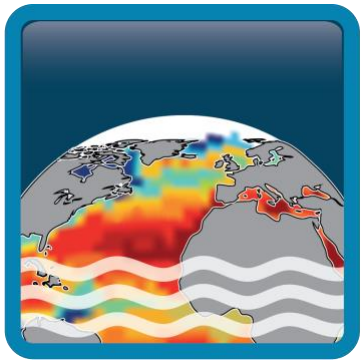
Climate Change Initiative+ (CCI+) Phase 1

Sea Surface Salinity



[D4.3] Product User Guide (PUG)

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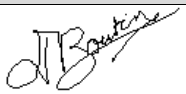
APPROVED BY	Jacqueline Boutin (Science Leader) LOCEAN		05-03-2020
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Amendment Record Sheet

	Document Change Record	
Date / Issue	Description	Section / Page
29/06/2019	Delivery to ESA	New document
29/11/2019	AR update	
05/03/2020 / v1.2	Comments from ESA before publication	

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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 v1.8 delivered at the end of the first-year exercise consist in two Level-4 datasets:

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

Input data used to produce the dataset are levels 2 for SMOS and 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 CATDS SSS produced with version 6.22 of the Level 2 OS processor (corresponding to CATDS RE05 reprocessed data until 31/03/2017 and near-real time CPDC products after)
- Aquarius Level 3 SSS produced with version v5.0
- SMAP Level 2 SSS produced with version v3.0

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 scientist 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; in particular in term of product format [DSTD].

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 first version of the document addressing Year 1 activity. More accomplished versions will be proposed in Year 2 and 3 accounting for acquired experience and feedback received by the users of the products.

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
- ✓ Annex 1: Level 4 netCDF structure

1.4 Applicable Document

DSTD	CCI Data Standards, CCI-PRGM-EOPS-TN-13-0009	V2.1, 25/03/2019
SRD	System Requirement Document	SSS_cci-D3.1-SRD-i1r5
SSD	System Specification Document	SSS_cci-D3.2-SSD-i1r0
URD	User Requirement Document	SSS_cci-D1.1-URD-i1r0
DARD	Data Access Requirement Document	SSS_cci-D1.3-DARD-v1r3
PSD	Product Specification Document	SSS_cci-D1.2-PSD-v1r4
SoW	CCI+ Statement of Work	
ATBD	Algorithm Theoretical Baseline Document	SSS_cci-D2.3-ATBD_L3_L4-i1r0_v1.2
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_L3OS_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://cci.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

Table 2 – Reference documents

1.6 Acronyms

AD	Applicable Document
ADP	Algorithm Development Plan
ATBD	Algorithm Theoretical Basis Document
C3S	Copernicus Climate Change Service
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

Salinity plays a fundamental role in the density-driven global ocean circulation, the water cycle, and climate. Therefore, salinity is considered to be 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.

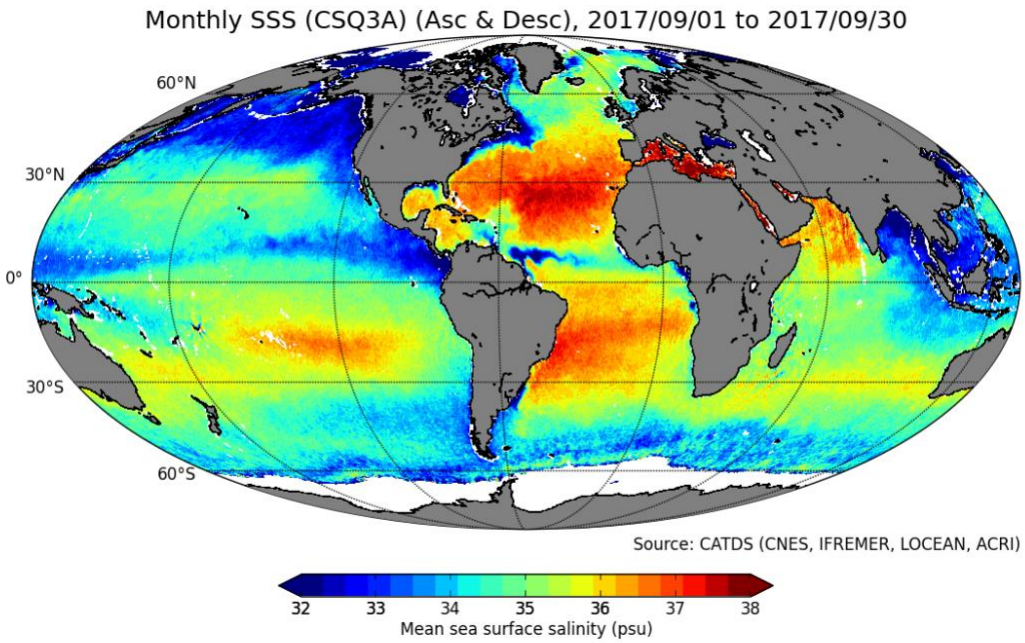


Figure 1 – Example of monthly SMOS Sea Surface Salinity map (salinity units using practical salinity scale, PSS) from SMOS data processed at Centre Aval de Traitement des Données SMOS (after applying a debiasing procedure similar to Boutin et al.(2018))

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 the SSS data set will be considered starting in Year 2 of the project.

2.1 The L-Band missions

2.1.1 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 0600 local time in ascending node and 1800hr in descending node along a sun-synchronous orbit.

2.1.2 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.

2.1.3 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.

2.2 The C-Band missions

During the first Year, the C-band missions are not considered.

2.3 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].

2.3.1 L-Band Input data

For the first Year (June-2018 to June-2019) of the project, the input data used to compute the time series are levels 2 for SMOS and SMAP or Level 3 for Aquarius sensor:

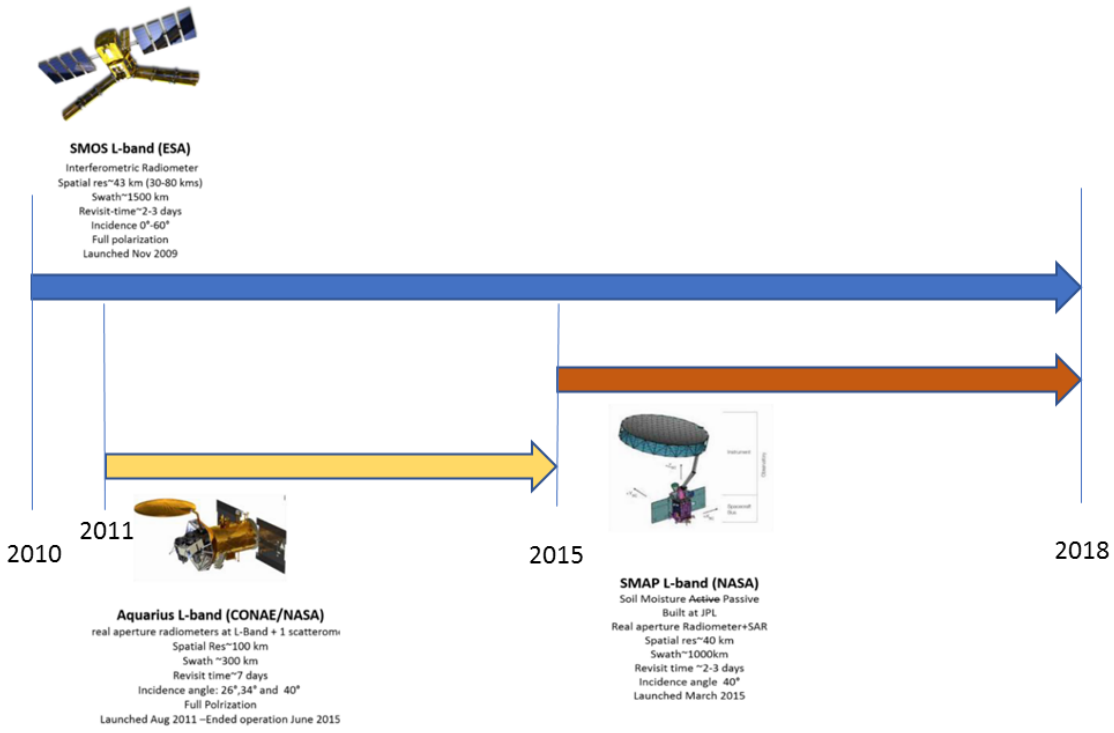


Figure 2 – L-Band missions time coverage in Year 1 of the project

- ✓ SMOS Level 2 from CATDS (from RE05 reprocessing TDS and operational data). ATBD is available in reference [ALGO_L2_SMOS]. Data is available from 2010 onwards.
- ✓ SMAP Level 2 from RSS (version 3.0). 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.

  ftp://ftp.remss.com/smap/SSS/V03.0/FINAL/L2C/40km

- ✓ 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 1, daily average datasets are used. 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.

  ftp://podaac-ftp.jpl.nasa.gov/allData/aquarius/L3/mapped/V5/7day_running/SCI

2.3.2 Level 4 user products

Only Level 4 products are disseminated to users during the first-Year exercise.

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

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 coastal and seasonal latitudinal systematic errors

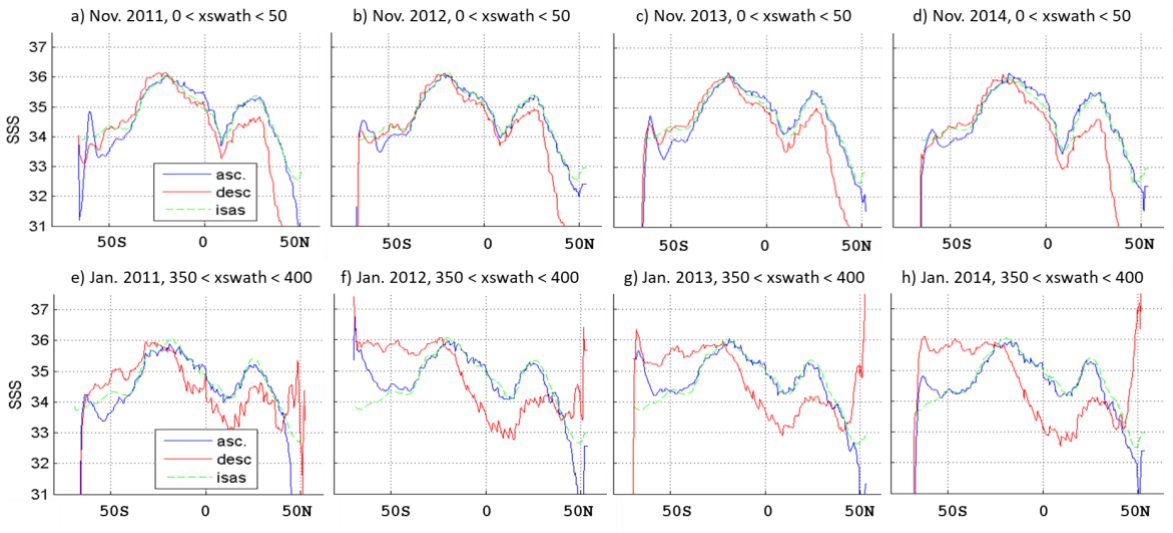


Figure 3 : Examples of seasonally-varying latitudinal systematic error. SSS averaged over the Pacific Ocean further than 800 km from coast: green: ISAS, blue: SMOS ascending orbits; red: SMOS descending orbits: a-d) November; middle of the swath (0-50 km from the centre of the swath); e-h) January; edge of the swath (350-400 km from the centre of the swath); a & e) 2011; b & f) 2012; c & g) 2013; d & h) 2014.

- Estimation of representativity errors, 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 9-year mean of the CCI SSS is adjusted to the 9-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 (e.g. river plumes).

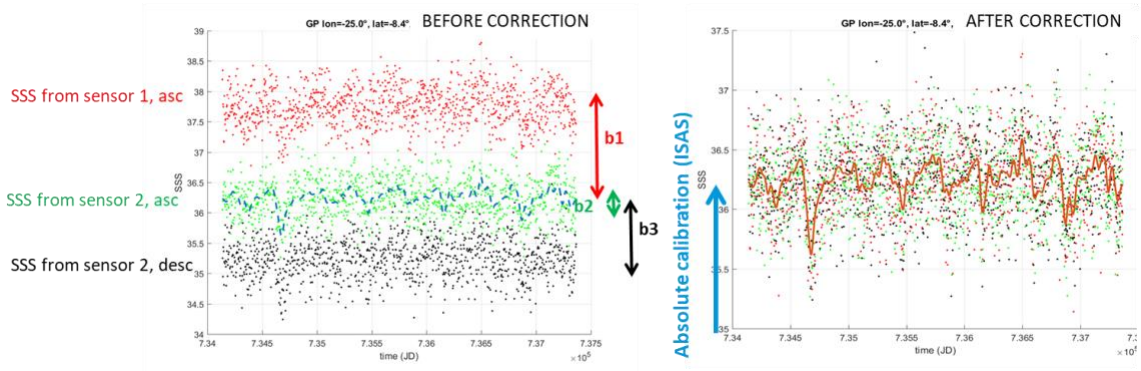


Figure 4 Example of systematic error adjustment: time series over the 9 Year time period of SSS retrieved from 2 sensors with different orbit orientation for a pixel close to coast, showing a shift between the various time series.

2.3.2.1 Processing chain

The following Figure 5 summarizes the different processing steps of the algorithm. Full details are provided in [ATBD].

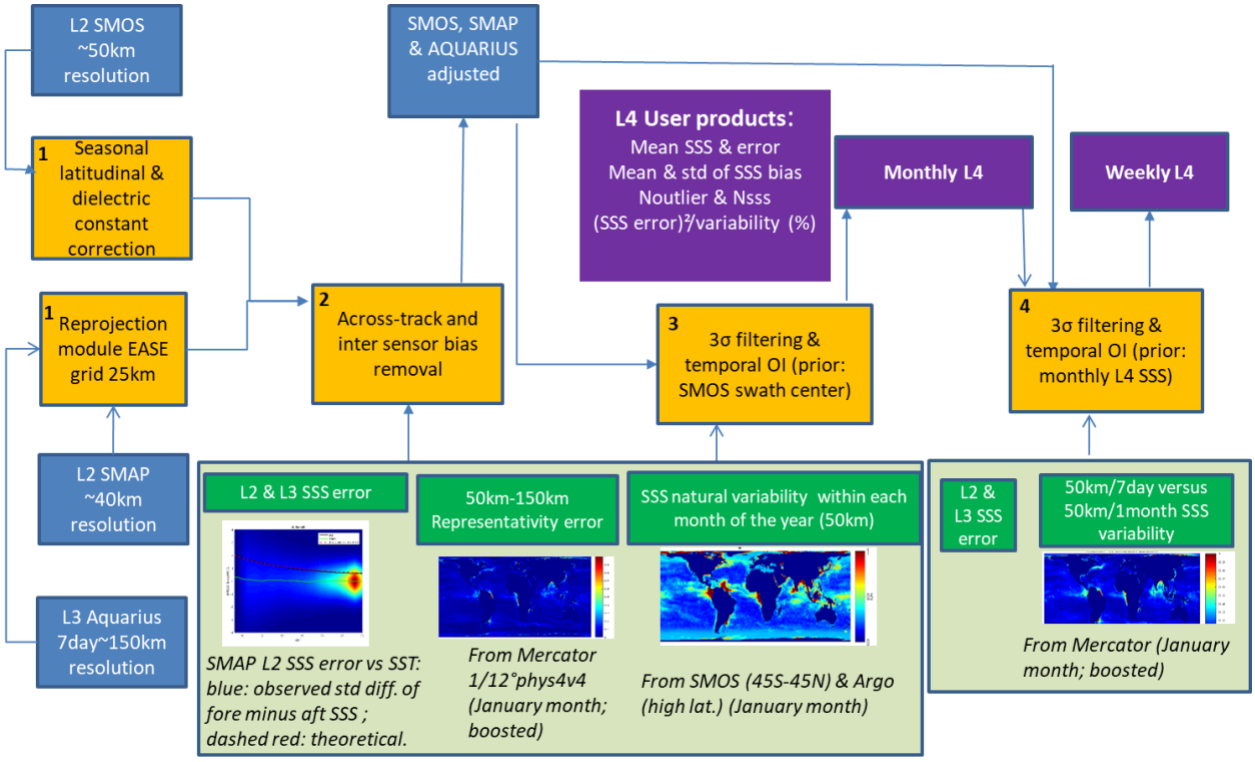


Figure 5: Level 4 processing scheme

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. Across-track and inter sensor bias removal
3. 3-sigma filtering and temporal Optimal Interpolation to generate monthly SSS. Error propagation.

   3-sigma filtering and temporal OI to generate weekly SSS using monthly SSS as prior. Error propagation.

2.3.2.2 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.

2.3.2.3 Weekly products

To estimate the weekly SSS, the biases calculated at 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 given by Mercator model. This eliminates outliers that deviate too far from what is expected.

3 Specification of the products

3.1 Dataset version

The version of the dataset corresponds to Year 1 activity.

Version	Production date	Publication date
1.8	April, 23rd 2019	November, 21st 2019

Table 3 – Dataset version

3.2 Disclaimer

This first version of the CCI+SSS products is a preliminary version issued for evaluation purposes by voluntary scientists and for framing future CCI+SSS products. This product has not been fully validated yet and may contain flaws.

The following caveats must be considered:

- The SSS random error in the weekly product is overestimated by a factor ~1.4.
- The Number of outliers is wrongly set to 'NaN' in the case where it is equal to zero.
- Products have not yet been not optimised for some issues encountered at high latitudes (i.e. remaining ice, RFI pollution, biases due to land-sea contamination and dielectric constant in cold waters).
- The criteria for flagging data close to land (including islands) are conservative and likely to be too restrictive in places.
- There is a systematic global underestimation (-0.08) of SSS starting at the beginning of the data set, and gradually disappearing at the end of 2010.
- There is a seasonal varying bias (~0.1, peaking in the middle of the year) in the Pacific North of 25°N".

In case you discover some inconsistencies, we (Mngt_CCI-Salinity@argans.co.uk) are very keen to get your feedback. In case you would like to use them in a presentation or publication, please contact us to get their correct reference . A DOI has been minted to the dataset:

http://dx.doi.org/10.5285/9ef0ebf847564c2eabe62cac4899ec41

3.3 Dataset time coverage

	Weekly	**Monthly**
Start date	January 6th 2010	January 1st 2010
End date	November 1st 2018	November 1st 2018

Table 4 – Dataset time coverage

3.4 Volume of data

The dataset are generated with a level 4 netCDF internal compression.

	Weekly	**Monthly**
Volume per product (uncompressed)	21.1 Mb	21.1 Mb
Volume per product (**compressed**)	9.8 Mb	9.8 Mb
Number of products	One product per day 3222 products	Two products per Month 214 Products
Total volume (compressed)	30 Gb	2.1 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/v01.8/

Table 6 – Data access

The full directory structure is the following (Figure 6):

Index of /neodc/esacci/sea_surface_salinity/data/v01.8/

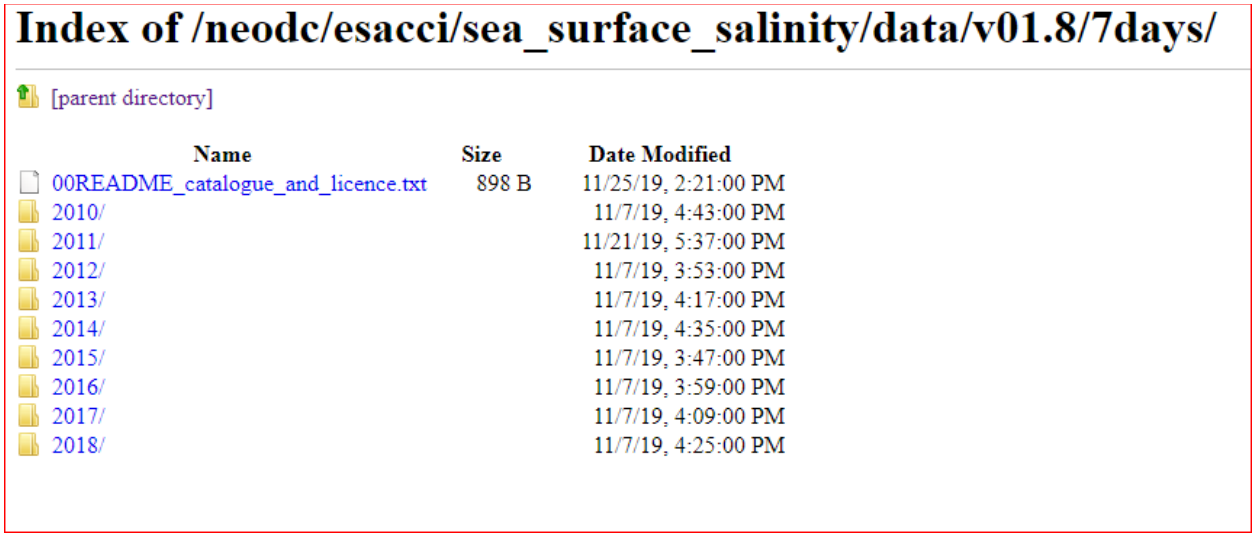
[parent directory]

Name	Size	Date Modified
30days/		11/25/19, 2:21:00 PM
7days/		11/25/19, 2:21:00 PM

Index of /neodc/esacci/sea_surface_salinity/data/v01.8/30days/

[parent directory]

Name	Size	Date Modified
00README_catalogue_and_licence.txt	899 B	11/25/19, 2:21:00 PM
2010/		11/6/19, 5:42:00 PM
2011/		11/6/19, 5:34:00 PM
2012/		11/6/19, 5:38:00 PM
2013/		11/6/19, 5:39:00 PM
2014/		11/6/19, 5:41:00 PM
2015/		11/6/19, 5:37:00 PM
2016/		11/6/19, 5:38:00 PM
2017/		11/6/19, 5:39:00 PM
2018/		11/6/19, 5:40:00 PM



Index of /neodc/esacci/sea_surface_salinity/data/v01.8/7days/

[parent directory]

Name	Size	Date Modified
00README_catalogue_and_licence.txt	898 B	11/25/19, 2:21:00 PM
2010/		11/7/19, 4:43:00 PM
2011/		11/21/19, 5:37:00 PM
2012/		11/7/19, 3:53:00 PM
2013/		11/7/19, 4:17:00 PM
2014/		11/7/19, 4:35:00 PM
2015/		11/7/19, 3:47:00 PM
2016/		11/7/19, 3:59:00 PM
2017/		11/7/19, 4:09:00 PM
2018/		11/7/19, 4:25:00 PM

Figure 6 CCI+SSS dataset directory tree structure

3.6 File format

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

- the CCI Data Standard version 2.1 [DSTD]
- the Climate and Forecasting (CF) convention version 1.7
- 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	fv1.8
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].

Annexe 1 - Level 4 products content

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

A.1 7 days running mean

Example of filename:

ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_7DAY_RUNNINGMEAN_DAILY_25km-20151225-fv1.8.nc

```
netcdf ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_7DAY_RUNNINGMEAN_DAILY_25km-20151225-fv1.8 {
dimensions:
        lat = 584 ;
        lon = 1388 ;
        time = 1 ;
variables:
        short total_nobs(time, lat, lon) ;
                total_nobs:long_name = "Number of SSS in the time interval" ;
                total_nobs:valid_max = 10000s ;
                total_nobs:valid_min = 0s ;
                total_nobs:_FillValue = -1s ;
        short noutliers(time, lat, lon) ;
                noutliers:long_name = "Count of the Number of Outliers within this bin cell" ;
                noutliers:valid_max = 10000s ;
                noutliers:valid_min = 0s ;
                noutliers:_FillValue = -1s ;
        float lat(lat) ;
                lat:long_name = "latitude" ;
                lat:units = "degrees_north" ;
                lat:standard_name = "latitude" ;
                lat:valid_range = -90.f, 90.f ;
        float lon(lon) ;
                lon:long_name = "longitude" ;
                lon:units = "degrees_east" ;
                lon:standard_name = "longitude" ;
                lon:valid_range = -180.f, 180.f ;
        float time(time) ;
                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:standard_name = "sea_surface_salinity" ;
                sss:valid_min = 0. ;
                sss:valid_max = 50. ;
        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. ;
        float sss_bias_std(time, lat, lon) ;
                sss_bias_std:_FillValue = NaNf ;
                sss_bias_std:long_name = "Standard Deviation of the Bias in Sea Surface Salinity" ;
                sss_bias_std:valid_min = 0. ;
                sss_bias_std:valid_max = 100. ;
        float sss_bias(time, lat, lon) ;
                sss_bias:_FillValue = NaNf ;
                sss_bias:long_name = "Bias in Sea Surface Salinity" ;
                sss_bias:valid_min = -100. ;
                sss_bias:valid_max = 100. ;
        float pct_var(time, lat, lon) ;
                pct_var:_FillValue = NaNf ;
```

```
                pct_var:long_name = "Percentage of Explained Sea Surface Salinity Variance by the Sea
Surface Salinity Standard Error" ;
                pct_var:units = "%" ;
                pct_var:valid_min = 0. ;
                pct_var:valid_max = 100. ;
        short sss_qc(time, lat, lon) ;
                sss_qc:long_name = "Sea Surface Salinity Quality, 0=Good; 1=Bad" ;
                sss_qc:valid_min = 0s ;
                sss_qc:valid_max = 1s ;

// global attributes:
                :creation_time = "25-Feb-2019 09:18:52" ;
                :institution = "ACRI-ST; LOCEAN" ;
                :Conventions = "CF-1.7" ;
                :keywords = "Ocean, Ocean Salinity, Sea Surface Salinity, Satellite" ;
                :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_url = "http://cci.esa.int/salinity" ;
                :project = "Climate Change Initiative - European Space Agency" ;
                :license = "ESA CCI Data Policy: free and open access" ;
                :standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention version
1.7" ;
                :platform = "PROTEUS; SAC-D; SMAP" ;
                :sensor = "SMOS/MIRAS; Aquarius; SMAP" ;
                :spatial_resolution = "50km" ;
                :geospatial_lat_units = "degrees_north" ;
                :geospatial_lon_units = "degrees_east" ;
                :date_modified = "" ;
                :tracking_id = "c9084d41-f887-45de-91bc-925140bb24a2" ;
                :creator_email = "jean-luc.vergely@acri-st.fr" ;
                :time_coverage_duration = "P7D" ;
                :geospatial_lat_min = -90. ;
                :geospatial_lat_max = 90. ;
                :geospatial_lon_min = -180. ;
                :geospatial_lon_max = 180. ;
                :date_created = "20190419T155320Z" ;
                :time_coverage_start = "20151222T000000Z" ;
                :title = "ESA CCI Sea Surface Salinity ECV produced at a spatial resolution of 50 km and
time resolution of 1 week and spatially resampled on 25 km EASE grid and 1 day of time sampling" ;
                :source = "SMOS CATDS-PDC L3OS 2P - DOI:10.12770/77edd308-4296-4774-b6f3-5b38301cee18,
SMAP L2 RSS v3.0 - DOI:10.5067/SMP30-2SOCS, Aquarius L3 v5.0 - DOI:10.5067/AQR50-3SQCS" ;
                :references                =                "http://cci.esa.int/salinity                -
DOI:10.5285/9ef0ebf847564c2eabe62cac4899ec41" ;
                :comment = "This is the first version of the CCI+SSS products. It is a preliminary version
issued for evaluation purposes by voluntary scientists and for framing future CCI+SSS products. In case
you discover some flaws not listed below, we (Mngt_CCI-Salinity@argans.co.uk) are very keen to get your
feedback. The caveats identified by CCI+SSS team are as follows. SSS random error in the weekly product
is overestimated by a factor ~1.4. The Number of outliers is wrongly set to \'NaN\' in case it is equal
to zero. Products have not yet been not optimised for some issues encountered at high latitudes (i.e.
remaining ice, RFI pollution, biases due to land-sea contamination and dielectric constant in cold waters).
The criteria for flagging data close to land (including islands) are conservative and likely to be too
restrictive in places. There is a systematic global underestimation (-0.08) of SSS starting at the
beginning of the data set, and gradually disappearing at the end of 2010. There is a seasonal varying
bias (~0.1, peaking in the middle of the year) in the Pacific North of 25 deg N" ;
                :product_version = "01.08" ;
                :id = "ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_7DAY_RUNNINGMEAN_DAILY_25km-20151225-
fv1.8.nc" ;
                :time_coverage_resolution = "P1D" ;
                :geospatial_lat_resolution = 0.25f ;
                :geospatial_lon_resolution = 0.25f ;
                :spatial_grid = "25km EASE 2 grid" ;
                :geospatial_vertical_min = 0.f ;
                :geospatial_vertical_max = 0.f ;
                :summary = "ESA CCI Sea Surface Salinity" ;
                :time_coverage_end = "20151228T000000Z" ;
                :history = " " ;
}
```

A.2 Monthly running mean

Example of filename:

ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_Monthly_CENTRED_15Day_25km-20141115-fv1.8.nc

```
netcdf ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_Monthly_CENTRED_15Day_25km-20141115-fv1.8 {
dimensions:
        lat = 584 ;
        lon = 1388 ;
        time = 1 ;
variables:
        short total_nobs(time, lat, lon) ;
                total_nobs:long_name = "Number of SSS in the time interval" ;
                total_nobs:valid_max = 10000s ;
                total_nobs:valid_min = 0s ;
                total_nobs:_FillValue = -1s ;
        short noutliers(time, lat, lon) ;
                noutliers:long_name = "Count of the Number of Outliers within this bin cell" ;
                noutliers:valid_max = 10000s ;
                noutliers:valid_min = 0s ;
                noutliers:_FillValue = -1s ;
        float lat(lat) ;
                lat:long_name = "latitude" ;
                lat:units = "degrees_north" ;
                lat:standard_name = "latitude" ;
                lat:valid_range = -90.f, 90.f ;
        float lon(lon) ;
                lon:long_name = "longitude" ;
                lon:units = "degrees_east" ;
                lon:standard_name = "longitude" ;
                lon:valid_range = -180.f, 180.f ;
        float time(time) ;
                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:standard_name = "sea_surface_salinity" ;
                sss:valid_min = 0. ;
                sss:valid_max = 50. ;
        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. ;
        float sss_bias_std(time, lat, lon) ;
                sss_bias_std:_FillValue = NaNf ;
                sss_bias_std:long_name = "Standard Deviation of the Bias in Sea Surface Salinity" ;
                sss_bias_std:valid_min = 0. ;
                sss_bias_std:valid_max = 100. ;
        float sss_bias(time, lat, lon) ;
                sss_bias:_FillValue = NaNf ;
                sss_bias:long_name = "Bias in Sea Surface Salinity" ;
                sss_bias:valid_min = -100. ;
                sss_bias:valid_max = 100. ;
        float pct_var(time, lat, lon) ;
                pct_var:_FillValue = NaNf ;
                pct_var:long_name = "Percentage of Explained Sea Surface Salinity Variance by the Sea
Surface Salinity Standard Error" ;
                pct_var:units = "%" ;
                pct_var:valid_min = 0. ;
                pct_var:valid_max = 100. ;
        short sss_qc(time, lat, lon) ;
                sss_qc:long_name = "Sea Surface Salinity Quality, 0=Good; 1=Bad" ;
                sss_qc:valid_min = 0s ;
                sss_qc:valid_max = 1s ;
```

```
// global attributes:
                :creation_time = "23-Feb-2019 11:34:36" ;
                :institution = "ACRI-ST; LOCEAN" ;
                :Conventions = "CF-1.7" ;
                :keywords = "Ocean, Ocean Salinity, Sea Surface Salinity, Satellite" ;
                :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_url = "http://cci.esa.int/salinity" ;
                :project = "Climate Change Initiative - European Space Agency" ;
                :license = "ESA CCI Data Policy: free and open access" ;
                :standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention
version 1.7" ;
                :platform = "PROTEUS; SAC-D; SMAP" ;
                :sensor = "SMOS/MIRAS; Aquarius; SMAP" ;
                :spatial_resolution = "50km" ;
                :geospatial_lat_units = "degrees_north" ;
                :geospatial_lon_units = "degrees_east" ;
                :date_modified = "" ;
                :tracking_id = "1014de50-d0d7-4f79-846a-430ac24bace9" ;
                :creator_email = "jean-luc.vergely@acri-st.fr" ;
                :time_coverage_duration = "P1M" ;
                :geospatial_lat_min = -90. ;
                :geospatial_lat_max = 90. ;
                :geospatial_lon_min = -180. ;
                :geospatial_lon_max = 180. ;
                :date_created = "20190419T114826Z" ;
                :time_coverage_start = "20141031T000000Z" ;
                :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" ;
                :source = "SMOS CATDS-PDC L3OS 2P - DOI:10.12770/77edd308-4296-4774-b6f3-5b38301cee18,
SMAP L2 RSS v3.0 - DOI:10.5067/SMP30-2SOCS, Aquarius L3 v5.0 - DOI:10.5067/AQR50-3SQCS" ;
                :references = "http://cci.esa.int/salinity -
DOI:10.5285/9ef0ebf847564c2eabe62cac4899ec41" ;
                :comment = "This is the first version of the CCI+SSS products. It is a preliminary
version issued for evaluation purposes by voluntary scientists and for framing future CCI+SSS products.
In case you discover some flaws not listed below, we (Mngt_CCI-Salinity@argans.co.uk) are very keen to
get your feedback. The caveats identified by CCI+SSS team are as follows. SSS random error in the
weekly product is overestimated by a factor ~1.4. The Number of outliers is wrongly set to \'NaN\' in
case it is equal to zero. Products have not yet been not optimised for some issues encountered at high
latitudes (i.e. remaining ice, RFI pollution, biases due to land-sea contamination and dielectric
constant in cold waters). The criteria for flagging data close to land (including islands) are
conservative and likely to be too restrictive in places. There is a systematic global underestimation
(-0.08) of SSS starting at the beginning of the data set, and gradually disappearing at the end of
2010. There is a seasonal varying bias (~0.1, peaking in the middle of the year) in the Pacific North
of 25 deg N" ;
                :product_version = "01.08" ;
                :id = "ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_Monthly_CENTRED_15Day_25km-20141115-
fv1.8.nc" ;
                :time_coverage_resolution = "P15D" ;
                :geospatial_lat_resolution = 0.25f ;
                :geospatial_lon_resolution = 0.25f ;
                :spatial_grid = "25km EASE 2 grid" ;
                :geospatial_vertical_min = 0.f ;
                :geospatial_vertical_max = 0.f ;
                :summary = "ESA CCI Sea Surface Salinity" ;
                :time_coverage_end = "20141130T000000Z" ;
                :history = " " ;
}
```

End of Document