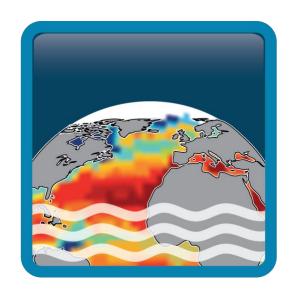
Sea Surface Salinity Climate Change Initiative Phase 1 **Product Specification Document**





Product Specification Document (PSD)

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1 Introduction

1.1 Purpose and Scope

- 3 The purpose of this document is to convert the user requirements, summarized in the User
- 4 Requirement Document (URD, [AD01]), into a detailed set of Sea Surface Salinity (SSS) product
- 5 specifications of the Seasurface Surface Salinity Climate Change Initiative (CCI+SSS) project.
- 6 The PSD provides results from a detailed analysis of the requirements of current and future
- 7 users of satellite SSS. The survey aims to involve users in the development process of the
- 8 CCI+SSS product and to understand their needs prior to the start of the product development.
- 9 The PSD connects the recommendations from the URD with the aim to produce a detailed set
- 10 of product specifications that respond to the user needs and are continuously assessed
- 11 against their needs.

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1.2 Recommendations for Product Specification

- 14 The survey conducted by the project was very detailed and the requirements are widely
- 15 spread. Therefore, not all aspects of user requirements are covered by the first phase of
- 16 CCI+SSS. (which coincides with the third programmatic phase of the whole CCI Program).
- 17 The goal is to design products that meet as many requirements as possible taking into account
- 18 the available options. The recommendations derived here from the user consultation relate
- 19 to the need for a growing and diverse user community and their needs:
 - 1) make high-resolution data available, to account for the high diversity of requirements for spatio-temporal resolution of the products. The survey results show, that the resolution needs strongly depend on the analyzed phenomena ranging from original spatial sampling to 10° and temporal resolution from weekly (daily sampling) to monthly (15 day sampling).
 - 2) Error specification for L4 SSS product, along with error estimation details, to account for the need of broad uncertainty specification. The CCI+SSS product will contain the random error, systematic error, standard deviation of the bias, as well as good/bad flags computed from different indicators (Xi2, number of outliers).
 - 3) Compatibility between products (L2,L3,L4, other CCI products)



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30 1.3 References

1.3.1 Applicable Documents

ID	Document	Reference
AD01	User Reference Document (URD)	SSS_cci_D1.1_URD-i1r4

32 1.3.2 Reference Documents

33 List here all the document that must be read in the conjunction of this document.

ID	Document	Reference
RD01	End-to-End ECV Uncertainty Budget	E3UB
RD02	CCI Data Standards 2.0 (17/09/2018)	CCI-PRGM-EOPS-TN-13-009

34 1.4 Acronyms

35	AD	Applicable Document
36	ADP	Algorithm Development Plan
37	ATBD	Algorithm Theoretical Basis Document
38 39 40	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
41 42	CCI+	Climate Change Initiative Extension (CCI+), is an extension of the CCI over the period 2017–2024
43	CMUG	Climate Modelling User Group
44	DARD	Data Access Requirements Document
45	DOI	Digital Object Identifier
46	E3UB	End-to-End ECV Uncertainty Budget
47	EC	European Commission
48	ECV	Essential Climate Variable
49	EO	Earth Observation
50	EOV	Essential Ocean Variable (of the OOPC)



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Sea Surface Salinity Climate Change Initiative Phase 1 (ESA CCI Phase 3)

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51	ESM	Earth System Model
52	NASA	National Aeronautics and Space Administration
53	ODP	Open Data Portal
54	PSD	Product Specification Document
55	PUG	Product User Guide
56	PVASR	Product Validation and Algorithm Selection Report
57	PVIR	Product Validation and Intercomparison Report
58	PVP	Product Validation Plan
59	RD	Reference Document
60	SMAP	Soil Moisture Active Passive [mission of NASA)
61	SMOS	Soil Moisture and Ocean Salinity [satellite of ESA]
62	SRD	System Requirements Document
63	SSD	System Specification Document
64	SSS	Sea Surface Salinity
65	SVR	System Verification Report
66 67	UCR/CECR	Uncertainty Characterisation Report (formerly known as the Comprehensive Error Characterisation Report)
68	URD	User Requirements Document
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2 Product format and metadata

72 2.1 Data format

- 73 Users expressed a clear preference for data in NetCDF format [AD01]. NetCDF has many
- advantages, since it is a self-describing, machine independent data format used in a number
- of other projects.

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- 76 Consequently, the primary format of CCI+SSS dataset will be NetCDF. CCI, in general produce
- 77 data according to the CCI Data Standards Requirements in netCDF-4 classic format using
- 78 Climate and Forecasting (CF) Metadata convention [RD02].
- 79 NetCDF format allows the use of various programming languages and tools to read and
- 80 analyze the data, for example MATLAB, the preferred language chosen by the users. File
- 81 format and name convention follows the common CCI conventions.
- The detailed internal format of the NetCDF structure to be used has not been defined yet (this
- requires decisions on product names etc.) and will follow in the next version of this document.

84 2.2 Filename convention

- A common CCI filename convention has been developed and CCI+SSS will follow these.
- 86 ESACCI-<CCI project>--processing level>-<data type>--type>--ct
- 87 string>[-<additional segregator>]-<indicative date>-
- 88 [<indicative time>]-fv<file version|.nc
- 89 For example, a SSS product with a timestep of one day and a spatial grid size of 25 km Version
- 90 1.0 for the first November 2018, created from satellite SSS measurements would be named:
- 91 ESACCI-SEASURFACESALINITY-L4-SSS-MERGED-OI-7DAY-RUNNINGMEAN-
- 92 DAILY-25km-20181101-fv1.6.nc
- 93 Monthly SSS product with a spatial grid size of 25 km with the centered date at the first
- 94 November would be named:
- 95 ESACCI-SEASURFACESALINITYSSS-L4-SSS-MERGED-OI-Monthly-CENTRED-
- 96 15Day-25km-20181101-fv1.6.nc



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- 97 The same product but with the centred date at the 15th November:
- 98 ESACCI-SEASURFACESALINITYSSS-L4-SSS-MERGED-OI-Monthly-CENTRED-
- 99 15Day-25km-20181115-fv1.6.nc
- 100 2.2.1 CCI Project
- 101 The project identifier is set to SSS
- 2.2.2 Processing level
- During the first phase of the CCI+SSS project a Level 4 (L4) product will be provided, a data
- 104 product created from the analysis of lower level satellite data from SMOS, Aquarius and SMAP
- that result in gridded high-quality products.

Level	<processing level=""> Code</processing>	Description	
Level 0	LO	Unprocessed and payload data at full resolution. No CCI recommendations regarding formats or content for data at this processing level	
Level 1A	L1A	Reconstructed unprocessed instrument data at full resolution, time referenced and annotated with ancillary information, including radiometric and geometric calibration coefficients and georeferencing parameters, computed and appended, but not applied, to LO data	
Level 1B	L1B	Level 1A data processed to sensor units	
Level 1C	L1C	Further processed Level 1B data (e.g. correcting radiances, mapping onto a spatial grid)	
Level 2	L2	Retrieved environmental variables at the same resolution and location as the level 1 source	
Level 2 Pre- processed	L2P	Geophysical variables derived from Level 1 source data at the same resolution and location as Level 1 data, typically in a satellite projection with geographic information. These data are the fundamental basis for higher level CCI products.	
Level 3	L3	L2 variables mapped on a defined grid with reduced ancillary data requirements:	
Level 3	L3U	Uncollated L3U: L2 data granules remapped to a space grid without combining any observations from overlapping orbits.	



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Level 3	L3C	Collated L3C: Observations combined from a single instrument into a space-time grid	
Level 3	L3S	Super-collated L3S: Observations combined from multiple instruments into a space-time grid	
Level 4	L4	Data set created from an analysis of lower level data that result in gridded, gab-free products	

Table 1 Details of processing level naming conventions taken from [RD02]

107

108 2.2.3 Data Type

Here, the main data type in the dataset is described, SSS for Sea Surface Salinity.

110 2.2.4 Product String

- 111 The product string depends on the processing level. During the first year it is planned to
- submit L4 data, therefore, the product string should be MERGED.

2.2.5 Additional Segregator

114 The additional segregator describes an optional part of the filename.

115 **2.3 Data access**

- Based on the User Requirement Survey [AD01], the user community prefer accessing data
- using a File Transfer Protocol (FTP) with a dedicated FTP connection. Furthermore, users
- require data products available at multiple resolutions. In the first year, two L4 products will
- be provided with 1) daily time step based on a 7-day running mean and 2) a monthly mean.

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2.4 Attributes 123

- 124 Attributes are metadata stored in the NetCDF files. Here, a distinction is made between global
- 125 and variable attributes. The latter are specific for each variable and differ between data- and
- 126 NetCDF files. On the other hand, global attributes apply to the whole content of the NetCDF
- 127

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2.4.1 Global attributes

Name	Data Type	Description	CCI+SSS Definition
title	string	description of the data set	ESA SMOS CCI Sea Surface Salinity Product
institution	string	Institution where the data was produced	ACRI-ST; LOCEAN
source	string	Original data sources	Source data were: SMOS ESAL2OSv622/CATDS RE05, Aquarius L3 v5.0, SMAP L2 RSS v3.0
history	string	processing history of data set	CCI processing
references	string	references to ATBD	http://cci.esa.int/salinity
tracking_id	string	a Universal Unique Identifier value	
conventions	string	the CF version	CF-1.7
product_version	string	Product version of this data file	n{1,}[.n{1,}], e.g. 01.5
summary	string	a paragraph describing the data set	ESA CCI Sea Surface Salinity
keywords	string	a comma separated list of keywords and phrases	Ocean; Ocean Salinity; Sea Surface Salinity; Satellite
id	string	file name, file identification	e.g. ESACCI- SEASURFACESALINIT YSSS-L4-SSS-MERGED-OI- 7DAY-RUNNINGMEAN-



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			DAILY-25km-YYYYMMDD- fv1.6.nc
naming authority	string		European Space Agency - ESA Climate Office
keywords_vocabulary	string		NASA Global Change Master Directory (GCMD) Science Keywords
cdm_data_type	string	The THREDDS data type appropriate for this data set.	Grid
comment	string	Various information about the data set	Data are based on a 7-day running mean objectively interpolated
date_created	string	the date on which the data was created	yyyymmddThhmmssZ
date_modified	string	the date on which the data was modified	
creator_name	string	Name of the creator	ACRI-ST; LOCEAN
creator_url	string	Contact of the creator	http://cci.esa.int/salinity
creator_email	string	Contact of the creator	TBD
project	string	the scientific project that produced the data: "Climate Change Initiative – European Space Agency"	Climate Change Initiative - European Space Agency
geospatial_lat_min	float	Decimal degrees North, Range: - 90 to 90	-90.0
geospatial_lat_max	float	Decimal degrees North, Range: - 90 to 90	90.0
geospatial_lon_min	float	Decimal degrees East, Range: - 180 to 180	-180.0
geospatial_lon_max	float	Decimal degrees East, Range: - 180 to 180	180.0



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			1
time_coverage_start string		Time of the first measurement in the data file. Time format is ISO 8601.	yyyymmddThhmmssZ
time_coverage_end	string	Time of the last measurement in the data file. Time format is ISO 8601.	yyyymmddThhmmssZ
time_coverage_duration	string	Length of time coverage	7 days - indicative date as centred date
time_coverage_resolut ion	string	Time resolution	1 day
standard_name_vocab ulary	string	the name of the controlled vocabulary from which variable standard names are taken	NetCDF Climate and Forecast (CF) Metadata Conventions Version 1.7
licence	string	describe the restrictions to data access and distribution	ESA CCI Data Policy: free and open access

Table 2 List of global attributes. The contents of the first four columns of this table are reproduced from CCI DataStandards Issue 2.0 [RD02].

131 In the following Table 3, the CCI project specific attributes are listed:

Name	Data Type	Description	CCI+SSS Definition
platform	string	Name of the Satellites	MIRAS; SAC-D
sensor	string	Sensor name	SMOS; Aquarius; SMAP
spatial_resolution	string	approximate resolution of the product	25 km
geospatial_lon_resolution	string	Decimal degrees	0.25
geospatial_lat_resolution	string	Decimal degrees	0.25
geospatial_lat_units	string	Degrees North	degrees_north



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geospatial_lon_units	string	Degrees East	degrees_east

Table 3 Specific attributes to the CCI+SSS

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2.4.2 Variable attributes

Name	Data Type	Description	CCI+SSS Definition
standard_name	string	the standard name of the variable following the CF convention	sea_surface_salinity,longitude, latitude
_FillValue	same as variable data type	a value used to indicate array elements containing no valid data	NaN or a number?
units	string	Description of the units (text). Preferable S.I.	psu, degrees_east, degreas_north
scale_factor	same as variable data type	a factor needed to convert the variable into S.I. units	
add_offset	same as variable data type	offset needed to convert variable into S.I. units	
long_name	string	a free text descriptive variable name	
valid_min	same as variable data type	Minimum valid value for this variable	
valid_max	same as variable data type	Maximum valid value for this variable	
valid_range	same as variable data type	Range of valid values for this variable	
comment	string	important information about the variable	
source	string	original data source	

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grid-mapping	string	This attribute is attached to data variables so that variables with different mappings may be present in a single file.	
auxiliary_data_N	string	A string describing additional data used to produce this variable	

- Table 4 List of variable attributes. The contents of the first three columns of this table are reproduced from CCI Data Standards 2.0 Document [RD02].
- 137 Based on these conventions, the file will contain a
- 138 1. map of SSS
- a corresponding map of uncertainties (random, systematic error, standard deviation
 of the bias)
- 3. a corresponding map of quality flags (good/bad flags computed from Xi2 and numberof outliers)
 - 4. a corresponding map of the number of outliers
- 5. Explained Variance PCTVAR= SSS_error/SSS_variability?
- 145 6. global attributes

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- The L4 files will contain a regular lat-lon map, the products at the different time steps (daily, monthly) files share the same names for variables that appear in both products as well as dimensions (latitude, longitude, SSS, QF etc.):
- 150 Dimensions:

1	51	time =	1
т.	JI	uiiic –	_

152 lat = 584

153 lon = 1388

154

155 lat

156 Size: 584x1

157 Dimensions: lat

158 Datatype: single



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159	Att	ributes:		
160		_FillValu	ie =	NaN
161		long_na	me =	'latitude'
162		units	=	'degrees_north'
163		standar	d_name	= 'latitude'
164	valid_rang	e = -90.f, 90.	f	
165				
166	lon			
167	Size	e: 1388x1		
168	Din	nensions: lor	1	
169	Dat	atype: sing	le	
170	Att	ributes:		
171		_FillValu	ie =	NaN
172		long_na	me =	'longitude'
173		units	=	'degrees_east'
174		standar	d_name	= 'longitude'
175	valid_rang	e = -180.f,18	0.f	
176				
177	time			
178	Size	e: 1x1		
179	Din	nensions: tin	ne	
180	Dat	atype: sing	le	
181	Att	ributes:		
182		_FillValu	ie =	NaN



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183	long_name = 'time'
184	units = 'days since 1970-01-01 00:00:00 UTC'
185	standard_name = 'time'
186	
187	
188	total_nobs
189	Size: 1388x584
190	Dimensions: lon,lat
191	Datatype: int16
192	Attributes:
193	_FillValue =0
194	<pre>long_name = Number of SSS in time interval'</pre>
195	coordinates = ' lon lat'
196	units = 'NA'
197	standard_name = 'number_of_observations'
198	valid_min =0
199	valid_max=10000
200	valid_range=0.f, 10000.f
201	scale_factor=1
202	add_offset=0
203	
204	SSS
205	Size: 1388x584
206	Dimensions: Ion,lat



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207	Datat	ype: single	
208	Attrib	utes:	
209		_FillValue	= NaN
210		long_name	= 'Unbiased merged Sea Surface Salinity
211		coordinates	= ' lon lat'
212		units	= 'pss'
213		standard_nar	me = 'sea_surface_salinity'
214		valid_min =0	
215		valid_max=50)
216		valid_range=0	0.f, 50.f
217		scale_factor=	1
218		add_offset=0	
219	sss_bias		
220	Size:	1388x584	
221	Dimer	nsions: ,lon,lat	
222	Datat	ype: single	
223	Attrib	utes:	
224		_FillValue	= NaN
225		long_name	= 'Bias in Sea Surface Salinity.'
226		coordinates	=' time lon lat'
227		standard_nar	me = 'sea_surface_salinity_bias'
228		units	= 'pss'
229		valid_min =-1	.00
230		valid_max=10	00



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231	valid_range=-100.f, 100.f
232	scale_factor=1
233	add_offset=0
234	
235	sss_bias_std
236	Size: 1x1440x720
237	Dimensions: time,lon,lat
238	Datatype: float
239	Attributes:
240	_FillValue = NaN
241	long_name = 'Standard Deviation of the Bias in Sea Surface Salinity.'
242	coordinates = 'time Ion Iat'
243	standard_name = 'sea_surface_salinity_bias_std'
244	units = 'pss'
245	valid_min =0
246	valid_max=100
247	valid_range=0.f, 100.f
248	scale_factor=1
249	add_offset=0
250	
251	
252	
253	
254	



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255		
256		
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259		
260		
261		
262		
263		
264		
265	SSS	_random_error
266	Size:	1388x584
267		Dimensions:,lon,lat
268		Datatype: single
269		Attributes:
270		_FillValue = NaN
271		long_name = 'Sea Surface Salinity Random Error'
272		coordinates = ' lon lat'
273		standard_name = 'sea_surface_salinity_random_error'
274		units = 'pss'
275		valid_min =0
276		valid_max=100
277		valid_range=0.f, 100.f
278		scale_factor=1



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279 add_offset=0 280 281 282 noutliers 283 Size: 1388x584 284 Dimensions: lon,lat Datatype: int16 285 286 Attributes: 287 _FillValue = 0 = "Count of the Number of Outliers within this bin cell" 288 long_name coordinates = 'lon lat' 289 = 'number_of_outliers' 290 standard_name 291 units = 'NA' 292 valid_min =0 valid max=10000 293 valid_range=0.f, 10000.f 294 scale_factor=1 295 add_offset=0 296 297 298 pct_var 299 Size: 1388x584 300 Dimensions: lon,lat 301 Datatype: single 302 Attributes:



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303		_FillValue = NaN
304 305	Sea Su	long_name = 'Percentage of Explained Sea Surface Salinity Variance by the urface Salinity Standard Error'
306		coordinates = ' time Ion Iat'
307		standard_name = 'percentage_variance'
308		units = '%'
309		valid_min =0
310		valid_max=100
311		valid_range=0.f, 100.f
312		scale_factor=1
313		add_offset=0
314		
315		
316	SSS	_qc
317	Size:	1388x584
318		Dimensions: lon,lat
319		Datatype: int16
320		Attributes:
321		_FillValue = 0
322		long_name = 'Sea Surface Salinity Quality. 1=good; 0=Bad'
323		coordinates =' lon lat'
324		
325		valid_min =0
326		valid_max=1



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Sea Surface Salinity Climate Change Initiative Phase 1 (ESA CCI Phase 3)

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3 Spatial and temporal resolution, grid 330 format and projection 331 The majority of users have spoken out for a high resolution on temporal and spatial scale with 332 333 the highest accuracy possible at this resolution. Here some users wanted highly processed 334 data products (L3 and L4) while other users prefer to have low level products (L2). 335 Within Phase 1, the CCI+SSS project want to make highly processed L4 data accessible. Lower processed data products based on the different satellites can be accessed via ESA or other 336 337 websites. Within Phase 2 the CCI+SSS project is planning to provide also debiased L2 and L3 data products. 338 3.1 Spatial resolution 339 To analyze at least mesoscale processes, many users require higher spatial resolution (1-100 340 341 km) than users, who focus on large scale processes (> 100 km). Based on the URD and based on the capabilities of the different L-Band sensors, a specification of interpolated 25 km 342 343 resolution data based on 75 km resolution seems achievable. 3.2 Temporal resolution 344 Corresponding to the requirements regarding spatial resolution, the requirements for 345 temporal resolution varied dependent on the research interest. There was no clear majority 346 347 for the gueried resolutions but a tendency to at least weekly data products. 348 Based on the URD and the capabilities of the sensors (SMOS & SMAP - 3 day observing cycle, 349 Aquarius 7 days), it seem sensible to offer a product with daily timesteps with a 7-day window. For users who require lower temporal resolution a second product will be available with a 350 resolution of one month centred 1) at the first of each month and 2) centred at the 15th of 351 each month. The latter is comparable with climatological means. 352

The majority of users have spoken out for data with a global coverage on a regular latitude-

longitude grid. The first CCI+SSS product files will be delivered on the global (Cylindrical) Equal-Area Scalable Earth Grid 2.0 (EASE 2), since it is used for other satellite SSS products

3.3 Grid format, map projection and coverage

and therefore favors the compatibility between different data products.



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4 Error budget and uncertainties

In order to characterize errors in the final product, analysis of the various sources of error 359 360 need to be conducted. Divergent user responses indicate that there is no one way of 361 communicating uncertainties that will suit everyone. But the majority of users require random noise and systematic errors for each grid point as 362 363 well as detailed information about the error budget and bias correction. 4.1 Characterizing error and error budgeting 364 Error characterization and budgeting is described in the End-to-End ECV Uncertainty Budget 365 document, but to summarize, the uncertainty can be generally grouped into the following 366 primary categories: 367 368 uncertainties due to the measurement instrument 369 systematic errors in the retrieval algorithm 370 unknown uncertainties (e.g., spatial-temporal sampling errors) 371 Errors in each of these sources need to be propagated through the processing pixel by pixel 372 resulting in an error budget for each SSS grid point. During the first phase of the CCI+SSS project, data sets will include information about random 373 374 noise and systematic errors, number of outliers and standard deviation of the bias. Error 375 estimation for the L4 CCI+SSS product is described in the End to End ECV Uncertainty

4.2 Data format for uncertainty information

The uncertainty products will be stored directly alongside the product in NetCDF, encoding the uncertainty information as additional variable in NetCDF and bin them to their associated variable by attributes and naming convention. This will be compatible with the CF conventions.

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5 Quality indicators and flags

5.1 Quality indicators

Based on the user requirements [AD001], the L4 CCI+SSS product must have quality indicators. Users prefer to have data flagged dependent on their quality. In the case of the L4 product released during the first phase of the CCI+SSS project it is not possible to specify each quality flag since the data sets are created from lower level data that result in gridded, higher quality products. For production, a detailed documentation is needed including all steps in the data and product delivery chain. Furthermore, uncertainty information is essential for the users.

5.2 Flags

The detailed composition of the list of flags has not been defined yet and will follow in the next version of this document.

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597 6 Summary

- The aim of this document was to transform the user requirements summarized in the URD into a set of product specifications for input into Task 2 (algorithm development etc.) of the CCI+SSS project.
 - 1. Two CCI+SSS products on a regular latitude longitude grid will be provided during the first year of the CCI+SSS project (Table 5).
 - 2. Data products will include uncertainty information (random noise + systematic error (bias), standard deviation of the systematic error, number of outliers, Chi2 of applied correction to homogenize SMOS, SMAP and Aquarius).
 - 3. Additional information (SST, Sea Ice) will not be provided with the products at this stage of the project.
 - 4. Quality indicators will be provided in the L4 data.
 - 5. At each step of processing, the error will be quantified, propagated through the processing chain and well documented.
 - 6. Updates of the products will be given 2 times during the first year of the CCI+SSS project.
 - 7. Data will be produced in CF-compliant NetCDF-v4 format
- 414 8. The NetCDF data will be distributed through an FTP site.

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Level	Decorrelation timescales	Spatial Smoothing scale	Temporal timesteps	Spatial grid size	Coverage
L2	-	-	-	-	-
L3	-	-	-	-	-
L4	weekly	50 km (TBC)	daily (based on 7-day running means)	25 km	global 01/2010-10/2018
L4	30 days	50 km (TBC)	centred at each 1st and 15th day of the month	25 km	global 01/2010-10/2018

Table 5 Summary of the specifications of the first dataset CCI+SSS project (dataset year1). L2 and L3 products will be provided during the second delivery.

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End of Document