CCI Phase 1 (SST)
Product Specification Document (PSD)

SST_CCI-PSD-UKMO-001 Issue 3

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Abstract: This document contains the Product Specification for the ESA SST_cci project.

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EUROPEAN SPACE AGENCY CONTRACT REPORT

The work described in this report was done under ESA contract. Responsibility for the contents resides in the author or organisation that prepared it.



AMENDMENT RECORD

This document shall be amended by releasing a new edition of the document in its entirety. The Amendment Record Sheet below records the history and issue status of this document.

AMENDMENT RECORD SHEET

ISSUE	DATE REASON FOR CHANGE						
1	01 Apr 2011	First issue					
2	11 Nov 2011	Amended following comments from ESA (Craig Donlon)					
3	15 Mar 2013	Amended by S. Good following comments from project team					



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1. INTRODUCTION

1.1 Purpose and Scope

1.1.1 Purpose

This document provides descriptions and specifications of products that shall be produced by the sea surface temperature (SST) climate change initiative project (SST_cci), which is part of the European Space Agency (ESA) Climate Change Initiative (CCI). The specifications were developed from user requirements defined in the SST_cci User Requirements Document [RD.171]. SST_cci plans to produce two types of SST products as follows:

- Long term essential climate variable (ECV) products, where the priorities are for a long, stable climate record formed from two series of sensors.
- Demonstration ECV products, based on wider use of the modern satellite observing system to increase completeness and/or frequency of coverage.

The specifications contained in this Product Specification Document (PSD) provide a complete description of the products, including the definition of file level metadata. Specifications are defined for level 2, 3 and 4 data files. These are all based on the Group for High Resolution SST (GHRSST) Data Specification version 2.0 (GDS2.0; document revision 2.007) [AD.1], are specified to be compatible with the climate and forecasting (CF) conventions [RD.177] and include the metadata specified by the CCI Data Standards Working Group (DSWG; [RD.215]).

1.1.2 Scope

This document covers the following aspects of requirement SST-TR-12 from the CCI statement of work, annex G [RD.165]:

- File metadata format and structure (Sections 2 and 4).
- Discovery metadata contained in the files and their structure (Sections 2 and 4)
- Long-term document revision control procedures (Section 1.2).
- Any other requirements relevant to SST ECV product specification (for example file format and naming convention; Sections 2.2 and 3.2).

This document does not include in its scope the analysis of the error budget for translating input data to ECV products [RD.164]. This is to be reported in a separate document [RD.174].

Information is included to allow the reader to trace the product specifications defined in this document back to the user requirements, both directly by referring to the user requirements document, [RD.171], and through performance metrics obtained by analysis of the user requirements as detailed in a technical note [RD.189].

This document is to be subjected to review by the international scientific community (SST-TR-13) [RD.165]. The main focus of this review will be discussions with the GHRSST community.



1.2 Document revision control

Document revision control is necessary to manage any changes to the product specifications and to retain a permanent record of when and where updates were made. The following principles will be followed in order to ensure that this occurs:

- Every release of the product specification document should be archived in a central project archive. The files should be protected from accidental change or deletion and backed up to a separate location.
- For every new release the version number should be incremented. The
 document naming convention established for the SST_cci should be used to
 ensure a unique file name for every version of the document.
- A summary of changes to the document and the person responsible for making the changes should be recorded in the relevant place at the beginning of the document.

Each new release must be approved by the project science leader or a person nominated by the project science leader.

1.3 Applicable Documents

The following is a list of documents that must be read in conjunction with this document. Where referenced in the text, these are identified as AD.n, where 'n' is the number in the list below:

AD.1 GHRSST Science Team, cited 2010: The Recommended GHRSST Data Specification (GDS) Revision 2.0 Technical Specifications. [Available online at http://www.ghrsst.org/modules/documents/documents/GDS2.0_TechnicalSpecifications_v2.0.pdf.]

1.4 Referenced Documents

The following is a list of documents with a bearing on the content of this report. Where referenced in the text, these are identified as RD.n, where 'n' is the number in the list below:

- RD.164 ESA Climate Change Initiative phase 1 scientific user consultation and detailed specification statement of work, Issue 1.4, Revision 1, 09/11/2009, Reference EOP-SEP/SOW/0031-09/SP; http://earth.eo.esa.int/workshops/esa_cci/ao6207SoW.pdf
- RD.165 Annex G to RD.164, Sea Surface Temperature ECV (SST_cci)
- RD.166 Taylor, K.E. and C. Doutriaux (2010), CMIP5 Model Output Requirements: File Contents and Format, Data Structure and Metadata; http://cmip-pcmdi.llnl.gov/cmip5/docs/CMIP5_output_metadata_requirements.pdf
- RD.167 Rew, R., G. Davis, S. Emmerson, H. Davies, E. Hartnett and D. Heimbigner (2010), The NetCDF Users Guide; http://www.unidata.ucar.edu/software/netcdf/docs/netcdf.pdf
- RD.168 Climate Modelling User Group (2010), Requirement Baseline Document;



http://dialspace.dial.pipex.com/prod/dialspace/town/estate/gtp89/cmug/D1.2_U
RD_v1.3.pdf
·

- RD.169 ESA Climate Change Initiative CCI project guidelines, Issue 1, Revision 0, 05/11/2010, Reference EOP-DTEX-EOPS-SW-10-0002
- RD.170 NetCDF Attribute Convention on Dataset Discovery (ACDD): http://www.unidata.ucar.edu/software/netcdfjava/formats/DataDiscoveryAttConvention.html
- RD.171 CCI Phase 1 (SST) (2010), User Requirements Document, Reference SST_CCI-URD-UKMO-001; http://www.esa-sst-cci.org/sites/default/files/documents/admin/public/SST_cci%20URD%20UKMO-001%20Issue%202.pdf
- RD.172 CCI Phase 1 (SST), Data Access Requirements Document (in preparation)
- RD.173 CCI Phase 1 (SST), Product Validation Plan (in preparation)
- RD.174 CCI Phase 1 (SST), Error Characterisation (in preparation)
- RD.176 Olsen, L.M., G. Major, K. Shein, J. Scialdone, R. Vogel, S. Leicester, H. Weir, S. Ritz, T. Stevens, M. Meaux, C. Solomon, R. Bilodeau, M. Holland, T. Northcutt and R. A. Restrepo (2007), NASA/Global Change Master Directory (GCMD) Earth Science Keywords Version 6.0.0.0.0; http://gcmd.nasa.gov/Resources/valids/
- RD.177 NetCDF Climate and Forecast (CF) Metadata Convention; http://cf-pcmdi.llnl.gov/
- RD.178 The UDUNITS-2 package; http://www.unidata.ucar.edu/software/udunits/udunits-2/udunits2.html
- RD.189 CCI Phase 1 (SST): Technical note on product metrics derived from the user requirements document
- RD.215 Bennett, V. (2010), Format and Metadata Guidelines for CCI Data Products (draft).
- RD.219 Donlon, C.J. et al. (2009), The GODAE High Resolution Sea Surface Temperature Pilot Project, Oceanography, 22(3), 34-45.

1.5 Definitions of Terms

The following terms have been used in this report with the meanings shown.

Term	Definition
AATSR	Advanced ATSR.
ACDD	Attribute Convention for Dataset Discovery.



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AMSR-E Advanced Microwave Scanning Radiometer – Earth Observing System.

ATSR Along Track Scanning Radiometer; the ATSR series of instruments

comprises ATSR-1, ATSR-2 and AATSR.

AVHRR Advanced Very High Resolution Radiometer.

BEAM Earth observation toolbox and development platform.

CDL Network Common Data form Language.

CF Climate and Forecasting [conventions for metadata].

CMIP Climate Model Intercomparison Project.

DM Demonstration

DSWG CCI Data Standards Working Group

ECMWF European Centre for Medium-range Weather Forecasts.

ECV Essential Climate Variable.

ERA-Interim ECMWF reanalysis 'interim' product.

ERS European Remote Sensing satellite series (ERS-1, ERS-2).

GAC Global Area Coverage.

GCMD Global Change Master Directory.

GDS GHRSST Data Specification.

GMPE GHRSST Multi-Product Ensemble

GHRSST Group for High Resolution SST.

HDF5 Hierarchical Data Format version 5

IDL Interactive Data Language.

ISO International Organisation for Standardisation

L1B Level 1 B data; the data collected by the satellite sensor with

processing (for example calibration) applied.

L2P Level 2 pre-processed data; geophysical variables at the full resolution

of the instrument, in a satellite projection with associated geographical

information.

L3U Level 3 uncollated data; gridded version of L2P data.

L3C Level 3 collated data; L2P data from a single instrument that have been

combined and mapped onto a space-time grid.

L3S Level 3 super-collated data; L2P data from multiple instruments that

have been combined and mapped onto a space-time grid.



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L4 Level 4 data; a dataset formed by analysing lower level data to create a

gridded product with no data gaps. The use of an infilling procedure to

remove data gaps distinguishes L4 data from lower level data.

LT Long-term

MATLAB Matrix Laboratory

MSG Meteosat Second Generation

NetCDF Network Common Data Format.

NWP Numerical Weather Prediction.

OSI SAF Ocean and Sea Ice Satellite Applications Facility.

OSTIA Operational Sea surface Temperature and sea Ice Analysis.

RDAC Regional Data Assembly Centre.

SSES Single Sensor Error Statistics.

SST Sea Surface Temperature.

SST_cci SST climate change initiative [project].

SEVIRI Spinning Enhanced Visible and Infrared Imager.

TBC To be confirmed

TMI TRMM Microwave Imager.

TRMM Tropical Rainfall Measuring Mission.

URL Uniform Resource Locator.

UUID Universally Unique Identifier.

WGS World Geodetic System.

XML Extensible Mark-up Language.



2. PRODUCT OVERVIEW

2.1 Summary of products

Table 1. Summary of SST_cci products, the source and level of data to be produced. L2 and L3 products contain data from a single sensor; L4 products will include data from all sensors used in the product.

Category of product and description	Satellite sensors & data to be used	Level of data to be produced for each sensor (resolution/grid spacing)			
Long term ECV. A long term, stable data	ATSR series (ATSR-1, ATSR-2, AATSR) (Envisat format)	L3U (0.05°)	L4 (0.05°)		
record formed from data from the ATSR and AVHRR series of instruments. Will cover the period Aug 1991 to Dec 2010.	AVHRR series global area coverage (GAC) data	L2P (4 km)			
Demonstration ECV.	AATSR (Envisat format)	L2P (1 km)	L4 (0.05°)		
A product that will demonstrate what can be	AVHRR from Metop-A (internal gridded format)	L3C (0.05°)			
achieved using a broader sample of the SST satellite observing system. To be	SEVIRI (GDS2.0 compliant L3C/internal gridded format)	nt L3C (0.05°)			
produced for two three- month demonstration	AMSR-E (L2P)	L2P (0.25°)			
periods only in CCI Phase One.	TMI (L2P)	L2P (0.25°)			

An overview of the products to be produced by the SST_cci project is shown in Table 1. The table also records which satellite sensors will be used to create the products and the format of the input data. The final column indicates the level of data to be produced from each sensor and the resolution/grid spacing of the data in the files.

The table indicates that the project will produce data at levels L2P, L3U, L3C and L4. These are all defined below. User requirements indicate that all will be useful to users (SST_CCI-UR-QUF-33, [RD.171]). As the project will receive some data at data level L1B, this is also defined below.

- L1B Level 1 B data; the data collected by the satellite sensor with processing (for example calibration) applied.
- L2P Level 2 pre-processed data; geophysical variables at the full resolution of the instrument, in a satellite projection with associated geographical information.
- L3U Level 3 uncollated data; gridded version of L2P data.
- L3C Level 3 collated data; L2P data from a single instrument that have been combined and mapped onto a space-time grid.



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Level 4 data; a dataset formed by analysing lower level data to create a gridded product with no data gaps. The use of an infilling procedure to remove data gaps distinguishes L4 data from lower level data.

Each entry in Table 1 is expanded in Table 2. This table provides full details of each product. This includes aspects such as the file names, the file sizes, the target for stability etc.

The headings to the columns in Table 2 define unique names for each product. These shall be appended in brackets with the name of an individual sensor if it is necessary to distinguish between sensors in a series. For example the individual components of the LT ATSR product shall be referred to as LT ATSR (ATSR-1), LT ATSR (ATSR-2) and LT ATSR (AATSR).

Note that – dependent on user requirements – a toolbox will be created that will also allow different varieties of data to be created from the level 2 and level 3 data (for example level 3 files with different grid spacing at multiples of 0.05° or containing a blend of data from different sensors).



Table 2. Detailed description of the SST_cci products. The column headings define unique names for each product. Where it is necessary to distinguish between data from individual sensors in products that contain a series of sensors the name of the sensor shall be appended to the product name in brackets. For example the ATSR-1 part of the LT ATSR product shall be referred to as LT ATSR (ATSR-1). File size estimates are based on the following grid sizes: AATSR L2P – 512 x 28,000, AVHRR – 625 x 7000, AMSR-E L2P – 243 x 4180, TMI – 104 x 3000, L3 and L4 data - 7,200 x 3,600 and one time step per file. User requirements for each aspect of the products are included and are referenced as codes beginning with SST_CCI-UR-; full details of these requirements are in [RD.171].

Product	LT ATSR	LT AVHRR	LT Analysis	DM AATSR	DM AVHRR	DM SEVIRI	DM AMSR-E	DM ТМІ	DM Analysis	
Product group	Long term			Demonstration	Demonstration					
Satellite sensors used	ATSR series (ATSR-1, ATSR-2, AATSR)	AVHRR series GAC data	ATSR series and AVHRR series	AATSR	AVHRR	SEVIRI	AMSR-E	ТМІ	AATSR, AVHRR, SEVIRI, AMSR-E, TMI	
Satellite sensor type	Infrared	Infrared	Infrared	Infrared	Infrared	Infrared	Passive microwave	Passive microwave	Infrared and passive microwave	
Satellite platform	ERS-1, ERS- 2, Envisat	NOAA platforms, Metop-A	ERS-1, ERS- 2, Envisat, NOAA platforms, Metop-A	Envisat	Metop-A	MSG	Aqua	TRMM	Envisat, Metop-A, MSG, Aqua, TRMM	
Satellite orbit	Polar	Polar	Polar	Polar	Polar	Geostationar y	Polar	Low inclination low Earth orbit	Low Earth orbit (polar and low inclination), geostationary	



Product	LT ATSR	LT AVHRR	LT Analysis	DM AATSR	DM AVHRR	DM SEVIRI	DM AMSR-E	ом тмі	DM Analysis
Input data source	ESA	NOAA	SST_cci (LT ATSR and LT AVHRR products)	ESA	ESA	Meteo- France	RSS	RSS	SST_cci (DM AATSR, DM AVHRR, DM SEVIRI, DM AMSR-E, and DM TMI products)
Input data format	Envisat format	AVHRR GAC	NetCDF compliant with this document	Envisat format	Internal gridded format	Internal gridded format	NetCDF compliant with GDS2.0	NetCDF compliant with GDS2.0	NetCDF compliant with this document
Input data level	L1B	L1B	L3U (LT ATSR) and L2P (LT AVHRR)	L1B	L1B	L3C	L2P	L2P	L2P (DM AATSR, DM AMSR-E, DM TMI), L3C (DM AVHRR), L3C (DM SEVIRI)
Input data frequency	One file per orbit per sensor (typically 14 orbits per day, one sensor operating)	One file per orbit per sensor (typically 14 orbits per day, more than one sensor operating)	Typically 28 orbits per day, one file per orbit	One file per orbit (typically 14 per day)	12 hourly	One file per day	One file per orbit (typically 14 per day)	One file per orbit (typically 16 per day)	Typically 47 files per day



Product	LT ATSR	LT AVHRR	LT Analysis	DM AATSR	DM AVHRR	DM SEVIRI	DM AMSR-E	ом тмі	DM Analysis		
Input data grid	0.05° grid	4 km spaced irregular grid	0.05° grid (LT ATSR) and 4 km irregular grid (LT AVHRR)	1 km spaced irregular grid	0.05° grid	0.05° grid	0.25° grid	0.25° grid	Range from 1 km spaced irregular grid to 0.25° grid		
Input data spatial coverage	Global	Global	Global	Global	Global	Fixed view of the Earth centred at 0° longitude and latitude	Global	Tropics	Various		
Processing to be applied by the project	SST retrieval; cloud and ice screening; depth and time adjustment to SSTs; uncertainty estimates	SST retrieval; cloud and ice screening; depth and time adjustment to SSTs; uncertainty estimates	Analysis	SST retrieval; cloud and ice screening	SST retrieval; cloud and ice screening	Reformatting to L3C format compliant with this document	Uncertainty estimates to be added to the files	Uncertainty estimates to be added to the files	Analysis		
Output data level	L3U	L2P	L4	L2P	L3C	L3C	L2P	L2P	L4		
Output data level user requirement	SST_CCI-UR-	SST_CCI-UR-QUF-33: indicates that all the levels of data to be produced by the project (levels 2, 3 and 4) will be useful to users.									



Product	LT ATSR	LT AVHRR	LT Analysis	DM AATSR	DM AVHRR	DM SEVIRI	DM AMSR-E	DM ТМІ	DM Analysis		
Output data frequency	One file per orbit per sensor (typically 14 orbits per day, one sensor operating)	One file per orbit per sensor (typically 14 orbits per day, more than one sensor operating)	One file per day	One file per orbit per sensor (typically 14 orbits per day)	One file per day	One file per day	One file per orbit (typically 14 per day)	One file per orbit (typically 16 per day)	One file per day		
Output data frequency user requirement		SST_CCI-UR-QUF-38: the most common requirements for data frequency at a location are monthly (threshold), daily (breakthrough) and 3 hourly (objective). See also [RD.189] Tables 4 and 19.									
Output grid	0.05° grid	4 km spaced irregular grid	0.05° grid	1 km spaced irregular grid	0.05° grid	0.05° grid	0.25° grid	0.25° grid	0.05° grid		
Output grid user requirement		o users' applicat					his grid spacing portion of applica				
File size estimate (assuming no compression)	593 MB	125 MB	173 MB	410 MB	593 MB	593 MB	29 MB	9 MB	173 MB		
File size user requirement	SST_CCI-UR-0 [RD.189] Table		ment for maxim	um file size varie	es considerably l	between users, I	petween <100 K	B and >10 GB. \$	See also		



Product	LT ATSR	LT AVHRR	LT Analysis	DM AATSR	DM AVHRR	DM SEVIRI	DM AMSR-E	DM ТМІ	DM Analysis			
Output file format	CF compliant N	NetCDF										
Output file format user requirement	SST_CCI-UR-0	QUF-89: CF con	npliant NetCDF	is required.								
Spatial coverage	Global	pal										
Spatial coverage user requirement	SST_CCI-UR-0	ST_CCI-UR-QUF-42: global coverage is required.										
Product start date	August 1991			2007 and Jan	2012 (start date:	s of two separat	e three month pe	eriods)				
Product end date	December 201	0		2007 and Mar	2012 (end dates	of two separate	e three month pe	eriods)				
Product length	19 years	19 years 6 months (comprising two separate three month periods)										
Product length user requirement							is not possible, a of the ATSR seri					



Product	LT ATSR	LT AVHRR	LT Analysis	DM AATSR	DM AVHRR	DM SEVIRI	DM AMSR-E	DM ТМІ	DM Analysis			
SST depth	Skin and 20 cm	Skin and 20 cm	20 cm	Skin	Skin	Skin	Subskin	Subskin	20 cm (2007 period) / Foundation (2012 period)			
SST depth user requirement		SST_CCI-UR-QUF-46: skin SST is the most common requirement, followed by SSTs at depths roughly corresponding to the range of traditional in situ observations (20 cm and 5 m). See also [RD.189] Tables 17 and 32.										
SST time of day	Platform dependent time and adjusted to 10.30 am and pm local time	Platform dependent time and adjusted to 10.30 am and pm local time	Representati ve of daily average	10 am and pm	Daily average	Daily average	1.30 am and pm	Various	SST from which the diurnal cycle grows			
SST time of day user requirement	does not matcl		bserving system	. SST_CCI-UR-	QUF-40: Tempo		so [RD.189] Table acceptable to the					
Target accuracy	0.1°C when ev	aluated over le	ngth scales of \leq	1000 km		Not applicable control of the p	 the accuracy oroject. 	of the input data	are out of the			
Acceptable level of bias user requirement	the us	SST_CCI-UR-QUF-48: the highest acceptable bias level is 0.1°C, and, SST_CCI-UR-QUF-49: 0.1°C is the required precision. While the user requirement is that the achievement of both should be demonstrated over spatial scales of 100 km, the achievable scales are controlled by the density of comparison data, and will usually be longer than this. See also [RD.189] Tables 9, 10, 11, 12, 24, 25, 26, 27.										
Target stability	0.1°C/decade						duct. The stabilit		ta from			



Product	LT ATSR	LT AVHRR	LT Analysis	DM AATSR	DM AVHRR	DM SEVIRI	DM AMSR-E	ом тмі	DM Analysis				
Stability user requirement	SST_CCI-UR-	SST_CCI-UR-QUF-50: 0.1°C per decade, to be demonstrated on spatial scales of 100 km. See also [RD.189] Tables 13, 14, 28, 29.											
Ancillary data to be included	Surface wind s ERA-Interim re		Sea ice concentration and uncertainties; taken from OSI SAF data	Surface wind speed from the ERA-Interim reanalysis			No ancillary data to be added by the SST_cci project		Sea ice concentration and uncertainties; taken from OSI SAF data				
Ancillary data user requirement	SST_CCI-UR-	QUF-70	SST_CCI- UR-QUF-69				Not applicable		SST_CCI- UR-QUF-69				
File names –	<indicative date=""><indicative time="">-ESACCI-</indicative></indicative>												
read from top	L3U	L2P	L4	L2P	L3C	L3C	L2P	L2P	L4				
obtain the file name for	_GHRSST-	_GHRSST-											
Definitions of the fields contained in chevrons (<>) are in	SSTskin- [ATSR1, ATSR2 or AATSR]-LT	SSTskin- AVHRR <x>_ G-LT</x>	SSTdepth- OSTIA- GLOB_LT	SSTskin- AATSR-DM	SSTskin- AVHRRMTA- DM	SSTskin- SEVIRI_SST -DM	SSTsubskin- AMSRE-DM	SSTsubskin- TMI-DM	SSTdepth- OSTIA- GLOB_DM / SSTfnd- OSTIA- GLOB_DM				
Section 3.2.	-v2.0-fv <fileve< td=""><td>ersion>.nc</td><td>,</td><td>,</td><td>,</td><td>,</td><td>,</td><td>,</td><td>,</td></fileve<>	ersion>.nc	,	,	,	,	,	,	,				



2.2 Improvements over existing data

The new products to be produced by the SST_cci project will address a number of the weaknesses of existing SST data that are perceived by users and take advantage of their strengths. These strengths and weaknesses are described in full in [RD.171]; some points of relevance to the SST_cci products are summarised below:

- Long term records of SST are available from the ATSR and AVHRR series of sensors. ATSR series data are viewed as weak in spatial sampling and the frequency of observations. However, its bias characteristics and stability are seen as strengths. Frequency of observations is seen as a strength of AVHRR series data but its bias characteristics received mixed responses from users.
 - By using new algorithms and cross referencing the AVHRR data to the ATSR data the SST_cci project will produce SST products that have the bias characteristics and stability approaching that of ATSR alone with the coverage of AVHRR (the long term ECV products).
- Characterisation of uncertainties is generally viewed as being weak.
 - The project will improve this situation by providing uncertainty estimates split into components with different spatial and temporal correlation characteristics.
- The modern satellite observing system includes infrared sensors (on polar orbiting and geostationary platforms) and microwave sensors and these all have individual strengths and weaknesses. For example the microwave sensor AMSR-E is seen as having good spatial sampling and frequency of observations but its bias characteristics and characterisation of uncertainties are perceived as weaknesses.
 - A system will be created that uses AATSR, AVHRR and data from other instruments to demonstrate the improved data coverage that can be achieved with the additional sensors (the demonstration ECV products). The accuracy of AATSR will still underpin the dataset and new uncertainty estimates for AMSR-E will be developed.



3. FILE FORMAT AND METADATA

3.1 Rationale

The format of the data files shall be Network Common Data Format (NetCDF) and shall follow Climate and Forecasting (CF) conventions. This is the format preferred by the majority of potential users of the products (user requirement SST_CCI-UR-QUF-89, [RD.171]). The use of NetCDF also allows the use of a variety of different tools/languages to manipulate and view the data, for example BEAM and the tools available within languages such as the Interactive Data Language (IDL), the Matrix Laboratory (MATLAB) and Python.

CF compliant NetCDF files are already very well established in the SST user community owing to the success of the GHRSST project ([RD.219]; https://www.ghrsst.org/). GHRSST provides SST data products in a CF compliant NetCDF data format, the latest version being the GDS2.0 [AD.1]. The GDS2.0 already includes much of the data and metadata that users require and that SST_cci wish to include in the files, but also has the flexibility of allowing additional data fields to be added as required. The user requirements gathered by the SST_cci project shows some limited support for the GDS2.0 for the NetCDF files (SST_CCI-UR-QUF-89, [RD.171]). It is not clear from the results whether this limited support is due to lack of awareness of the specification or a desire for an alternative. Adopting the GDS2.0 specification would provide benefits to users as some will already have experience with the files and may have existing software and tools to work with the data. It will also ensure easy incorporation of the SST_cci products into the GHRSST framework. ESA have mandated use of GDS2.0 for this project.

It would also be desirable for the SST_cci data to be available in a form that is familiar to climate modellers to allow ease of comparison of observational data with climate model data [RD.168]. There exists a format specification for the Climate Model Intercomparison Project 5 (CMIP5) that details a standard structure for NetCDF files containing model data [RD.166]. This was developed for storing model data rather than observations and also has some differences to the way that the storage of data in NetCDF format is implemented by GHRSST. These differences mean that it is not possible to produce data files that are consistent with both the GHRSST and CMIP5 specifications. The SST_cci project shall produce files that are consistent with the GDS2.0 specification.

The format of NetCDF used for GDS2.0 data files is preferentially 'NetCDF-4 classic' and therefore this shall be used for SST_cci files. The term 'NetCDF-4 classic' combines two aspects of the files: the underlying file format and the data model. These are explained briefly below:

Three different underlying formats could be used:

- 'classic': this is compatible with all versions of the NetCDF library;
- '64-bit offset': this allows larger datasets to be written but is not compatible with versions of the NetCDF library prior to 3.6.0;
- NetCDF-4; this uses Hierarchical Data Format version 5 (HDF5) as its base format and gives access to desirable features such as internal per variable compression; it is compatible with the NetCDF library from version 4.

Although the NetCDF-4/HDF5 format is not compatible with older versions of the library, the additional features such as its compression abilities gives clear advantages over the other options.



There are two NetCDF data models: 'classic' and 'enhanced' [RD.167]. The classic data model has a number of limitations compared to enhanced, for example the enhanced data model includes a greater number of allowed storage types. Either can be written using the NetCDF-4/HDF5 underlying format. The advantage of using the classic model is that it maintains compatibility with legacy software.

In summary:

- The SST_cci files shall be NetCDF-4/HDF5 format and shall use the NetCDF classic data model.
- The file specifications shall follow CF conventions.
- The files will be based on and be consistent with the GHRSST GDS2.0 [AD.1].

3.2 Filename convention

SST_cci shall follow the file naming convention specified in [AD.1], i.e.:

<Indicative Date><Indicative Time>-<RDAC>-<Processing Level>_GHRSST-<SST
Type>-<Product String>-<Additional Segregator>-v<GDS Version>-fv<FileVersion>.<File
Type>

The components to this list are summarised in [AD.1] Table 7-1 with further explanatory information in the text of that document. That table is reproduced here in Table 3 with an additional column (headed SST_cci definition) that details the implementation of the filenaming convention that shall be used by the SST_cci project. All the information required to define the SST_cci files is contained within this document. However, note that references in the Description column of the table are to sections in the [AD.1] document and these shall be referred to if further explanation is desired. In places, clarifications to the [AD.1] version of the text have been made and these are indicated in italics.



Table 3. Components of the filenames; based on [AD.1] section 7.1 – refer there for more details. The final column details the implementation for the SST_cci project. In the Description column the references refer to sections of [AD.1]. All references in the SST_cci column are to parts of this document.

Name	Definition	Description	SST_cci definition
<indicative Date></indicative 	YYYYMMDD	The identifying date for this data set. See Section 7.2 in [AD.1]. The section states that: YYYY is the four-digit year, MM is the two-digit month from 01 to 12, and DD is the two-digit day of month from 01 to 31 and The date used should best represent the observation date for the dataset.	As stated in Description column.
<indicative Time></indicative 	HHMMSS	The identifying time for this data set. The time used is dependent on the <processing level=""> of the data set:</processing>	As stated in Description column.
		L2P: start time of granule	
		L3U: start time of granule	
		L3C and L3S: centre time of the collation window	
		L4 and GMPE: nominal time of analysis	
		All times should be given in UTC. See Section 7.3 in [AD.1]. The section states that: HH is the two-digit hour from 00 to 23, MM is the two-digit minute from 00 to 59, and SS is the two-digit second from 00 to 59 and All times should be given in UTC and should be chosen to best represent the observation time for this dataset. Note: RDACs should ensure the applications they use to determine UTC properly account for leap seconds.	
<rdac></rdac>	The RDAC where the file was created.	The Regional Data Assembly Centre (RDAC) code.	For the SST_cci products, this is:
<processing< td=""><td>The data</td><td>The data processing level code, defined in</td><td>See Table 1 in</td></processing<>	The data	The data processing level code, defined in	See Table 1 in
Level>	processing level code (L2P, L3U, L3C, L3S, or L4)	Section 7.5 in [AD.1].	this document.
<sst type=""></sst>	The type of SST data included in the file.	Conforms to the GHRSST definitions for SST, defined in Section 7.6 in [AD.1].	This should be set to be the primary SST stored in the file. See Table 4.



Name	Definition	Description	SST_cci definition
<product String></product 	A character string identifying the SST product set. The string is used uniquely within an RDAC but may be shared across RDACs.	The unique "name" within an RDAC of the product line. See Section 7.7 <i>in [AD.1]</i> for the product string lists, one each for L2P, L3, L4, and GMPE products. See Section 7.7 <i>in [AD.1]</i> .	See Table 5 in this document.
<additional Segregator></additional 	Optional text to distinguish between files with the same <product string="">. Dashes are not allowed within this element.</product>	This text is used since the other filename components are sometimes insufficient to uniquely identify a file. For example, in L2P or L3U (un-collated) products this is often the original file name or processing algorithm. Note, underscores should be used, not dashes. For L4 files, this element should begin with the appropriate regional code as defined in Section 7.8. This component is optional but must be used in those cases where non-unique filenames would otherwise result.	For L2 and L3 products this should be set to LT (for long-term reprocessed) or DM (meaning "delayed mode", for demonstration outputs) to distinguish between products. For L4 products either GLOB_LT or GLOB_DM (GLOB is required to indicate spatial coverage)
<gds Version></gds 	nn.n	Version number of the GDS used to process the file. For example, GDS 2.0 = "02.0".	To be set to "02.0".
<file Version></file 	xx.x	Version number for the file, for example, "01.0".	As stated in Description column.
<file type=""></file>	NetCDF data file suffix (nc) or ISO metadata file suffix (xml).	Indicates this is a NetCDF file containing data or its corresponding ISO-19115 metadata record in XML.	Will be nc for SST_cci files.



Table 4. Values and definitions of <SST type>. Based on [AD.1] section 7.6 – refer there for more details.

SST type	Description
SSTskin	SST sensed by infrared instruments (at depth of approximately 10 µm).
SSTsubskin	SST sensed by microwave instruments (at depth of approximately 1 mm).
SSTdepth	Temperature at a specific depth. The depth shall be included in the file metadata.
SSTfnd	Temperature from which the diurnal thermocline develops each day.

Table 5: Product strings for data to be processed; based on [AD.1] Tables 7-5 to 7-7 refer there for more details.

Sensor/analysis	Platform (if applicable)	Product String	Comment
ATSR	ERS-1	ATSR1	
ATSR	ERS-2	ATSR2	
AATSR	Envisat	AATSR	
AMSRE	Aqua	AMSRE	
AVHRR_GAC	NOAA- <x> or MetOpA</x>	AVHRR <x>_G</x>	<x> is either.</x>
			if the satellite hosting the AVHRR is a NOAA platform, <x> is the satellite number,</x>
			or,
			if the AVHRR is on Metop-A, <x> is 'MTA'.</x>
			To be used for L2P outputs (long-term).
AVHRR	MetOpA	AVHRRMTA	To be used for L3C outputs (demonstration).
SEVIRI	MSG1 or 2	SEVIRI_SST	
ТМІ	TRMM	ТМІ	
OSTIA		OSTIA	L4 analysis using the OSTIA system

3.3 Global attributes

Attributes are metadata that are stored in a NetCDF file. Global attributes contain information that applies to the whole contents of the NetCDF file.

All GHRSST format data files share the same set of global attributes. These are listed in [AD.1] Table 8-1. The CCI DSWG also specify a set of global attributes that should be included in the SST_cci data files([RD.215]), some of which are not in the GHRSST specification. In addition an attribute called "creator_processing_institution" has been included to indicate the institution that created products as part of the SST_cci project



Table 6 contains a list of the global attributes. Much of this is reproduced from Table 8-1 in [AD.1]. However, annotations to the table have been made in places in order to clarify the text; these are indicated by italics. The additional attributes specified by the CCI DSWG are also included. These are the entries that include 'CCI DSWG' in the Source column of the table. The "creator_processing_institute" attribute has SST_cci within the Source column. Other points to note are:

- The definition of the shading of the rows in the table is given in Table 7.
- All references in the Description column refer to the contents of [AD.1]. Although
 all the information required to create the SST_cci files is contained here, these
 can be used to obtain more information about GDS2.0 files.
- The final column, headed 'SST_cci definition' contains information about the implementation of the attributes for the SST_cci files. All references in this column are to parts of this document.

As revealed by the column headed 'Source', the definition of the attributes was based on CF conventions, the Unidata Attribute Convention for Dataset Discovery (ACDD) [RD.170], the requirements of the GHRSST project [AD.1] and the specifications provided by the CCI DSWG.

Table 6. Global attributes that are included in all GHRSST format data files and additional attributes specified by the CCI DSWG. Much of the contents of this table is reproduced from [AD.1] and further information can be found there. Annotations and changes to the original text are made in places and these are written in italics. The meaning of the colours is given in Table 7. Note that attributes described as having the format 'string' shall actually be stored in the NetCDF file as an array of characters. References in the Description column are to parts of [AD.1]; references in the SST_cci definition column are to parts of this document.

Global Attribute Name	Format	Description	Source	SST_cci definition
Conventions	string	A text string identifying the netCDF conventions followed. This attribute should be set to the version of CF used and should also include the ACDD. For example: "CF-1.4, Unidata Observation Dataset v1.0".	CF	CF-1.5, Unidata Observation Dataset v1.0
title	string	A descriptive title for the GHRSST data set	CF, ACDD	See examples in Section 4 and Appendix A.
summary	string	A paragraph describing the dataset.	ACDD	See examples in Section 4 and Appendix A.
references	string	Published or web-based references that describe the data or methods used to produce it.	CF	Include any relevant publications or webpages.



Global Attribute Name	Format	Description	Source	SST_cci definition
institution	string	GHRSST RDAC code where the data were produced. See Table 7-2 in [AD.1] for available codes (this version of the GDS does not, however, include the SST_cci RDAC code).	CF, ACDD	The RDAC code for the SST_cci products is ESACCI
history	string	History of all applications that have modified the original data to create this file.	CF, ACDD	Appendix A contains a basic example of this.
comment	string	Miscellaneous information about the data or methods used to produce it.	CF, ACDD	Used to indicate the centre where the data were produced. Set to: These data were produced at <institution> as part of the ESA SST CCI project.</institution>
license	string	Describe any restrictions to data access, use, and distribution. GHRSST data sets should be freely and openly available to comply with the R/GTS framework, with no restrictions. However, if a user should submit a simple registration via a web form, for example, the URL could be given here. Default to "GHRSST protocol describes data use as free and open."	ACDD	TBC
id	string	The unique GHRSST character string for this product. All GHRSST SST products have one, and they are listed in Table 7-10 in [AD.1].	ACDD	See Section 3.5 for the list of strings to be used by the SST_cci project.
naming_ authority	string	Fixed as "org.ghrsst" following ACDD convention.	ACDD	org.ghrsst
product_version	string	The product version of this data file, which may be different than the file version used in the file naming convention (Section 7 in [AD.1]).	GDS	See Section 3.2 of this document



Global Attribute Name	Format	Description	Source	SST_cci definition
uuid	string	A Universally Unique Identifier (UUID). Numerous, simple tools can be used to create a UUID, which is inserted as the value of this attribute. See http://en.wikipedia.org/wiki/Universally_Unique_Identifier for more information and tools.	GDS	[RD.169] suggests the use of http://www.ossp. org/pkg/lib/uuid/, and this will be followed.
tracking_id	string	Identical to uuid (i.e. this shall contain the same value as uuid).	CCI DSWG	As stated in Description column. This is an alternative name for the UUID as used in the CMIP5 specification [RD.166].
gds_version_id	string	GDS version used to create this data file. For example, "2.0".	GDS	The GDS version used for the SST_cci product specification was 2.0.
netcdf_ version_id	string	Version of netCDF libraries used to create this file. For example, "4.1.1"	GDS	As stated in Description column.
date_created	string	The date and time the data file was created in the form "yyyymmddThhmmssZ". This time format is ISO 8601 compliant.	ACDD	As stated in Description column.
file_quality_ level	integer	A code value: 0 = unknown quality 1 = extremely suspect (frequent problems, e.g. with known satellite problems) 2 = suspect (occasional problems, e.g. after launch) 3 = excellent (no known problems)	GDS	As stated in Description column.



Global Attribute Name	Format	Description	Source	SST_cci definition
spatial_ resolution	string	A string describing the approximate resolution of the product. For example, "1.1km at nadir"	GDS	Value depends on the product. See Table 1 or Table 2.
start_time	string	Date and time of the first measurement in the data file in the form "yyyymmddThhmmssZ". This time format is ISO 8601 compliant.	GDS	As stated in Description column.
time_coverage_ start	string	Identical to start_time. Included for increased ACDD compliance.	ACDD	As stated in Description column.
stop_time	string	Date and time of the last measurement in the data file in the form "yyyymmddThhmmssZ". This time format is ISO 8601 compliant.	GDS	As stated in Description column.
time_coverage_ end	string	Identical to stop_time. Included for increased ACDD compliance.	ACDD	As stated in Description column.
time_coverage_ duration	string	Duration of time coverage in ISO 8601 compliant format; the difference between time_coverage_end and time_coverage_start.	CCI DSWG, ACDD	In the form PdDThHmMsS where d is the number of days, h is the number of hours, m is the number of minutes, s is the number of seconds, omitting dD etc. if the number is zero.
time_coverage_ resolution	string	Time resolution of the data in the file in ISO 8601 compliant format.	CCI DSWG, ACDD	Orbit repeat period (for single orbit files) or frequency of data files.
northernmost_ latitude	float	Decimal degrees north, range - 90 to +90. This is equivalent to ACDD geospatial_lat_max.	GDS	As stated in Description column; see also examples in Appendix A.



Global Attribute Name	Format	Description	Source	SST_cci definition
geospatial_lat_ max	float	Identical to northernmost_latitude.	CCI DSWG, ACDD	As stated in Description column.
southernmost_ latitude	float	Decimal degrees north, range - 90 to +90. This is equivalent to ACDD geospatial_lat_min.	GDS	As stated in Description column; see also examples in Appendix A.
geospatial_lat_ min	float	Identical to southernmost_latitude.	CCI DSWG, ACDD	As stated in Description column.
easternmost_ longitude	float	Decimal degrees east, range - 180 to +180. This is equivalent to ACDD geospatial_lon_max.	GDS	As stated in Description column; see also examples in Appendix A.
geospatial_lon_ max	float	Identical to easternmost_longitude.	CCI DSWG, ACDD	As stated in Description column.
westernmost_ longitude	float	Decimal degrees east, range - 180 to +180. This is equivalent to ACDD geospatial_lon_min.	GDS	As stated in Description column; see also examples in Appendix A.
geospatial_lon_ min	float	Identical to westernmost_longitude.	CCI DSWG, ACDD	As stated in Description column.
geospatial_ vertical_min	float	Minimum of the vertical extent of the data; positive values indicate distances above the surface.	CCI DSWG, ACDD	To be set to the representative depth of the deepest SST in the file.
geospatial_ vertical_max	float	Maximum of the vertical extent of the data; positive values indicate distances above the surface.	CCI DSWG, ACDD	To be set to the representative depth of the shallowest SST in the file.



Global Attribute Name	Format	Description	Source	SST_cci definition
source	string	Comma separated list of all source data present in this file. List SST sources first, followed by Auxiliary sources. If the source is a GHRSST product, use the GHRSST unique string listed in Table 7-10. For other sources, following the best practice described in Section 7.9 in [AD.1].	CF	See Section 3.5 in this document for the source codes relevant to the SST_cci products.
platform	string	Satellite(s) used to create this data file. Select from the entries found in the Satellite Platform column of Table 7-5 in [AD.1] and provide as a comma separated list if there is more than one.	GDS	See Table 5 in this document for the platforms relevant to the SST_cci products.
sensor	string	Sensor(s) used to create this data file. Select from the entries found in the Satellite Sensor column of Table 7-5 in [AD.1] and provide as a comma separated list if there is more than one.	GDS	See Table 5 in this document for the platforms relevant to the SST_cci products.
metadata_ conventions	string	Unidata Dataset Discovery v1.0	ACDD	As stated in Description column.
metadata_link	string	Link to collection metadata record at archive	ACDD	http://www.esa- cci.org
keywords	string	Typically GCMD Science Keyword: "Oceans > Ocean Temperature > Sea Surface Temperature"	ACDD	As stated in Description column.
keywords_ vocabulary	string	"NASA Global Change Master Directory (GCMD) Science Keywords" as defined in [RD.176].	ACDD	As stated in Description column.
standard_ name_ vocabulary	string	"NetCDF Climate and Forecast (CF) Metadata Convention"	ACDD	As stated in Description column.
geospatial_ lat_units	string	Units of the latitudinal resolution. Typically "degrees_north"	ACDD	degrees_north



Global Attribute Name	Format	Description	Source	SST_cci definition
geospatial_lat_ resolution	float	Latitude Resolution in units matching geospatial_lat_units.	ACDD	See examples in Appendix A.
geospatial_lon_ units	string	Units of the longitudinal resolution. Typically "degrees_east"	ACDD	degrees_east
geospatial_lon_ resolution	float	Longitude Resolution in units matching geospatial_lon_resolution.	ACDD	See examples in Appendix A.
acknowledgmen t	string	Information about funding source and how to cite the use of these data.	ACDD	Funded by ESA.
creator_name	string	Provide a name and email address for the most relevant	ACDD	SST_cci
creator_ email	string	point of contact at the producing RDAC, as well as a URL relevant to this data set.	ACDD	science.leader @esa-sst- cci.org
creator_url	string		ACDD	http://www.esa- sst-cci.org
creator_ processing_ institution	string	Contains additional information about the institution that created the product within the CCI project.	SST_cci	These data were produced at <institution> as part of the ESA SST CCI project.</institution>
project	string	"Group for High Resolution Sea Surface Temperature"	ACDD	ESA climate Change Initiative SST Project
publisher_ name	string	The name of the data publisher; for GHRSST data this is The GHRSST Project Office	ACDD	ESACCI
publisher_ url	string	The web address of the data published; for GRHSST data this is http://www.ghrsst.org	ACDD	http://www.esa- sst-cci.org
publisher_ email	string	The email address of the data publisher; for GHRSST data this is ghrsst-po@nceo.ac.uk	ACDD	science.leader @esa-SST- cci.org



Global Attribute Name	Format	Description	Source	SST_cci definition
processing_ level	string	GHRSST definitions are the options: L2P, L3U, L3C, L3S, L4 and GMPE	ACDD	Value depends on the product. See Table 1 or Table 2.
cdm_data_ type	string	"swath" or "grid"	ACDD, GDS	"swath" if L2P file, otherwise "grid"

Table 7. Key to colours used in Table 6 and Table 8. Based on Table 4-2 in [AD.1].

Colour	Meaning	
Blue	Mandatory item.	
Violet	An item that is mandatory for only certain situations.	

3.4 Variable attributes

In the context of a NetCDF file a variable refers to an array of data stored within the file. Each variable can have attributes associated with it. [AD.1] defines attributes that should be provided with variables. As for the global attributes, the table of variable attributes from [AD.1] (Table 8-2) is reproduced here (Table 8). Annotations to the original text are indicated by italics. References within the table in the Description column refer to the contents of [AD.1] or to other external references. The SST_cci implementation of the variables is given in the column headed 'SST_cci definition'. All references in this column are to parts of this document. There are some differences to the attributes to be used that depends on the nature of the data being stored; these are identified using violet shading (see Table 7).

Table 8. List of variable attributes. The contents of the first four columns of this table are reproduced from [AD.1] and further information can be found there. References in those columns refer to parts of [AD.1]. Annotations and changes to the [AD.1] text are identified by italics. The final column contains the SST_cci implementation of the attributes. All references in that column refer to parts of this document. The meaning of the colours is given in Table 7. Note that attributes described as having the format 'string' shall actually be stored in the NetCDF file as an array of characters.

Variable attribute name	Format	Description	Source	SST_cci definition
_FillValue	Must be same as the variable type	A value used to indicate array elements containing no valid data. This value must be of the same type as the storage (packed) type; should be set as the minimum value for this type. Note that some netCDF readers are unable to cope with signed bytes and may, in these cases, report fill as 128. Some cases will be reported as unsigned bytes 0 to 255.	CF	As stated in Description column.
units	string	Text description of the units, preferably S.I., and must be compatible with the Unidata UDUNITS-2 package [RD.178]. For a given variable (e.g. wind speed), these must be the same for each dataset.	CF, ACDD	See specifications in Section 4.
scale_ factor	Must be expressed in the unpacked data type	To be multiplied by the variable to recover the original value. Defined by the producing RDAC. Valid values within valid_min and valid_max should be transformed by scale_factor and add_offset, otherwise skipped to avoid floating point errors.	CF	See specifications in Section 4. The type of this attribute defines the type of the unpacked data.
add_offset	Must be expressed in the unpacked data type	To be added to the variable after multiplying by the scale factor to recover the original value. If only one of scale_factor or add_offset is needed, then both should be included anyway to avoid ambiguity, with scale_factor defaulting to 1.0 and add_offset defaulting to 0.0. Defined by the producing RDAC.	CF	See specifications in Section 4. The type of this attribute defines the type of the unpacked data.
long_name	string	A free-text descriptive variable name.	CF, ACDD	See specifications in Section 4.



Variable attribute name	Format	Description	Source	SST_cci definition
valid_min	Expressed in same data type as variable	Minimum valid value for this variable once they are packed (in storage type). The fill value should be outside this valid range. Note that some netCDF readers are unable to cope with signed bytes and may, in these cases, report valid min as 129. Some cases as unsigned bytes 0 to 255. Values outside of valid_min and valid_max will be treated as missing values.	CF	See specifications in Section 4.
valid_max	Expressed in same data type as variable	Maximum valid value for this variable once they are packed (in storage type). The fill value should be outside this valid range. Note that some netCDF readers are unable to cope with signed bytes and may, in these cases, report valid min as 127.	CF	See specifications in Section 4.
standard_ name	string	Where defined, a standard and unique description of a physical quantity. For the complete list of standard name strings, see [RD.177]. Do not include this attribute if no standard_name exists.	CF, ACDD	See specifications in Section 4.
comment	string	Miscellaneous information about the data or the methods used to produce it.	CF	As stated in Description column. See examples in Appendix A.
source	string	For L2P and L3 files: For a data variable with a single source, use the GHRSST unique string listed in Table 7-10 in [AD.1] if the source is a GHRSST SST product. For other sources, following the best practice described in Section 7.9 in [AD.1] to create the character string. If the data variable contains multiple sources, set this string to be the relevant "sources of" variable name. For example, if multiple wind speed sources are used, set source = sources_of_wind_speed. For L4 and GMPE files: follow the source convention used for the global attribute of the same name, but	CF	String containing the source of data, or comma separated list if there are multiple sources. Section 3.5 details the sources of data to be used by the SST_cci products and the names for these that shall be used to fill this attribute.



Variable attribute name	Format	Description	Source	SST_cci definition
		provide in the comma-separated list only the sources relevant to this variable.		
references	string	Published or web-based references that describe the data or methods used to produce it. Note that while at least one reference is required in the global attributes (See Table 8-1 in [RD.87], references to this specific data variable may also be given.	CF	As stated in Description column. Note that the equivalent in this document to the table that is referred to is Table 6.
axis	string	For use with coordinate variables only. The attribute 'axis' may be attached to a coordinate variable and given one of the values "X", "Y", "Z", or "T", which stand for a longitude, latitude, vertical, or time axis respectively. See: http://cf-conventions/1.4/cf-conventions.html .	CF	See specifications in Section 4.
positive	string	For use with a vertical coordinate variables only. May have the value "up" or "down". For example, if an oceanographic netCDF file encodes the depth of the surface as 0 and the depth of 1000 meters as 1000 then the axis would set positive to "down". If a depth of 1000 meters was encoded as -1000, then positive would be set to "up". See the section on vertical-coordinate in the CF conventions document [RD.177].	CF	This is not used in SST_cci files.
coordinates	string	Identifies auxiliary coordinate variables, label variables, and alternative coordinate variables. See the section on coordinate-system in the CF conventions document [RD.177].	CF	As stated in Description column.



Variable attribute name	Format	Description	Source	SST_cci definition
grid_ mapping	string	Use this for data variables that are on a projected grid. The attribute takes a string value that is the name of another variable in the file that provides the description of the mapping via a collection of attached attributes. That named variable is called a grid mapping variable and is of arbitrary type since it contains no data. Its purpose is to act as a container for the attributes that define the mapping. See the section on mappings-and-projections in the CF conventions document [RD.177].	CF	This is not used in SST_cci files.
flag_ meanings	string	Space-separated list of text descriptions. Words within a phrase should be connected with underscores. Used only for flag and "sources_of_xxx" variables.	CF	See specifications in Section 4.
flag_values	Array of the data type of variable (Note that this is listed incorrectly as 'string' in [AD.1])	Comma-separated array of valid, mutually exclusive variable values (required when the bit field contains enumerated values). Used only for flag and "sources_of_xxx" variables.	CF	See specifications in Section 4.
flag_masks	Array of the data type of variable (Note that this is listed incorrectly as 'string' in [AD.1])	Array of valid variable masks (required when the bit field contains independent Boolean conditions). Used only for flag and "sources_of_xxx" variables.	CF	See specifications in Section 4.

3.5 Unique product identifiers

Some of the attributes described in Table 6 and Table 8 contain identifiers for the data that have been used to create the file. Section 7.9 of [AD.1] describes these strings. For completeness a brief summary can be found below. In Table 9 all the source data to be used by the project are listed together with the unique text strings that shall be used by to refer to these in the SST_cci files. The entries to the table are based on the information in [AD.1] and [RD.172].



The format of the text is:

<Product String>-<RDAC>-<Processing Level>-<Additional Segregator>-v<Product Version>

The definition of these elements can be found in Table 3, with the exception of the following points:

- <Product Version> this specifies the version of the dataset and should have the form x.y, where x is the major and y the minor version number.
- <Additional Segregator> for wind speed data, <Additional Segregator> should be set to WSP, and to ICE for sea ice fraction.
- If there is no predefined GHRSST RDAC for a data source an appropriate acronym can be substituted instead.

[AD.1] includes a number of predefined text strings. An example of relevance to SST_cci is SEVIRI_SST-OSISAF-L3C-v1.0. Some existing text strings predate the format described above and hence do not conform.

Table 9. Table of source data and unique product identifiers.

Source data	Unique text string	Comment
ATSR1 Level 1	ATSR1-ESA-L1-v2.0	
ATSR2 Level 1	ATSR2-ESA-L1-v2.0	
AATSR Level 1	AATSR-ESA-L1-v2.0	
AVHRR GAC Level 1	AVHRR <x>_G-NOAA-L1-v<y></y></x>	<x> is the satellite number; <y> is the format version number in form x.y where x is the major format version (1, 2, 3, 4 or 5) and y is used to denote format changes where the major format number is unchanged (possible values are 0, 1 and 2).</y></x>
AVHRR MetOp Level 1	AVHRRMTA-OSISAF-L1B-vA1.0p1.0	Version number format is non-standard.
SEVIRI Level 3	SEVIRI_SST-OSISAF-L3C-vA0.0p0.1	
AMSR-E Level 2	REMSS-L2P_GRIDDED_25-AMSRE	
TMI Level 2	REMSS-L2P_GRIDDED_25-TMI	
NWP wind speed	ERA_INTERIM-ECMWF-WSP-v1.0	
OSI SAF sea ice fractions	EUMETSAT_OSI-SAF-ICE-v1.1	This is an adaptation of the source field used in current OSTIA files
Land mask	NAVOCEANO_landmask_v1.0	
Lake mask	ARCLake_lakemask	
Data files created by SST_cci	<product string="">-ESACCI-<processing level="">-v<version number=""></version></processing></product>	See text for definition of these fields.



4. PRODUCT SPECIFICATION

This section contains detailed specifications for the files to be produced by the SST_cci project. The structure of the files is fully specified, including the geophysical variables, the metadata and aspects of the data such as the grid.

In addition to the tables in this section, Network Common Data Form Language (CDL) format listing of the headers of example L2P, L3U and L4 NetCDF files are provided in Appendix A. These have been tested using the CF compliance checker at http://puma.nerc.ac.uk/cgi-bin/cf-checker.pl to confirm that they comply with the CF conventions version 1.5.

4.1 Format of the product description tables

Tables are used to describe the detailed structure of the data files in the following subsections. An example of the layout of the tables is shown in Table 10. The points to note are:

- Colours are used to show the start and end of sections of the file structure.
- The column headed 'T' contains the storage type of the variables and attributes; the abbreviations used are explained in Table 11.
- The column headed 'D' contains the dimensionality of the variables. Dimensions
 are ordered as in the network Common Data form Language (CDL) definition i.e.
 with the fastest changing dimension last.
- The 'Bytes' column indicates the storage requirement for each item.

Table 10. Example of a table showing file structure. Colours are used to denote the beginning and end of sections of the structure.

Element name	Description	Range/value	Unit	Т	D	Bytes
Dataset	Begin of dataset					
dimensions	Begin of dimensions					
dimension1						
dimension2						
dimensionN						
dimensions	End of dimensions					
variables	Begin of variables					
variable	Begin of variable					
variable_name						
attributes	Begin of attributes					
attribute1						
attribute2						
attributeN						
attributes	End of attributes					
variable	End of variable					



Element name	Description	Range/value	Unit	Т	D	Bytes
	More variable definition	ons as required				
variables	End of variables					
attributes	Begin of global attributes					
Global attributes that have	e values that are consisten	t between data le	vels are d	efine	d in Ta	ble 13.
global_attribute1						
global_attribute2						
global_attributeN						
attributes	End of global attributes					
dataset	End of dataset					

4.2 Storage type definitions

Storage types and abbreviations used to refer to them are listed in Table 11. Storage types are limited to those available in the classic NetCDF format. For information the names given to these types in [AD.1] are also listed.

Note that although the abbreviation 'st' is used to indicate text strings, in the NetCDF classic data model there is actually no 'string' storage type [RD.167]. This type of data is instead stored as an array of characters.

Type Description Name used in [AD.1] Comment sc 8-bit signed integer byte The NetCDF data type names match 16-bit signed integer short SS those used in [AD.1] for these types. sl 32-bit signed integer int (or long) fl 32-bit floating point float db 64-bit floating point double To be stored in the st Character array string NetCDF file as an array of characters (8-bit unsigned integers)

Table 11. Abbreviations used for storage types.

4.3 L2P data

4.3.1 Description

L2P data files contain swath based SST data. In the context of the SST_cci project, they will be produced from:

- AVHRR Global Area Coverage (GAC) data for the long term ECV, and,
- AATSR data for the demonstration ECV.

Additionally, passive microwave data will be received by the project in L2 form and will have additional data added.



Each file shall contain a single orbit of data. The pixel geometry used is instrument and data source dependent:

- For AATSR, it is the regridded 1 km geometry present in L1B.
- For AVHRR-GAC it is the sub-sampled geometry of GAC with its variable resolution across the swath.

L2P files shall include confidence information and single sensor error statistics (SSES) (bias and standard deviation).

Multiple different types of retrieval are possible using different views and channels. The L2P files shall contain the best available retrievals. No specific user requirement has been identified for files containing the other retrievals. However, in case such a requirement becomes apparent a method of storing these data is defined in Appendix B.

4.3.2 Summary of contents

The files produced by SST_cci will meet the specification of the 'L2Pcore' files defined in [AD.1]. The SSES mean bias traditionally provides a bias correction to apply to the data. This is not appropriate in the case of SST_cci products, so SSES bias will be populated with zeros. SSES standard deviations will contain the total uncertainty of each data point of the best available skin/subskin SSTs. One variable from the list of auxiliary fields (L2Paux), wind speed, is also included within the SST_cci L2P files. In addition, six experimental variables are included:

- SST adjusted for time and depth (not applicable for all demonstration product data),
- large scale correlated uncertainty (highly correlated between pixels over long spatiotemporal scales),
- synoptically correlated uncertainty (highly correlated between pixels over synoptic scales),
- uncorrelated uncertainty (uncorrelated or weakly correlated between pixels), and,
- uncertainty in time and depth adjustment (a systematic uncertainty; not applicable for demonstration ECV).
- total uncertainty for the SST adjusted for time and depth (not applicable for all demonstration product data).

Information about how to combine the uncertainties is provided in the comment attributes within the files and correlation length and time scales are provided for the synoptically correlated components. CF standard name modifiers do not exist for individual uncertainty components and so no standard names are defined for them. It is suggested that these should be proposed in the future if it becomes clear that there is a general need for uncertainties that are decomposed in this way.

A summary of the data fields is given in Table 12.



Table 12. Variables to be included within the L2P data files; some of the name and description information in this table is reproduced from Section 9.1 of [AD.1]. The shading (see Table 7) and the OCC column indicate the number of occurrences of each variable. These are either mandatory (1, blue shading) or optional (0..1, violet shading).

Name	Description	OCC
lat	Coordinate variable; central latitude of each spatial point of the data arrays	1
lon	Coordinate variable; central longitude of each spatial point of the data arrays	1
time	Coordinate variable; time of each temporal point of the data arrays; the start time of the granule	1
sea_surface_temperature	Best available skin/subskin SST retrievals (unadjusted for time and depth); fill values to be provided where there is land, cloud or total sea ice cover	1
sst_dtime	Time differences of SST retrievals from the base time in the time coordinate variable	1
sses_bias	SST single sensor error statistic measurement bias estimate (to contain zeroes)	1
sses_standard_deviation	SST single sensor error statistic measurement standard deviation estimate (to contain the total of the large scale correlated, synoptically correlated and uncorrelated uncertainties)	1
l2p_flags	Flags specific to each L2P dataset that help users interpret data	1
quality_level	A quality level for each measurement	1
wind_speed	An estimate of surface wind speed (from the ERA-Interim reanalysis)	1
sea_surface_temperature_depth	Sea surface temperature at standard depth and time (adjusted version of the sea_surface_temperature variable)	01
large_scale_correlated_uncertainty	Systematic uncertainty that is highly correlated between pixels over large scales	1
synoptically_correlated_uncertainty	Systematic uncertainty that is highly correlated between pixels over synoptic scales only	1
uncorrelated_uncertainty	Non-systematic uncertainty (uncorrelated or weakly correlated between pixels)	1
adjustment_uncertainty	Uncertainty in adjustment to standard depth and time (correlated between pixels over synoptic scales)	01
sst_depth_total_uncertainty	To contain the total of the large scale correlated, synoptically correlated, uncorrelated and adjustment uncertainties.	01



The contents of these files meet the following user requirements:

- The inclusion of wind speed meets user requirement SST_CCI-URD-QUF-70 [RD.171].
- The SST that is adjusted for time and depth will correspond to 10.30 am or pm and a depth of 20 cm. This is the (joint) second most popular choice of depth with users according to requirement SST_CCI-UR-QUF-46 [RD.171]. Note that the most popular choice (skin SST) corresponds to the SST viewed by infrared instruments and so will also be included in the files for data from that type of sensor.
- The separate uncertainty components and correlation scales provide information to the user about the correlation structure of the uncertainties (requirement SST_CCI-UR-QUF-57, [RD.171]).
- When the uncertainty components are combined they give an estimate of total uncertainty (requirement SST_CCI-UR-QUF-53, [RD.171]).
- The files also include a simple quality flag (SST_CCI-URD-QUF-58, [RD.171]).

4.3.3 Detailed contents

The detailed contents of the L2P products are defined in Table 13 and Table 14. The former is used to specify the global attributes that have common values in files for all data levels. Together the tables specify the structure of the NetCDF files. Examples of what the attributes might contain in a real file can be found in Appendix A.

Table 13. Global attributes common to all data files. Contents were taken from [AD.1] Table 8-1 and adapted for the SST_cci data files.

Element name	Description	Range/ value	Unit	Т	D	Bytes
attributes	Beginning of global attributes					
Conventions	The version of the netCDF conventions followed.	CF-1.5, Unidata Observation Dataset v1.0		st		
title	Insert satellite sensor name and data level into the string to create a descriptive name for the data.	ESA SST CCI <product String> <data level=""> product</data></product 		st		
summary	Insert satellite sensor name, data level and algorithm name/brief description.	<product string=""> <data level=""> product from the ESA SST CCI project, produced using <algorithm name="">.</algorithm></data></product>		st		



Element name	Description	Range/ value	Unit	Т	D	Bytes
references	Published or web- based references.			st		
institution	RDAC code.	ESACCI		st		
history	To contain a history of applications that have been used to process the data. For example this can be used to record the version of the retrieval algorithm applied to the data, the identity of intermediate files used in the processing etc.			st		
license	The GHRSST standard data license.	GHRSST protocol describes data use as free and open		st		
id	Unique text string for this product. See Section 3.5.			st		
naming_authority	Defined in [RD.87] as org.ghrsst.	org.ghrsst		st		
product_version	Product version (see Section 3.5).			st		
uuid	Universally Unique Identifier. For example see http://www.ossp.or g/pkg/lib/uuid/ [RD.169]			st		
tracking_id	Identical to uuid (i.e. this shall contain the same value as uuid)			st		
gds_version_id	Version of [GDS] that files are based on.	2.0		st		
netcdf_version_id	NetCDF library.	Format example: 4.1.1		st		
date_created	File creation	Format: yyyymmddTh hmmssZ		st		



Element name	Description	Range/ value	Unit	Т	D	Bytes
file_quality_level	Select from:	[0, 3]		sl		4
	0 = unknown quality					
	1 = extremely suspect (frequent problems, e.g. with known satellite problems)					
	2 = suspect (occasional problems, e.g. after launch)					
	3 = excellent (no known problems)					
spatial_resolution	A string describing the approximate resolution of the product. For example, "1.1km at nadir". See Table 1 for values to use.	[1 km at nadir, 0.05°]		st		
start_time	Date and time of the first measurement in the data file.	Format: yyyymmddTh hmmssZ		st		
time_coverage_start	Identical to start_time.	Format: yyyymmddTh hmmssZ		st		
stop_time	Date and time of the last measurement in the data file in the form.	Format: yyyymmddTh hmmssZ		st		
time_coverage_end	Identical to stop_time.	Format: yyyymmddTh hmmssZ		st		
time_coverage_duration	Difference between time_coverage_ end and time_coverage_ start in the form PdDThHmMsS, replacing the lower case letters with the appropriate numbers.	Format: PdDThHmMs S (see description column for more details)		st		



Element name	Description	Range/ value	Unit	Т	D	Bytes
time_coverage_resolution	Temporal resolution of data in the file i.e. the orbit repeat period or the frequency of L3/L4 data.	Format: PdDThHmMs S (see description of time_ coverage_ duration for more details)		st		
source	Comma separated list of all source data present in this file. List SST sources first, followed by auxiliary sources. See Section 3.5 for source data names.			st		
platform	Satellite(s) used to create this data file. Select from the entries found in Table 5			st		
sensor	Satellite(s) used to create this data file. Select from the entries found in Table 5			st		
metadata_conventions		Unidata Dataset Discovery v1.0		st		
metadata_link	Link to collection metadata record at archive.	http://www.es a-cci.org		st		
keywords	Standard words that describe the data, taken from the source specified in keywords_ vocabulary.	Oceans > Ocean Temperature > Sea Surface Temperature		st		
keywords_vocabulary	Defines the source of the text in the keywords attribute; [RD.176].	NASA Global Change Master Directory (GCMD) Science Keywords		st		



Element name	Description	Range/ value	Unit	Т	D	Bytes
standard_name_vocabulary	Defines the source of the standard names for the variables; [RD.177].	NetCDF Climate and Forecast (CF) Metadata Convention		st		
geospatial_lat_units	Units of the latitudinal resolution.	degrees_nort h		st		
geospatial_lat_resolution	Latitude resolution in units matching geospatial_lat_unit s. See values in Table 1.	[0.009, 0.05]		fl		4
geospatial_lon_units	Units of the longitudinal resolution.	degrees_ east		st		
geospatial_lon_resolution	Longitude resolution in units matching geospatial_lon _units. See values in Table 1.	[0.009, 0.05]		fl		4
geospatial_vertical_min	Depth of the deepest SST in the file (negative value as the direction is downwards) – see Table 4	-10 ⁻⁶ or -0.001 or - 0.2 or -10		fl		4
geospatial_vertical_max	Depth of the shallowest SST in the file (negative value as the direction is downwards) – see Table 4	-10 ⁻⁶ or -0.001 or - 0.2 or -10		fl		4
acknowledgment	Information about funding source and how to cite the use of these data.	Funded by ESA		st		
creator_name	Description of data creators.	ESA SST CCI		st		
creator_email		science.lead er@esa-sst- cci.org		st		
creator_url		http://www.es a-sst-cci.org/		st		



Element name	Description	Range/ value	Unit	Т	D	Bytes
creator_processing_ institution	Contains additional information about the institution that created the product within the CCI project. Insert institution name (for example 'the University of Edinburgh' or 'the Met Office') to indicate where the data were produced.	These data were produced at <institution> as part of the ESA SST CCI project.</institution>		st		
project	The name of the project.	Climate Change Initiative – European Space Agency		st		
publisher_name	Information about	ESACCI		st		
publisher_url	the data publisher.	http://www.es a-sst-cci.org		st		
publisher_email		science.lead er@esa- SST-cci.org		st		
attributes	End of global attributes					

Table 14. Detailed specification of the SST_cci L2P files.

Element name	Description	Range/value	Unit	Т	D	Bytes
dataset	Begin of dataset					
dimensions	Begin of dimensions					
ni	Across track dimension.			sl	1	4
nj	Along track dimension.			sl	1	4
time	Time dimension; must be 1 for L2P data.	1		sl	1	4
dimensions	End of dimensions					
variables	Begin of variables					
variable	Begin of variable					



Element name	Description	Range/value	Unit	Т	D	Bytes
lat	Latitude coordinates.	[-90, 90]		fl	nj, ni	nj x ni x 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_nort h		st		
long_name	A free-text descriptive variable name.	Latitude coordinates		st		
standard_name	Unique descriptive name for data.	latitude		st		
valid_min	Minimum valid value for this variable.	-90.0		fl		4
valid_max	Maximum valid value for this variable.	90.0		fl		4
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
comment	Miscellaneous information about the data or the methods used to produce it.			st		
	(Optional.)					
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
lon	Longitude coordinates.	[-180, 180]		fl	nj, ni	nj × ni × 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_east		st		
long_name	A free-text descriptive variable name.	Longitude coordinates		st		
standard_name	Unique descriptive name for data.	longitude		st		
valid_min	Minimum valid value for this variable.	-180.0		fl		4
valid_max	Maximum valid value for this variable.	180.0		fl		4



Element name	Description	Range/value	Unit	Т	D	Bytes
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
comment	Miscellaneous information about the data or the methods used to produce it.			st		
	(Optional.)					
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
time	Time coordinate; the start time of the granule	[0, 2 ³¹]		sl	time	time × 4
attributes	Begin of attributes					
units	Text description of the units.	seconds since 1981- 01-01 00:00:00		st		
long_name	A free-text descriptive variable name.	reference time of sst file		st		
standard_name	Unique descriptive name for data.	time		st		
calendar	Defines the calendar used to define the times.	gregorian		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sea_surface_temperature	Best available sea surface temperature retrievals; to contain fill values if land, cloud or full sea ice cover.	[271.15, 323.15] (after scaling)	К	SS	time, nj, ni	time × nj × ni × 2



Element name	Description	Range/value	Unit	Т	D	Bytes
attributes	Beginning of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	273.15		fl		4
long_name	A free-text descriptive variable name. First option is for infrared data, second for passive microwave data; see also Table 4.	sea surface skin temperature or sea surface subskin temperature		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-200		SS		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		SS		2
standard_name	Unique descriptive name for data. Choose appropriate value from Table 4.	sea_surface_ skin_ temperature or sea_surface_ subskin_ temperature		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
comment	Miscellaneous information about the data or the methods used to produce it. Includes method of calculating total uncertainty.	Temperature of the skin of the ocean; total uncertainty = sqrt(large_sc ale_correlate d_uncertainty ^2+synoptical ly_correlated _uncertainty^2+uncorrelat ed_uncertaint y^2)		st		
source	See Table 9.			st		
references	Published or web- based references that describe the data or methods used to produce it.			st		
depth	Effective depth of the sea_surface_temperature variable. Choose appropriate value from Table 4.	10 micrometres or 1 millimetre		st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sst_dtime	Time differences of SST retrievals from the reference time.	[-32767, 32767]	secs	ss	time, nj, ni	time × nj × ni × 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	seconds		st		
scale_factor	To be multiplied by the variable to recover the original value.	1.0		fl		4



Element name	Description	Range/value	Unit	Т	D	Bytes
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	time difference from reference time		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-32767		SS		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	32767		SS		2
comment	Miscellaneous information about the data or the methods used to produce it.	time plus sst_dtime gives seconds after 1981-01-01 00:00:00		st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sses_bias	Single sensor error statistic bias error.	Zero for all SST values	К	sc	time, nj, ni	time x nj x ni
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4



Element name	Description	Range/value	Unit	Т	D	Bytes
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	SSES bias estimate		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-127		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	127		SC		1
comment	Miscellaneous information about the data or the methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sses_standard_deviation	Single sensor error statistic standard deviation.	Total uncertainty from combining uncertainties as described in the comment attribute to the sea_surface_ temperature variable	К	sc	time, nj, ni	time × nj × ni
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1



Element name	Description	Range/value	Unit	Т	D	Bytes
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	1.27		fl		4
long_name	A free-text descriptive variable name.	SSES standard deviation		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-127		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	127		sc		1
comment	Miscellaneous information about the data or the methods used to produce it. Only include the text ', adjustment_uncertainty' if this is to be included in the file (i.e. do not include if it is a demonstration ECV file).	Uncertainty data are also contained in the variables large_scale_ correlated_ uncertainty, synoptically_ correlated_ uncertainty, uncorrelated_ uncertainty, adjustment_ uncertainty.		st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					



Element name	Description	Range/value	Unit	Т	D	Bytes
l2p_flags	Specifies type of input data and provide flags and information to the user. See Table 15.	[0, 255] (this may change if extra flags are defined)		SS	time × nj × ni	time × nj × ni × 2
attributes	Begin of attributes					
long_name	A free-text descriptive variable name.	L2P flags		st		
comment	Miscellaneous information about the data or the methods used to produce them.	These flags are important to properly use the data		st		
coordinates	Identifies coordinate variables.	lon lat		st		
flag_meanings	Meaning attached to each flag value.	microwave land ice lake river spare views channels		st		
flag_masks	Bit masks corresponding to the flags described in flag_meanings.	1, 2, 4, 8, 16, 32, 64, 128		SS		2
attributes	End of attributes					
variable	Begin of variable					
quality_level	Indicator of the quality of each SST.	[0, 5]		sc	time × nj × ni	time × nj × ni
attributes	Begin of attributes					
long_name	A free-text descriptive variable name.	quality level of SST pixel		st		
comment	Miscellaneous information about the data or the methods used to produce it.	These are the overall quality indicators and are those used for all GHRSST SSTs		st		
coordinates	Identifies coordinate variables.	lon lat		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
flag_meanings	Meaning attached to each flag value.	no_data bad_data worst_quality low_quality acceptable_q uality best_quality		st		
flag_values	Values that correspond to the flags described in flag_meanings. The b after the numbers is to indicate that they are single byte numbers.	0b, 1b, 2b, 3b, 4b, 5b		sc		1
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
wind_speed	Surface wind speed at 10 m height. Resolution should be no less than 1 m s ⁻¹ and has been defined here to be 0.1 m s ⁻¹ . The range of wind speeds that can be represented is 0 – 25.4 m s ⁻¹ ; values higher than this should be set to the maximum.	[0, 25.4] (after scaling)	ms ⁻¹	sc	time, nj, ni	time × nj × ni
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
units	Text description of the units.	m s-1		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.1		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	12.7		fl		4



Element name	Description	Range/value	Unit	Т	D	Bytes
long_name	A free-text descriptive variable name.	10m wind speed		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-127		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	127		sc		1
standard_name	Unique descriptive name for data.	wind_speed		st		
comment	Miscellaneous information about the data or the methods used to produce it.	Wind speeds sourced from ECMWF ERA Interim reanalysis; wind speeds greater than 25.4 m/s are set to 25.4.		st		
source	See Table 9.			st		
references	Published or web- based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
height	Height that the wind values correspond to.	10 m		st		
time_offset	Difference in hours between the SST reference time and the time of the wind speed value.			fl		4
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					



Element name	Description	Range/value	Unit	Т	D	Bytes
sea_surface_temperature_ depth	SSTs adjusted to 10.30 local time (either morning or evening, whichever is closest) and 20 cm.	[271.15, 323.15] (after scaling)	К	SS	time, nj, ni	time x nj x ni x 2
attributes	Beginning of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	273.15		fl		4
long_name	A free-text descriptive variable name.	sea surface temperature at 0.2 m		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-200		SS		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		SS		2
standard_name	Unique descriptive name for data.	sea_water_ temperature		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
comment	Miscellaneous information about the data or the methods used to produce it. Includes method of calculating total uncertainty.	Temperature of the ocean at 20 cm depth; total uncertainty = sqrt(large_sc ale_correlate d_uncertainty ^2+synoptical ly_correlated _uncertainty ^2+uncorrelat ed_uncertaint y^2+adjustm ent_uncertain ty^2)		st		
source	See Table 9.			st		
references	Published or web- based references that describe the data or methods used to produce it.			st		
depth	Effective depth of the SST data.	0.2 metre		st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
large_scale_correlated_ uncertainty	Component of uncertainty that is highly correlated between SST retrievals separated by larger than sub-synoptic spatio-temporal scales.	[0, 50] (after scaling)	К	SS	time × nj × ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty from errors likely to be correlated over large scales		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		SS		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		SS		2
comment	Miscellaneous information about the data or the methods used to produce it.	Component of uncertainty that is correlated over large scales; can be combined with other uncertainty estimates to form a total uncertainty		st		
references	Published or web- based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes			_		
variable	End of variable					
variable	Begin of variable					



Element name	Description	Range/value	Unit	Т	D	Bytes
synoptically_correlated_ uncertainty	Component of uncertainty that is highly correlated between SST retrievals separated by subsynoptic spatiotemporal scales.	[0, 50] (after scaling)	К	SS	time × nj × ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty from errors like to be correlated over synoptic scales		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		SS		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		SS		2



Element name	Description	Range/value	Unit	Т	D	Bytes
comment	Miscellaneous information about the data or the methods used to produce it.	Component of uncertainty that is correlated over synoptic scales; can be combined with other uncertainty estimates to form a total uncertainty		st		
references	Published or web- based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
correlation_length_scale	Estimate of the correlation length scale of the uncertainties.	100 km		st		
correlation_time_scale	Estimate of the correlation time scale of the uncertainties	1 day		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
uncorrelated_uncertainty	Component of uncertainty that is uncorrelated between SST retrievals separated by any spatio-temporal scales.	[0, 50] (after scaling)	К	SS	time × nj × ni	time × nj × ni × 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty from errors likely to be uncorrelated between SSTs		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		SS		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		SS		2
comment	Miscellaneous information about the data or the methods used to produce it.	Component of uncertainty that is uncorrelated between SSTs; can be combined with other uncertainty estimates to form a total uncertainty		st		
references	Published or web- based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					



Element name	Description	Range/value	Unit	Т	D	Bytes
adjustment_uncertainty	Uncertainty in adjustment for depth and time, correlated between SST estimates separated by subsynoptic spatiotemporal scales.	[0, 50] (after scaling)	К	SS	time × nj × ni	time × nj × ni × 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Time and depth adjustment uncertainty		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		SS		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		SS		2
comment	Miscellaneous information about the data or the methods used to produce it.	Adjustment uncertainty; can be combined with other uncertainty estimates to form a total uncertainty		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
references	Published or web- based references that describe the data or methods used to produce it.			st		
coordinates	Identifies coordinate variables.	lon lat		st		
correlation_length_scale	Estimate of the correlation length scale of the uncertainties.	100 km		st		
correlation_time_scale	Estimate of the correlation time scale of the uncertainties	1 day		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sst_depth_total_uncertainty	Combination of all uncertainty components.	Total uncertainty from combining uncertainties as described in the comment attribute to the sea_surface_ temperature_ depth variable	К	SS	time, nj, ni	time × nj × ni × 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original	0.00		fl		4



Element name		Description	Range/value	Unit	Т	D	Bytes
		value.					
long_name		A free-text descriptive variable name.	Total uncertainty in sea_surface_ temperature_ depth		st		
	valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		SS		2
	valid_max	Maximum valid value for this variable once they are packed (in storage type).	5000		SS		2
	comment	Miscellaneous information about the data or the methods used to produce it.	Total uncertainty in each sea_surface_temperature_depth data point		st		
С	coordinates	Identifies coordinate variables.	lon lat		st		
attributes		End of attributes					
variable		End of variable					
variables		End of variables					
attributes		Begin of global attributes					
	G	lobal attributes as des	cribed in Table 6	ô.			
	comment	To contain any miscellaneous information about the data and methods. Delete the 'and sea_surface_ temperature_depth' part of the second sentence if the sea_surface_ temperature_depth variable is not included in the file.	For information about uncertainty estimates see the comment attributes to the sea_surface temperature and sea_surface_temperature_depth variables.		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
northernmost_latitude	Decimal degrees north, range -90 to +90. May vary from orbit to orbit.	[-90, 90]		fl		4
geospatial_lat_max	Identical to northernmost_ latitude	[-90, 90]		fl		4
southernmost_latitude	Decimal degrees north, range -90 to +90. May vary from orbit to orbit.	[-90, 90]		fl		4
geospatial_lat_min	Identical to southernmost_ latitude	[-90, 90]		fl		4
easternmost_longitude	Decimal degrees east, range -180 to +180. May vary from orbit to orbit.	[-180, 180]		fl		4
geospatial_lon_max	Identical to easternmost_longitude	[-180, 180]		fl		4
westernmost_longitude	Decimal degrees east, range -180 to +180. May vary from orbit to orbit.	[-180, 180]		fl		4
geospatial_lon_min	Identical to westernmost_longitude	[-180, 180]		fl		4
processing_level	Data level.	L2P		st		
cdm_data_type	"swath" or "grid"	swath		st		
attributes	End of global attributes					
dataset	End of dataset					



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Table 15. Meaning of each bit in a l2p_flags field. Reformatted version of Table 9-19 of [AD.1] with additional entries denoted by italics. Bits 6-15 are available for use by the SST_cci project; two of these are used to describe the retrieval.

Bit	Description	Meaning if 0	Meaning if 1			
0	Type of sensor	Infrared	Microwave			
1	Ocean or land indicator	Over the ocean	Over land			
2	Sea ice indicator	Not sea ice contaminated	Sea ice contaminated			
3	Lake indicator (if known)	Not over lake	Over lake			
4	River indicator (if known)	Not over river	Over river			
5	Reser	ved for future use				
6	Number of satellite views used in retrieval (or, if no retrieval possible, what it would have been if a retrieval had been performed))	Single (nadir only) view	Dual view			
7	Number of channels used in retrieval (or, if no retrieval possible, what it would have been if a retrieval had been performed)	Two channels	Three channels			
8-15	Available for use by SST_cci					

Table 16. Quality level indicators for SST data. To simplify the flags SST_cci shall use only values of 0, 1 and 5. Reproduced from Section 9.18 of [AD.1] with shading added to indicate flags that will not be used by SST_cci.

Value	Meaning
0	Missing data
1	These data are not valid and should not be used
2	Data are of the lowest quality that still could be usable
3	Low quality data
4	Acceptable quality data
5	Best quality data

4.4 L3U and L3C data

4.4.1 Description

Level 3 data files contain gridded SST data (but not analysis data, i.e. they do not include values where no retrieval could be made). In the context of the data to be produced by SST cci these will be:

- Uncollated (L3U) data files these contain a single orbit of data from a single sensor (i.e. a gridded version of L2P data.
 - o L3U files will be produced for ATSR series data for the long term ECV.
- Collated (L3C) data files these contain data from multiple orbits of a single sensor combined onto a space and/or time grid.
 - L3C files will be produced for Metop AVHRR data for the demonstration ECV.
 - SEVIRI input data will also be converted into a L3C file as defined in this
 document

The grid used shall be a regular 0.05° latitude-longitude grid (SST_CCI-UR-QUF-36, [RD.171]). As with L2P files, the level 3 files shall contain the best available SST data. See Appendix B for specifications of files that could be used to hold data obtained using other retrievals should a user requirement arise. L3C files will be daily collations of data from a sensor.

The contents of the files are very similar to those of L2P files and hence meet the same user requirements described in Section 4.3.2.

4.4.2 Summary of contents

The files are almost identical to the L2P files. They differ in the specification of the grid and in some of the attributes. Note that the time dimension in level 3 (and 4) files is set to be unlimited. In practice only one time field is contained in each file, but this allows utilities that operate on the files to concatenate the data [AD.1].

Table 17. Fields within a L3 data file; some of the name and description information in this table is reproduced from Section 9.1 of [AD.1]. The shading (see Table 7) and the OCC column indicate the number of occurrences of each variable. These are either mandatory (1, blue shading) or optional (0..1, violet shading).

Name	Description	occ
lat	Vector specifying the central latitude of each spatial point in the data grid	1
lat_bnds	Latitude bounds of each grid cell; included from [RD.166].	1
Ion	Vector specifying the central longitude of each spatial point in the data grid	1
lon_bnds	Longitude bounds of each grid cell; included from [RD.166].	1



time	Vector specifying the reference time of each temporal point in the data grid; this is either the start time of the L3U granule or the mid-point of the collation window for L3C (the midpoint of the day the data represent)	1
time_bnds	Time bounds of each time point (either start and end times of the data collection for L3U or start and end of the day for L3C); included from [RD.166]	1
sea_surface_temperature	Best available sea surface temperature retrievals (unadjusted for time and depth); fill values to be provided where there is land, cloud or total sea ice cover	1
sst_dtime	Time differences of SST retrievals from the reference time	1
sses_bias	SST single sensor error statistic measurement bias estimate (to contain zeroes)	1
sses_standard_deviation	SST single sensor error statistic measurement standard deviation estimate (to contain the total of the large scale correlated, synoptically correlated and uncorrelated uncertainties)	1
l2p_flags	Flags that help users interpret data	1
quality_level	A quality level for each SST	1
wind_speed	An estimate of surface wind speed (from the ERA-Interim reanalysis)	1
sea_surface_temperature_depth	Sea surface temperature adjusted to standard time and depth	01
large_scale_correlated_uncertainty	Systematic uncertainty that is highly correlated between pixels over large scales	1
synoptically_correlated_uncertainty	Systematic uncertainty that is highly correlated between pixels over synoptic scales only	1
uncorrelated_uncertainty	Non-systematic uncertainty (uncorrelated or weakly correlated between pixels)	1
adjustment_uncertainty	Uncertainty in adjustment to standard depth and time (correlated between pixels over synoptic scales)	01
sst_depth_total_uncertainty	To contain the total of the large scale correlated, synoptically correlated, uncorrelated and adjustment uncertainties.	01



4.4.3 Detailed contents

The detailed contents of the products are defined in Table 18. The table specifies the structure of the NetCDF files. Much of this is done with reference to Table 14. However, note that in keeping with the examples in [AD.1] the spatial dimensions are given different names in level 3 files compared to L2P (lat and lon in the former, ni and nj in the latter). Example of how these contents would look in a real file are given in Appendix A.

Table 18. Description of L3 file contents; this follows the specification defined in [AD.1].

Element name	Description	Range/value	Unit	Т	D	Bytes
dataset	Begin of dataset					
dimensions	Begin of dimensions					
lon	Zonal dimension.	7200		sl		4
lat	Meridional dimension.	3600		sl		4
time	Time dimension; in practice will be 1.	Unlimited		sl		4
bnds	Dimension for the latitude, longitude and time bounds.	2		sl		4
dimensions	End of dimensions					
variables	Begin of variables					
variable	Begin of variable					
lat	Latitude coordinates	[-90, 90]		fl	lat	lat × 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_ north		st		
long_name	A free-text descriptive variable name.	Latitude		st		
standard_name	Unique descriptive name for data.	latitude		st		
valid_min	Minimum valid value for this variable.	-90.0		fl		4
valid_max	Maximum valid value for this variable.	90.0		fl		4
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
axis	Set to X for longitudinal axis, Y for latitudinal axis, T for time.	Y		st		
bounds	Indicates the variable containing the latitude cell boundaries	lat_bnds		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
comment	Miscellaneous information about the data or the methods used to produce it.			st		
	(Optional.)					
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
lat_bnds	Bounds of the latitude cells	[-90, 90]		fl	bnds × lat	bnds ×lat × 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_nort h		st		
long_name	A free-text descriptive variable name.	Latitude cell boundaries		st		
valid_min	Minimum valid value for this variable.	-90.0		fl		4
valid_max	Maximum valid value for this variable.	90.0		fl		4
comment	Miscellaneous information about the data or the methods used to produce it.	Contains the northern and southern boundaries of the grid cells.		st		
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
lon	Longitude coordinates	[-180, 180]		fl	lon	lon × 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_east		st		
long_name	A free-text descriptive variable name.	Longitude		st		
standard_name	Unique descriptive name for data.	longitude		st		
valid_min	Minimum valid value for this variable.	-180.0		fl		4
valid_max	Maximum valid value for this variable.	180.0		fl		4



Element name	Description	Range/value	Unit	Т	D	Bytes
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
axis	Set to X for longitudinal axis, Y for latitudinal axis, T for time.	X		st		
bounds	Indicates the variable containing the longitude cell boundaries	lon_bnds		st		
comment	Miscellaneous information about the data or the methods used to produce it.			st		
	(Optional.)					
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable			-		
lon_bnds	Bounds of the longitude cells	[-180, 180]		fl	bnds × lon	bnds x lon x 4
attributes	Begin of attributes					
units	Text description of the units.	degrees_east		st		
long_name	A free-text descriptive variable name.	Longitude cell boundaries		st		
valid_min	Minimum valid value for this variable.	-180.0		fl		4
valid_max	Maximum valid value for this variable.	180.0		fl		4
comment	Miscellaneous information about the data or the methods used to produce it.	Contains the eastern and western boundaries of the grid cells.		st		
reference_datum	Information about the coordinates.	geographical coordinates, WGS84 projection		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
time	Time coordinate	[0, 2 ³¹]		sl	time	time ×
attributes	Begin of attributes					



Element name	Description	Range/value	Unit	Т	D	Bytes	
units	Text description of the units.	seconds since 1981- 01-01 00:00:00		st			
long_name	A free-text descriptive variable name.	reference time of sst file		st			
standard_name	Unique descriptive name for data.	time		st			
axis	Set to X for longitudinal axis, Y for latitudinal axis, T for time.	Т		st			
calendar	Defines the calendar used to define the times.	gregorian		st			
bounds	Indicates the variable containing the time cell boundaries	time_bnds		st			
comment	Miscellaneous information about the data or the methods used to produce it.			st			
	(Optional.)						
attributes	End of attributes						
variable	End of variable						
variable	Begin of variable						
time_bnds	Bounds of the time cells	[0, 2 ³¹]		fl	bnds × time	bnds × time × 4	
attributes	Begin of attributes						
units	Text description of the units.	seconds since 1981- 01-01 00:00:00		st			
long_name	A free-text descriptive variable name.	Time cell boundaries		st			
comment	Miscellaneous information about the data or the methods used to produce it.	Contains the start and end times for the time period the data represent.		st			
attributes	End of attributes						
variable	End of variable						
variable	Begin of variable						
sea_surface_temperat ure		As specified in Table 14 (except that the coordinates attribute is not required)					



Element name	Description	Range/value	Unit	Т	D	Bytes
variable	End of variable					
variable	Begin of variable					
sst_dtime	As specified in Table 14 (except that the coordinates attribute is not required, the storage type is fill value is -2 ³¹ and valid min and valid max are -43200 and 43200 respectively since 43200 is half a day in units of seconds)					3200
variable	End of variable					
variable	Begin of variable					
sses_bias	As (except that the	s specified in Tal coordinates attri		ot re	quired)	
variable	End of variable					
variable	Begin of variable					
sses_standard_ deviation	As (except that the	s specified in Tal coordinates attri		ot re	quired)	
variable	End of variable					
variable	Begin of variable					
l2p_flags	As specified in Table 14 (except that the coordinates attribute is not required and if a L3C file do not include 'views' and 'channels' in the flag_meanings attribute and also remove', 64, 128' from the flag_masks attribute – these are not appropriate for a L3C file since a grid cell could contain data from a mix or retrievals)					
					hese are	not
variable		ince a grid cell c			hese are	not
variable variable	appropriate for a L3C file s	ince a grid cell c			hese are	not
	appropriate for a L3C file since End of variable Begin of variable	ince a grid cell coretrievals) s specified in Tal	ould con	tain (hese are data from	not
variable	appropriate for a L3C file since End of variable Begin of variable As	ince a grid cell coretrievals) s specified in Tal	ould con	tain (hese are data from	not
variable quality_level	appropriate for a L3C file so End of variable Begin of variable As (except that the	ince a grid cell coretrievals) s specified in Tal	ould con	tain (hese are data from	not
variable quality_level variable	appropriate for a L3C file sile. End of variable Begin of variable As (except that the End of variable Begin of variable	retrievals) s specified in Tal coordinates attri	ould con	ot re	hese are data from quired)	not
variable quality_level variable variable	appropriate for a L3C file si End of variable Begin of variable As (except that the End of variable Begin of variable As A	retrievals) s specified in Tal coordinates attri	ould con	ot re	hese are data from quired)	not
variable quality_level variable variable wind_speed	appropriate for a L3C file so End of variable Begin of variable As (except that the End of variable Begin of variable As (except that the except that the	retrievals) s specified in Tal coordinates attri	ould con	ot re	hese are data from quired)	not
variable quality_level variable variable wind_speed variable	appropriate for a L3C file sile. End of variable Begin of variable As (except that the End of variable) Begin of variable As (except that the End of variable) End of variable End of variable Begin of variable	retrievals) s specified in Talcoordinates attri	ole 14 bute is not bute is not but bute is not but but but but but but but but but bu	not re	hese are data from quired)	not
variable quality_level variable variable wind_speed variable variable variable sea_surface_temperat ure	appropriate for a L3C file since the second of variable segments of vari	retrievals) s specified in Talcoordinates attri	ole 14 bute is not bute is not but bute is not but but but but but but but but but bu	not re	hese are data from quired)	not
variable quality_level variable variable wind_speed variable variable variable sea_surface_temperat uredepth	appropriate for a L3C file sile. End of variable Begin of variable As (except that the End of variable Begin of variable As (except that the End of variable End of variable Begin of variable As (except that the End of variable) As (except that the except that t	retrievals) s specified in Talcoordinates attri	ole 14 bute is not bute is not but bute is not but but but but but but but but but bu	not re	hese are data from quired)	not
variable quality_level variable variable wind_speed variable variable variable sea_surface_temperat uredepth variable	appropriate for a L3C file so End of variable Begin of variable As (except that the End of variable Begin of variable As (except that the End of variable Begin of variable Begin of variable As (except that the End of variable Begin of variable As (except that the End of variable)	s specified in Tal coordinates attri	ould con ole 14 bute is n ole 14 bute is n ole 14 bute is n	not re	quired) quired)	not
variable quality_level variable variable wind_speed variable variable sea_surface_temperat uredepth variable variable variable large_scale_correlated	appropriate for a L3C file sile. End of variable Begin of variable As (except that the End of variable Begin of variable As (except that the End of variable Begin of variable Begin of variable As (except that the End of variable Begin of variable As (except that the End of variable As (except that the End of variable Begin of variable As End of variable Begin of variable	s specified in Tal coordinates attri	ould con ole 14 bute is n ole 14 bute is n ole 14 bute is n	not re	quired) quired)	not



Element name	Description	Range/value	Unit	Т	D	Bytes
synoptically_correlated _uncertainty	As (except that the	s specified in Tal coordinates attri		ot re	equired)	
variable	End of variable					
variable	Begin of variable					
uncorrelated_uncertain ty	As (except that the	s specified in Tal coordinates attri		ot re	quired)	
variable	End of variable					
variable	Begin of variable					
adjustment_ uncertainty	As (except that the	s specified in Tal coordinates attri		ot re	equired)	
variable	End of variable					
variable	Begin of variable					
sst_depth_total_ uncertainty		s specified in Tal coordinates attri		ot re	equired)	
variable	End of variable					
variables	End of variables					
attributes	Begin of global attributes					
	Global attributes as des	cribed in Table 1	3.			
comment	To contain any miscellaneous information about the data and methods. Delete the 'and sea_surface_temperature _depth' part of the second sentence if the sea_surface_temperature _depth variable is not included in the file.	For information about uncertainty estimates see the comment attributes to the sea_surface temperature and sea_surface_temperature_depth variables.		st		
northernmost_latitude	Decimal degrees north, range -90 to +90.	90.0		fl		4
geospatial_lat_max	Identical to northernmost_ latitude	90.0		fl		4
southernmost_latitude	Decimal degrees north, range -90 to +90.	-90.0		fl		4
geospatial_lat_min	Identical to southernmost_ latitude	-90.0		fl		4
easternmost_longitude	Decimal degrees east, range -180 to +180.	180.0		fl		4



Element name	Description	Range/value	Unit	Т	D	Bytes
geospatial_lon_max	Identical to easternmost_ longitude	180.0		fl		4
westernmost_longitud e	Decimal degrees east, range -180 to +180.	-180.0		fl		4
geospatial_lon_min	Identical to westernmost_ longitude	-180.0		fl		4
processing_level	Data level.	L3U or L3C		st		
cdm_data_type	"swath" or "grid"	grid		st		
attributes	End of global attributes					
dataset	End of dataset					

4.5 L4 data

4.5.1 Description

Level 4 data – SST data that have been analysed to remove data gaps – are to be produced by the SST_cci project using the Operational Sea surface Temperature and sea Ice Analysis (OSTIA) system for both the demonstration and long term ECVs. The contents of these files are largely as defined in [AD.1]. A summary of the specification is included here for completeness.

4.5.2 Summary of contents

As described in [AD.1], the contents of the L4 files include SSTs, uncertainties and information about locations of land and sea ice. These are summarised in Table 19.

The contents of the files meets user requirements:

- Provision of a product that does not contain data gaps, such as a L4 product, is required (SST_CCI-UR-QUF-39, [RD.171]).
- SST_CCI-UR-QUF-46 [RD.171]: the LT Analysis product will contain SSTs corresponding to 20 cm depth, which is the joint second most popular choice with potential users. The foundation temperature provided in the DM Analysis product is relevant to over half of the user's applications.
- SST_CCI-UR-QUF-53 [RD.171]: an estimate of total uncertainty, as provided in the L4 files, is the most popular way of communicating uncertainty with potential users.
- Sea ice fraction and sea ice flags are provided in the L4 files (SST_CCI-UR-QUF-60 and SST_CCI-UR-QUF-69, [RD.171]).



Table 19. Variables to be included within the SST_cci L4 data files; some of the name and description information in this table is reproduced from Section 11.2 of [AD.1]; see [AD.1] for more details. The shading (see Table 7) and the OCC column indicate the number of occurrences of each variable. All variables listed are mandatory (1, shaded blue).

Name	Description	OCC
lat	Central latitude of each spatial point of the data arrays	1
lat_bnds	Latitude bounds of each grid cell; included from [RD.166].	1
lon	Central longitude of each spatial point of the data arrays	1
lon_bnds	Longitude bounds of each grid cell; included from [RD.166].	1
time	Time of each temporal point of the data arrays; time should be the middle of the day that the data represents	1
time_bnds	Time bounds of each time point (start and end of the day); included from [RD.166]	1
analysed_sst	Sea surface temperature data; this will either be a foundation SST (demonstration ECV) or 20 cm depth SST (long term ECV); fill values to be used where there is land; where there is total sea ice cover the analysis will contain temperatures that relax over time towards -1.8°C.	1
analysis_error	Analysis uncertainty (one error standard deviation)	1
sea_ice_fraction	Sea ice concentration; taken from OSI SAF data	1
sea_ice_fraction_error	Estimated error standard deviation of sea ice fraction; taken from OSI SAF data	01
mask	Indicates if a location is land, sea-ice or lake	1



4.5.3 Detailed contents

The detailed contents of the files are specified in Table 20. An example of how these contents would look in a real file is given in Appendix A.

Table 20. Detailed contents of the SST_cci L4 files.

Element name		Description	Range/value	Unit	Т	D	Bytes
dataset		Begin of dataset					
dimensions		Begin of dimensions					
	lon	Zonal dimension	7200		sl	1	4
	lat	Meridional dimension	3600		sl	1	4
	time	Time dimension; in practice will be 1.	Unlimited		sl	1	4
	bnds	Dimension for the latitude, longitude and time bounds.	2		sl		4
dimensions		End of dimensions					
variables		Begin of variables					
variable		Begin of variable					
	lat		As Table	18.			
variable		End of variable					
variable		Begin of variable					
	lat_bnds		As Table	18.			
variable		End of variable					
variable		Begin of variable					
	lon		As Table	18.			
variable		End of variable					
variable		Begin of variable					
	lon_bnds		As Table	18.			
variable		End of variable					
variable		Begin of variable					
	time		As Table	18.			
variable		End of variable					
variable		Begin of variable					
	time_bnds		As Table	18.			
variable		End of variable					
variable		Begin of variable					



Element name	Description	Range/value	Unit	Т	D	Bytes
analysed_sst	SST values	[270.15, 318.15] (after scaling)	K	ss	time × lat × lon	time × lat × lon × 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	273.15		fl		4
long_name	A free-text descriptive variable name.	analysed sea surface temperature		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	-300		SS		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	4500		SS		2
standard_name	If demonstration ECV set to "sea_surface_ foundation_ temperature" and include the type attribute; if long term ECV set to "sea_water_ temperature" and include the depth attribute.	sea_surface_ _foundation_t emperature or sea_water_te mperature		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
source	Set to comma separated list of the values of the global source attribute in the input files; see Section 3.5.			st		
depth	Include only if standard_name is set to sea_water_temperature. Effective depth of the SST data.	20 cm		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Start of variable					
analysis_error	Uncertainty in the SSTs	[0, 327.68] (after scaling)	К	SS	time x lat x lon	time x lat x lon x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	estimated error standard deviation of analysed_sst		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		SS		2
valid_max	Maximum valid value for this variable once they are packed (in storage type).	32767		SS		2
standard_name	Unique descriptive name for data.	sea_surface_ foundation_ temperature standard_ error or sea_surface_ water_ temperature standard_ error		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sea_ice_fraction	Sea ice concentration	[0, 1]	Fract ion	sc	time × lat × lon	time × lat × lon
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		SC		1
units	Text description of the units.	1		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4



Element name	Description	Range/value	Unit	Т	D	Bytes
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	sea ice area fraction		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	100		SC		1
standard_name	Unique descriptive name for data.	sea_ice_area _fraction		st		
source	Source of the sea ice concentrations, including version number (to be confirmed).	EUMETSAT_ OSI-SAF- ICE-v1.1		st		
comment	Miscellaneous information about the data or the methods used to produce it. (Optional.)			st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
sea_ice_fraction_error	Sea ice concentration	[0, 1]	Fract ion	sc	time x lat x lon	time x lat x lon
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
units	Text description of the units.	1		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	sea ice area fraction error estimate		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	0		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	100		SC		1
standard_name	Unique descriptive name for data.	sea_ice_area _fraction standard_err or		st		
source	Source of the sea ice concentrations, including version number (to be confirmed).	EUMETSAT_ OSI-SAF- ICE-v1.1		st		
comment	Miscellaneous information about the data or the methods used to produce it.	Estimated error standard deviation of sea ice fraction		st		
attributes	End of attributes					
variable	End of variable					
variable	Start of variable					
mask	Specifies if a location is land, sea-ice or lake	[1, 31]	None	sc	time × lat × lon	time × lat × lon
attributes	Begin of attributes					



Element name	Description	Range/value	Unit	Т	D	Bytes
_FillValue	A value used to indicate array elements containing no valid data.	-128		sc		1
long_name	A free-text descriptive variable name.	sea/land/lake /ice field composite mask		st		
valid_min	Minimum valid value for this variable once they are packed (in storage type).	1		sc		1
valid_max	Maximum valid value for this variable once they are packed (in storage type).	31		sc		1
source	Source of the mask, including version numbers.	NAVOCEAN O_landmask _v1.0, EUMETSAT_ OSI- SAF_icemas k, ARCLake_lak emask		st		
comment	Miscellaneous information about the data or methods used to produce them.	b0: 1=grid cell is open sea water b1: 1=grid cell is land b2: 1=grid cell is lake surface b3: 1=grid cell is sea ice b4-b7: reserved for future grid mask data		st		
flag_meanings	Meaning attached to each flag value.	water land optional_lake _surface sea_ice optional_river _surface		st		
flag_masks	Values that correspond to the flags described in flag_meanings.	1b, 2b, 4b, 8b, 16b		sc		1



Element name	Description	Range/value	Unit	Т	D	Bytes
attributes	End of attributes					
variable	End of variable					
variables	End of variables					
attributes	Begin of global attributes					
	As Table	13.				
comment	To contain any miscellaneous information about the data and methods.			st		
northernmost_latitude	Decimal degrees north, range -90 to +90.	90.0		fl		4
geospatial_lat_max	Identical to northernmost_ latitude	90.0		fl		4
southernmost_latitude	Decimal degrees north, range -90 to +90.	-90.0		fl		4
geospatial_lat_min	Identical to southernmost_ latitude	-90.0		fl		4
easternmost_longitude	Decimal degrees east, range -180 to +180.	180.0		fl		4
geospatial_lon_max	Identical to easternmost_ longitude	180.0		fl		4
westernmost_longitude	Decimal degrees east, range -180 to +180.	-180.0		fl		4
geospatial_lon_min	Identical to westernmost_longitude	-180.0		fl		4
processing_level	Data level.	L4		st		
cdm_data_type	"swath" or "grid"	grid		st		
attributes	End of global attributes					
dataset	End of dataset					



5. FILE SIZE ESTIMATES

An estimate of product size per file for each file type is provided in Table 21. The product sizes are broken down into components with different dimensionality and the number of bytes used for each component is recorded. For example the table reveals that a level 2 file stores data with dimensionality $ni \times nj$ and the total amount of storage required per element of the arrays with these dimensions is 8 bytes (these are the arrays containing the latitudes and longitudes of the data, which are both stored as floating point numbers and use 4 bytes per value). The total storage requirement for these data are therefore $ni \times nj \times 8$ bytes, The total file size can be estimated by assuming values for the dimensions and totalling the storage requirements for all the components.

The size estimates give an indication of the data processing and writing requirements. However, they exclude storage for arrays of characters, which use negligible space compared to the data arrays.

Note that these sizes are for uncompressed files. The sizes for L2 data will vary according to sensor but are representative of the largest files that might be expected. In practice the compression capability of the NetCDF-4/HDF5 format will result in much smaller files. However, even if there were no compression the maximum file size would be ~500 MB, which is usable by a high percentage (71%) of users [RD.189].

Table 21. File size estimates in bytes unless otherwise stated, divided into components with different dimensionality. Total size estimate assumes that ni = 512, nj = 28,000, lon = 7,200, lat = 3,600, time = 1, bnds = 2. Size of level 2 files will vary from sensor to sensor and level 3/4 file sizes depend on the grid that is used.

Dimensionality	Level 2	Level 3	Level 4
Scalars (attributes)	232	252	176
ni <i>or</i> lon	0	4	4
nj <i>or</i> lat	0	4	4
time	4	4	4
(ni <i>or</i> lon) × bnds	0	4	4
(nj <i>or</i> lat) × bnds	0	4	4
time × bnds	0	4	4
(ni or lon) × (nj or lat)	8	0	0
(ni or lon) x (nj or lat) x time	22	24	7
Total uncompressed size estimate	410 MB	593 MB	173 MB



6. ISSUES FOR FUTURE RELEASES OF THIS DOCUMENT

It is recommended that future releases of this product specification should resolve the following issues:

- Currently there is no indication in the file metadata about which version of the
 product specification document was followed when creating each file. It is
 recommended that a new global attribute is added to the specification for each
 data level to provide this information.
- The definition of product strings and filename additional segregators are currently not consistent with those defined by the ESA CCI data standards working group.
 These need to be resolved in the future in a way that allows the SST CCI product specifications to remain consistent with the GDS.



APPENDIX A. CDL LISTINGS OF NETCDF HEADERS

This appendix contains Network Common Data Form Language (CDL) examples of the contents of L2P, L3U and L4 files that conform to the specifications defined in this document.

A.1 L2P example

```
netcdf 20100701000000-ESACCI-L2P GHRSST-SSTskin-AATSR-DM-v02.0-fv01.0 {
dimensions:
      ni = 512 ;
      nj = 28000 ;
      time = 1;
variables:
      float lat(nj, ni) ;
            lat:units = "degrees_north" ;
            lat:long name = "Latitude coordinates" ;
            lat:standard name = "latitude" ;
            lat:valid min = -90.f;
            lat:valid_max = 90.f ;
            lat:reference datum = "geographical coordinates, WGS84
projection";
      float lon(nj, ni) ;
            lon:units = "degrees east" ;
            lon:long name = "Longitude coordinates" ;
            lon:standard name = "longitude" ;
            lon:valid min = -180.f;
            lon:valid max = 180.f ;
            lon:reference datum = "geographical coordinates, WGS84
projection";
      int time(time) ;
            time:units = "seconds since 1981-01-01 00:00:00";
            time:long name = "reference time of sst file" ;
            time:standard name = "time" ;
            time:calendar = "gregorian" ;
      short sea surface temperature(time, nj, ni);
            sea_surface_temperature:_FillValue = -32768s ;
            sea surface temperature:units = "kelvin" ;
            sea_surface_temperature:scale_factor = 0.01f ;
            sea_surface_temperature:add_offset = 273.15f ;
            sea_surface_temperature:long_name = "sea surface skin
temperature";
            sea surface temperature:valid min = -200s ;
            sea surface temperature:valid max = 5000s ;
            sea surface temperature:standard name =
"sea surface skin temperature" ;
            sea_surface_temperature:comment = "Temperature of the skin
of the ocean; total uncertainty =
sqrt(large_scale_correlated_uncertainty^2+synoptically correlated uncert
ainty^2+uncorrelated uncertainty^2)";
            sea_surface_temperature:source = "AATSR-ESA-L1-v2.0" ;
            sea surface temperature:references = "Insert published or
web-based references that describe the data or methods used to produce
them";
            sea surface temperature:depth = "10 micrometres" ;
            sea surface temperature:coordinates = "lon lat" ;
      short sst dtime(time, nj, ni) ;
```



```
sst dtime: FillValue = -32768s;
            sst dtime:units = "seconds" ;
            sst dtime:scale factor = 1.f ;
            sst dtime:add offset = 0.f ;
            sst_dtime:long_name = "time difference from reference time"
;
            sst_dtime:valid_min = -32767s;
            sst_dtime:valid_max = 32767s ;
            sst_dtime:comment = "time plus sst_dtime gives seconds after
1981-01-01 00:00:00";
            sst_dtime:coordinates = "lon lat" ;
      byte sses_bias(time, nj, ni) ;
            sses_bias:_FillValue = -128b ;
            sses bias:units = "kelvin" ;
            sses bias:scale factor = 0.01f ;
            sses_bias:add_offset = 0.f ;
            sses_bias:long_name = "SSES bias estimate" ;
            sses_bias:valid_min = -127b ;
            sses_bias:valid_max = 127b ;
            sses bias:comment = "Populated with zeroes" ;
            sses bias:coordinates = "lon lat" ;
      byte sses standard deviation(time, nj, ni);
            sses standard deviation: FillValue = -128b ;
            sses standard deviation:units = "kelvin" ;
            sses standard deviation:scale factor = 0.01f ;
            sses standard deviation:add offset = 1.27f ;
            sses standard deviation:long name = "SSES standard
deviation" :
            sses standard deviation:valid min = -127b;
            sses standard deviation:valid max = 127b;
            sses_standard_deviation:comment = "Total uncertainty in each
sea surface temperature data point" ;
            sses standard deviation:coordinates = "lon lat" ;
      short l2p_flags(time, nj, ni) ;
            12p_flags:long_name = "L2P flags" ;
            12p_flags:comment = "These flags are important to properly
use the data" ;
            12p flags:coordinates = "lon lat" ;
            12p flags:flag meanings = "microwave land ice lake river
spare views channels";
            12p flags:flag masks = 1s, 2s, 4s, 8s, 16s, 32s, 64s, 128s;
      byte quality_level(time, nj, ni) ;
            quality_level:long_name = "quality level of SST pixel" ;
            quality_level:comment = "These are overall quality
indicators and are those used for all GHRSST SSTs";
            quality level:coordinates = "lon lat";
            quality level:flag meanings = "no data bad data
worst quality low quality acceptable quality best quality";
            quality_level:flag_values = 0b, 1b, 2b, 3b, 4b, 5b ;
      byte wind_speed(time, nj, ni) ;
            wind speed: FillValue = -128b;
            wind_speed:units = "m s-1" ;
            wind_speed:scale factor = 0.1f ;
            wind speed:add offset = 12.7f ;
            wind speed:long name = "10m wind speed" ;
            wind_speed:valid_min = -127b ;
            wind_speed:valid_max = 127b ;
            wind speed:standard name = "wind speed" ;
            wind speed:comment = "Wind speeds sourced from ECMWF ERA
Interim reanalysis; wind speeds greater than 25.4 m/s are set to 25.4";
```



```
wind speed:source = "ERA INTERIM-ECMWF-WSP-v1.0" ;
            wind speed:references = "Insert published or web-based
references that describe the data or methods used to produce them" ;
            wind speed:coordinates = "lon lat" ;
           wind speed:height = "10 m" ;
           wind speed:time offset = 1.f ;
      short sea_surface_temperature_depth(time, nj, ni) ;
            sea_surface_temperature_depth:_FillValue = -32768s ;
            sea_surface_temperature_depth:units = "kelvin" ;
            sea_surface_temperature_depth:scale_factor = 0.01f ;
            sea_surface_temperature_depth:add_offset = 273.15f ;
            sea surface temperature depth:long name = "sea surface
temperature at 0.2 m";
            sea surface temperature depth:valid min = -200s ;
            sea_surface_temperature_depth:valid_max = 5000s ;
            sea_surface_temperature_depth:standard_name =
"sea_water_temperature" ;
           sea_surface_temperature_depth:comment = "Temperature of the
ocean at 20 cm depth; total uncertainty =
sqrt(large scale correlated uncertainty^2+synoptically correlated uncert
ainty^2+uncorrelated uncertainty^2+adjustment uncertainty^2)" ;
            sea surface temperature depth:source = "AATSR-ESA-L1-v2.0" ;
            sea surface temperature depth:references = "Insert published
or web-based references that describe the data or methods used to
produce them" ;
            sea surface temperature depth:depth = "0.2 metre";
            sea surface temperature depth:coordinates = "lon lat" ;
      short large scale correlated uncertainty(time, nj, ni) ;
            large scale correlated uncertainty: FillValue = -32768s ;
            large scale correlated uncertainty:units = "kelvin" ;
            large scale correlated uncertainty:scale factor = 0.01f ;
            large scale correlated uncertainty:add offset = 0.f ;
            large scale correlated uncertainty:long name = "Uncertainty
from errors likely to be correlated over large scales";
           large scale correlated uncertainty:valid min = 0s ;
            large_scale_correlated_uncertainty:valid_max = 5000s ;
            large_scale_correlated_uncertainty:comment = "Component of
uncertainty that is correlated over large scales; can be combined with
other uncertainty estimates to form a total uncertainty";
            large scale correlated uncertainty:references = "Insert
published or web-based references that describe the data or methods used
to produce them";
            large_scale_correlated_uncertainty:coordinates = "lon lat" ;
      short synoptically_correlated_uncertainty(time, nj, ni) ;
            synoptically_correlated_uncertainty:_FillValue = -32768s ;
            synoptically correlated uncertainty:units = "kelvin" ;
            synoptically_correlated_uncertainty:scale_factor = 0.01f ;
            synoptically_correlated_uncertainty:add_offset = 0.f ;
            synoptically_correlated_uncertainty:long_name = "Uncertainty
from errors likely to be correlated over synoptic scales";
            synoptically_correlated_uncertainty:valid_min = 0s ;
            synoptically_correlated_uncertainty:valid_max = 5000s ;
            synoptically correlated uncertainty:comment = "Component of
uncertainty that is correlated over synoptic scales; can be combined
with other uncertainty estimates to form a total uncertainty";
            synoptically correlated uncertainty:references = "Insert
published or web-based references that describe the data or methods used
to produce them" ;
            synoptically correlated uncertainty:coordinates = "lon lat"
```



```
synoptically correlated uncertainty:correlation length scale
= "100 km";
           synoptically correlated uncertainty:correlation time scale =
"1 day" ;
      short uncorrelated uncertainty(time, nj, ni);
           uncorrelated_uncertainty:_FillValue = -32768s ;
           uncorrelated_uncertainty:units = "kelvin" ;
           uncorrelated_uncertainty:scale_factor = 0.01f ;
           uncorrelated_uncertainty:add_offset = 0.f ;
           uncorrelated_uncertainty:long_name = "Uncertainty from
errors likely to be uncorrelated between SSTs";
           uncorrelated uncertainty:valid min = 0s ;
           uncorrelated_uncertainty:valid_max = 5000s ;
           uncorrelated uncertainty:comment = "Component of uncertainty
that is uncorrelated between SSTs; can be combined with other
uncertainty estimates to form a total uncertainty";
           uncorrelated_uncertainty:references = "Insert published or
web-based references that describe the data or methods used to produce
them";
           uncorrelated uncertainty:coordinates = "lon lat" ;
      short adjustment uncertainty(time, nj, ni) ;
           adjustment uncertainty: FillValue = -32768s;
           adjustment uncertainty:units = "kelvin" ;
            adjustment uncertainty:scale factor = 0.01f;
            adjustment uncertainty:add offset = 0.f;
           adjustment uncertainty:long name = "Time and depth
adjustment uncertainty";
           adjustment uncertainty:valid min = 0s;
            adjustment uncertainty:valid max = 5000s;
           adjustment uncertainty:comment = "Adjustment uncertainty;
can be combined with other uncertainty estimates to form a total
uncertainty";
           adjustment uncertainty:references = "Insert published or
web-based references that describe the data or methods used to produce
them";
            adjustment uncertainty:coordinates = "lon lat" ;
           adjustment uncertainty:correlation length scale = "100 km";
            adjustment uncertainty:correlation time scale = "1 day" ;
      short sst_depth_total_uncertaintytime, nj, ni) ;
           sst_depth_total_uncertainty:_FillValue = -32768s ;
           sst_depth_total_uncertainty:units = "kelvin" ;
            sst_depth_total_uncertainty:scale_factor = 0.01f ;
            sst_depth_total_uncertainty:add_offset = 0.f ;
            sst_depth_total_uncertainty:long_name = "Total uncertainty
in sea_surface_temperature_depth" ;
            sst depth total uncertainty:valid min = 0s;
            sst depth total uncertainty:valid max = 5000s;
            sst depth total uncertainty:comment = "Total uncertainty in
each sea surface temperature depth data point";
            sst depth total uncertainty:coordinates = "lon lat" ;
// global attributes:
            :Conventions = "CF-1.5, Unidata Observation Dataset v1.0";
            :title = "ESA SST CCI AATSR L2P product" ;
            :summary = "AATSR L2P product from the ESA SST CCI project,
produced using <algorithm name>." ;
           :references = "Insert published or web-based references that
describe the data or methods used to produce them";
            :institution = "ESACCI";
```



```
:history = "SST CCI processor XXX.YY";
            :licence = "TBC" ;
            :id = "AATSR-ESACCI-L2P-v<Version Number>";
            :naming_authority = "org.ghrsst" ;
            :product_version = "1.0" ;
            :uuid = "D7A88FA8-7421-4039-807C-B551D638EDC6";
            :tracking_id = "D7A88FA8-7421-4039-807C-B551D638EDC6";
            :gds_version_id = "2.0" ;
            :netcdf_version_id = "4.1.1" ;
            :date_created = "20110616T152207Z" ;
            :file_quality_level = 3 ;
            :spatial resolution = "1.1km at nadir";
            :start time = "20100701T000000Z";
            :time_coverage_start = "20100701T000000Z" ;
            :stop time = "20100701T013000Z";
            :time_coverage_end = "20100701T013000Z";
            :time_coverage_duration = "PT1H30M" ;
            :time_coverage_resolution = "PT1S" ;
            :source = "AATSR-ESA-L1-v2.0, ERA_INTERIM-ECMWF-WSP-v1.0";
            :platform = "Envisat" ;
            :sensor = "AATSR" ;
            :metadata conventions = "Unidata Dataset Discovery v1.0" ;
            :metadata link = "http://www.esa-cci.org" ;
            :keywords = "Oceans > Ocean Temperature > Sea Surface
Temperature";
            :keywords vocabulary = "NASA Global Change Master Directory
(GCMD) Science Keywords";
            :standard name vocabulary = "NetCDF Climate and Forecast
(CF) Metadata Convention";
            :geospatial lat units = "degrees north" ;
            :geospatial lat resolution = "0.009";
            :geospatial lon units = "degrees east" ;
            :geospatial_lon_resolution = "0.009";
            :geospatial_vertical_min = -0.2f ;
            :geospatial_vertical_max = -1.e-05f ;
            :acknowledgment = "Funded by ESA" ;
            :creator_name = "ESA SST CCI" ;
            :creator email = "science.leader@esa-sst-cci.org";
            :creator url = "http://www.esa-sst-cci.org" ;
            :creator processing institution = "These data were produced
at <institution> as part of the ESA SST CCI project."
            :project = "European Space Agency Sea Surface Temperature
Climate Change Initiative";
            :publisher_name = "ESACCI" ;
            :publisher_url = "http://www.esa-sst-cci.org" ;
            :publisher email = "science.leader@esa-SST-cci.org";
            :comment = "See the comment attributes to the
sea surface temperature and sea surface temperature depth variables for
information about uncertainty estimates.";
            :northernmost_latitude = 90.f ;
            :southernmost latitude = -90.f;
            :easternmost_longitude = -180.f ;
            :westernmost_longitude = 180.f ;
            :geospatial_lat_max = 90.f ;
            :geospatial_lat_min = -90.f ;
            :geospatial_lon_max = -180.f ;
            :geospatial_lon_min = 180.f ;
            :processing level = "L2P" ;
            :cdm data type = "swath" ;
}
```



A.2 L3U example

```
netcdf 20100701000000-ESACCI-L3U GHRSST-SSTskin-AATSR-LT-v02.0-fv01.0 {
dimensions:
      lon = 7200 ;
      lat = 3600 ;
      bnds = 2 ;
      time = UNLIMITED ; // (1 currently)
variables:
      float lat(lat) ;
            lat:units = "degrees north" ;
            lat:long name = "Latitude" ;
            lat:standard name = "latitude" ;
            lat:valid min = -90.f ;
            lat:valid max = 90.f ;
            lat:reference_datum = "geographical coordinates, WGS84"
projection";
            lat:axis = "Y" ;
            lat:bounds = "lat_bnds" ;
      float lat bnds(lat, bnds) ;
            lat bnds:units = "degrees north" ;
            lat_bnds:long_name = "Latitude cell boundaries" ;
            lat bnds:valid min = -90.f ;
            lat bnds:valid max = 90.f ;
            lat bnds:comment = "Contains the northern and southern
boundaries of the grid cells.";
            lat bnds:reference datum = "geographical coordinates, WGS84
projection";
      float lon(lon) ;
            lon:units = "degrees east" ;
            lon:long name = "Longitude" ;
            lon:standard name = "longitude" ;
            lon:valid min = -180.f ;
            lon:valid max = 180.f ;
            lon:reference datum = "geographical coordinates, WGS84
projection";
            lon:axis = "X" ;
            lon:bounds = "lon bnds" ;
      float lon bnds(lon, bnds) ;
            lon bnds:units = "degrees east" ;
            lon bnds:long name = "Longitude cell boundaries" ;
            lon bnds:valid min = -180.f ;
            lon bnds:valid max = 180.f ;
            lon bnds:comment = "Contains the eastern and western
boundaries of the grid cells.";
            lon_bnds:reference_datum = "geographical coordinates, WGS84
projection";
      int time(time) ;
            time:units = "seconds since 1981-01-01 00:00:00";
            time:long name = "reference time of sst file" ;
            time:standard name = "time" ;
            time:axis = \overline{T};
            time:calendar = "gregorian" ;
            time:bounds = "time_bnds" ;
      int time_bnds(time, bnds) ;
            time bnds:units = "seconds since 1981-01-01 00:00:00";
            time bnds:long name = "Time cell boundaries" ;
```



```
time bnds:comment = "Contains the start and end times for
the time period the data represent";
      short sea_surface_temperature(time, lat, lon) ;
            sea_surface_temperature:_FillValue = -32768s ;
            sea_surface_temperature:units = "kelvin" ;
            sea_surface_temperature:scale_factor = 0.01f ;
            sea_surface_temperature:add_offset = 273.15f ;
            sea_surface_temperature:long_name = "sea surface skin
temperature" ;
            sea_surface_temperature:valid_min = -200s ;
            sea_surface_temperature:valid_max = 5000s ;
            sea_surface_temperature:standard_name =
"sea surface skin temperature" ;
            sea surface temperature:comment = "Temperature of the skin
of the ocean; total uncertainty =
sqrt(large scale correlated uncertainty^2+synoptically correlated uncert
ainty^2+uncorrelated_uncertainty^2)";
            sea_surface_temperature:source = "AATSR-ESA-L1-v2.0" ;
            sea_surface_temperature:references = "Insert published or
web-based references that describe the data or methods used to produce
them";
            sea surface temperature:depth = "10 micrometres" ;
      int sst dtime(time, lat, lon) ;
            sst dtime: FillValue = 0 ;
            sst dtime:units = "seconds" ;
            sst dtime:scale factor = 1. ;
            sst dtime:add offset = 0.;
            sst dtime:long name = "time difference from reference time"
            sst dtime:valid min = -43200;
            sst dtime:valid max = 43200 ;
            sst dtime:comment = "time plus sst dtime gives seconds after
1981-01-01 00:00:00";
      byte sses bias(time, lat, lon);
            sses_bias:_FillValue = -128b ;
            sses_bias:units = "kelvin" ;
            sses_bias:scale_factor = 0.01f ;
            sses bias:add offset = 1.27f ;
            sses bias:long name = "SSES bias estimate" ;
            sses_bias:valid_min = -127b ;
            sses_bias:valid_max = 127b ;
            sses_bias:comment = "Populated with zeroes" ;
      byte sses standard deviation(time, lat, lon);
            sses_standard_deviation:_FillValue = -128b ;
            sses_standard_deviation:units = "kelvin" ;
            sses standard deviation:scale factor = 0.01f ;
            sses standard deviation:add offset = 0.f ;
            sses standard deviation:long name = "SSES standard
deviation";
            sses standard deviation:valid min = -127b ;
            sses standard deviation:valid max = 127b ;
            sses standard deviation:comment = " Total uncertainty in
each sea surface temperature data point";
            sses standard deviation:coordinates = "lon lat" ;
      short 12p flags(time, lat, lon) ;
            12p_flags:long_name = "L2P flags" ;
            12p flags:comment = "These flags are important to properly
use the data" ;
            12p_flags:flag_meanings = "microwave land ice lake river
spare views channels";
```



```
12p flags:flag masks = 1s, 2s, 4s, 8s, 16s, 32s, 64s, 128s;
      byte quality level(time, lat, lon);
            quality level:long name = "quality level of SST pixel" ;
            quality_level:comment = "These are overall quality
indicators and are those used for all GHRSST SSTs";
            quality_level:flag_meanings = "no_data bad_data
worst_quality low_quality acceptable_quality best_quality" ;
           quality_level:flag_values = 0b, 1b, 2b, 3b, 4b, 5b;
      byte wind_speed(time, lat, lon) ;
           wind_speed:_FillValue = -128b ;
           wind speed:units = "m s-1" ;
           wind speed:scale factor = 0.1f ;
           wind speed:add offset = 12.7f ;
           wind_speed:long_name = "10m wind speed" ;
           wind speed:valid min = -127b;
           wind_speed:valid_max = 127b ;
           wind speed:standard name = "wind speed" ;
           wind speed:comment = "Wind speeds sourced from ECMWF ERA
Interim reanalysis; wind speeds greater than 25.4 m/s are set to 25.4";
           wind speed:source = "ERA INTERIM-ECMWF-WSP-v1.0" ;
           wind speed:references = "Insert published or web-based
references that describe the data or methods used to produce them" ;
           wind speed:height = "10 m";
           wind speed:time offset = 1.f;
      short sea surface temperature depth(time, lat, lon);
           sea surface temperature depth: FillValue = -32768s;
            sea surface temperature depth:units = "kelvin" ;
            sea surface temperature depth:scale factor = 0.01f ;
            sea surface temperature depth:add offset = 273.15f ;
           sea surface temperature depth:long name = "sea surface
temperature at 0.2 m";
           sea surface temperature depth:valid min = -200s;
            sea_surface_temperature depth:valid max = 5000s ;
            sea_surface_temperature_depth:standard_name =
"sea_water_temperature" ;
           sea_surface_temperature_depth:comment = "Temperature of the
ocean at 20 cm depth; total uncertainty =
sqrt(large scale correlated uncertainty^2+synoptically correlated uncert
ainty^2+uncorrelated uncertainty^2+adjustment uncertainty^2) " ;
            sea_surface_temperature_depth:source = "AATSR-ESA-L1-v2.0" ;
            sea surface temperature depth:references = "Insert published
or web-based references that describe the data or methods used to
produce them" ;
            sea_surface_temperature_depth:depth = "0.2 metre" ;
      short large_scale_correlated_uncertainty(time, lat, lon) ;
           large scale correlated uncertainty: FillValue = -32768s ;
            large_scale_correlated_uncertainty:units = "kelvin" ;
            large_scale_correlated_uncertainty:scale_factor = 0.01f ;
            large_scale_correlated_uncertainty:add_offset = 0.f ;
           large_scale_correlated_uncertainty:long name = "Uncertainty
from errors likely to be correlated over large scales";
            large scale correlated uncertainty:valid min = 0s ;
            large scale correlated uncertainty:valid max = 5000s ;
           large scale correlated uncertainty:comment = "Component of
uncertainty that is correlated over large scales; can be combined with
other uncertainty estimates to form a total uncertainty";
           large scale correlated uncertainty:references = "Insert
published or web-based references that describe the data or methods used
to produce them";
      short synoptically correlated uncertainty(time, lat, lon) ;
```



```
synoptically correlated uncertainty: FillValue = -32768s;
            synoptically_correlated_uncertainty:units = "kelvin" ;
            synoptically_correlated_uncertainty:scale_factor = 0.01f ;
            synoptically_correlated_uncertainty:add_offset = 0.f ;
            synoptically_correlated_uncertainty:long_name = "Uncertainty
from errors likely to be correlated over synoptic scales";
            synoptically_correlated_uncertainty:valid_min = 0s ;
            synoptically_correlated_uncertainty:valid_max = 5000s ;
            synoptically_correlated_uncertainty:comment = "Component of
uncertainty that is correlated over synoptic scales; can be combined
with other uncertainty estimates to form a total uncertainty";
            synoptically_correlated_uncertainty:references = "Insert
published or web-based references that describe the data or methods used
to produce them";
            synoptically correlated uncertainty:correlation length scale
= "100 km";
            synoptically correlated uncertainty:correlation time scale =
"1 day" ;
      short uncorrelated_uncertainty(time, lat, lon) ;
           uncorrelated uncertainty: FillValue = -32768s;
           uncorrelated uncertainty:units = "kelvin" ;
           uncorrelated uncertainty:scale factor = 0.01f ;
           uncorrelated uncertainty:add offset = 0.f ;
           uncorrelated_uncertainty:long name = "Uncertainty from
errors likely to be uncorrelated between SSTs";
           uncorrelated uncertainty: valid min = 0s;
           uncorrelated uncertainty:valid max = 5000s;
           uncorrelated uncertainty:comment = "Component of uncertainty
that is uncorrelated between SSTs; can be combined with other
uncertainty estimates to form a total uncertainty";
           uncorrelated_uncertainty:references = "Insert published or
web-based references that describe the data or methods used to produce
them" ;
      short adjustment_uncertainty(time, lat, lon) ;
           adjustment_uncertainty:_FillValue = -32768s ;
            adjustment uncertainty:units = "kelvin" ;
            adjustment_uncertainty:scale_factor = 0.01f ;
            adjustment uncertainty:add offset = 0.f;
           adjustment uncertainty:long name = "Time and depth
adjustment uncertainty";
           adjustment uncertainty:valid min = 0s ;
            adjustment uncertainty:valid max = 5000s;
            adjustment uncertainty:comment = "Adjustment uncertainty;
can be combined with other uncertainty estimates to form a total
uncertainty";
            adjustment uncertainty:references = "Insert published or
web-based references that describe the data or methods used to produce
them";
            adjustment uncertainty:correlation length scale = "100 km";
            adjustment uncertainty:correlation time scale = "1 day" ;
      short sst depth total uncertaintytime, nj, ni);
            sst_depth_total_uncertainty:_FillValue = -32768s ;
            sst_depth_total_uncertainty:units = "kelvin" ;
            sst_depth_total_uncertainty:scale_factor = 0.01f ;
            sst_depth_total_uncertainty:add_offset = 0.f ;
            sst_depth_total_uncertainty:long_name = "Total uncertainty
in sea_surface_temperature_depth" ;
            sst_depth_total_uncertainty:valid_min = 0s ;
            sst_depth_total_uncertainty:valid max = 5000s ;
```



```
sst depth total uncertainty:comment = "Total uncertainty in
each sea surface temperature depth data point";
// global attributes:
            :Conventions = "CF-1.5, Unidata Observation Dataset v1.0";
            :title = "ESA SST CCI AATSR L3U product" ;
            :summary = "AATSR L3U product from the ESA SST CCI project,
produced using <algorithm name>.";
            :references = "Insert published or web-based references that
describe the data or methods used to produce them";
            :institution = "ESACCI" ;
            :history = "SST CCI processor XXX.YY" ;
            :licence = "TBC" ;
            :id = "AATSR-ESACCI-L3U-v<Version Number>";
            :naming_authority = "org.ghrsst" ;
            :product version = "1.0";
            :uuid = "D7A88FA8-7421-4039-807C-B551D638EDC6" ;
            :tracking id = "D7A88FA8-7421-4039-807C-B551D638EDC6";
            :gds_version_id = "2.0" ;
            :netcdf version id = "4.1.1" ;
            :date created = "20110616T152612Z" ;
            :file quality level = 3;
            :spatial resolution = "1.1km at nadir" ;
            :start time = "20100701T000000Z";
            :time coverage start = "20100701T000000Z";
            :stop time = "20100701T013000Z";
            :time coverage end = "20100701T013000Z";
            :time coverage duration = "PT1H30M";
            :time coverage resolution = "PT1S" ;
            :source = "AATSR-ESA-L1-v2.0, ERA INTERIM-ECMWF-WSP-v1.0";
            :platform = "Envisat" ;
            :sensor = "AATSR" ;
            :metadata conventions = "Unidata Dataset Discovery v1.0" ;
            :metadata link = "http://www.esa-cci.org" ;
            :keywords = "Oceans > Ocean Temperature > Sea Surface
Temperature";
            :keywords_vocabulary = "NASA Global Change Master Directory
(GCMD) Science Keywords";
            :standard name vocabulary = "NetCDF Climate and Forecast
(CF) Metadata Convention";
            :geospatial_lat_units = "degrees_north" ;
            :geospatial_lat_resolution = "0.05";
            :geospatial_lon_units = "degrees_east";
:geospatial_lon_resolution = "0.05";
            :geospatial_vertical_min = -0.2f ;
            :geospatial vertical max = -1.e-05f;
            :acknowledgment = "Funded by ESA" ;
            :creator_name = "ESA SST CCI" ;
            :creator email = "science.leader@esa-sst-cci.org";
            :creator url = "http://www.esa-sst-cci.org" ;
            :creator processing institution = "These data were produced
at <institution> as part of the ESA SST CCI project."
            :project = "European Space Agency Sea Surface Temperature
Climate Change Initiative";
            :publisher name = "ESACCI" ;
            :publisher url = "http://www.esa-sst-cci.org";
            :publisher email = "science.leader@esa-SST-cci.org";
            :comment = "See the comment attributes to the
sea_surface_temperature and sea_surface_temperature_depth variables for
information about uncertainty estimates.";
```



```
:northernmost_latitude = 90.f ;
:southernmost_latitude = -90.f ;
:easternmost_longitude = -180.f ;
:westernmost_longitude = 180.f ;
:geospatial_lat_max = 90.f ;
:geospatial_lat_min = -90.f ;
:geospatial_lon_max = -180.f ;
:geospatial_lon_min = 180.f ;
:processing_level = "L3U" ;
:cdm_data_type = "grid" ;
}
```

A.3 L4 example

```
netcdf 20100701000000-ESACCI-L4 GHRSST-SSTdepth-OSTIA-GLOB LT-v02.0-
fv01.0 {
dimensions:
      lon = 7200 ;
      lat = 3600 ;
      bnds = 2;
      time = UNLIMITED ; // (1 currently)
variables:
      float lat(lat) ;
            lat:units = "degrees north" ;
            lat:long name = "Latitude" ;
            lat:standard name = "latitude" ;
            lat:valid min = -90.f ;
            lat:valid_max = 90.f ;
            lat:reference datum = "geographical coordinates, WGS84"
projection";
            lat:axis = "Y" ;
            lat:bounds = "lat bnds" ;
      float lat bnds(lat, bnds) ;
            lat bnds:units = "degrees north" ;
            lat bnds:long name = "Latitude cell boundaries" ;
            lat bnds:valid min = -90.f ;
            lat bnds:valid max = 90.f ;
            lat bnds:comment = "Contains the northern and southern
boundaries of the grid cells.";
            lat_bnds:reference_datum = "geographical coordinates, WGS84"
projection";
      float lon(lon) ;
            lon:units = "degrees east" ;
            lon:long name = "Longitude" ;
            lon:standard name = "longitude" ;
            lon:valid min = -180.f ;
            lon:valid max = 180.f ;
            lon:reference datum = "geographical coordinates, WGS84"
projection";
            lon:axis = "X" ;
            lon:bounds = "lon bnds" ;
      float lon bnds(lon, bnds);
            lon bnds:units = "degrees east" ;
            lon_bnds:long_name = "Longitude cell boundaries" ;
            lon bnds:valid min = -180.f ;
            lon_bnds:valid_max = 180.f ;
            lon bnds:comment = "Contains the eastern and western
boundaries of the grid cells.";
```



```
lon bnds:reference datum = "geographical coordinates, WGS84
projection";
      int time(time) ;
            time:units = "seconds since 1981-01-01 00:00:00";
            time:long name = "reference time of sst file" ;
            time:standard name = "time" ;
            time:axis = \overline{T};
            time:calendar = "gregorian" ;
            time:bounds = "time bnds" ;
      float time_bnds(time, bnds) ;
            time bnds:units = "seconds since 1981-01-01 00:00:00";
            time bnds:long name = "Time cell boundaries" ;
            time bnds:comment = "Contains the start and end times for
the time period the data represent";
      short analysed_sst(time, lat, lon) ;
            analysed_sst:_FillValue = -32768s ;
            analysed sst:units = "kelvin" ;
            analysed sst:scale factor = 0.01f ;
            analysed_sst:add_offset = 273.15f ;
            analysed sst:long name = "analysed sea surface temperature"
;
            analysed sst:valid min = -300s ;
            analysed sst:valid max = 4500s;
            analysed sst:standard name = "sea water temperature" ;
            analysed sst:source = "AATSR-ESACCI-L3U-LT-v01.0, AVHRR19 G-
ESACCI-L2P-LT-v01.0";
            analysed sst:depth = "20 cm";
      short analysis error(time, lat, lon);
            analysis error: FillValue = -32768s;
            analysis error:units = "kelvin" ;
            analysis error:scale factor = 0.01f ;
            analysis_error:add_offset = 0.f ;
            analysis_error:long_name = "estimated error standard
deviation of analysed sst";
            analysis error:valid min = 0s;
            analysis_error:valid_max = 32767s ;
            analysis_error:standard_name = "sea_water_temperature
standard error";
      byte sea ice fraction(time, lat, lon);
            sea ice fraction: FillValue = -128b ;
            sea ice fraction:units = "1" ;
            sea ice fraction:scale factor = 0.01f ;
            sea_ice_fraction:add_offset = 0.f ;
            sea_ice_fraction:long_name = "sea ice area fraction" ;
            sea_ice_fraction:valid_min = 0s ;
            sea ice fraction:valid max = 100s ;
            sea ice fraction:standard name = "sea ice area fraction" ;
            sea_ice_fraction:source = "EUMETSAT_OSI-SAF-ICE-v1.1" ;
      byte sea_ice_fraction_error(time, lat, lon) ;
            sea ice fraction: FillValue = -128b;
            sea ice fraction:units = "1" ;
            sea ice fraction:scale factor = 0.01f;
            sea_ice_fraction:add offset = 0.f ;
            sea ice fraction:long name = "sea ice area fraction error
estimate";
            sea_ice_fraction:valid min = 0s ;
            sea_ice_fraction:valid_max = 100s ;
            sea ice fraction:standard name = "sea ice area fraction
standard error"
            sea ice fraction:source = "EUMETSAT OSI-SAF-ICE-v1.1" ;
```



```
byte mask(time, lat, lon) ;
            mask: FillValue = -128b ;
            mask:long name = "sea/land/lake/ice field composite mask" ;
            mask:valid min = 1b ;
            mask:valid max = 31b ;
            mask:source = "NAVOCEANO landmask v1.0, EUMETSAT OSI-
SAF icemask, ARCLake_lakemask" ;
            mask:comment = "b0: 1=grid cell is open sea water b1: 1=grid
cell is land b2: 1=grid cell is lake surface b3: 1=grid cell is sea ice
b4-b7: reserved for future grid mask data";
            mask:flag meanings = "water land optional lake surface sea-
ice optional river surface" ;
            mask:flag masks = 1b, 2b, 4b, 8b, 16b;
// global attributes:
            :Conventions = "CF-1.5, Unidata Observation Dataset v1.0";
            :title = "ESA SST CCI OSTIA L4 product" ;
            :summary = "OSTIA L4 product from the ESA SST CCI project,
produced using <algorithm name>." ;
            :references = "Insert published or web-based references that
describe the data or methods used to produce them" ;
            :institution = "ESACCI";
            :history = "SST CCI processor XXX.YY" ;
            :licence = "TBC" ;
            :id = "OSTIA-ESACCI-L4-v<Version Number>";
            :naming authority = "org.ghrsst" ;
            :product version = "1.0";
            :uuid = "D7A88FA8-7421-4039-807C-B551D638EDC6";
            :tracking id = "D7A88FA8-7421-4039-807C-B551D638EDC6";
            :qds version id = "2.0";
            :netcdf version id = "4.1.1" ;
            :date created = "20110616T152836Z";
            :file_quality_level = 3 ;
            :spatial resolution = "1.1km at nadir";
            :start time = "20100701T000000Z";
            :time_coverage_start = "20100701T000000Z";
            :stop_time = "20100701T235959Z" ;
            :time_coverage_end = "20100701T235959Z";
            :time_coverage_duration = "P1D" ;
            :time coverage resolution = "P1D";
            :source = "AATSR-ESACCI-L3U-v1.0, AVHRR-ESACCI-L2P-v1.0,
EUMETSAT OSI-SAF-ICE-v1.1" ;
            :platform = "Envisat, NOAA-<X>";
            :sensor = "AATSR" ;
            :metadata_conventions = "Unidata Dataset Discovery v1.0" ;
            :metadata link = "http://www.esa-cci.org" ;
            :keywords = "Oceans > Ocean Temperature > Sea Surface
Temperature";
            :keywords vocabulary = "NASA Global Change Master Directory
(GCMD) Science Keywords";
            :standard name vocabulary = "NetCDF Climate and Forecast
(CF) Metadata Convention";
            :geospatial_lat_units = "degrees_north" ;
            :geospatial_lat_resolution = "0.05";
            :geospatial_lon_units = "degrees_east" ;
            :geospatial_lon_resolution = "0.05";
            :geospatial_vertical_min = -0.2f ;
            :geospatial_vertical_max = -0.2f ;
            :acknowledgment = "Funded by ESA" ;
            :creator_name = "ESA SST CCI" ;
```



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```
:creator email = "science.leader@esa-sst-cci.org";
            :creator url = "http://www.esa-sst-cci.org";
            :creator_processing_institution = "These data were produced
at the Met Office as part of the ESA SST CCI project."
            :project = "European Space Agency Sea Surface Temperature
Climate Change Initiative";
            :publisher_name = "ESACCI" ;
            :publisher_url = "http://www.esa-sst-cci.org" ;
            :publisher_email = "science.leader@esa-SST-cci.org";
            :comment = "";
            :northernmost_latitude = 90.f ;
            :southernmost_latitude = -90.f ;
            :easternmost_longitude = -180.f ;
            :westernmost_longitude = 180.f ;
            :geospatial_lat_max = 90.f ;
            :geospatial_lat_min = -90.f ;
            :geospatial_lon_max = -180.f;
            :geospatial_lon_min = 180.f ;
            :processing_level = "L4" ;
            :cdm data type = "grid" ;
}
```



APPENDIX B. SPECIFICATION OF FILES TO STORE SSTS FROM INDIVIDUAL RETRIEVALS

The SST_cci products will contain SSTs derived using the best available retrievals. For example a retrieval that makes use of three channels would be preferred to a two channel retrieval. No user requirement has been identified for the 'non-best' retrievals. However, it is possible that a user requirement may arise and so a specification for files to hold these retrievals is presented here. These are referred to as auxiliary files.

Auxiliary files are defined to contain each individual retrieval type and the adjustments that can be used to translate the SSTs to represent a standard depth and time (produced for the long term ECV only). As defined here, these can only be used in combination with the SST_cci files containing the best retrievals as they do not contain variables that do not vary with retrieval type. By not including these variables, storage requirements are reduced. The user would obtain any data and metadata that are not included in the auxiliary file from the file containing the best retrievals. However, this clearly has the disadvantage that the complexity of managing the data is increased.

B.1 L2P auxiliary files

Two basic auxiliary file structures are specified as containers for:

- 1. types of retrievals additional to the 'best available' retrievals in the L2P files, and,
- 2. adjustments to convert the SSTs to a standard depth and time (20 cm depth at 10.30 am or pm).

The first type of auxiliary file will store the results from different (alternative) retrieval algorithms. The adjustments to convert to standard depth and time are independent of retrieval type and so are stored separately in the second type of auxiliary file. The contents of these are designed to be minimal to reduce storage space. They are only usable in combination with their corresponding L2P file. Attributes in the file informs the user of the name of the full L2P file that corresponds to the auxiliary file and its universally unique identifier.

Files for the different retrievals

File name

The file name shall be identical to the name of the L2P file except the <Additional Segregator> component shall additionally be used to distinguish between retrievals. The form of this shall be:

<Additional Segregator> = <LT or DM>_Aux_<Retrieval_><View_><Channels>

<Retrieval_> is used to record the nature of the retrieval algorithm; for example "OE1_", "OE2_".

<View_> is used to record the number of views used in the retrieval; possible values are "Nadir_" and "Dual_". Only include this for ATSR data as it is not applicable to other sensors.

<Channels> is used to record the number of channels used in the retrieval; possible values are "2_channel" and "3_channel".



File structure

The structure of the file is described in Table 22. It comprises components that have changed relative to the L2P file. The adjusted SST for the alternative retrieval can be calculated by the user from the information in the auxiliary file containing the adjustments. Global attributes are provided to link the file to its L2P counterpart and to the file containing the adjustments using with the filenames or the universally unique identifiers. The full set of global attributes from the full L2P file is also included.

Table 22. Specification of auxiliary files that can be used to store alternative retrievals to those held in the L2P file.

Element name	Description	Range/value	Unit	Т	D	Bytes
dataset	Begin of dataset	3				,
dimensions	Begin of dimensions					
ni	Across track dimension.			sl	1	4
nj	Along track dimension.			sl	1	4
time	Time dimension; must be 1 for L2P data.	1		sl	1	4
dimensions	End of dimensions					
variables	Begin of variables					
variable	Begin of variable					
sea_surface_temperature	Sea surface temperature retrievals	[271.15, 323.15] (after scaling)	K	SS	time, nj, ni	time x nj x ni x 2
attributes	Beginning of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	273.15		fl		4
long_name	A free-text descriptive variable name. Insert	sea surface skin temperature				



Element name	Description	Range/value	Unit	Т	D	Bytes
	algorithm name as appropriate.	retrieved using <algorithm></algorithm>				
standard_name	Unique descriptive name for data.	sea_surface_ skin_tempera ture				
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
l2p_flags	Specifies type of input data and provide flags and information to the user.	[0, 255] (this may change if extra flags are defined)		SS	time × nj × ni	time x nj x ni x 2
long_name	A free-text descriptive variable name.	L2P flags		st		
flag_meanings	Meaning attached to each flag value.	microwave land ice lake river spare views channels		st		
flag_masks	Bit masks corresponding to the flags described in flag_meanings.	1, 2, 4, 8, 16, 32, 64, 128		SS		2
variable	End of variable					
variable	Begin of variable					
quality_level	Indicator of the quality of each SST.	[0, 5]		sc	time × nj × ni	time × nj × ni
long_name	A free-text descriptive variable name.	quality level of SST pixel		st		
flag_meanings	Meaning attached to each flag value.	no_data bad_data worst_quality low_quality acceptable_q uality best_quality		st		
flag_values	Values that correspond to the flags described in flag_meanings. The b after the numbers is to indicate that they are single byte	0b, 1b, 2b, 3b, 4b, 5b		SC		1



Element name	Description	Range/value	Unit	Т	D	Bytes
	numbers.					
variable	End of variable					
variable	Begin of variable					
large_scale_correlated _uncertainty	Component of uncertainty that is highly correlated between SST retrievals separated by larger than sub-synoptic spatio-temporal scales.	[0, 50] (after scaling)	К	SS	time × nj × ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty from errors likely to be correlated over large scales		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
synoptically_correlated _uncertainty	Component of uncertainty that is highly correlated between SST retrievals separated by subsynoptic spatiotemporal scales.	[0, 50] (after scaling)	К	SS	time × nj × ni	time × nj × ni × 2
attributes	Begin of attributes					



Element name	Description	Range/value	Unit	Т	D	Bytes
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty from errors like to be correlated over synoptic scales		st		
correlation_length_scale	Estimate of the correlation length scale of the uncertainties.	100 km		st		
correlation_time_scale	Estimate of the correlation time scale of the uncertainties	1 day		st		
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
uncorrelated_uncertainty	Component of uncertainty that is uncorrelated between SST retrievals separated by any spatio-temporal scales.	[0, 50] (after scaling)	К	SS	time × nj × ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of	kelvin		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
	the units.					
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Uncertainty from errors likely to be uncorrelated between SSTs		st		
attributes	End of attributes					
variable	End of variable					
variables	End of variables					
attributes	Begin of global attribute					
Global a	attributes as for the full	L2P files (see Ta	able 14)			
full_file	The name of the L2P file that these data correspond to.			st		
full_file_uuid	The universally unique identifier of the full file.					
adj_file	The name of the auxiliary file containing the adjustments to standard depth and time and the corresponding uncertainties.			st		
	Only needs to be inserted where tos is included in the L2P file.					
adj_file_uuid	The universally unique identifier of the adjustments auxiliary file.			st		
attributes	End of global attributes					
dataset	End of dataset					



Files for the adjustments

File name

The file name shall be identical to the name of the L2P file except the <Additional Segregator> component shall additionally be used to distinguish between retrievals. The form of this shall be:

<Additional Segregator> = <LT or DM>_Adj_<Algorithm_>00.2m_10.30

<Algorithm_> is used to for text that distinguishes between different methods of obtaining adjustments.

File structure

The structure of the file is described in Table 23. It comprises only the adjustments to convert the SSTs to the standard depth and time. Adjustments shall be defined anywhere that an SST retrieval is possible. Global attributes are provided to link the file to its L2P counterpart using either the file name or the universally unique identifier. The global attributes from the L2P file are all also included.

Table 23. Specification of auxiliary files that can be used to store adjustments convert SSTs to a standard depth and time.

Element name	Description	Range/value	Unit	Т	D	Bytes
dataset	Begin of dataset					
dimensions	Begin of dimensions					
ni	Across track dimension.	7200		sl	1	4
nj	Along track dimension.	3600		sl	1	4
time	Time dimension; must be 1 for L2P data.	1		sl	1	4
dimensions	End of dimensions					
variables	Begin of variables					
variable	Begin of variable					
sst_adjustments		[-32767, 32767]	K	SS	time, nj, ni	time x nj x ni x 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Adjustment for SSTs to make them correspond to 10.30 local time and depth of 20 cm				
attributes	End of attributes					
variable	End of variable					
variable	Begin of variable					
adjustment_uncertainty	Uncertainty in adjustment for depth and time, correlated between SST estimates separated by subsynoptic spatiotemporal scales.	[0, 50] (after scaling)	К	SS	time × nj × ni	time × nj × ni × 2
attributes	Begin of attributes					
_FillValue	A value used to indicate array elements containing no valid data.	-32768		SS		2
units	Text description of the units.	kelvin		st		
scale_factor	To be multiplied by the variable to recover the original value.	0.01		fl		4
add_offset	To be added to the variable after multiplying by the scale factor to recover the original value.	0.0		fl		4
long_name	A free-text descriptive variable name.	Time and depth adjustment		st		



Element name	Description	Range/value	Unit	Т	D	Bytes
		uncertainty				
correlation_length_scale	Estimate of the correlation length scale of the uncertainties.	100 km		st		
correlation_time_scale	Estimate of the correlation time scale of the uncertainties	1 day		st		
attributes	End of attributes					
variable	End of variable					
variables	End of variables					
attributes Begin of global attribute						
Global attributes as for the full L2P files (see Table 14).						
full_file The name of the L2P file that these data correspond to.				st		
adj_file_uuid	The universally unique identifier of the adjustments auxiliary file.			st		
attributes	End of global attributes					
dataset End of dataset						

B.2 L3 auxiliary files

The SST_cci L3 files (L3U and L3C) are to hold the best available retrievals of SST. As with L2 data, auxiliary files are defined to hold other retrievals and the adjustment to standard depth and time. The same definitions as for L2 data are used; these are defined in Table 22 and Table 23. As with the L2P and L3 file specification, dimensions are named lon and lat in place of ni and nj. The global attributes shall follow the L3 definition given in Table 18, rather than the L2P definitions from Table 14.

B.2.1 Auxiliary file size estimates

Estimates of the sizes of the auxiliary files are given in Table 24. See Section 5 for more details about the contents of this table.



Table 24. File size estimates in bytes unless otherwise stated, divided into components with different dimensionality. Total size estimate assumes that ni = 512, nj = 28,000, lon = 7,200, lat = 3,600, time = 1, bnds = 2. Size of level 2 files will vary from sensor to sensor and level 3 file sizes depend on the grid that is used.

Dimensionality	Level 2 auxiliary – alternate retrievals	Level 2 auxiliary – adjustments	Level 3 auxiliary — alternate retrievals	Level 3 auxiliary – adjustments
Scalars (attributes)	107	84	107	84
ni <i>or</i> lon	0	0	0	0
nj <i>or</i> lat	0	0	0	0
time	0	0	0	0
(ni <i>or</i> lon) × bnds	0	0	0	0
(nj <i>or</i> lat) × bnds	0	0	0	0
time × bnds	0	0	0	0
(ni <i>or</i> lon) × (nj <i>or</i> lat)	0	0	0	0
(ni <i>or</i> lon) × (nj <i>or</i> lat) × time	11	4	11	4
Total uncompressed size estimate	150 MB	55 MB	272 MB	99 MB

B.2.2 CDL listings of NetCDF headers for the auxiliary files

As described in Appendix A, CDL listings of the NetCDF headers of example files are provided.

B.2.2.1 L2P auxiliary file containing SST retrievals

```
netcdf 20100701000000-ESACCI-L2P GHRSST-SSTskin-AATSR-
DM Aux_OE1_Nadir_2_channel-v02.0-fv01.0 {
dimensions:
     ni = 512;
      nj = 28000 ;
      time = 1;
variables:
      short sea surface temperature(time, nj, ni);
            sea surface temperature: FillValue = -32768s;
            sea surface temperature:units = "kelvin" ;
            sea_surface_temperature:scale factor = 0.01f ;
            sea_surface_temperature:add_offset = 273.15f ;
            sea_surface_temperature:long_name = "sea surface temperature"
retrieved using 2-channels, dual view";
            sea surface temperature:standard name =
"sea_surface_skin_temperature" ;
      short l2p_flags(time, nj, ni) ;
```



```
12p flags:long name = "L2P flags";
            12p flags:flag meanings = "microwave land ice lake river
spare views channel" ;
            12p flags:flag masks = 1s, 2s, 4s, 8s, 16s, 32s, 64s, 128s;
      byte quality level(time, nj, ni) ;
            quality_level:long_name = "quality level of SST pixel" ;
            quality_level:flag_meanings = "no_data bad_data
worst_quality low_quality acceptable_quality best_quality" ;
            quality_level:flag_values = 0b, 1b, 2b, 3b, 4b, 5b ;
      short large_scale_correlated_uncertainty(time, nj, ni) ;
            large_scale_correlated_uncertainty:_FillValue = -32768s ;
            large_scale_correlated_uncertainty:units = "kelvin" ;
            large_scale_correlated_uncertainty:scale_factor = 0.01f ;
            large_scale_correlated_uncertainty:add_offset = 0.f ;
            large_scale_correlated_uncertainty:long_name = "Uncertainty
from errors likely to be correlated over large scales";
      short synoptically_correlated_uncertainty(time, nj, ni) ;
            synoptically_correlated_uncertainty:_FillValue = -32768s ;
            synoptically_correlated_uncertainty:units = "kelvin" ;
            synoptically correlated uncertainty:scale factor = 0.01f;
            synoptically correlated uncertainty:add offset = 0.f ;
            synoptically correlated uncertainty:long name = "Uncertainty
from errors likely to be correlated over synoptic scales";
           synoptically correlated uncertainty:correlation length scale
= "100 km";
           synoptically correlated uncertainty:correlation time scale =
"1 day" ;
      short uncorrelated uncertainty(time, nj, ni);
           uncorrelated uncertainty: FillValue = -32768s;
           uncorrelated uncertainty:units = "kelvin" ;
            uncorrelated uncertainty:scale factor = 0.01f;
            uncorrelated uncertainty:add offset = 0.f ;
           uncorrelated uncertainty:long name = "Uncertainty from
errors likely to be uncorrelated between SSTs";
// global attributes:
            :Conventions = "CF-1.5, Unidata Observation Dataset v1.0";
            :title = "ESA SST CCI AATSR L2P product" ;
            :summary = "AATSR L2P product from the ESA SST CCI project,
produced using <algorithm name>." ;
           :references = "Insert published or web-based references that
describe the data or methods used to produce them" ;
            :institution = "ESACCI";
            :history = "SST CCI processor XXX.YY" ;
            :licence = "TBC" ;
            :id = "AATSR-ESACCI-L2P-v<Version Number>";
            :naming authority = "org.ghrsst" ;
            :product version = "1.0";
            :uuid = "E7A88FA8-7421-4039-807C-B551D638EDC6" ;
            :tracking id = "E7A88FA8-7421-4039-807C-B551D638EDC6";
            :gds version id = "2.0";
            :netcdf version id = "4.1.1" ;
            :date created = "20110616T152318Z";
            :file_quality_level = 3;
            :spatial resolution = "1.1km at nadir";
            :start time = "20100701T000000Z";
            :time coverage start = "20100701T000000Z";
            :stop time = "20100701T013000Z" ;
            :time coverage end = "20100701T013000Z";
            :time coverage duration = "PT1H30M" ;
```



```
:time coverage resolution = "PT1S";
            :source = "AATSR-ESA-L1-v2.0, ERA INTERIM-ECMWF-WSP-v1.0";
            :platform = "Envisat" ;
            :sensor = "AATSR" ;
            :metadata_conventions = "Unidata Dataset Discovery v1.0" ;
            :metadata link = "http://www.esa-cci.org" ;
            :keywords = "Oceans > Ocean Temperature > Sea Surface
Temperature";
            :keywords vocabulary = "NASA Global Change Master Directory
(GCMD) Science Keywords";
            :standard name vocabulary = "NetCDF Climate and Forecast
(CF) Metadata Convention";
            :geospatial_lat_units = "degrees_north" ;
            :geospatial_lat_resolution = "0.009";
            :geospatial_lon_units = "degrees_east" ;
            :geospatial_lon_resolution = "0.009";
            :geospatial_vertical_min = -1.e-05f ;
            :geospatial_vertical_max = -1.e-05f ;
            :acknowledgment = "Funded by ESA" ;
            :creator name = "ESA SST CCI" ;
            :creator email = "science.leader@esa-sst-cci.org";
            :creator url = "http://www.esa-sst-cci.org" ;
            :creator processing institution = "These data were produced
at <institution> as part of the ESA SST CCI project."
            :project = "European Space Agency Sea Surface Temperature
Climate Change Initiative";
            :publisher name = "ESACCI" ;
            :publisher url = "http://www.esa-sst-cci.org";
            :publisher email = "science.leader@esa-SST-cci.org" ;
            :comment = "See the comment attributes to the
sea surface temperature and sea surface temperature depth variables for
information about uncertainty estimates.";
            :northernmost latitude = 90.f ;
            :southernmost latitude = -90.f;
            :easternmost longitude = -180.f;
            :westernmost_longitude = 180.f ;
            :geospatial_lat_max = 90.f ;
            :geospatial lat min = -90.f;
            : geospatial lon max = -180.f;
            :geospatial lon min = 180.f ;
            :processing level = "L2P" ;
            :cdm_data_type = "swath" ;
            :full file = "20100701000000-ESACCI-L2P GHRSST-SSTskin-
AATSR-DM-v02.0-fv01.0.nc";
            :full_file_uuid = "D7A88FA8-7421-4039-807C-B551D638EDC6" ;
            :adj file = "20100701000000-ESACCI-L2P GHRSST-SSTskin-AATSR-
DM Adj <Algorithm>00.2m 10.30-v02.0-fv01.0.nc";
            :adj file uuid = "F7A88FA8-7421-4039-807C-B551D638EDC6" ;
```

B.2.2.2 L2P auxiliary file containing SST adjustments

```
netcdf 20100701000000-ESACCI-L2P_GHRSST-SSTskin-AATSR-
DM_Adj_Algorithm_00.2m_10.30-v02.0-fv01.0 {
    dimensions:
        ni = 512 ;
        nj = 28000 ;
        time = 1 ;
    variables:
```



```
short sst adjustments(time, nj, ni) ;
            sst adjustments: FillValue = -32768s;
            sst adjustments:units = "kelvin" ;
            sst adjustments:scale factor = 0.01f ;
            sst adjustments:add offset = 0.f ;
            sst_adjustments:long_name = "Adjustment for SSTs to make
them correspond to 10.30 local time and depth of 20 cm";
      short adjustment_uncertainty(time, nj, ni) ;
            adjustment_uncertainty:_FillValue = -32768s ;
            adjustment_uncertainty:units = "kelvin" ;
            adjustment_uncertainty:scale_factor = 0.01f ;
            adjustment_uncertainty:add_offset = 0.f ;
            adjustment_uncertainty:long_name = "Time and depth
adjustment uncertainty";
            adjustment_uncertainty:correlation_length_scale = "100 km" ;
            adjustment_uncertainty:correlation_time_scale = "1 day" ;
// global attributes:
            :Conventions = "CF-1.5, Unidata Observation Dataset v1.0";
            :title = "ESA SST CCI AATSR L2P product" ;
            :summary = "AATSR L2P product from the ESA SST CCI project,
produced using <algorithm name>." ;
            :references = "Insert published or web-based references that
describe the data or methods used to produce them" ;
            :institution = "ESACCI";
            :history = "SST CCI processor XXX.YY";
            :licence = "TBC" ;
            :id = "AATSR-ESACCI-L2P-v<Version Number>";
            :naming authority = "org.ghrsst" ;
            :product version = "1.0";
            :uuid = "F7A88FA8-7421-4039-807C-B551D638EDC6" ;
            :tracking id = "F7A88FA8-7421-4039-807C-B551D638EDC6";
            :gds version id = "2.0";
            :netcdf_version_id = "4.1.1" ;
            :date_created = "20110616T152330Z" ;
            :file_quality_level = 3;
            :spatial_resolution = "1.1km at nadir" ;
            :start time = "20100701T000000Z";
            :time coverage start = "20100701T000000Z";
            :stop time = "20100701T013000Z";
            :time_coverage_end = "20100701T013000Z";
            :time_coverage_duration = "PT1H30M" ;
            :time_coverage_resolution = "PT1S";
            :source = "AATSR-ESA-L1-v2.0, ERA INTERIM-ECMWF-WSP-v1.0";
            :platform = "Envisat" ;
            :sensor = "AATSR" ;
            :metadata conventions = "Unidata Dataset Discovery v1.0";
            :metadata link = "http://www.esa-cci.org" ;
            :keywords = "Oceans > Ocean Temperature > Sea Surface
Temperature";
            :keywords vocabulary = "NASA Global Change Master Directory
(GCMD) Science Keywords";
            :standard name vocabulary = "NetCDF Climate and Forecast
(CF) Metadata Convention";
            :geospatial_lat_units = "degrees_north" ;
            :geospatial_lat_resolution = "0.009";
            :geospatial_lon_units = "degrees_east" ;
            :geospatial_lon_resolution = "0.009";
            :geospatial_vertical_min = -0.2f ;
            :geospatial_vertical_max = -1.e-05f ;
```



```
:acknowledgment = "Funded by ESA" ;
            :creator name = "ESA SST CCI" ;
            :creator_email = "science.leader@esa-sst-cci.org" ;
            :creator url = "http://www.esa-sst-cci.org" ;
            :creator processing institution = "These data were produced
at <institution> as part of the ESA SST CCI project."
            :project = "European Space Agency Sea Surface Temperature
Climate Change Initiative";
            :publisher_name = "ESACCI" ;
            :publisher_url = "http://www.esa-sst-cci.org" ;
            :publisher_email = "science.leader@esa-SST-cci.org" ;
            :comment = "See the comment attributes to the
sea_surface_temperature and sea_surface_temperature_depth variables for
information about uncertainty estimates.";
            :northernmost_latitude = 90.f ;
            :southernmost_latitude = -90.f ;
            :easternmost_longitude = -180.f ;
            :westernmost_longitude = 180.f ;
            :geospatial_lat_max = 90.f ;
            :geospatial lat min = -90.f;
            : geospatial lon max = -180.f;
            :geospatial lon min = 180.f;
            :processing level = "L2P" ;
            :cdm data type = "swath" ;
            :full file = "20100701000000-ESACCI-L2P GHRSST-SSTskin-
AATSR-DM-v02.0-fv01.0.nc";
            :full file uuid = "D7A88FA8-7421-4039-807C-B551D638EDC6";
}
```

B.2.2.3 L3U auxiliary file containing SST retrievals

```
netcdf 20100701000000-ESACCI-L3U GHRSST-SSTskin-AATSR-
LT_Aux_OE1_Nadir_2_channel-v02.0-fv01.0 {
dimensions:
      lon = 7200 ;
      lat = 3600 ;
      time = UNLIMITED ; // (1 currently)
variables:
      short sea surface temperature(time, lat, lon) ;
            sea surface temperature: FillValue = -32768s ;
            sea_surface_temperature:units = "kelvin" ;
            sea_surface_temperature:scale_factor = 0.01f ;
            sea surface temperature:add offset = 273.15f ;
            sea surface temperature:long name = "sea surface temperature
retrieved using 2-channels, dual view";
            sea surface temperature:standard name =
"sea surface skin temperature";
      short 12p flags(time, lat, lon);
            12p flags:long name = "L2P flags" ;
            12p flags:flag meanings = "microwave land ice lake river
spare views channel";
            12p flags:flag masks = 1s, 2s, 4s, 8s, 16s, 32s, 64s, 128s;
      byte quality level(time, lat, lon);
            quality level:long name = "quality level of SST pixel" ;
            quality level:flag meanings = "no data bad data
worst quality low quality acceptable quality best quality";
            quality_level:flag_values = 0b, 1b, 2b, 3b, 4b, 5b ;
      short large scale correlated uncertainty(time, lat, lon) ;
            large scale correlated uncertainty: FillValue = -32768s ;
```



```
large scale correlated uncertainty:units = "kelvin" ;
            large scale correlated uncertainty:scale factor = 0.01f ;
            large_scale_correlated_uncertainty:add_offset = 0.f ;
            large_scale_correlated_uncertainty:long_name = "Uncertainty
from errors likely to be correlated over large scales";
      short synoptically_correlated_uncertainty(time, lat, lon) ;
            synoptically_correlated_uncertainty:_FillValue = -32768s ;
            synoptically_correlated_uncertainty:units = "kelvin" ;
            synoptically_correlated_uncertainty:scale_factor = 0.01f ;
            synoptically_correlated_uncertainty:add_offset = 0.f ;
            synoptically_correlated_uncertainty:long_name = "Uncertainty
from errors likely to be correlated over synoptic scales";
           synoptically correlated uncertainty:correlation length scale
= "100 km" ;
           synoptically_correlated_uncertainty:correlation_time_scale =
"1 day" ;
      short uncorrelated uncertainty(time, lat, lon);
           uncorrelated_uncertainty:_FillValue = -32768s ;
           uncorrelated_uncertainty:units = "kelvin" ;
           uncorrelated uncertainty:scale factor = 0.01f ;
            uncorrelated uncertainty:add offset = 0.f ;
           uncorrelated_uncertainty:long_name = "Uncertainty from
errors likely to be uncorrelated between SSTs";
// global attributes:
            :Conventions = "CF-1.5, Unidata Observation Dataset v1.0";
            :title = "ESA SST CCI AATSR L3U product";
            :summary = "AATSR L3U product from the ESA SST CCI project,
produced using <algorithm name>." ;
            :references = "Insert published or web-based references that
describe the data or methods used to produce them" ;
            :institution = "ESACCI";
            :history = "SST CCI processor XXX.YY";
            :licence = "TBC" ;
            :id = "AATSR-ESACCI-L3U-v<Version Number>" ;
            :naming_authority = "org.ghrsst" ;
            :product version = "1.0";
            :uuid = "E7A88FA8-7421-4039-807C-B551D638EDC6" ;
            :tracking id = "E7A88FA8-7421-4039-807C-B551D638EDC6";
            :gds_version_id = "2.0" ;
            :netcdf_version_id = "4.1.1" ;
            :date created = "20110616T152756Z";
            :file_quality_level = 3;
            :spatial resolution = "1.1km at nadir" ;
            :start_time = "20100701T000000Z" ;
            :time coverage start = "20100701T000000Z";
            :stop time = "20100701T013000Z";
            :time_coverage_end = "20100701T013000Z";
            :time_coverage_duration = "PT1H30M" ;
            :time_coverage_resolution = "PT1S" ;
            :source = "AATSR-ESA-L1-v2.0, ERA INTERIM-ECMWF-WSP-v1.0";
            :platform = "Envisat" ;
            :sensor = "AATSR" ;
            :metadata_conventions = "Unidata Dataset Discovery v1.0" ;
            :metadata_link = "http://www.esa-cci.org" ;
            :keywords = "Oceans > Ocean Temperature > Sea Surface
Temperature";
            :keywords_vocabulary = "NASA Global Change Master Directory
(GCMD) Science Keywords";
```



```
:standard name vocabulary = "NetCDF Climate and Forecast
(CF) Metadata Convention";
            :geospatial_lat_units = "degrees_north" ;
            :geospatial_lat_resolution = "0.05";
            :geospatial_lon_units = "degrees_east" ;
            :geospatial_lon_resolution = "0.05";
            :geospatial_vertical_min = -1.e-05f ;
            :geospatial_vertical_max = -1.e-05f ;
            :acknowledgment = "Funded by ESA" ;
            :creator_name = "ESA SST CCI" ;
            :creator email = "science.leader@esa-sst-cci.org";
            :creator url = "http://www.esa-sst-cci.org" ;
            :creator_processing_institution = "These data were produced
at <institution> as part of the ESA SST CCI project."
            :project = "European Space Agency Sea Surface Temperature
Climate Change Initiative";
            :publisher_name = "ESACCI" ;
            :publisher url = "http://www.esa-sst-cci.org" ;
            :publisher_email = "science.leader@esa-SST-cci.org" ;
            :comment = "See the comment attributes to the
sea surface temperature and sea surface temperature depth variables for
information about uncertainty estimates.";
            :northernmost latitude = 90.f ;
            :southernmost latitude = -90.f;
            :easternmost longitude = -180.f;
            :westernmost longitude = 180.f;
            :geospatial lat max = 90.f;
            :geospatial lat min = -90.f;
            : geospatial lon max = -180.f;
            :geospatial lon min = 180.f;
            :processing level = "L3U" ;
            :cdm data type = "grid" ;
            :full file = "20100701000000-ESACCI-L3U_GHRSST-SSTskin-
AATSR-LT-v02.0-fv01.0.nc";
            :full_file_uuid = "F7A88FA8-7421-4039-807C-B551D638EDC6" ;
            :adj file = "20100701000000-ESACCI-L3U GHRSST-SSTskin-AATSR-
LT_Adj_<Algorithm>00.2m_10.30-v02.0-fv01.0.nc";
```

B.2.2.4 L3U auxiliary file containing SST adjustments

```
netcdf 20100701000000-ESACCI-L3U GHRSST-SSTskin-AATSR-
LT_Adj_Algorithm 00.2m 10.30-fv01.0 {
dimensions:
     lon = 7200 ;
      lat = 3600 ;
      time = 1 ;
variables:
      short sst adjustments(time, lat, lon);
            sst adjustments: FillValue = -32768s;
            sst adjustments:units = "kelvin" ;
            sst adjustments:scale factor = 0.01f;
            sst adjustments:add offset = 0.f ;
            sst adjustments:long name = "Adjustment for SSTs to make
them correspond to 10.30 local time and depth of 20 cm";
      short adjustment uncertainty(time, lat, lon);
            adjustment uncertainty: FillValue = -32768s;
            adjustment uncertainty:units = "kelvin" ;
            adjustment uncertainty:scale factor = 0.01f;
```



```
adjustment uncertainty:add offset = 0.f;
            adjustment uncertainty:long name = "Time and depth
adjustment uncertainty";
            adjustment_uncertainty:correlation_length_scale = "100 km" ;
            adjustment uncertainty:correlation time scale = "1 day" ;
// global attributes:
            :Conventions = "CF-1.5, Unidata Observation Dataset v1.0";
            :title = "ESA SST CCI AATSR L3U product" ;
            :summary = "AATSR L3U product from the ESA SST CCI project,
produced using <algorithm name>." ;
            :references = "Insert published or web-based references that
describe the data or methods used to produce them" ;
            :institution = "ESACCI" ;
            :history = "SST CCI processor XXX.YY" ;
            :licence = "TBC" ;
            :id = "AATSR-ESACCI-L3U-v<Version Number>";
            :naming_authority = "org.ghrsst" ;
            :product_version = "1.0";
            :uuid = "F7A88FA8-7421-4039-807C-B551D638EDC6" ;
            :tracking id = "F7A88FA8-7421-4039-807C-B551D638EDC6";
            :gds version id = "2.0";
            :netcdf version id = "4.1.1" ;
            :date created = "20110616T152822Z";
            :file quality level = 3;
            :spatial resolution = "1.1km at nadir";
            :start time = "20100701T000000Z";
            :time coverage start = "20100701T000000Z";
            :stop time = "20100701T013000Z";
            :time_coverage_end = "20100701T013000Z";
            :time coverage duration = "PT1H30M";
            :time coverage resolution = "PT1S" ;
            :source = "AATSR-ESA-L1-v2.0, ERA_INTERIM-ECMWF-WSP-v1.0";
            :platform = "Envisat" ;
            :sensor = "AATSR" ;
            :metadata_conventions = "Unidata Dataset Discovery v1.0" ;
            :metadata_link = "http://www.esa-cci.org" ;
            :keywords = "Oceans > Ocean Temperature > Sea Surface
Temperature";
            :keywords vocabulary = "NASA Global Change Master Directory
(GCMD) Science Keywords";
            :standard_name_vocabulary = "NetCDF Climate and Forecast
(CF) Metadata Convention";
            :geospatial_lat_units = "degrees_north" ;
            :geospatial_lat_resolution = "0.05";
            :geospatial_lon_units = "degrees_east" ;
            :geospatial lon resolution = "0.05";
            :geospatial_vertical_min = -0.2f ;
            :geospatial_vertical_max = -1.e-05f ;
            :acknowledgment = "Funded by ESA" ;
            :creator name = "ESA SST CCI" ;
            :creator email = "science.leader@esa-sst-cci.org" ;
            :creator url = "http://www.esa-sst-cci.org" ;
            :creator_processing_institution = "These data were produced
at <institution> as part of the ESA SST CCI project."
            :project = "European Space Agency Sea Surface Temperature
Climate Change Initiative";
            :publisher_name = "ESACCI" ;
            :publisher_url = "http://www.esa-sst-cci.org" ;
            :publisher email = "science.leader@esa-SST-cci.org";
```



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```
:comment = "See the comment attributes to the
sea_surface_temperature and sea_surface_temperature_depth variables for
information about uncertainty estimates.";
    :northernmost_latitude = 90.f;
    :southernmost_latitude = -90.f;
    :easternmost_longitude = -180.f;
    :westernmost_longitude = 180.f;
    :geospatial_lat_max = 90.f;
    :geospatial_lat_min = -90.f;
    :geospatial_lon_max = -180.f;
    :geospatial_lon_min = 180.f;
    :processing_level = "L3U";
    :cdm_data_type = "grid";
    :full_file = "20100701000000-ESACCI-L3U_GHRSST-SSTskin-
AATSR-LT-v02.0-fv01.0.nc";
    :full_file_uuid = "D7A88FA8-7421-4039-807C-B551D638EDC6";
}
```



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