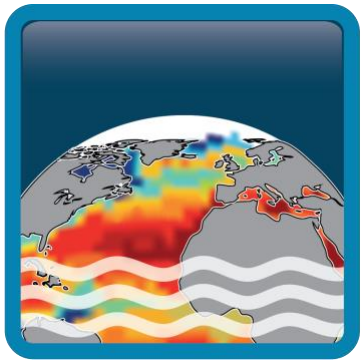
Climate Change Initiative+ (CCI+) Phase 1

Sea Surface Salinity



Product User Guide (PUG)

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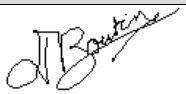
APPROVED BY	Jacqueline Boutin (Science Leader) LOCEAN		28-07-2021
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Amendment Record Sheet

	Document Change Record	
Date / Issue	Description	Section / Page
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13/01/2021 / v2.2	MS#4	New document
28/07/2021 / v3.1	Phase 1 final version including final ESA revision	All

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1 Introduction

1.1 Executive Summary

The Product User Guide (PUG) serves to define the Sea Surface Salinity 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-CCI-PRGM-EOPS-SW-17-0032) 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 Year together with each CRDP release.

The SSS ECV products v3.21 delivered at the end of the third-Year activities 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 at one day time sampling

Input data used to produce the datasets are:

- Level 1C for SMOS produced by ESA official ground segment (DPGS) with version 6.20 of the L1C processor. Level 2 OS products are generated using the CCI processing facilities.

- Level 2 for SMAP and Level 3 for Aquarius sensor coming directly from official space agency dedicated centres. They are therefore not generated by the CCI processing chains.

Data are the following for each sensor:

- SMOS L2 SSS produced with version 6.71 of the ESA Level 2 OS processor, with a configuration peculiar to the CCI project, over the full SMOS period considered in Year 3.
- Aquarius Level 3 SSS produced daily for ascending and descending passes separately with version v5.0
- SMAP Level 2 SSS produced with version v4.0

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

- CCI L4 algorithm:
  - Representativity error derived from Mercator model (monthly climatology)
  - In each pixel, adjustment of absolute SSS value using 8-year mean ISAS SSS
- Individual sensor calibration:

- SMOS – ***geographical dependency correction***: Ocean Target Transformation (OTT) - Mean SMOS Tb in a SE Pacific Ocean box (45S-5S) over ~10days adjusted to mean Tb derived from ISAS-Argo Surface Salinity (S).
- Aquarius – ***geographical dependency correction***: Ocean Target Calibration (OTC) - Mean global Aquarius Ta adjusted every 7day to mean global Ta derived from Scripps-Argo (or HYCOM if Argo not available) surface salinity (S)
- SMAP – ***latitudinal dependency correction***: weekly latitudinal correction based on Scripps-Argo (or Hycom model if Argo not available)

These data are all projected on the same EASE-2 cylindrical equal area grid at a spatial sampling of 25 km. 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 SSS natural variability as inferred from Mercator ocean model. 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 1 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.

- It capitalizes on the multiple sources of data available at the time of processing and further acquired during the 3 Years of phase 1 exercise: 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 exposed in the project [URD]. It results from the requirements established in the [SRD].

This is the third version of the document addressing Phase 1 activities and leading to v3 (namely v3.21, see section 3) of the dataset. This dataset constitutes the last version of the products generated in phase 1 of the project. It accounts for acquired experience and feedback received by the users during the 3 Years exercise.

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 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 (present 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-D3.2-SSD-i3r0
URD	User Requirement Document	SSS_cci-D1.1-URD-i2r0
DARD	Data Access Requirement Document	SSS_cci-D1.3-DARD-v1r3
PSD	Product Specification Document	SSS_cci-D1.2-PSD-v2.0
SoW	CCI+ Statement of Work	
ATBD	Algorithm Theoretical Baseline Document	SSS_cci-D2.3-ATBD-v3.0
SMAP_L2C	NASA/RSS SMAP Salinity: Version 3.0 Validated Release - RSS Technical Report 101518 October 15, 2018.	
ALGO_L2_SMOS	CATDS (2017). CATDS-PDC L3OS 2P Algorithm Theoretical Basis Document. Available at: https://www.catds.fr/content/download/78841/file/ATBD_L3OS_v3.0.pdf	ATBD_L30S_v3.0
ALGO_L2_SMAP	RSS SMAP Level 2 Sea Surface Salinity V3.0 40km Validated Dataset. Available at: ftp://podaac-ftp.jpl.nasa.gov/allData/smap/docs/V3/	RSS Technical Report 101518
ALGO_L2_AQUA	Aquarius Official Release Level 2 Sea Surface Salinity v5.0 ATBD. Available at: ftp://podaac-ftp.jpl.nasa.gov/allData/aquarius/docs/v5/	RSS Technical Report 120117
ALGO_L3_AQUA	Aquarius Official Release Level 3 Sea Surface Salinity v5.0. Aquarius L2 to L3 Processing Document.ATBD. Available at: ftp://podaac-ftp.jpl.nasa.gov/allData/aquarius/docs/v5/	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.

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) is formally known as the Global Monitoring for Essential Climate Variables (GMECV) element of the European Earth Watch programme
CCI+	Climate Change Initiative Extension (CCI+), is 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 - 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 [mission of NASA]
SMOS	Soil Moisture and Ocean Salinity [satellite of ESA]
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 that contribute to the 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.

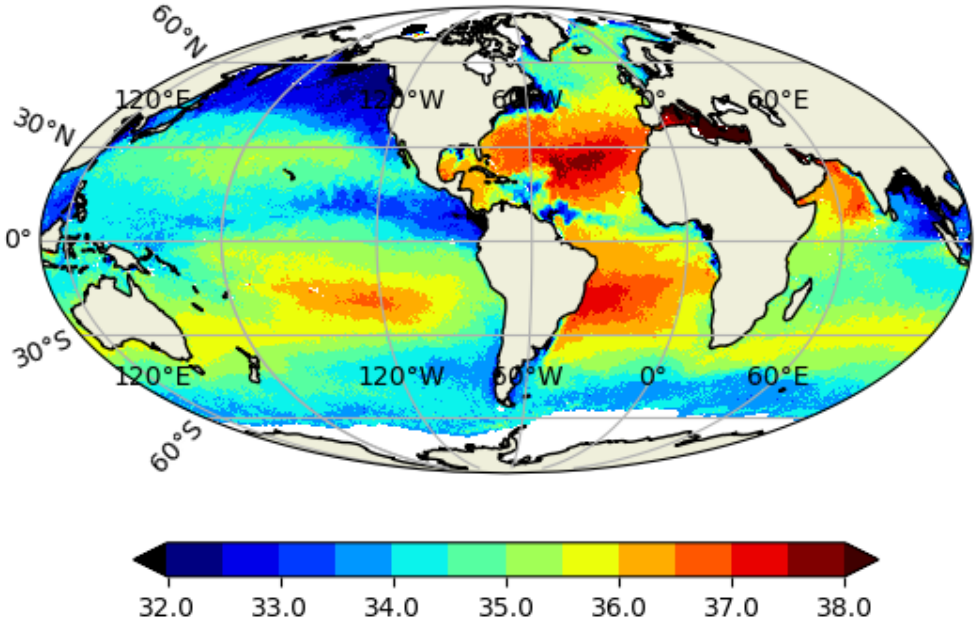

Figure 1 – Example of monthly CCI L4 Sea Surface Salinity map (salinity units using practical salinity scale, PSS) (October 2019, v3.21).

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 tool for improving monitoring methods. The possibility of using C- and X-band radiometers to extend backward the SSS data set will be considered in Phase 2 of the project.

2.2 General remarks

At L-Band (frequency of 1.4GHz), the penetration depth (the skin depth) is about 1cm. In most situation, this depth represents well the first meters of the upper ocean (where in-situ measurements are usually taken), except for a few hours after a rainfall or in very 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' depths 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 v3.21 SSS using a relationship between salinity freshening and satellite rain rate [30]. 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 eg 1m and 10m depth) in river plumes, but strong differences between the 1cm satellite SSS and 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 PIMEP (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 ~50km 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 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 ~40km. It also crosses the equator at the same local time as SMOS but in the opposite phase.

2.4 The C-Band missions

During the phase 1, the C-band missions are not considered.

2.5 The algorithms

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

Main updates in version 3 of the dataset (namely v 3.21, see section 3) with respect to version 2 (namely v 2.31) are as follows:

- SSS from SMOS have been generated from a complete L2 reprocessing with the following updates: OTT correction computed from ISAS-Argo instead of WOA climatology; Specific RFI filtering; ERA5 reanalysis auxiliary data instead of ECMWF forecast data. Dielectric constant model of [RD-33] (instead of [RD-34] in v2.3).

- Ice mask has been computed from SMOS retrieved pseudo dielectric constant (so called, Acard parameter) estimated over the whole period.

- SMOS seasonal/latitudinal biases have been computed by using Pacific + Atlantic region (whilst only Atlantic was used in v2.3)

- Instantaneous rain effect has been corrected, relating surface salinity freshening to IMERG rain rate following [RD-32], before estimating bias correction and before L4 merging for SMOS and SMAP SSS. Bulk SSS is now available in the L4 product.

- SSS random uncertainty computation has been updated.

- Aquarius SSS have been resampled on the EASE 2 grid using an interpolation with a distance weighting (instead of a closest neighbour algorithm used in the v2.3)

- SSS is now provided much closer to coast, but additional pixels are flagged with the same land-sea mask as in v2.3. So, users who wish to ensure using same pixels as in v2.3 should use this flag; users interested in Salinity variability very close to coast, should not apply this flag but should use data close to coast with care.

- Representativity uncertainties considering the various spatio-temporal scales covered by the various sensors are taken into account for all sensors (only for Aquarius in v2.3) when estimating L4 fields.

2.5.1 L-Band Input data

In v3.21, the input data used to compute the time series are levels 1 for SMOS, level 2 for SMAP or Level 3 for Aquarius sensor:

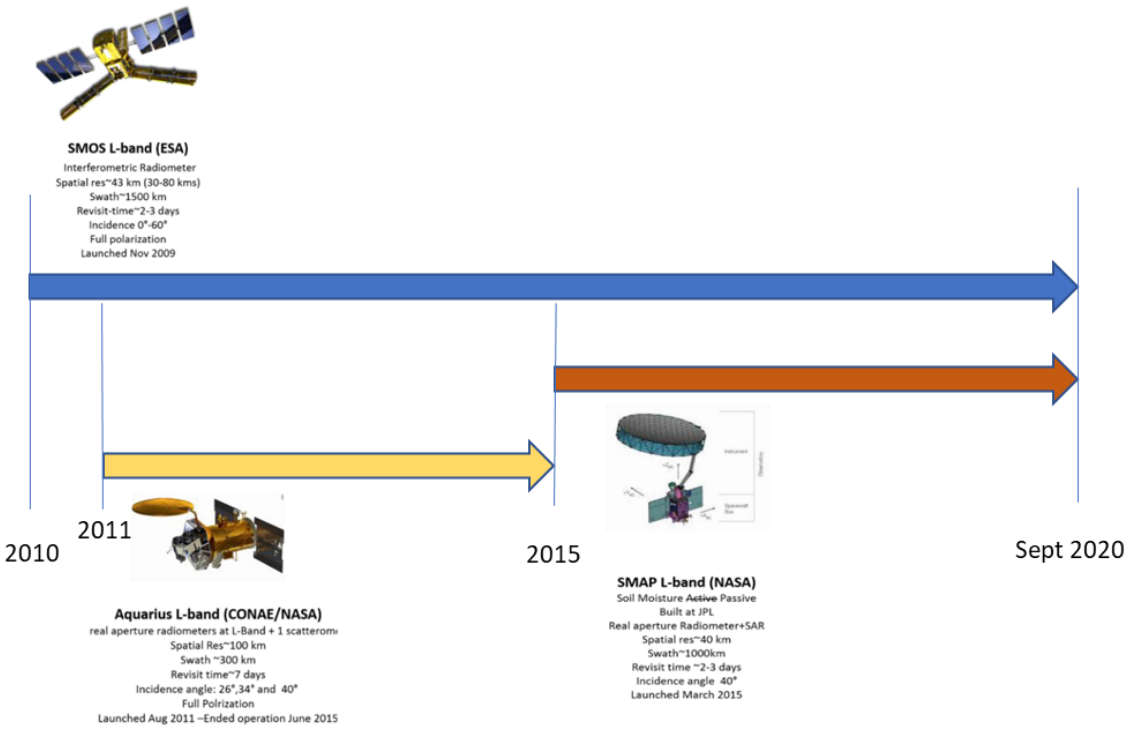

Figure 2 – L-Band missions time coverage in Year 1 to 3 of the project

- ✓ Level 1C for SMOS produced by ESA official ground segment (DPGS) with version 6.20 of the L1C processor. This dataset is used in a first place in the CCI+ project to generate the Level 2 OS products with version 6.71 of the L2 OS processor. ATBD is available in reference [ALGO_L2_SMOS]. Data is available from 2010 onwards.
- ✓ SMAP Level 2 from RSS (version 4.0). 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://podaac-tools.jpl.nasa.gov/drive/files/allData/smap/L2/RSS/V4/SCI

- ✓ 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 of year 2, 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://podaac-tools.jpl.nasa.gov/drive/files/allData/aquarius/L3/mapped/CAPv5/7day/SCI

2.5.2 Level 4 user products

Only Level 4 products are disseminated to users during phase 1 exercise.

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 bias 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 mean 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 30/7days 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 resolution is 25km, but the satellite native footprints are ~50km (SMOS and SMAP). So, the products are oversampled over a grid at 25km, but each grid point is representative of a SSS integrated over 50x50km^2.

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

2.5.2.1 Processing chain

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

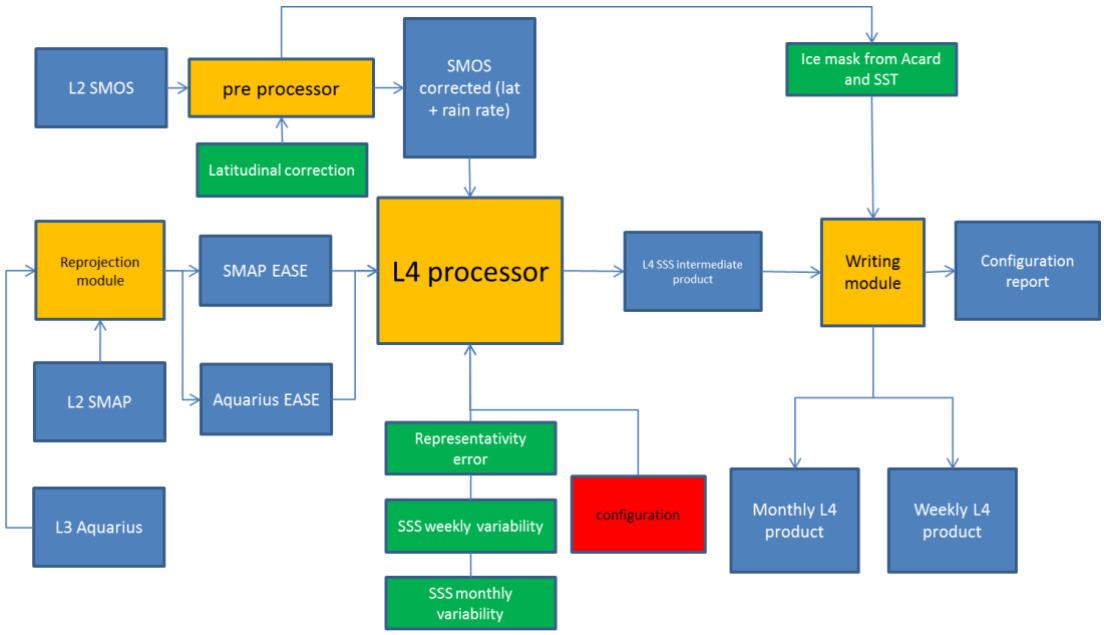

Figure 3: Level 4 processing scheme

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 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.

2.5.2.2 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 the SMOS central across swath location as a priori.

2.5.2.3 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 far from expected values.

3 Specification of the products

3.1 Dataset version

The version of the dataset corresponds to Year 3 activity.

Version	Production date	Publication date
3.21	April 27th 2021	September 30th 2021

Table 3 – Dataset version

3.2 Disclaimer

The following caveats must be considered:

- Products have not been fully optimised for very high latitudes.
- There is a systematic global underestimation of ~0.1 pss in early 2010 (SMOS Commissioning Phase) that gradually disappears over the year.
- 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	September 29th 2020	September 29th 2020

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 (uncompressed)	19.6 Mb	19.6 Mb
Volume per product (**compressed**)	~5.2 Mb	~5.2 Mb
Number of products	One product per day 3916 products	Two products per Month 257 Products
Total volume (compressed)	19 Gb	1.3 Gb

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/v03.21/

Table 6 – Data access

Example for Year 2 v02.31 dataset full directory structure is shown on Figure 4:

Index of /neodc/esacci/sea_surface_salinity/data/v02.31/

[parent directory]

Name	Size	Date Modified
30days/		9/12/20, 3:02:00 AM
7days/		9/12/20, 3:02:00 AM

Index of /neodc/esacci/sea_surface_salinity/data/v02.31/30days/

[parent directory]

Name	Size	Date Modified
00README_catalogue_and_licence.txt	919 B	9/12/20, 3:02:00 AM
2010/		7/8/20, 2:00:00 AM
2011/		7/8/20, 2:00:00 AM
2012/		7/8/20, 2:00:00 AM
2013/		7/8/20, 2:00:00 AM
2014/		7/8/20, 2:00:00 AM
2015/		7/8/20, 2:00:00 AM
2016/		7/8/20, 2:00:00 AM
2017/		7/8/20, 2:00:00 AM
2018/		7/8/20, 2:00:00 AM
2019/		7/8/20, 2:00:00 AM

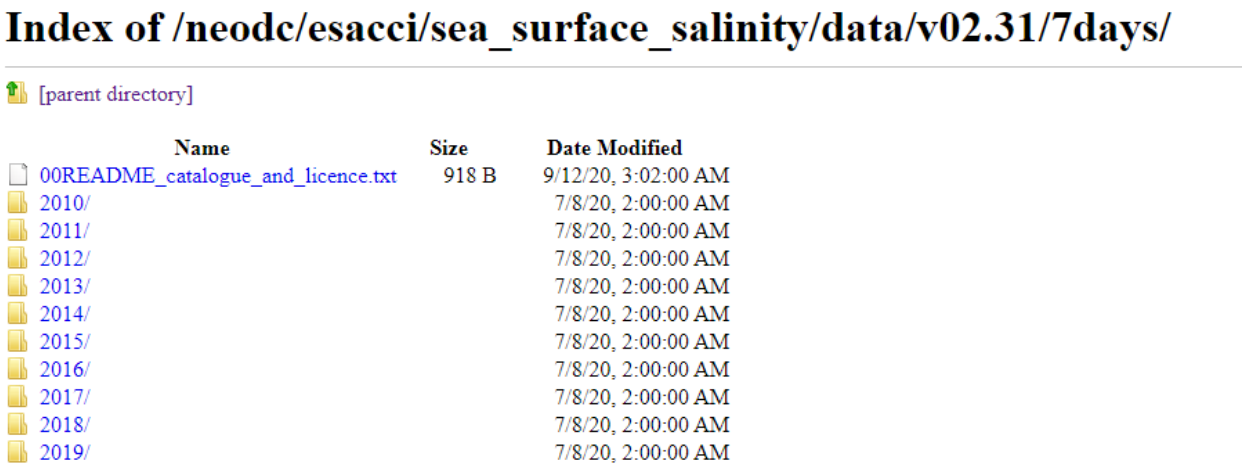

Figure 4 CCI+SSS dataset directory tree structure (for Year 2)

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	MERGED
additional segregator	Field describing the product: - OI: Optimal Interpolation - Time sampling - Spatial resolution	OI_Monthly_CENTRED_15Day_25km
		OI_7DAY_RUNNINGMEAN_DAILY_25km
indicative date	Product coverage date: YYYYmmdd	Every 15 days for the monthly
		Daily for the 7 days
indicative time	Product coverage time (optional) N/A for L4	-
file version	Version of the file	fv3.21
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-MERGED_OI_7DAY_RUNNINGMEAN_DAILY_25km-20100111-fv3.21.nc

```
netcdf ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_7DAY_RUNNINGMEAN_DAILY_25km-20100111-fv3.21 {
dimensions:
        lat = 584 ;
        lon = 1388 ;
        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 = "Multi-Satellite Sea Surface Salinity" ;
                sss:standard_name = "sea_surface_salinity" ;
                sss:valid_min = 0. ;
                sss:valid_max = 50. ;
                sss:ancillary_variables = "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:valid_min = 0. ;
                sss_random_error:valid_max = 100. ;
                sss_random_error:ancillary_variables = "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 ;
                noutliers:_FillValue = -1s ;
        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 ;
                total_nobs:_FillValue = -1s ;
        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 = "27-Apr-2021 00:38:55" ;
                :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 25 km EASE grid and 1 day of time sampling" ;
                :institution = "ACRI-ST,LOCEAN" ;
                :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" ;
                :creator_name = "ACRI-ST,LOCEAN" ;
                :creator_email = "jean-luc.vergely@acri-st.fr" ;
                :project = "Climate Change Initiative - European Space Agency" ;
                :geospatial_lat_min = -83.5171356201172 ;
                :geospatial_lat_max = 83.5171356201172 ;
                :geospatial_lon_min = -179.870315551758 ;
                :geospatial_lon_max = 179.870315551758 ;
                :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 = "20210427T003855Z" ;
                :date_modified = "" ;
                :time_coverage_start = "20100107T000000Z" ;
                :time_coverage_end = "20100114T235959Z" ;
                :time_coverage_duration = "P7D" ;
                :time_coverage_resolution = "P1D" ;
                :tracking_id = "10a4596b-d449-4dba-a01b-b13d24ea0717" ;
                :spatial_grid = "25km EASE 2 cylindrical grid" ;
                :source = "SMOS CCI v3 L2OS reprocessing (ERA5,ref OTT SSS:ISAS, RFI filtering) from DPGS
L1 v620, L2OS v671 modified as in DOI:10.1109/tgrs.2020.3030488, SMAP L2 RSS v4.0 - DOI:10.5067/SMP40-
2SOCS, Aquarius L3 v5.0 - DOI:10.5067/AQR50-3SQCS" ;
                :references      =      "https://climate.esa.int/fr/projects/sea-surface-salinity/      -
DOI:10.5285/5920a2c77e3c45339477acd31ce62c3c" ;
                :product_version = "3.21" ;
                :format_version = "CCI Data Standards v2.3" ;
                :comment = "The following caveats must be considered: 1) Products have not been fully
optimised for very high latitudes, 2) There is a systematic global underestimation of ~0.1 pss early 2010
that gradually disappears over the year, 3) 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" ;
                :creator_url = "https://climate.esa.int/fr/projects/sea-surface-salinity/" ;
                :id = "ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_7DAY_RUNNINGMEAN_DAILY_25km-20100111-
fv3.21.nc" ;
                :history = " " ;
}
```

4.2 Monthly running mean

Example of filename:

ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_Monthly_CENTRED_15Day_25km-20100201-fv3.21.nc

```
netcdf ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_Monthly_CENTRED_15Day_25km-20100201-fv3.21 {
dimensions:
        lat = 584 ;
        lon = 1388 ;
        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 = "Multi-Satellite Sea Surface Salinity" ;
                sss:standard_name = "sea_surface_salinity" ;
                sss:valid_min = 0. ;
                sss:valid_max = 50. ;
                sss:ancillary_variables = "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:valid_min = 0. ;
                sss_random_error:valid_max = 100. ;
                sss_random_error:ancillary_variables = "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 ;
                noutliers:_FillValue = -1s ;
        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 ;
                total_nobs:_FillValue = -1s ;
        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 = "27-Apr-2021 00:36:29" ;
                :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 25 km EASE grid and 15 days of time sampling" ;
                :institution = "ACRI-ST,LOCEAN" ;
                :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" ;
                :creator_name = "ACRI-ST,LOCEAN" ;
                :creator_email = "jean-luc.vergely@acri-st.fr" ;
                :project = "Climate Change Initiative - European Space Agency" ;
                :geospatial_lat_min = -83.5171356201172 ;
                :geospatial_lat_max = 83.5171356201172 ;
                :geospatial_lon_min = -179.870315551758 ;
                :geospatial_lon_max = 179.870315551758 ;
                :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 = "20210427T003629Z" ;
                :date_modified = "" ;
                :time_coverage_start = "20100118T000000Z" ;
                :time_coverage_end = "20100216T235959Z" ;
                :time_coverage_duration = "P1M" ;
                :time_coverage_resolution = "P15D" ;
                :tracking_id = "d9836c74-bacf-4a6d-b747-546bb2e38293" ;
                :spatial_grid = "25km EASE 2 cylindrical grid" ;
                :source = "SMOS CCI v3 L2OS reprocessing (ERA5,ref OTT SSS:ISAS, RFI filtering) from DPGS
L1 v620, L2OS v671 modified as in DOI:10.1109/tgrs.2020.3030488, SMAP L2 RSS v4.0 - DOI:10.5067/SMP40-
2SOCS, Aquarius L3 v5.0 - DOI:10.5067/AQR50-3SQCS" ;
                :references      =      "https://climate.esa.int/fr/projects/sea-surface-salinity/      -
DOI:10.5285/5920a2c77e3c45339477acd31ce62c3c" ;
                :product_version = "3.21" ;
                :format_version = "CCI Data Standards v2.3" ;
                :comment = "The following caveats must be considered: 1) Products have not been fully
optimised for very high latitudes, 2) There is a systematic global underestimation of ~0.1 pss early 2010
that gradually disappears over the year, 3) 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" ;
                :creator_url = "https://climate.esa.int/fr/projects/sea-surface-salinity/" ;
                :id  =  "ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_Monthly_CENTRED_15Day_25km-20100201-
fv3.21.nc" ;
                :history = " " ;
}
```

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