology Satellite Applications Facility
HDD	Hard disk
IOC	Intergovernmental Oceanographic commission (of UNESCO)
IODD	Input Output Data Definition
IP	Implementation Plan
IPCC	Intergovernmental Panel on Climate Change
ISAS	In Situ Analysis System
ISDB	in situ database (of Fiducial Reference Measurements and satellite measurements)
JAXA	Japan Aerospace Exploration Agency
JCOMM	Joint Commission on Oceanography and Marine Meteorology
KO	Kick-off
MOOC	Massive Open Online Course
NASA	National Aeronautics and Space Administration
NOAA	National Oceanic and Atmospheric Administration
NOP	Numerical Ocean Prediction
NWP	Numerical Weather Prediction
Obs4MIPs	Observations for Model Intercomparison Projects
ODP	Open Data Portal
OOPC	Ocean Observation Panel for Climate
PMP	Project Management Plan
PSD	Product Specification Document
PUG	Product User Guide
PVASR	Product Validation and Algorithm Selection Report
PVIR	Product Validation and Intercomparison Report
PVP	Product Validation Plan
QA4EO	Quality Assurance Framework for Earth Observation
QSR	Quarterly Status Report
RAM	Random Access Memory
R&D	Research and Development
RCP	Representative Concentration Pathways
RD	Reference Document
RSS	Remote Sensing Systems

SAF	Satellite Applications Facility
SAR	Synthetic Aperture Radar
SISS	Satellite and In situ [Working Group]
SLP	Sea Level Pressure
SMAP	Soil Moisture Active Passive [NASA mission]
SMOS	Soil Moisture and Ocean Salinity [ESA mission]
SoW	Statement of Work
SRAL	SAR Radar Altimeter (of Sentinel-3)
SRD	System Requirements Document
SSD	System Specification Document
SSS	Sea Surface Salinity
SVR	System Verification Report
SWIM	Surface Waves Investigation and Monitoring (instrument of CFOSAT)
SWH	Significant Wave Height (see also Hs)
TOPC	Terrestrial Observation Panel for Climate
TR	Technical Requirement
UCR/CECR	Uncertainty Characterisation Report (formerly known as the Comprehensive Error Characterisation Report)
URD	User Requirements Document
WCRP	World Climate Research Programme

2 Sea Surface Salinity

2.1 Introduction

Salinity plays a fundamental role in the density-driven global ocean circulation, the water cycle, and climate. Therefore, salinity is considered an Essential Climate Variable (ECV) that has to be monitored along with other variables to contribute to the generation of Climate Data Records (CDR). With remote sensing technology, Earth Observation (EO) from satellites extends our current knowledge of Sea Surface Salinity (SSS) by providing continuous and regular monitoring of this variable across the oceans.

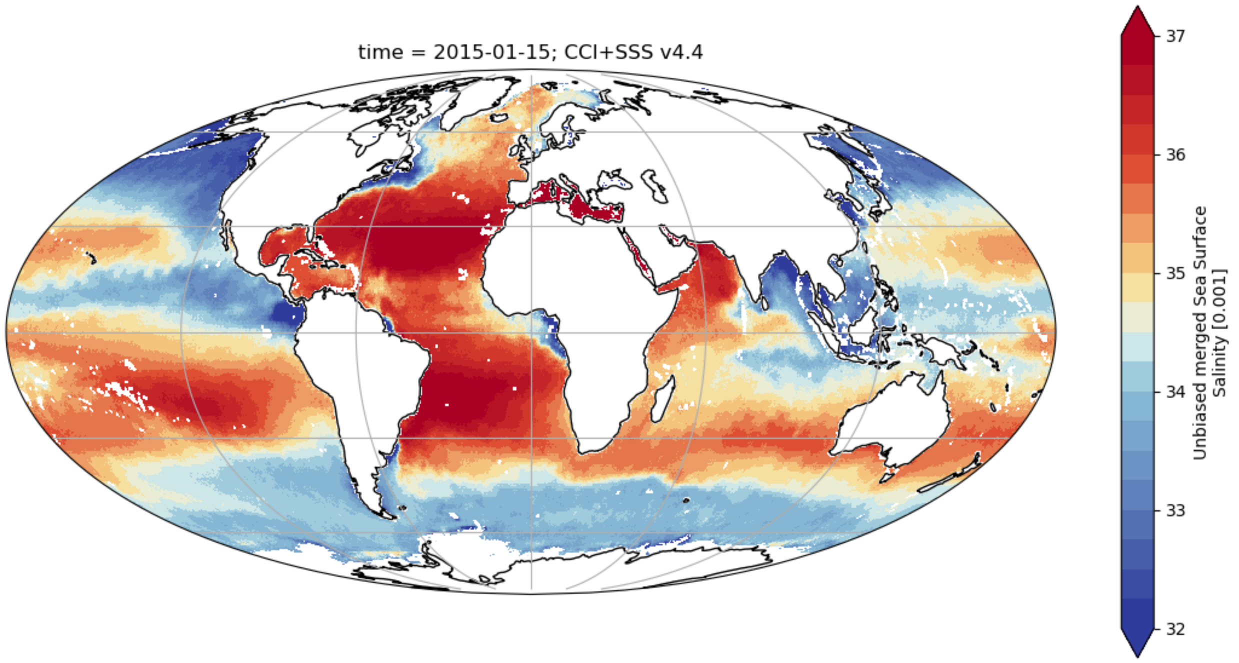

Figure 1 – Example of monthly CCI L4 Sea Surface Salinity map (salinity units using practical salinity scale, PSS) (January 2015, v04.41).

Through the Climate Change Initiative (CCI) program, ESA aims to produce the longest global SSS Climate Data Record by combining all past and present satellite missions capable of retrieving this variable from space. This includes all L-band satellites. The resulting data set provides an essential asset for scientific and climatic studies.

2.2 General remarks

At L-Band (frequency of 1.4GHz), the penetration depth (the skin depth) is about 1cm. In most situations, this depth can be considered as representative of the top few meters of the upper ocean (where in-situ measurements are usually taken), except for a few hours after rainfall or in highly stratified regions like river plumes. In rainy areas, the SSS retrieved from L-Band radiometers is fresher than the ones measured at a few meters' depth or in the non-rainy surrounding regions. On monthly SSS averaged over a longitudinal band centred on the ITCZ this effect is estimated to be up to 0.1, smaller in other regions [32]. The salinity freshening associated with instantaneous rain rate has been corrected or filtered out in satellite salinities entering in CCI L4 v4.41 SSS using a relationship between salinity freshening and satellite rain rate and wind speed [ATBD]. This leads to more consistent comparisons with in situ sub-surface salinity in rainy areas. The representativeness of satellite SSS relative to in situ SSS is studied in [31]. There can be also strong stratification in the upper layers of the ocean (between e.g. 1m and 10m depth) in river plumes, but strong differences between the 1cm satellite SSS and the 1m depth in situ measurements are rarely observed.

Validation of CCI products is available in [PVIR]; detailed comparisons with respect to various in situ measurements are available at the Pi-MEP Platform (see https://www.salinity-pimep.org/).

2.3 The L-Band missions

2.3.1 SMOS

Sea surface salinity satellite missions began with ESA's Soil Moisture and Ocean Salinity (SMOS) which has provided the longest record for SSS measurements from space over the global ocean (2010 – present) at a ~43km average spatial resolution. SMOS carries an L-band Microwave Interferometric Radiometer with Aperture Synthesis (MIRAS), the first L-band radiometer observing from space, and crosses the equator at 0600hr local time in ascending node and 1800hr in descending node along a sun-synchronous orbit.

2.3.2 Aquarius

NASA's Aquarius satellite successfully collected global SSS data from 2011 until the spacecraft ceased operating due to power failure in 2015. SSS in global L3 products has a spatial resolution of ~150km.

2.3.3 SMAP

The Soil Moisture Active Passive (SMAP) mission started measurements in April 2015. Spatial resolution is ~43km. It also crosses the equator at the same local time as SMOS but in the opposite phase.

2.4 The algorithms

This section synthetically draws the rationale within CCI+ SSS project to obtain the Level 4 user products. Fully detailed algorithms are provided in [ATBD].

Main algorithm steps in CCI+SSS processing are as follows (Boutin et al. 2021):

- Reprojection of L2 or L3 products on the same grid. Before aggregation, the SMOS, SMAP and Aquarius data must appear on the same grid. It is therefore a question of interpolating the salinities from one grid to another by using closest neighbours or linear interpolation. Note that a representativeness error is added to the Aquarius measurement error to take into account its lower spatial resolution.

- Correction of L2/L3 SSS from different biases [E3UB].
- Estimation of the inter-sensor biases and 30-day SSS are done simultaneously. The inter-sensor systematic errors are considered constant for each month and evaluated assuming SSS varies slowly over a month. These systematic errors depend on the acquisition geometry of each sensor (ascending/descending orbits, across swath location for SMOS, aft/fore antenna for SMAP). This computation is carried out by an optimal interpolation whose cost function is described in ATBD section 2.2.2.3.
- Estimation of uncertainties of the monthly SSS and detection of outliers.
- Correction of individual SSS and computation of a weekly-averaged SSS field. In this step, the bias correction is fixed and the 30-day SSS field is taken as a priori. We estimate fluctuations around this monthly field to achieve a time resolution of 7 days.
- Estimation of uncertainties of the weekly SSS.
- Absolute calibration of SSS.

Main updates in version 4 of the dataset (namely v 04.41, see section 3) with respect to the v3 are as follows [E3UB]:

- Extension of the time coverage
- Extension of the spatial coverage especially in the Arctic and Antarctic regions (thanks to a change of criteria for ice detection)
- Use of v700 SMOS products and v5.0 SMAP products. Use of SMAP v5.0 uncertainties.
- Regular 0.25° grid for global product (instead of EASE global grid). EASE2 25km polar grids for polar products, hence providing a smaller product than the global one. Polar products are obtained from global ones by nearest neighbour interpolation.
- SSS correction depending on SST and on latitude and season for SMAP and Aquarius.
- Impact of instantaneous rain on SMOS SSS corrected with a dependency to the wind speed.
- Remaining impact of roughness/foam on retrieved SMOS SSS corrected as a function of wind speed and sea state.
- SMOS SSS corrected from RFI contamination over three areas (near Samoa and Barbados islands, Gulf of Guinea).
- Change of the dielectric constant model for SMOS.

2.4.1 L-Band Input data

In v4.41, the input data used to compute the time series are Levels 2 for SMOS and SMAP, or Level 3 for Aquarius sensor:

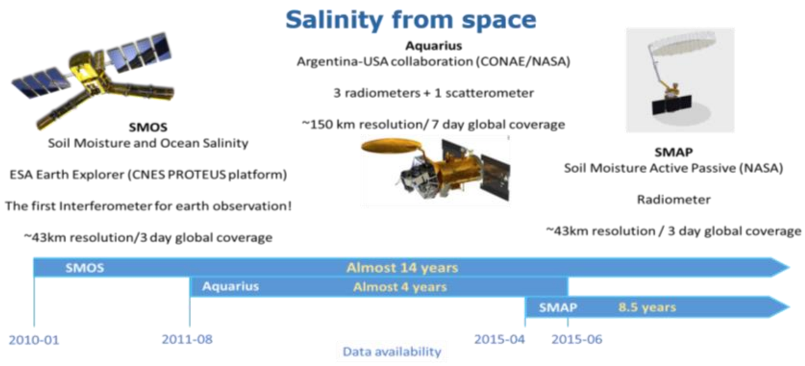

Figure 2 – L-Band missions time coverage in CCI v4

- ✓ Level 2 OS products with version 700 of the L2 OS processor. ATBD is available in reference [ALGO_L2_SMOS]. Data are available from 2010 onwards.
- ✓ SMAP Level 2 from RSS (version 5.0). The data is split into ascending and descending products and between the fore and aft views. See [ALGO_L2_SMAP] for details. Data is available from 2015 onwards.

  https://archive.podaac.earthdata.nasa.gov/podaac-ops-cumulus-docs/smap/open/docs/V5/SMAP_NASA_RSS_Salinity_Release_V5.0.pdf
- ✓ Aquarius Level 3 from NASA (version 5) which is the official end-of-mission public data release from the Aquarius/SAC-D mission. Aquarius Level 3 sea surface salinity (SSS) standard mapped image data contain gridded 1-degree spatial resolution SSS averaged over daily, 7 day, monthly, and seasonal time scales. For generating the CCI-SSS L4 dataset, daily datasets are used (ascending and descending separated). An average of ascending and descending products over the 3 radiometer footprints is performed. The algorithms for L2 and L3 products are detailed in [ALGO_L2_AQUA] and [ALGO_L3_AQUA]. Data is available from 2011 to 2015.
  https://archive.podaac.earthdata.nasa.gov/podaac-ops-cumulus-docs/aquarius/open/docs/v5/AQ-010-UG-0008_AquariusUserGuide_DatasetV5.0.pdf

2.4.2 Level 4 user products

Only Level 4 products are disseminated to users.

The aggregation of the input products from the different sensors requires a step of homogenization of the data which in turn requires:

- Qualification and removal of land-sea contamination and seasonal latitudinal systematic errors.
- Estimation of representativity uncertainties, e.g. variability of SSS between SMOS, SMAP resolution (40-50km) and Aquarius resolution (150km).

The bias corrections are of different kinds:

- Instrumental.
- Related to errors in the forward emissivity models used for the retrieval (mainly dielectric constant at high latitudes, roughness corrections, etc.).
- Linked to biased auxiliary geophysical data.
- Related to measurement contamination (Tb) by anthropogenic sources (RFI).

One of the important sources of systematic error is related to the contamination of the instrument side lobes around the coasts (for real aperture radiometers) or by the land signal in the reconstruction of oceanic scene (for the SMOS interferometric radiometer). For all instruments and geometries, the systematic errors are estimated relative to SMOS SSS at the centre of the swath; after recalibration, in each pixel, the 10-year mean of the CCI SSS is adjusted to the 10-year mean of In-Situ Analysed Salinity (ISAS) SSS (high quantiles are used instead of median in regions with large dissymmetry in the statistical distributions, such as river plumes).

CCI L4 products are running means weighted by a gaussian autocorrelation function (see ATBD), hence data outside 30/7 days are used but with a much lower weight. The number of data in 7-day or one-month window is only given as indicative.

The grid sampling is 0.25°, but the satellite native footprints are ~43km (SMOS and SMAP). So, the products are oversampled over a grid at 0.25°, but each grid point is representative of a SSS integrated over ~50x50km^2.

Detailed information about the L4 algorithm can be found in [ATBD].

2.4.2.1 Processing chain

The following figure summarizes the different processing steps of the algorithm.

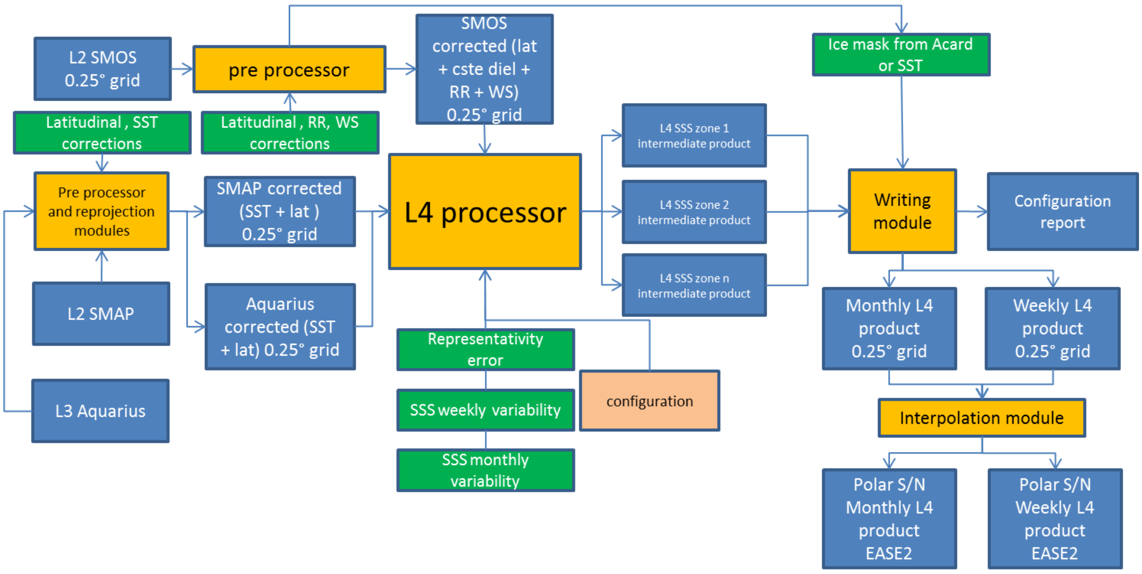

Figure 3: Level 4 processing scheme

The main processing steps are listed hereafter:

1. Pre-processing of the SSS L2/L3 products from the different sensors; Latitudinal correction and reprojection on the regular or EASE-2 grid
2. 3-sigma filtering and temporal Optimal Interpolation to generate monthly SSS without inter sensor bias removal
3. 3-sigma filtering and temporal Optimal Interpolation to generate weekly SSS without inter sensor bias removal
4. Across-track and inter sensor bias removal
5. 3-sigma filtering and temporal Optimal Interpolation to generate monthly SSS. Error propagation
6. 3-sigma filtering and temporal OI to generate weekly SSS using monthly SSS as prior. Error propagation.

2.4.2.2 Monthly products

The monthly SSS are evaluated in 3 steps:

1) A first estimation of the biases and time series of SSS, grid node by grid node is performed.

2) A 3-sigma filtering of the observed SSS in comparison with the estimated SSS is done.

3) A second estimate of SSS biases and time series after removing outliers.

The relative biases used to derive monthly SSS are estimated taking the averaged SSS from ISAS as a priori.

2.4.2.3 Weekly products

To estimate the weekly SSS, the biases calculated on the monthly SSS are used. The weekly fluctuations are estimated around the monthly SSS as a priori. A 3-sigma filter is used where:

$$sigma = sqrt(error\_L2OS^2 + variability^2).$$

The variability is estimated from Mercator model. This eliminates outliers that deviate too much from expected values.

3 Specification of the products

3.1 Dataset version

The version of the dataset corresponds to the first cycle in this second phase.

Version	Production date	Publication date
04.41	May 21th 2023	February 16th 2024

Table 3 – Dataset version

3.2 Disclaimer

The following caveats must be considered:

- There is a systematic global underestimation (0.1 pss) of SSS starting at the beginning of the dataset (SMOS Commissioning Phase), and gradually disappearing at the end of 2010.
- There is a seasonal varying bias (< 0.1 pss) in the Northern Hemisphere which decreases after 2015.
- In the North Atlantic, between April and August 2015, CCI v4 data are saltier by more than 0.2 pss; this is due to known issues in SMAP v5.0 which have been ingested for CCI v4 generation. This will be corrected for next CCI version.
- Products are in general of better quality after 2015 due to the inclusion of SMAP data and reduced contaminations (RFI, sun) on SMOS data.

We (Mngt_CCI-Salinity@argans.co.uk) are very keen to get users feedbacks about these products.

3.3 Dataset time coverage

	Weekly	Monthly
Start date	January 1st 2010	January 1st 2010
End date	October 30th 2022	October 30th 2022

Table 4 – Dataset time coverage

3.4 Volume of data

The dataset is generated with a level 6 netCDF internal compression in a netCDF 4 classic model.

	Weekly	**Monthly**
Volume per product (**compressed**)	GLOBAL: 6-13 Mb NH/SH: 1.3-1.8 Mb	GLOBAL: 7-13 Mb NH/SH: 1.3-1.8 Mb
Number of products	One product per day 4685 products	Two products per Month 307 Products
Total volume (compressed)	GLOBAL: 39 Gb NH: 5.8 Gb SH: 7.5 Gb	GLOBAL: 2.7 Gb NH: 390 Mb SH: 514 Mb

Table 5 – Data volume

3.5 Data access

The archive of SSS ECV data product is accessible through an FTP server hosted by CEDA using the following parameters:

Parameter	**Value**
Ftp server name	ftp://anon-ftp.ceda.ac.uk
Login name/passwd	anonymous
Full path	neodc/esacci/sea_surface_salinity/data/v04.41/ doi:10.5285/f2ca631f29a24c47a7e98654ddf2c7d9 catalogue.ceda.ac.uk/uuid/f2ca631f29a24c47a7e98654ddf2c7d9

Table 6 – Data access

3.6 File format

The SSS ECV user products are stored in netCDF-4 (classic) format. They conform with:

- the CCI Data Standard version 2.3 [DSTD]
- the Climate and Forecasting (CF) convention version 1.8
- Attribute Convention for Data Discovery (ACDD) version 1.3
- Infrastructure for Spatial Information in the European Community (INSPIRE) metadata records

3.7 Naming convention

The SSS ECV filename convention complies with the following CCI standard format.

```
ESACCI-<CCI project>-<processing level>-<data type>-<product string>[-<additional segregator>]-<indicative date>-[<indicative time>]-fv<file version>.nc
```

Where:

Field	Description	Value
CCI project	Project name within CCI	SEASURFACESALINITY
processing level	Data sets created from the analysis of lower level data that result in gridded, gap-free products	L4
data type	Short term describing the main data type in the data set	SSS
product string	Field describing the product L4 is a combination of 3 sensors	GLOBAL-MERGED
		POLAR-MERGED
additional segregator	Field describing the product: - OI: Optimal Interpolation - Time sampling	OI_Monthly_CENTRED_15Day_0.25deg
		OI_7DAY_RUNNINGMEAN_DAILY_0.25deg
		OI_Monthly_CENTRED_15Day_25kmEASE2-NH

	- Spatial resolution - <NH or SH>	OI_7DAY_RUNNINGMEAN_DAILY_25kmEASE2-NH
		OI_Monthly_CENTRED_15Day_25kmEASE2-SH
		OI_7DAY_RUNNINGMEAN_DAILY_25kmEASE2-SH
`indicative date`	Product coverage date: YYYYmmdd	Monthly for the 1st and the 15th
		Daily for the 7 days
`indicative time`	Product coverage time (optional) N/A for L4	-
`file version`	Version of the file	fv4.41
`extension`	Extension of the product	.nc

Table 7 – Naming convention fields

3.8 Product structure

The SSS ECV products are in netCDF-4 format. They include:

- A global metadata section
- A list of variables with attributes

The full details of the netCDF structures are provided in [PSD].

4 Level 4 products structure

A dump of the two types of netCDF L4 products is provided below.

4.1 7 days running mean

Example of filename:

ESACCI-SEASURFACESALINITY-L4-SSS-GLOBAL-MERGED_OI_7DAY_RUNNINGMEAN_DAILY_0.25deg-20100102-fv4.41.nc

```
netcdf  ESACCI-SEASURFACESALINITY-L4-SSS-GLOBAL-MERGED_OI_7DAY_RUNNINGMEAN_DAILY_0.25deg-20100102-fv4.41
{
dimensions:
        lat = 720 ;
        lon = 1440 ;
        time = UNLIMITED ; // (1 currently)
variables:
        float lat(lat) ;
                lat:_FillValue = NaNf ;
                lat:long_name = "latitude" ;
                lat:units = "degrees_north" ;
                lat:standard_name = "latitude" ;
                lat:valid_min = -90. ;
                lat:valid_max = 90. ;
        float lon(lon) ;
                lon:_FillValue = NaNf ;
                lon:long_name = "longitude" ;
                lon:units = "degrees_east" ;
                lon:standard_name = "longitude" ;
                lon:valid_min = -180. ;
                lon:valid_max = 180. ;
        float time(time) ;
                time:_FillValue = NaNf ;
                time:long_name = "time" ;
                time:units = "days since 1970-01-01 00:00:00 UTC" ;
                time:standard_name = "time" ;
                time:calendar = "standard" ;
        float sss(time, lat, lon) ;
                sss:_FillValue = NaNf ;
                sss:long_name = "Unbiased merged Sea Surface Salinity" ;
                sss:units = "0.001" ;
                sss:standard_name = "sea_surface_salinity" ;
                sss:valid_min = 0. ;
                sss:valid_max = 50. ;
                sss:ancilliary = "noutliers total_nobs sss_qc" ;
        float sss_random_error(time, lat, lon) ;
                sss_random_error:_FillValue = NaNf ;
                sss_random_error:long_name = "Sea Surface Salinity Random Error" ;
                sss_random_error:units = "0.001" ;
                sss_random_error:valid_min = 0. ;
                sss_random_error:valid_max = 100. ;
                sss_random_error:ancilliary = "pct_var" ;
        short noutliers(time, lat, lon) ;
                noutliers:long_name = "Count of the Number of Outliers within this bin cell" ;
                noutliers:valid_min = 0s ;
                noutliers:valid_max = 10000s ;
        short total_nobs(time, lat, lon) ;
                total_nobs:long_name = "Number of SSS in the time interval" ;
                total_nobs:valid_min = 0s ;
                total_nobs:valid_max = 10000s ;
        float pct_var(time, lat, lon) ;
                pct_var:_FillValue = NaNf ;
                pct_var:long_name = "Percentage of SSS_variability that is expected to be not explained
by the products" ;
                pct_var:units = "%" ;
                pct_var:valid_min = 0. ;
                pct_var:valid_max = 100. ;
        byte sss_qc(time, lat, lon) ;
```

```
                sss_qc:long_name = "Sea Surface Salinity Quality, 0=Good; 1=Bad" ;
                sss_qc:valid_min = 0b ;
                sss_qc:valid_max = 1b ;
        byte lsc_qc(time, lat, lon) ;
                lsc_qc:long_name = "Land Sea Contamination Quality Check, 0=Good; 1=Bad" ;
                lsc_qc:valid_min = 0b ;
                lsc_qc:valid_max = 1b ;
        byte isc_qc(time, lat, lon) ;
                isc_qc:long_name = "Ice Sea Contamination Quality Check, 0=Good; 1=Bad" ;
                isc_qc:valid_min = 0b ;
                isc_qc:valid_max = 1b ;

// global attributes:
                :creation_time = "19-Dec-2023 08:44:09" ;
                :title = "ESA CCI Sea Surface Salinity ECV produced at a spatial resolution of 50 km and
time resolution of one week and spatially resampled on 0.25° rectangular grid and 1 day of time sampling"
;
                :institution = "ACRI-ST,LOCEAN" ;
                :source = "SMOS DPGSv700 L2OS reprocessing, SMAP L2 RSS v5.0 - DOI:10.5067/SMP50-2SOCS,
Aquarius L3 v5.0 - DOI:10.5067/AQR50-3SQCS" ;
                :history = " " ;
                :format_version = "CCI Data Standards v2.2" ;
                :Conventions = "CF-1.8" ;
                :summary = "ESA CCI Sea Surface Salinity" ;
                :keywords = "Ocean, Ocean Salinity, Sea Surface Salinity, Satellite" ;
                :key_variables = "sss,sss_random_error" ;
                :naming_authority = "European Space Agency - ESA Climate Office" ;
                :keywords_vocabulary = "NASA Global Change Master Directory (GCMD) Science Keywords" ;
                :cdm_data_type = "Grid" ;
                :comment = "Data are based on a 7-day running mean objectively interpolated" ;
                :creator_name = "ACRI-ST,LOCEAN" ;
                :creator_email = "jean-luc.vergely@acri-st.fr" ;
                :creator_url = "http://cci.esa.int/salinity" ;
                :project = "Climate Change Initiative - European Space Agency" ;
                :geospatial_lat_min = -89.875 ;
                :geospatial_lat_max = 89.875 ;
                :geospatial_lon_min = -179.875 ;
                :geospatial_lon_max = 179.875 ;
                :license = "ESA CCI Data Policy: free and open access" ;
                :standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention version
1.8" ;
                :platform = "PROTEUS,SAC-D,SMAP" ;
                :sensor = "SMOS/MIRAS,Aquarius,SMAP" ;
                :spatial_resolution = "50km" ;
                :geospatial_lat_units = "degrees_north" ;
                :geospatial_lon_units = "degrees_east" ;
                :geospatial_vertical_min = 0. ;
                :geospatial_vertical_max = 0. ;
                :date_created = "20231219T084409Z" ;
                :date_modified = "" ;
                :time_coverage_start = "20091229T000000Z" ;
                :time_coverage_end = "20100105T235959Z" ;
                :time_coverage_duration = "P7D" ;
                :time_coverage_resolution = "P1D" ;
                :tracking_id = "31718747-d827-49f2-9195-0debc7d3c4d1" ;
                :spatial_grid = "25km regular grid" ;
                :product_version = "4.41" ;
                :references = "http://cci.esa.ind/salinity -
DOI:10.5285/f2ca631f29a24c47a7e98654ddf2c7d9" ;
                :id = "ESACCI-SEASURFACESALINITY-L4-SSS-GLOBAL-MERGED_OI_7DAY_RUNNINGMEAN_DAILY_0.25deg-
20100102-fv4.41.nc" ;
}
```

4.2 Monthly running mean

Example of filename:

ESACCI-SEASURFACESALINITY-L4-SSS-GLOBAL-MERGED_OI_Monthly_CENTRED_15Day_0.25deg-20100115-fv4.41.nc

```
netcdf ESACCI-SEASURFACESALINITY-L4-SSS-GLOBAL-MERGED_OI_Monthly_CENTRED_15Day_0.25deg-20100115-fv4.41 {
dimensions:
        lat = 720 ;
        lon = 1440 ;
        time = UNLIMITED ; // (1 currently)
variables:
        float lat(lat) ;
                lat:_FillValue = NaNf ;
                lat:long_name = "latitude" ;
                lat:units = "degrees_north" ;
                lat:standard_name = "latitude" ;
                lat:valid_min = -90. ;
                lat:valid_max = 90. ;
        float lon(lon) ;
                lon:_FillValue = NaNf ;
                lon:long_name = "longitude" ;
                lon:units = "degrees_east" ;
                lon:standard_name = "longitude" ;
                lon:valid_min = -180. ;
                lon:valid_max = 180. ;
        float time(time) ;
                time:_FillValue = NaNf ;
                time:long_name = "time" ;
                time:units = "days since 1970-01-01 00:00:00 UTC" ;
                time:standard_name = "time" ;
                time:calendar = "standard" ;
        float sss(time, lat, lon) ;
                sss:_FillValue = NaNf ;
                sss:long_name = "Unbiased merged Sea Surface Salinity" ;
                sss:units = "0.001" ;
                sss:standard_name = "sea_surface_salinity" ;
                sss:valid_min = 0. ;
                sss:valid_max = 50. ;
                sss:ancilliary = "noutliers total_nobs sss_qc" ;
        float sss_random_error(time, lat, lon) ;
                sss_random_error:_FillValue = NaNf ;
                sss_random_error:long_name = "Sea Surface Salinity Random Error" ;
                sss_random_error:units = "0.001" ;
                sss_random_error:valid_min = 0. ;
                sss_random_error:valid_max = 100. ;
                sss_random_error:ancilliary = "pct_var" ;
        short noutliers(time, lat, lon) ;
                noutliers:long_name = "Count of the Number of Outliers within this bin cell" ;
                noutliers:valid_min = 0s ;
                noutliers:valid_max = 10000s ;
        short total_nobs(time, lat, lon) ;
                total_nobs:long_name = "Number of SSS in the time interval" ;
                total_nobs:valid_min = 0s ;
                total_nobs:valid_max = 10000s ;
        float pct_var(time, lat, lon) ;
                pct_var:_FillValue = NaNf ;
                pct_var:long_name = "Percentage of SSS_variability that is expected to be not explained
by the products" ;
                pct_var:units = "%" ;
                pct_var:valid_min = 0. ;
                pct_var:valid_max = 100. ;
        byte sss_qc(time, lat, lon) ;
                sss_qc:long_name = "Sea Surface Salinity Quality, 0=Good; 1=Bad" ;
                sss_qc:valid_min = 0b ;
                sss_qc:valid_max = 1b ;
        byte lsc_qc(time, lat, lon) ;
                lsc_qc:long_name = "Land Sea Contamination Quality Check, 0=Good; 1=Bad" ;
                lsc_qc:valid_min = 0b ;
                lsc_qc:valid_max = 1b ;
        byte isc_qc(time, lat, lon) ;
```

```
                isc_qc:long_name = "Ice Sea Contamination Quality Check, 0=Good; 1=Bad" ;
                isc_qc:valid_min = 0b ;
                isc_qc:valid_max = 1b ;

// global attributes:
                :creation_time = "19-Dec-2023 08:33:33" ;
                :title = "ESA CCI Sea Surface Salinity ECV produced at a spatial resolution of 50 km and
time resolution of 1 month and spatially resampled on 0.25° rectangular grid and 15 days of time sampling"
;
                :institution = "ACRI-ST,LOCEAN" ;
                :source = "SMOS DPGSv700 L2OS reprocessing, SMAP L2 RSS v5.0 - DOI:10.5067/SMP50-2SOCS,
Aquarius L3 v5.0 - DOI:10.5067/AQR50-3SQCS" ;
                :history = " " ;
                :format_version = "CCI Data Standards v2.2" ;
                :Conventions = "CF-1.8" ;
                :summary = "ESA CCI Sea Surface Salinity" ;
                :keywords = "Ocean, Ocean Salinity, Sea Surface Salinity, Satellite" ;
                :key_variables = "sss,sss_random_error" ;
                :naming_authority = "European Space Agency - ESA Climate Office" ;
                :keywords_vocabulary = "NASA Global Change Master Directory (GCMD) Science Keywords" ;
                :cdm_data_type = "Grid" ;
                :comment = "Data are based on a monthly running mean objectively interpolated" ;
                :creator_name = "ACRI-ST,LOCEAN" ;
                :creator_email = "jean-luc.vergely@acri-st.fr" ;
                :creator_url = "http://cci.esa.int/salinity" ;
                :project = "Climate Change Initiative - European Space Agency" ;
                :geospatial_lat_min = -89.875 ;
                :geospatial_lat_max = 89.875 ;
                :geospatial_lon_min = -179.875 ;
                :geospatial_lon_max = 179.875 ;
                :license = "ESA CCI Data Policy: free and open access" ;
                :standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention version
1.8" ;
                :platform = "PROTEUS,SAC-D,SMAP" ;
                :sensor = "SMOS/MIRAS,Aquarius,SMAP" ;
                :spatial_resolution = "50km" ;
                :geospatial_lat_units = "degrees_north" ;
                :geospatial_lon_units = "degrees_east" ;
                :geospatial_vertical_min = 0. ;
                :geospatial_vertical_max = 0. ;
                :date_created = "20231219T083333Z" ;
                :date_modified = "" ;
                :time_coverage_start = "20100101T000000Z" ;
                :time_coverage_end = "20100130T235959Z" ;
                :time_coverage_duration = "P1M" ;
                :time_coverage_resolution = "P15D" ;
                :tracking_id = "8f0ef834-403e-4067-bf3b-cc61e77c7c14" ;
                :spatial_grid = "25km regular grid" ;
                :product_version = "4.41" ;
                :references                =               "http://cci.esa.ind/salinity               -
DOI:10.5285/f2ca631f29a24c47a7e98654ddf2c7d9" ;
                :id = "ESACCI-SEASURFACESALINITY-L4-SSS-GLOBAL-MERGED_OI_Monthly_CENTRED_15Day_0.25deg-
20100115-fv4.41.nc" ;
}
```

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