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Project : **SST CCI Phase-II**

Title : **SST CCI Product User Guide**

Abstract : This document is the Product User Guide for the ESA CCI SST project.

Author(s) :

N. Rayner, Met Office
S. Good, Met Office
T. Block, Brockmann Consult
P. Evadzi, Brockmann Consult
O. Embury, U. of Reading

Approved by :

Chris Merchant,
Science Leader, U. of Reading

Accepted by :

Digitally signed by Craig Donlon
Date: 2019.04.19 14:18:28 +01'00'

Craig Donlon
ESA Technical Officer

ESTEC

Distribution : SST_cci team members

ESA (Craig Donlon)

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
v0.11	5 August 2015	Initial draft for comment
v0.13	19 September 2015	Version for review
Draft A	30 October 2015	Amended following internal review
Draft B	6 November 2015	Amended following review by SCL
Issue 1	14 December 2015	Amended following review by ESA. First issue.
V1.11	8 January 2019	Draft Issue 2 for ESA review
Issue 2	8 April 2019	Issue 2, incorporating ESA comments

RECORD OF CHANGES IN THIS ISSUE

Issue	Page/Sec.	Reason	Change
1.07			First complete draft.
1.09			Implemented comments from Chris Merchant, Owen Embury and Simon Good
1.10			Implemented further comments from Owen Embury and Tom Block.
1.11			Included Table 1 on product naming. Draft for ESA review.
1.12			Addressed ESA comments and completed placeholders

QUICK START GUIDE TO ESA SST CCI PRODUCTS

What products are available?

The following data products are now available:

- Stable, low-bias sea surface temperature (SST) data starting during August 1981 and continuing to 31 December 2016 (this version of the Product User Guide describes the Version 2 release).
- Data from the series of Along Track Scanning Radiometer (ATSR) sensors (1991 - 2012) and from the series of Advanced Very High Resolution Radiometer (AVHRR) sensors (1981 - 2016) are presented in three forms:
    - a single orbit per file on an irregular grid with grid cell spacing about 1 km (ATSR series) or 4 km (AVHRR series);
    - a single orbit per file on a 0.05° regular latitude-longitude grid; and
    - a 0.05° regular latitude-longitude grid which collates all orbits for a particular sensor for each day.

Each file contains two sets of SSTs. The first set provides a measure of the temperature of the skin of the water at the time it was observed; the second set are estimates of the temperature at 20 cm depth and at either 1030 h or 2230 h local time, times of day at which SST often closely approximates its daily mean. Each SST has associated with it a total uncertainty estimate, and uncertainty estimates for various contributions to that total uncertainty.

Daily, spatially complete fields of estimated daily mean SST are also available. These were obtained by combining orbit data, using a variational data assimilation technique to provide SSTs where there were no measurements (a single file per day; 0.05° regular latitude-longitude grid). These data start in September 1981 and end in December 2016.)

What tools are available for these products?

Tools have been developed to:

1) regrid any of the ESA SST CCI data to coarser spatial and temporal resolution and

2) perform regional averages of the ESA SST CCI data and generate time series.

How to obtain the data and tools

The Version 2 data are available from the CEDA archive (see http://data.ceda.ac.uk/neodc/esacci/sst/data/CDR_v2/). Contact us at science.leader@esa-SST-cci.org if you would like to use the tools.

How to read the ESA SST CCI data

The data are stored in NetCDF-4 format files. Information about the NetCDF format can be found at http://www.unidata.ucar.edu/software/netcdf/ and some example of reading the data are given in Section 7. Data arrays in NetCDF files are known as 'variables' and each variable has meta-data stored with it. The names of key variables in the product files are given in the table below.

Please also read the notes below the table before using the data, **particularly with regards to interpreting the quality/location type information - it is essential to check this information when using the data**.

Description of the content of key variables in the NetCDF files	Names of variables in files containing single or collated orbits of data	Names of variables in files containing infilled, combined data
Latitudes of the data points	lat	lat
Longitudes of the data points	lon	lon
Sea surface temperature at the skin*	sea_surface_temperature	N/A
Total uncertainty of the sea surface temperature at the skin*#	sses_standard_deviation	N/A
Sea surface temperature at 20 cm depth and 10.30 am and pm local time	sea_surface_temperature_depth	N/A
Infilled daily-mean estimate of sea surface temperature at 20 cm depth	N/A	analysed_sst**
Total uncertainty of the sea surface temperature at 20 cm depth #	sst_depth_total_uncertainty	analysis_uncertainty
Quality / location type (ocean / sea ice / lake etc.) information	l2p_flags and quality_level***	mask****

* Skin SST is the temperature of the radiating surface layer of the water, which is of 10 μm depth.

** 'analysis' is the term used for the combination/interpolation of the SSTs in the orbit files.

*** Good quality SSTs are those where the value in the SST data array is not -32768 and the value in the quality_level variable is 4 or 5.

**** Ocean SST values have mask = 1.

\# Also available in the files is uncertainty broken down into different components.

Important

- Check that the add_offset and scale_factor attributes are being applied when reading the variables. These must be used to convert the data stored in the file to the correct units. Many tools will do this automatically for NetCDF files, so no action may be necessary.

Further information and how to contact us

Table 1 gives the full SST CCI product names, a basic description to include in any written work carried out using the products and acceptable short forms of the names to include once the full name and description have been included early in the article or technical report.

Table 1. SST CCI product names and descriptions. Include in the name whichever of L2P, L2U or L3C has been used. *Use short product name after full product name has been included once. **Use short SST name after basic description has been included once.

Full name (CEDA page)	Full name with acronyms	Basic description	Short product	Short SST	Vs
European Space Agency Sea Surface Temperature Climate Change Initiative: Advanced Very High Resolution Radiometer level-2 Climate Data Record [version X]	ESA SST CCI AVHRR L2P [version X]	SSTs from AVHRR instruments in L2P format at GAC resolution covering 1981 – 2016	SST CCI AVHRR [vX.X]	CCI AVHRR SST	2.0
European Space Agency Sea Surface Temperature Climate Change Initiative: Along-Track Scanning Radiometer level-3 Uncollated Climate Data Record [version X]	ESA SST CCI ATSR L3U [version X]	SSTs from ATSR instruments in L3U format at 0.05° resolution covering 1991 – 2012	SST CCI ATSR [vX.X]	CCI ATSR SST	2.0
European Space Agency Sea Surface Temperature Climate Change Initiative: Analysis Climate Data Record [version X]	ESA SST CCI Analysis [version X]	Satellite-only SST-depth analysis created by OSTIA system from SST CCI ATSR and SST CCI AVHRR products, 0.05° resolution, daily files covering 1981 – 2016	SST CCI analysis [vX.X]	CCI analysis SST	2.0

For further help, first see the rest of this document. There is an extended introductory guide in Section 3 - "Getting started with the ESA SST CCI data" - and more detailed discussions of the data in other sections, plus references to documents that contain even more information. If these do not help, email science.leader@esa-sst-cci.org. We also welcome any feedback about the data to this address.

TABLE OF CONTENTS

1. DOCUMENT PURPOSE AND STRUCTURE

1.1 Purpose and scope

This document is the user guide for the Version 2 data products produced by the ESA SST CCI project. It also includes instructions for how to run tools that are made available by the project to regrid and to spatially and/or temporally average the data. A number of worked examples are provided to demonstrate how to get started with the data.

The main aim of the document is to aid a user in selecting a data product they require (including understanding its features and limitations) and to then enable them to read and use the data. A summary of how the data were produced is also included for those who are interested.

1.2 Document structure

At the beginning of the document is a quick start guide to the essential elements of getting started with using the data and some example plots of the data.

The remainder of this document has a more conventional structure for a technical report, summarised below.

Section 2	An overview of the ESA SST CCI project.
Section 3	A guide to getting started with using the ESA SST CCI data.
Section 4	Tables describing the features of each of the ESA SST CCI products.
Section 5	A detailed description of the ESA SST CCI data files.
Section 6	Description of tools that can be used to work on the data products including the tools developed by the ESA SST CCI project.
Section 7	Worked examples of how to use the data.
Section 8	Dictionary of acronyms, abbreviations and jargon that may be encountered when reading this document.
Section 9	List of references.
Section 10	Acknowledgments.
Appendix 1	A summary of the how the ESA SST CCI data are processed.
Appendix 2	Examples of the structure of the ESA SST CCI data files.

2. INTRODUCTION TO THE ESA SST CCI PROJECT

2.1 Background

Knowledge of the temperature at the surface of the oceans (known as sea surface temperature, or SST) is important to a variety of climate research applications. For example, it is required as a boundary condition for atmospheric reanalyses and it is used as a proxy for near-surface air temperature in surface temperature datasets such as ‘HadCRUT4’ [RD.313], which are used for climate change assessment.

SST information has been, and continues to be, provided from a variety of sources. These can be broadly grouped into *in situ* instruments (for example installed on drifting buoys or in ships’ engine room intakes) and satellite instruments (for example on platforms such as the European Space Agency (ESA) satellite Envisat). Of course, no observational record is perfect and there inevitably exist various uncertainties associated with them. For example, these may stem from issues such as changing instrumentation over time, with different instruments having different bias characteristics, and gaps in their coverage. The primary strength of satellite-derived records is in providing greater spatial and temporal detail than is available from *in situ* measurements, which is limited by the number of instruments operating. However, the different components of the observing system provide complementary information and there is therefore value in having alternative and independent records of surface temperature from satellite and *in situ* data. Each record can be used to confront the other and give confidence in it.

Instruments that are sensitive to the temperature of the surface of the Earth’s oceans have been flown on board satellites over the past 30+ years. The longest record comes from a series of instruments known as the Advanced Very High Resolution Radiometers (AVHRRs). These are based on polar orbiting platforms (the series of National Oceanic and Atmospheric Administration (NOAA) satellites and more recently on MetOp, which is operated by the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT)), which orbit the Earth about every 100 minutes, passing almost over the poles and viewing a narrow (~2500 km) strip of the surface each time. A second long-term record is provided by the Along Track Scanning Radiometer (ATSR) series of three instruments, which started in 1991 and ended in 2012. These sensors were also housed on polar orbiting platforms. Relative to AVHRRs, they gave more accurate data [RD.248, RD.296], but with less coverage (~500 km wide strips). In more recent years new types of data are available. While the AVHRRs and ATSRs are sensitive to the thermal infrared part of the electromagnetic spectrum, the Advanced Microwave Scanning Radiometer – Earth Observing System (AMSR-E and AMSR2) views the Earth in the microwave part of the spectrum, allowing them to ‘see’ through the majority of clouds. There are also data from sensors on geostationary satellites – which perform one orbit per day and stay over the same spot on the Earth all the time – such as the Spinning Enhanced Visible and Infrared Imager (SEVIRI) on Meteosat Second Generation (MSG), but these are not used here.

Although a large quantity of satellite data exists, working out the SST from those data is not simple. The signal emanating from the surface is altered – for example by absorption and scattering by the atmosphere – before it reaches the satellite and the magnitude of this effect must be estimated in order to ‘retrieve’ SST from the satellite measurements. There are also issues to deal with such as degradation of sensors over time and drift in the orbit of the satellites. It is therefore very difficult to produce a satellite-based record of SST that achieves ‘climate quality’ i.e. that meets very stringent requirements on aspects such as having little artificial change in the SST data over time. Existing long term satellite based SST records include the Pathfinder dataset derived from the AVHRR series of sensors [RD.205; RD.216] and the ATSR Reprocessing for Climate (ARC) data for the ATSR series [RD.296]. Notably, these are made up from only one series of sensors each.

In 2009 ESA instigated their Climate Change Initiative (CCI). Its goal is:

> "To realise the full potential of the long-term global Earth Observation archives that ESA together with its Member states have established over the last thirty years, as a significant and timely contribution to the ECV [essential climate variable] databases required by United Nations Framework Convention on Climate Change (UNFCCC)."

They established 13 projects that aimed to unlock the full potential for climate research of satellite-based records of variables such as ocean colour and land use type. Included in those variables is SST, the target of the ESA SST CCI project. The project team comprises the University of Reading (UK) as prime contractor, and partners in the Met Office (UK), the University of Leicester (UK), Météo France (France), Danmarks Meteorologiske Institut (Danish Meteorological Institute; DMI) (Denmark), the Norwegian Meteorological Institute (Norway), Brockmann Consult (Germany), National Oceanography Centre (UK) and Space ConneXions (UK).

A very significant outcome of the project is the bringing together of two long term series of satellite data (from ATSRs and AVHRRs) to produce an SST record that is maximally independent of *in situ* observations for the period since ATSRs have been available, and combines the strengths of each series while minimising their weaknesses. There are many other interesting aspects to the project and these are discussed in the following sections.

2.2 The ESA SST CCI project

The ESA SST CCI project began in August 2010, the initial phase lasted about three years. Phase 2 started in January 2014. Its scope includes user requirements gathering, algorithm development, algorithm benchmarking, data production and validation, disseminating those data, and obtaining user feedback. One of its major aims is to produce a system for refining and continuing data products into the future.

In the following subsections, some of the key components of the project are described in more detail.

2.2.1 User requirements gathering

A major effort to gather user requirements was undertaken in both Phase 1 and Phase 2. It included a review of requirements found in literature from bodies such as the Global Climate Observing System (GCOS), a review of lessons learned from other projects, an online questionnaire, and discussion sessions.

The primary source of information in both exercises was an online questionnaire, which covered a wide range of aspects of the use of SST data ranging from users' experiences with current SST datasets through to asking what requirements are for SST data in the future (such as the grid resolution required, data volumes and formats etc.) Users were also asked to describe the type of application for which they use SST data (such as monitoring of climate, and detection and attribution of climate change) and to identify their requirements at three levels: threshold requirements, which is the level at which a dataset is usable for an application; breakthrough, which is the level at which a significant improvement is realised for an application; and objective, which is the point at which there is no point in improving the SST data further because the application would not see any benefit. Complete sets of responses were received from 108 (Phase 1) and 132 (Phase 2) people from around the world.

The results were wide ranging and a full description can be found in the ESA SST CCI User Requirements Documents with further metrics obtained from the results also available [RD.385; RD.189; RD.393 available from http://www.esa-sst-cci.org/PUG/documents.htm].

Based on the user requirements, product specifications were defined that aimed to meet the majority of users' needs.

2.2.2 A multi-sensor matchup database

A matchup dataset (MD) is a set of near-coincident (in time and space) measurements from a satellite sensor and an *in situ* instrument (for example a drifting buoy). This can be used for various purposes including validation of SSTs retrieved from the satellite data and, if independence from *in situ* data is not required, to derive an algorithm to retrieve SSTs from the satellite data.

In Phase II of the ESA SST CCI project a set of multi-sensor matchup dataset (MMD) files have been generated for a variety of applications, which include satellite to satellite match-ups as well as satellite to *in situ*. A list of all available MMD files and their purpose is given in RD.375 and their content is described in RD.376.

2.2.3 Algorithm development

In order to achieve the best possible satellite climate data record, it is necessary to make use of the best available algorithm to retrieve SST from the measurements made by the satellite instruments. Algorithms used have been evolved from those employed in Phase 1 (see Appendix A).

The approach adjusts the data (satellite radiances) from the AVHRR series of instruments to be consistent with the better calibrated ATSR sensors, rather than the traditional approach of tuning AVHRR SSTs to drifting buoys. This achieves a key aim, which is to ensure independence of the satellite record from the *in situ* record.

2.2.4 The ESA SST CCI products

In Version 2 products of the ESA CCI SST project, the 'long term' products from the Version 1 release in Phase 1 have been updated. These consist of data from the long period ATSR and AVHRR series of instruments and span August 1981 through to April 2012 and the end of 2016 respectively. [Updates and ongoing extension of the version 2 products will be available via the ICDRv2 products created by the Copernicus Climate Change Service see https://cds.climate.copernicus.eu or http://data.ceda.ac.uk/neodc/c3s_sst/data/ICDR_v2/] The main objective of the SST CCI products is to provide stable, unbiased SSTs. Within the product family, SSTs are available from each individual orbit of the ATSR and AVHRR sensors.

2.2.5 Data dissemination

Version 2 products produced by the ESA SST CCI project are being made available via the CEDA archive (http://data.ceda.ac.uk/neodc/esacci/sst/data/CDR_v2/). Feedback from users is strongly encouraged to ensure that future refinements of the products meet users' needs.

Within the project the data products will be verified (to ensure they match the specifications), validated using *in situ* data as a reference and intercompared with other products. They will also be assessed for trends.

2.3 The future

A major outcome from the project is a system for processing SST data [RD.259]. This has enabled the ESA SST CCI algorithms to begin to be implemented operationally as part of the Copernicus Climate Change Service, enabling the data to be extended in time routinely in the future.

Additionally, feedback from users and from the verification, validation and intercomparison activities are likely to motivate further development of the ESA SST CCI products.

3. GETTING STARTED WITH THE ESA SST CCI DATA

A very brief guide to getting started with the ESA SST CCI data was given in pages 3-5. Here, an extended introduction to the data is provided including, in Section 3.5, a frequently asked questions section. This includes explanations for some of the terms that might be encountered when reading through this chapter and the other parts of this document. See also Section 8, which contains explanations of acronyms, abbreviations and jargon.

3.1 Which SST product do I need?

3.1.1 ESA SST CCI products

The ESA SST CCI project has produced four SST products in Version 2, three of which consist of sets of data from single satellite instruments (or series of instruments) and the other comprising a blended, globally-complete analysis of both sets of data. In brief, the products are:

Stable, low-bias SST data (i) starting during 1991 and continuing through to April 2012 (ATSR) and (ii) starting in August 1981 and continuing through to the end of 2016 (AVHRR), in the following forms:

- Level 2 pre-processed (L2P) data: single orbit of data per file on an irregular grid with grid cell spacing about 1 km (ATSR series) and about 4 km (AVHRR series);
- Level 3 uncollated (L3U) data: a single orbit of data per file on a 0.05° regular latitude-longitude grid;
- Level 3 collated (L3C) data: all orbits for a day (separated into daytime and nighttime files) gridded together on a 0.05° regular latitude-longitude grid; and
- Level 4 (L4) globally-complete daily analysis: combined data from both the ATSR and AVHRR series.

See Section 3.1.2 for more information about data levels.

Each file of three of the above four products (the L2P, L3U and L3C) contains two sets of SSTs. The first set provides a measure of the temperature of the skin of the water at the time it was observed; the second set are estimates of the temperature at 20 cm depth and at either 1030 h or 2230 h local time (provision of data at 20 cm depth was one of the requirements revealed by the user requirements gathering exercise [RD.385]). They have uncertainty estimates that have been broken down into different components and a total uncertainty for each SST value.

The SST data are suitable for many uses, such as the study of temporal and spatial variability and comparison to or initialisation of numerical models. Owing to the orbital drift of some satellites, the 20 cm SSTs are better suited to the study of long-term SST change than the skin SSTs as they have been adjusted so that they all represent the same point in the diurnal cycle.

The combined, globally-complete Level 4 analysis for September 1981 to December 2016 provides daily combinations of the orbit data from the Version 2 release, using a variational data assimilation system (run without use of a dynamical ocean model in this case) to provide SSTs where there were no observations. This results in a single file per day on a 0.05° regular latitude-longitude grid).

These Level 4 SSTs correspond approximately to the daily average of the temperature of the water at 20 cm depth. Uncertainty estimates are provided. An example use of these data is as a boundary condition for a numerical model.

Detailed descriptions of the products can be found in Section 4.

Please use the product names and descriptions found in Table 1 when documenting your work with the ESA SST CCI products.

3.1.2 What are data levels?

When dealing with satellite data it is common to encounter references to ’data levels’. The level of the data describes the amount of processing that has been performed. The higher the level the further the data are along the process of converting the raw data from the satellite instrument and into a geophysical product. In the context of the ESA SST CCI data products the following data levels are relevant:

- Level 2 pre-processed (L2P) – SSTs from a single orbit of a sensor, still arranged in the way that the satellite ‘saw’ them.
- Level 3: either
    - Level 3 uncollated (L3U) – as L2P except the SSTs have been re-gridded and/or averaged spatially.
    - Level 3 collated (L3C) – as L3U except combining multiple orbits/views of the Earth from the same instrument.
- Level 4 (L4) – SSTs (typically from multiple orbits and sensors) that have been combined and any gaps filled in using statistical techniques. L4 products have not been updated in this release.

The different data levels are illustrated in Figure 1. The L2P data are stored on an irregular grid and require separate two-dimensional longitude and latitude data arrays to determine the locations of the SST data. L3U and L3C data are stored on a regular latitude-longitude grid but with large areas unfilled – especially in L3U because only a single orbit of data is contained in each file. Level 4 data are similarly presented on a regular grid but no gaps in the data are present because multiple orbits and sensors are combined and any remaining gaps are filled in.

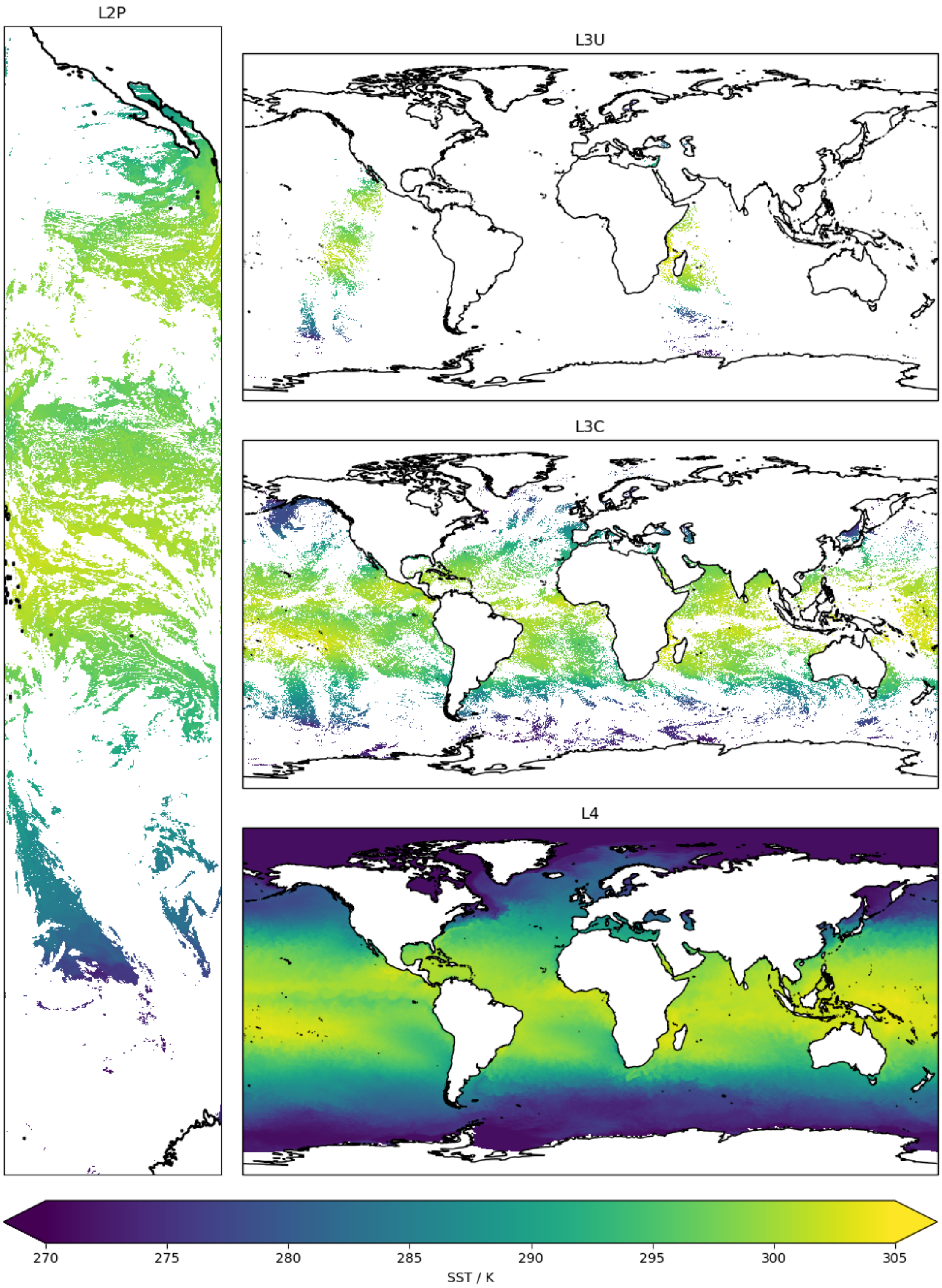


Figure 1. Illustration of how data are stored according to the 'level' of the data, using example ESA SST CCI data from one day. White areas correspond to locations with no SSTs. These occur, for example, due to cloud preventing an SST retrieval or because there was land or ice in the field of view of the instrument.

3.1.3 Other SST datasets

While the ESA SST CCI products will be ideal for many uses, it is important to note that there are many alternative SST products available, based on either *in situ* data, satellite data, or both. Each has its own features that may make it preferable for a particular application. Therefore, before selecting an ESA SST CCI product, it is useful to understand what alternatives are available. A list of some of the currently available SST datasets (not just from the ESA SST CCI project) is provided in Table 2. Each dataset has information with it about its time span, whether the dataset is updated in near real time (denoted by green shading) and references and/or webpages to go to for further information.

As a further aid to understanding the differences between the datasets, each dataset is categorised according to the length of its data record and how the data have been gridded or combined (i.e. the data 'level' - see Section 3.1.2). The diagram in Figure 2 illustrates how to choose the category of data according to these criteria. Note that for the criterion of how data should be gridded or combined, the types of data levels being produced by the ESA SST CCI project are listed with the category of data that they fit into. In Table 2, reading down the columns headed A to I yields the list of datasets that fall into those categories.

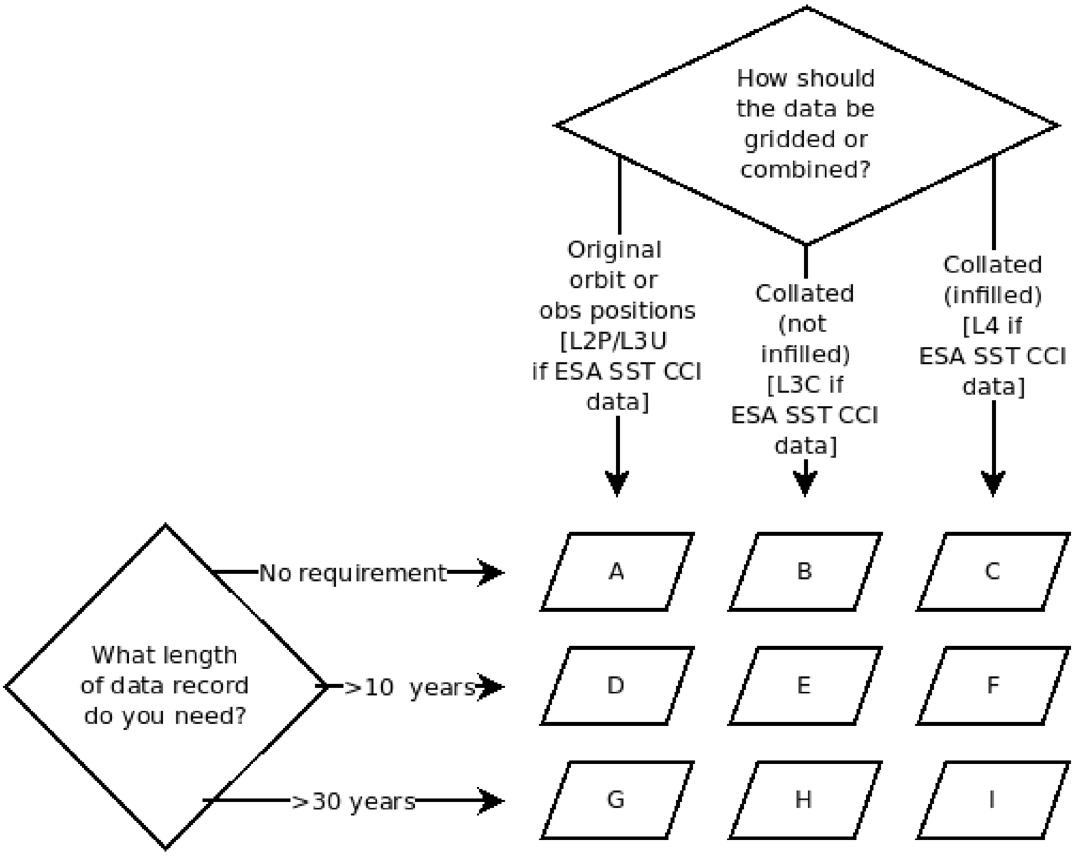


Figure 2. Guide to finding the category of data that you require. Products that meet these requirements are listed in Table 2.

If an ESA SST CCI product has been chosen, the rest of this document will give information about how to use the data. If an alternative product is required, the footnotes below the table give suggestions on where to go to find out more about it.

Please contact us if any information in Table 2 is inaccurate, or to add a new dataset – see Section 3.4 for contact information.

Table 2. SST data that meet the requirements shown in Figure 2 ordered by the starting date of the data record. The codes in the Type column are as follows: S – satellite data; I – *in situ* data; P – polar orbiting satellite; G – geostationary satellite; O – satellite in other orbit; IR – infrared radiometer; PMWR – passive microwave radiometer. Colours are used to denote: red – an ESA SST CCI product; blue – a product that is available in near real time. The numbers in the more info column relate to the list of references and webpages given in the footnotes at the bottom of the pages. See Section 8 for definitions of the acronyms used. Please contact us to correct any information in this table or to add a new dataset.

Product	Type	Period	More info	A	B	C	D	E	F	G	H	I
ICOADS	I	1800 – present	1	X	X		X	X		X	X	
HadSST3	I	1850 – present	2		X			X			X	
ERSST v5	I	1854 – present	3			X			X			X
Kaplan et al. (1998)	I	1856 – present	4			X			X			X
HadISST1	I, S	1870 – present	5			X			X			X
COBE-2	I	1850 – 2015	6			X			X			X
NOCS daily OI	I	1973 – 2017	7			X			X			X
AVHRR Pathfinder v5.3	S (P, IR)	1981 – present	8		X			X			X	
Other AVHRR	S (P, IR)	1981 – present	9	X			X			X		
Reynolds et al. daily OI (2007)	I, S	1981 – present	10			X			X			X
OSTIA	I, S	1985 – 2007 (reanalysis; near real time data also available)	11			X			X			

[1] http://icoads.noaa.gov/

[2] [RD.210; RD.211]; http://www.metoffice.gov.uk/hadobs/hadsst3

[3] [RD.403]; https://www.ncdc.noaa.gov/data-access/marineocean-data/extended-reconstructed-sea-surface-temperature-ersst-v5

[4] [RD.81]; http://www.esrl.noaa.gov/psd/data/gridded/data.kaplan_sst.html

[5] [RD.74]; http://www.metoffice.gov.uk/hadobs/hadisst

[6] [RD.404]; https://www.esrl.noaa.gov/psd/data/gridded/data.cobe2.html

[7] [RD.99]; https://noc.ac.uk/science/sustained-observations/noc-surface-flux-dataset

[8] [RD.205]; https://data.nodc.noaa.gov/cgi-bin/iso?id=gov.noaa.nodc:AVHRR_Pathfinder-NCEI-L3C-v5.3

[9] http://noaasis.noaa.gov/NOAASIS/ml/avhrr.html; http://www.ghrsst.org

[10] [RD.76]; https://www.ncdc.noaa.gov/oisst

[11] [RD.239]; https://podaac.jpl.nasa.gov/dataset/UKMO-L4HRfnd-GLOB-OSTIA

Product	Type	Period	More info	A	B	C	D	E	F	G	H	I
SST CCI ATSR, Version 2	S (P)	1991 – Apr 2012	[12]	X	X		X	X				
SST CCI AVHRR, Version 2	S (P)	August 1981 – 2016	[13]	X	X		X	X		X	X	
SST CCI analysis, Version 2	S (P)	September 1981 – 2016	[14]			X			X			X
ATSR series (processed using the 'SADIST' re-trieval method)	S (P, IR)	1991 – 2012	[15]	X			X					
ATSR Reprocess-ing for Climate, v1.1.1	S (P, IR)	1991 - 2012	[16]		X			X				
TMI	S (O, MW)	1997 – 2015	[17]	X			X					
RTG_SST_HR	I, S	2001 – present	[18]			X			X			
AMSR-E	S (P, PMWR)	2002 – 2010	[19]	X								
RSS MW Fu-sion	S (P, O, PMWR)	2002 – present (global cover-age)	[20]			X			X			
SEVIRI	S (G, IR)	2005 – present	[21]		X			X				
FNMOC 10 km high res analysis	I, S	2005 – present	[22]			X			X			

[12] See the rest of this document; **Error! Reference source not found.** gives a summary of the features of this data product

[13] See the rest of this document; **Error! Reference source not found.** gives a summary of the features of this data product

[14] See the rest of this document; **Error! Reference source not found.** gives a summary of the features of this data product

[15] https://earth.esa.int/web/guest/missions/esa-operational-eo-missions/envisat/content/-/article/status-of-envisat-products-4072

[16] [RD.405]; http://catalogue.ceda.ac.uk/uuid/a44cd6735b7046e13da2ca0bec33c7a9

[17] https://podaac.jpl.nasa.gov/dataset/TMI-REMSS-L2P-v4?ids=Platform&values=TRMM

[18] http://polar.ncep.noaa.gov/sst/rtg_high_res/

[19] https://podaac.jpl.nasa.gov/dataset/AMSRE_L3_SST_1DEG_1MO

[20] http://www.remss.com/measurements/sea-surface-temperature/

[21] http://www.osi-saf.org/?q=content/meteosat-sea-surface-temperature-a

[22] http://www.usgodae.org/cgi-bin/datalist.pl?summary=Go&dset=fnmoc_ghrsst

Product	Type	Period	More info	A	B	C	D	E	F	G	H	I
GAMSSA	I, S (P, IR, PMWR)	2008 – present	[23]			X			X			
CMC	I, S (P, IR, PMWR)	1991 - 2017	[24]			X			X			
JMA MGDSST		1982 - present	[25]			X			X			X

3.2 How do I get the data?

Version 2 products can be obtained from the CEDA archive (http://data.ceda.ac.uk/neodc/esacci/sst/data/CDR_v2/).

Version 1 products can be obtained from http://catalogue.ceda.ac.uk/uuid/1dc189bbf94209b48ed446c0e9a078af.

For non ESA SST CCI products, the references to the individual datasets (see above) provide access information.

3.3 How do I use the ESA SST CCI data?

3.3.1 The data files

The structure of the ESA SST CCI file names is described in detail in Section 6.1. In this summary, the explanation is restricted to probably the most useful parts of the filenames, which occur at the beginning in this form:

<Indicative date><Indicative time>-ESACCI-<Processing level>...

For example:

20000101000206-ESACCI-L2P_GHRSST-SSTskin-AVHRR15_G-CDR2.0-v02.0-fv01.0.nc

The first part, indicative date, is the date of the data using the ISO8601 basic format: YYYYMMDD (the 1st of January 2000 in the example). The second part, indicative time, is a time within that day using the ISO8601 basic format: HHMMSS (00 hours, 1 minute and 5 seconds in the example). The time used depends on the processing level of the dataset:

L2P: start time of granule

L3U: start time of granule

L3C: centre time of collation window (120000 for daily files, whether they are night or day)

[23] [RD.314]; https://podaac.jpl.nasa.gov/dataset/ABOM-L4LRfnd-GLOB-GAMSSA_28km

[24] https://podaac.jpl.nasa.gov/dataset/CMC0.2deg-CMC-L4-GLOB-v2.0

[25] https://ds.data.jma.go.jp/gmd/goos/data/rrtdb/file_list.php#a0

L4: nominal time of analysis (120000 for daily files)

Finally, the processing level of the data is given. This could be L2P (individual orbits of data, satellite projection; this is the type of data in the example filename), L3U (individual orbits of data, gridded), L3C (contain multiple L3U files from a single sensor combined into a longer time period[26]), or L4 (combined, gridded and infilled data). See Section 3.1.2 for more details on data levels.

The format of the data files is NetCDF-4. Within the files are data (known as variables) and metadata (known as attributes). A summary of the data within the product files is provided in Table 3. The notes below the table highlight some of the key attributes that are attached to the data.

Table 3. Summary of the key variables in the NetCDF files.

Description of the content of key variables in the NetCDF files	Names of variables in files containing single orbits of data	Names of variables in files containing infilled, combined data
Latitudes of the data points	lat	lat
Longitudes of the data points	lon	lon
Sea surface temperature at the skin*	sea_surface_temperature	Not applicable
Total uncertainty of the sea surface temperature at the skin*#	sses_standard_deviation	Not applicable
Sea surface temperature at 20cm depth and 10.30 am and pm local time	sea_surface_temperature_depth	analysed_sst**
Total uncertainty of the sea surface temperature at 20 cm depth and 10.30 am and pm local time#	sst_depth_total_uncertainty	analysis_uncertainty
Quality / location type (ocean / sea ice / lake etc.) information	l2p_flags and quality_level***	mask****

* Skin SST is the temperature of the radiating surface layer of the water, which is of 10 µm depth.

** SSTs in the infilled files are combined/interpolated estimates of the daily average SST at 20 cm depth

*** Good quality SSTs are those where the value in the SST data array is not -32768 and the value in the quality_level variable is 5.

**** Ocean SST values have mask = 1.

Also available in the files is uncertainty broken down into different components.

Important:

[26] The L3C products cover a single UTC day. L3C files contain data from multiple orbits giving more complete global coverage than L3U. However; coverage is still restricted to cloud free regions.

- Check that the add_offset and scale_factor attributes are being applied when reading the variables. These must be used to convert the data stored in the file to the correct units. Many tools will do this automatically for NetCDF files, so no action may be necessary. An example of how to apply the add_offset and scale_factor attributes can be found in Section 7.4.1.

3.3.2 Using the uncertainty estimates

L2P, L3U and L3C files contain uncertainties broken down into components from errors that correlate on different spatial and temporal scales (see RD.406 for details):

- uncorrelated_uncertainty – uncertainty from effects that are not correlated from location to location (such as random noise in the satellite sensors).

- synoptically_correlated_uncertainty – uncertainty from effects that are assumed (provisionally) to be correlated over distances of 100 km and 1 day (related to atmospheric conditions).

- large_scale_correlated_uncertainty – uncertainty from effects that can be assumed to be correlated everywhere and over long time scales (such as over all calibration of the satellite sensor).

- adjustment_uncertainty – only applicable if using SSTs that have been adjusted to the standard time (10.30/22.30 h) and depth (20 cm); (provisionally) assumed to be correlated over 100 km and 1 day.

For each individual SST, the total uncertainty can be obtained by summing each component in quadrature (i.e., square root of sum of squares). For the non-time-depth-adjusted SSTs (i.e., skin SSTs at time of observation), the total uncertainty is stored in the variable called sses_standard_deviation in the NetCDF files. For adjusted SSTs, the corresponding variable is called sst_depth_total_uncertainty. The former is a combination of the first three uncertainty components above; the latter combines all four.

For applications combining multiple SSTs such as performing a regional average of the data it is essential that the correlations in the uncertainties are taken into account when combining the uncertainty components. It is for this reason that the uncertainty components have been provided. An example of how to do this is given in Section 7.5.

L4 files contain a single uncertainty field called analysis_uncertainty, so it is not possible to consider different correlation length scales in this case.

3.3.3 Examples of reading the data and tools that can be used on the data

The ESA SST CCI files use NetCDF format and so they are readable using many tools and programming languages including C, Fortran, IDL, Matlab etc.

A recommendation for a tool for examining and analysing the files using a convenient graphical user interface is SNAP (http://step.esa.int/main/toolboxes/snap/).

The ESA SST CCI project has produced two tools for regridding and performing regional averages of data. These are highly recommended for these purposes as they will propagate the different uncertainty components automatically.

More information about tools is available in Section 4.

3.3.4 Dos and don'ts to be aware of when using the data

Do make sure the data read from the files are scaled to be in the correct units.

Do check for fill values in the data arrays **and** the quality information and/or data quality flags that say which locations contain usable SSTs.

Do make use of the uncertainty information.

Do make use of all the appropriate metadata and ancillary data (such as wind speed and sea ice) available in the files.

Do tell us what you think of the data!

Don't use the wrong SST and uncertainty fields. Remember there are two sets in the L2P, L3U and L3C files – one has been adjusted to a standard time and depth.

Don't forget, if averaging the data, to use the individual uncertainty components and propagate uncertainty as recommended.

Don't assume that because the grid spacing of the L4 products is 0.05° that SST features that fine are necessarily resolved. Observational information is spread spatially and temporally (to fill in gaps) during the processing. The length scales that govern this spreading of information are described in [RD.407].

3.4 Contact us

Our email address is science.leader@esa-sst-cci.org and our website is http://www.esa-sst-cci.org/.

We are happy to answer queries about the data and also very much welcome any feedback on the data.

3.5 Frequently asked questions

Here we provide explanations for some of the questions that you may have asked when reading the preceding text.

3.5.1 *In situ* SSTs

[RD.211] discusses many of the types of instruments that have been used to measure temperature by *in situ* instruments.

3.5.2 Satellite derived SSTs

Here we provide a brief summary of how satellite data are used to infer SST. Electromagnetic radiance emitted from the very top layer of the water travels up through the atmosphere and reaches the satellite instrument. The radiating layer is ~10 µm to ~1 mm deep for the wavelengths of interest for deriving SST. The amount of radiation reaching the satellite is partly determined by the skin temperature of the water. The amount of radiation also depends on the atmosphere, which both absorbs some radiation emitted from the surface and emits its own contribution. Where the atmosphere is cloudy, the atmospheric effect dominates. For clear sky areas, enough of the surface-emitted radiation reaches the sensor to allow a 'retrieval' of SST to be made. To retrieve the SST, measurements are made at multiple wavelengths and sometimes at different angles through the atmosphere. The differential atmospheric influence on each of these 'channels' is used to estimate (implicitly or explicitly, depending on the algorithm) the effects of the atmosphere and reveal the SST. Finding an adequate solution to obtaining SST data products that meet requirements for climate research is a particularly challenging retrieval problem, because of the accuracy and stability required.

3.5.3 Why is the depth of an SST important? What is foundation temperature, skin temperature etc?

The term SST can be used to refer to the temperature of water anywhere from the very point it touches the atmosphere down to depths of 10 m or more. The distinction is important because the influence of the sun and atmosphere are largest near the surface. For example, the SST in a particular location at a depth of 20 cm might exhibit a pronounced diurnal cycle, but not the SST in the same location at 10 m. There are therefore different types of SST that are sometimes referred to. For the ESA SST CCI data, the following types are relevant:

- Skin SST – the temperature in the top ~10 μm of water; this is nominally the layer of water that an instrument sensing in the infrared part of the electromagnetic spectrum would be sensitive to.
- Subskin SST – the temperature at a depth ~1 mm of water; nominally the mean depth that microwave sensing instruments are sensitive to.
- 20 cm SST – the SST at depth of 20 cm, which is the depth often associated with drifting buoy measurements (on average). Some ESA SST CCI products include SST data that have been adjusted to represent the temperature at this depth at a particular time of the day (10.30 in the morning or evening).
- Foundation SST – this is defined as the SST that is the starting point of the diurnal cycle that will develop over a day.

For more information about definitions of SST, in particular the concept of foundation SST, readers are encouraged to consult the Group for High Resolution SST (GHRSST) webpages at https://www.ghrsst.org/ghrsst-data-services/products/.

3.5.4 Who uses satellite derived SSTs?

Satellite derived SSTs have found many uses. For example, high resolution SST products are required for initialisation of numerical weather and ocean forecast models. Over the past decade efforts by GHRSST (https://www.ghrsst.org/) have made into reality the near real time availability of multiple satellite SST products for these kinds of purposes. Climate applications also make use of satellite SST data. For example, HadISST [RD.74; http://www.metoffice.gov.uk/hadobs/hadisst/] combines *in situ* and satellite data in a dataset spanning from 1870 to present and has been used for applications such as the reconstruction of past atmospheric conditions (e.g. the Twentieth Century Reanalysis; [RD.315; http://www.esrl.noaa.gov/psd/data/gridded/data.20thC_ReanV2.html]). An example of a satellite-only product is that produced by the Pathfinder project from data from the AVHRR series of instruments [RD.216; http://www.nodc.noaa.gov/SatelliteData/pathfinder4km/], which has found many applications [e.g. RD.316].

3.5.5 How were the ESA SST CCI data produced?

A summary of the algorithms and processing used to produce the ESA SST CCI data can be found in Appendix 1.

3.5.6 Why use ESA SST CCI data (and why not)?

3.5.6.1 Key features of ESA SST CCI data

The ESA SST CCI data product provides SSTs covering a 35-year period that are designed to be stable and accurate. The SSTs are retrieved largely independently of *in situ* measurements for the period after which good satellite reference sensors (ATSRs) became available, although there is tuning to *in situ* measurements during the 1980s. ESA SST CCI data are **not** blended with *in situ* measurements at level 4 (unlike most satellite and analysis SST datasets). ESA SST CCI products give a maximally independent set of SSTs that can be used to confront the *in situ* record, can be used to give an independent comparison point for ocean or climate models, etc. The data are from both the AVHRR and ATSR series of instruments. AVHRR radiances have been adjusted to the reference provided by the more stable and accurate ATSR instruments, with the aim of ensuring consistency in SST between these data sources.

The ESA SST CCI products are on fine grids, and can be re-gridded to resolutions that are multiples of 0.05°.

3.5.6.2 Limitations

The products currently start in August/September 1981 and terminate in December 2016 (AVHRR and L4, ATSR-only products are shorter), i.e. maximum length is approximately 35 years. Updates to the data will soon be available from the Copernicus Climate Change Service.

The ESA SST CCI data are on very fine grids, which is an advantage for some applications but also means that the file sizes are large (total size of the products for all the data levels is ~18 TB). However, data are provided separately with different levels of processing and individual files are provided for each day, so users can select the subset of data that is relevant to them. It is planned to make data available on a limited selection of coarser grids. Tools are available to regrid the data to coarser resolutions. However, this can currently only be done after first downloading the full resolution data.

The L4 data files do not have uncertainty correlation scale information embedded.

The best stability and precision are from 1991 onwards, the first ATSR in the series performing less well in these regards than the second and third.

Each pixel has an associated `quality_level` which indicates the general quality of that pixel – higher values being better. Quantitative analyses should use the higher quality levels (4 or 5). Quality levels 2 and 3 may be useful for qualitative analyses, but the pixels have an increased chance of being cloud contaminated.

A challenge to address has been the lack of an ATSR-class sensor (following the loss of Envisat in 2012) until the Sea and Land Surface Temperature Radiometer (SLSTR) became operational. A further challenge has also been the extension of the ESA SST CCI products back prior to the first ATSR using AVHRRs only, in a way that is consistent and gives good stability. Cross-referencing SSTs with *in situ* data has been necessary to extend the products with similar quality before 1991. From 2012 onwards the 2012 cross-referencing to AATSR has effectively been carried forward. Understanding of SLSTR-A will soon be mature enough that we expect to be able to use it as a reference sensor, but that was not possible in Version 2.

Known issues with the version 2.0 products:

- SSTs estimated from the AVHRR on-board NOAA-18 have a cold bias of ~-0.1 K

- Day-time AVHRR SSTs show a seasonal cycle of up to 0.2 K which is not thought to be attributable to seasonal artefacts the *in situ* data (i.e., is an artefact in the AVHRR SSTs)

- A trend artefact is present in daytime AVHRR data of NOAA-14

- Data between 01/10/1982 and 30/09/1983 should be treated with caution. Throughout this period, the AVHRR data are noisy. Embedded within this period are periods of a month or more where large calibration errors (several tenths K) are apparent. These latter biases are also found in the SST CCI analysis v2.0 product, as it relies on the AVHRR retrievals at this time.

- Daytime AVHRR uncertainty estimates are too large

- The ATSR1 3.7 µm channel failed in May 1992 so subsequent night-time data are produced using 2-channel retrieval (lessening consistency with the night-time data of later ATSRs)

- The ATSR2 scan mirror failed between December 1995 and July 1996 resulting in no ATSR2 data during a period when the available ATSR1 was degrading significantly

- The ATSR2 gyroscope failure in January 2001 means that locational accuracy is reduced until corrective measures were implemented in June 2001

3.5.6.3 Future developments

It is planned that the SST algorithms will be applied routinely as part of the Copernicus Climate Change Service, with the products extended to present observations after a short delay from the time of satellite observation.

3.5.7 How to cite the data

By accessing ESA SST CCI data, you agree to cite both the dataset and a journal article describing the dataset when publishing results obtained in whole or in part by use of ESA SST CCI products.

The dataset citation should reference the "ESA SST CCI" project, and from where the data were obtained. Accurate product descriptions and names to use in publications are given in Table 1 and should be used to avoid confusion and enable traceability.

The journal reference is: C.J. Merchant et al (2019) Satellite-based time-series of sea-surface temperature since 1981 for climate applications, in prep for Nature Science Data

4. TOOLS THAT CAN BE USED TO WORK WITH THE DATA

4.1 ESA SST CCI tools

The ESA SST CCI project provides two tools that automate regridding of data to a coarser resolution and calculating regional averages. An advantage to using the ESA SST CCI tools for these purposes is that uncertainty information is propagated automatically from the original data through to the output files. The tools will also incorporate an uncertainty component associated with incomplete sampling e.g. due to cloud preventing SST retrievals in some locations, which is not included in the product files. To use the tools it is necessary to download the ESA SST CCI data and also to download and install the tools software. Information about how to get and use the tools is given in the rest of this section.

4.1.1 Obtaining the ESA SST CCI tools

Contact us at science.leader@esa-SST-cci.org if you would like to use the tools.

4.1.2 Installing the ESA SST CCI tools

Three installation scripts are provided, for Linux, Windows and 64-bit Windows systems. After the software has been obtained, the installation scripts can be found by navigating to the sst-cci-tools-installers directory. To install the ESA SST CCI tools simply run the relevant script. This will invoke an interface to guide you through the rest of the installation process. Two executables will be produced: regrid and regavg in the bin directory in the directory chosen during the installation.

4.1.3 Running the tool to regrid onto a coarser grid

The tool that regrids the data to a reduced resolution uses the 'regrid' executable file. The tool is able to process any of the ESA SST CCI product files and also some files from the ARC project.

The information below gives the complete set of options that can be set when using the regrid tool (this information is produced by running the command **`regrid -h`**). An example of using this tool is provided in Section 7.2.

```
usage: regrid [OPTIONS]

The regrid tool is used to read in the ESA SST CCI L3U, L3C, and L4
products at daily 0.05° latitude by longitude resolution and output on
other spatio-temporal resolutions, which are a multiple of this and di-
vide neatly into 180 degrees. Output are SSTs and their uncertainties.

    --ARC_L3U.dir <DIR>          Directory that hosts the products of
type 'ARC_L3U'.

 -c,--config <FILE>              Reads a configuration (key-value pairs)
from given FILE.

    --CCI_L2P.dir <DIR>          Directory that hosts the products of
type 'CCI_L2P'.

    --CCI_L3C.dir <DIR>          Directory that hosts the products of
type 'CCI_L3C'.
```

```
    --CCI_L3U.dir <DIR>          Directory that hosts the products of
type 'CCI_L3U'.

    --CCI_L4.dir <DIR>           Directory that hosts the products of
type 'CCI_L4'.

    --climatologyDir <DIR>       The directory path to the reference
                                 climatology.  The  default  value  is
                                 './climatology'.

    --coverageUncertainty.StdDev <FILE>     A NetCDF file that provides
                                 lookup table 1/3 for coverage uncer-
                                 tainties.   The   default   value   is
                                 './conf/auxdata/20070321-UKMO-L4HRfnd-
                                 GLOB-v01-fv02-OSTIARANanom_stdev.nc'.

    --coverageUncertainty.x0Space  <FILE>    A  txt  file  that provides
                                 lookup table 3/3 for coverage uncer-
                                 tainties.   The   default   value   is
                                 './conf/auxdata/x0_space.txt'.

    --coverageUncertainty.x0Time  <FILE>     A  txt  file  that provides
                                 lookup table 2/3 for coverage uncer-
                                 tainties.   The   default   value   is
                                 './conf/auxdata/x0_time.txt'.

 -e,--errors                     Dumps a full error stack trace.

    --endDate <DATE>             The end date for the analysis given in
                                 the  format  YYYY-MM-DD.  The  default
                                 value is '2020-12-31'.

    --filenameRegex <REGEX>      The  input  filename  pattern.  REGEX  is
                                 Regular Expression that usually depends
                                 on  the  parameter  'productType'.  E.g.
                                 the default value for the product type
                                 'ARC_L3U'                             is
                                 'AT[12S]_AVG_3PAARC\d{8}_[DTEM]_[nd][ND
                                 ][23][bms][.]nc([.]gz)?'.  For  example,
                                 if  you  only  want  to  include  daily  (D)
                                 L3 AATSR (ATS) files with night obser-
                                 vations only, dual view, 3 channel re-
                                 trieval,  bayes  cloud  screening  (nD3b)
                                 you       could       use       the       regex
                                 'ATS_AVG_3PAARC\\d{8}_D_nD3b[.]nc[.]gz'
                                 .

 -h,--help                       Displays this help.

 -l,--logLevel <LEVEL>           Sets the logging level. Must be one of
                                 [off, error, warning, info, all]. level
                                 'all'  to  also  output  diagnostics.  The
                                 default value is 'info'.

    --maxTotalUncertainty <NUM>  The maximum relative total uncertainty
                                 allowed for non-missing output. The de-
                                 fault value is '1.0'.
```

--minCoverage <NUM>	The minimum fractional coverage required for non-missing output. (fraction of valid values in input per grid box in output) . The default value is '0.0'.
--outputDir <DIR>	The output directory. The default value is '.'.
--productType <NAME>	The product type. Must be one of [ARC_L3U, CCI_L2P, CCI_L3U, CCI_L3C, CCI_L4].
--region <REGION>	The sub-region to be used (optional). Coordinates in the format W,N,E,S. The default value is 'Global=-180,90,180,-90 (NAME=REGION)'.
--spatialRes <NUM>	The spatial resolution of the output grid in degrees. Must be one of [0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.4, 0.5, 0.6, 0.75, 0.8, 1.0, 1.2, 1.25, 2.0, 2.25, 2.4, 2.5, 3.0, 3.75, 4.0, 4.5, 5.0, 10.0]. The default value is '5.0'.
--sstDepth <DEPTH>	The SST depth. Must be one of [skin, depth_20, depth_100]. The default value is 'skin'.
--startDate <DATE>	The start date for the analysis given in the format YYYY-MM-DD. The default value is '1990-01-01'.
--temporalRes <NUM>	The temporal resolution. Must be one of [daily, weekly7d, weekly5d, monthly, seasonal, annual]. The default value is 'monthly'.
--totalUncertainty <BOOL>	A Boolean variable indicating whether total or separated uncertainties are written to the output file. Must be either 'true' or 'false'. The default value is 'false'.
-v,--version	Displays the version of this program and exits.

4.1.4 Running the tool to calculate regional averages

The tool that performs a regional average of data is run using the ‘regavg’ executable. The tool is able to process all the ESA SST CCI product files and also some data produced by the ARC project.

The information below gives the complete set of options that can be set when using the tool (this information is produced by running the command **`regavg -h`**). An example of using the regavg tool is provided in Section 7.2.

```
usage: regavg [OPTIONS]

The regavg tool is used to generate regional average time-series from
ARC (L2P, L3U) and SST_cci (L3U, L3P, L4) product files given a time in-
terval and a list of regions. An output NetCDF file will be written for
each region.

OPTIONS may be one or more of the following:

    --ARC_L3U.dir <DIR>          Directory that hosts the products of
                                 type 'ARC_L3U'.

 -c,--config <FILE>              Reads a configuration (key-value pairs)
                                 from given FILE.

    --CCI_L2P.dir <DIR>          Directory that hosts the products of
                                 type 'CCI_L2P'.

    --CCI_L3C.dir <DIR>          Directory that hosts the products of
                                 type 'CCI_L3C'.

    --CCI_L3U.dir <DIR>          Directory that hosts the products of
                                 type 'CCI_L3U'.

    --CCI_L4.dir <DIR>           Directory that hosts the products of
                                 type 'CCI_L4'.

    --climatologyDir <DIR>       The directory path to the reference
                                 climatology. The default value is
                                 './climatology'.

 -e,--errors                     Dumps a full error stack trace.

    --endDate <DATE>             The end date for the analysis given in
                                 the format YYYY-MM-DD. The default
                                 value is '2020-12-31'.

    --filenameRegex <REGEX>      The input filename pattern. REGEX is
                                 Regular Expression that usually depends
                                 on the parameter 'productType'. E.g.
                                 the default value for the product type
                                 'ARC_L3U'                            is
                                 'AT[12S]_AVG_3PAARC\d{8}_[DTEM]_[nd][ND
                                 ][23][bms][.]nc([.]gz)?'. For example,
                                 if you only want to include daily (D)
                                 L3 AATSR (ATS) files with night obser-
                                 vations only, dual view, 3 channel re-
                                 trieval, bayes cloud screening (nD3b)
                                 you      could      use      the      regex
                                 'ATS_AVG_3PAARC\\d{8}_D_nD3b[.]nc[.]gz'
                                 .

 -h,--help                       Displays this help.

 -l,--logLevel <LEVEL>           sets the logging level. Must be one of
                                 [off, error, warning, info, all]. Use
```

```
                                level 'all' to also output diagnostics.
                                The default value is 'info'.

    --lut1File <FILE>           A NetCDF file that provides lookup ta-
                                ble 1. The default value is
                                'conf/auxdata/coverage_uncertainty_para
                                meters.nc'.

    --lut2File <FILE>           A plain text file that provides lookup
                                table 2. The default value is
                                'conf/auxdata/RegionalAverage_LUT2.txt'
                                .

    --outputDir <DIR>           The output directory. The default value
                                is '.'.

    --productType <NAME>        The product type. Must be one of
                                [ARC_L3U, CCI_L2P, CCI_L3U, CCI_L3C,
                                CCI_L4].

    --regionList <NAME=REGION[;...]>   A semicolon-separated list of
                                NAME=REGION pairs. REGION may be given
                                as coordinates in the format W,N,E,S or
                                as name of a file that provides a re-
                                gion mask in plain text form. The re-
                                gion mask file contains 72 x 36 5-
                                degree grid cells. Columns correspond
                                to range -180 (first column) to +180
                                (last column) degrees longitude, while
                                lines correspond to +90 (first line) to
                                -90 (last line) degrees latitude. Cells
                                can be '0' or '1', where a '1' indi-
                                cates that the region represented by
                                the cell will be considered in the av-
                                eraging process. The default value is
                                'Global=-180,90,180,-90'.

    --sstDepth <DEPTH>          The SST depth. Must be one of [skin,
                                depth_20, depth_100]. The default value
                                is 'skin'.

    --startDate <DATE>          The start date for the analysis given
                                in the format YYYY-MM-DD. The default
                                value is '1990-01-01'.

    --temporalRes <NUM>         The temporal resolution. Must be one of
                                [daily, monthly, seasonal, annual]. The
                                default value is 'monthly'.

 -v,--version                   Displays the version of this program
                                and exits.

    --writeText                 Also writes results to a plain text
                                file 'regavg-output-<date>.txt'.
```

All parameter options may also be read from a key-value-pair file. The tool will always try to read settings in the default configuration file

`'./regavg.properties'. Optionally, a configuration file may be provided using the -c <FILE> option (see above). Command-line options overwrite the settings given by -c, which again overwrite settings in default configuration file.`

4.1.5 Format of the output from the tools

Both tools will output NetCDF data. The exact form of the data in the files can be clarified using a utility such as ncdump or using SNAP (see Section 4.2.1).

For the regional averaging tool there is also an option to write the output as a text file (see the writeText option).

4.2 Other tools

Many other tools can be used to analyse the ESA SST CCI files because the data are in a widely-used format (NetCDF) and follow international conventions. Some examples of these are given below.

4.2.1 ESA CCI Toolbox

The climate analysis toolbox of the ESA CCI (https://climatetoolbox.io/) is an open source software environment for ingesting, operating on and visualising all ESA CCI data. It can be used via the command line, via a Graphical User Interface, or via a python API. Installers are provided for Linux, Windows and Mac operating systems. A more detailed explanation and some real-life examples are given in section 7.2.

4.2.2 SNAP

The SNAP toolbox is recommended for viewing, interpreting, analysing and processing satellite imagery. This is free, open source software and can be downloaded from http://step.esa.int/main/toolboxes/snap/. SNAP can be used for viewing data fields and their associated metadata, for interpreting product flags, subsetting data, data analysis through statistics and histograms, comparison with other reference data and analysis of time series. Section 7.1 gives some worked examples for how SNAP can be used.

4.2.3 Generic NetCDF tools

Generic tools available for viewing and manipulating NetCDF files include:

- ncdump: provided with the NetCDF library, this produces a human readable version of the contents of a NetCDF file. More details can be found at http://www.unidata.ucar.edu/software/netcdf/.

- NetCDF operators: a set of command line utilities for performing various operations on NetCDF files such as concatenation, editing and mathematics. More details can be found at http://www.unidata.ucar.edu/software/netcdf/.

- ncview: a program to produce graphical displays of the contents of NetCDF files. More information can be found at http://meteora.ucsd.edu/~pierce/ncview_home_page.html.

A more complete list can be found at http://www.unidata.ucar.edu/software/netcdf/software.html.

4.2.4 Data analysis/programming languages

Numerous programming languages exist that can be used for reading and analysing NetCDF files. These include both compiled languages such as Java, Fortran and C, and languages that allow interactive analysis and plotting of data. Some examples of the latter are:

- Python (http://www.python.org/) with add on modules such as netCDF4 (https://github.com/Unidata/netcdf4-python), numpy (http://www.numpy.org/), matplotlib (http://matplotlib.org/) and iris (https://scitools.org.uk/iris/docs/latest/). Refer to Section 7.4 for worked examples.
- IDL (http://www.exelisvis.com/ProductsServices/IDL.aspx).
- Matlab (http://www.mathworks.co.uk/products/matlab/).
- GrADS (http://cola.gmu.edu/grads/).
- NCL (http://www.ncl.ucar.edu/).

5. ESA SST CCI PRODUCT FACT SHEETS

In this section, the key features of the ESA SST CCI data are listed. A table of features is provided for each instrument (or series of instruments) used in each of the ESA SST CCI Version 2 products.

The format of the table follows the template from the GHRSST Climate Data Record Technical Advisory Group described in [RD.408].

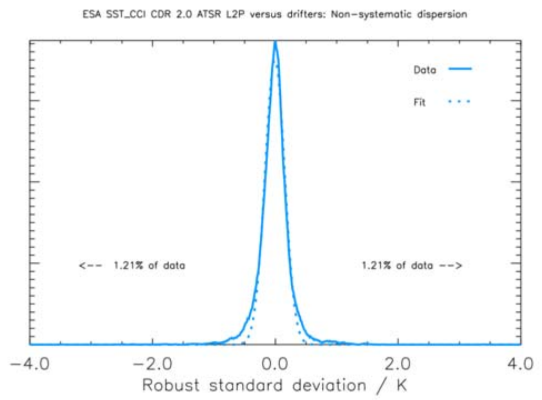
A summary of validation statistics is provided below. More details of these can be found in a journal article documenting the validation of the SST CCI v2 products [RD.412] and the ESA SST CCI Climate Assessment Report [RD.413], available from http://www.esa-sst-cci.org/PUG/documents.

Data between 01/10/1982 and 30/09/1983 should be treated with caution. Throughout this period, the AVHRR data are noisy. Embedded within this period are periods of a month or more where large calibration errors (several tenths K) are apparent. These latter biases are also found in the SST CCI analysis v2.0 product, as it relies on the AVHRR retrievals at this time.

5.1 ATSR

Table 4. Information evaluating the ESA SST CCI ATSR Version 2 product as a climate record.

SUMMARY	
Status of assessment	Dataset producer’s information
Dataset name and version	ESA SST CCI ATSR product version 2
Lead Investigator and/or Agency	Chris Merchant, University of Reading
Principal strengths of data set	Consistently processed data spanning all three ATSR sensors
Principal recommended applications	Climate research; particularly applications requiring long-term, stable, low-bias records of SST
KEY DESCRIPTIVE FEATURES	
Period covered	01-11-1991 to 08-04-2012
Geographic range	Global
Spatial resolution	1 km irregular grid and 0.05° regular latitude-longitude grid
Temporal resolution	Twice daily (not accounting for cloud cover)
Timeliness of new data	Data end in April 2012
Dataset volume	3.0 TB (L2P), 595 GB (L3U) and 208 GB (L3C)
Valid data fraction	SST from clear-sky observations only, this being ~14% of total data over oceans
Data level / grid	L2P (1 km irregular grid) and L3U/L3C (0.05° regular latitude-longitude grid)

Observation technology	The Along-Track Scanning Radiometer (ATSR) series of infrared sensors comprises three instruments: ATSR-1 on the ERS-1 platform (1991-1995); ATSR-2 on ERS-2 (1995-2001) and Advanced (A) ATSR on Envisat (2002-2012)
Dependence on other data	Numerical weather prediction fields (ERA Interim re-analysis)
Type(s) of SST	1. Skin SST (SST of upper ~10 μm depth). 2. SST at 0.2 m (standardised with respect to diurnal cycle). Diurnal variability modelling is used to estimate SST_{20cm} from SST_{skin}.
Traceability	Not yet established
Uncertainty info in product	Provided for each SST is total uncertainty and components of uncertainty from effects with different spatiotemporal correlation scales
QUANTITATIVE METRICS	
Difference relative to drifting buoys *Global median difference of satellite minus drifting buoy SST, across full dataset.*	0.01 K
Geographical variation in difference relative to drifting buoys *Geographical variation in the difference, as described by the standard deviation of median satellite minus drifting buoy SST differences on space scales of ~1000 km, across the full data-set*	0.04 K
Dispersion relative to drifting buoys *Spread of differences associated with non-systematic effects as quantified by a robust standard deviation of differences of satellite and drifting buoy data, after removing the geographical variations in differences quantified above*	0.17 K 
Stability *95% confidence interval for the relative multi-year trend between satellite SSTs and the Global Tropical Moored Buoy Array*	Daytime (1991-2012) in tropical Pacific: -2.1 mK/year < trend < 2.3 mK/year Nighttime (1991-2012) in tropical Pacific: -2.6 mK/year < trend < 0.4 mK/year

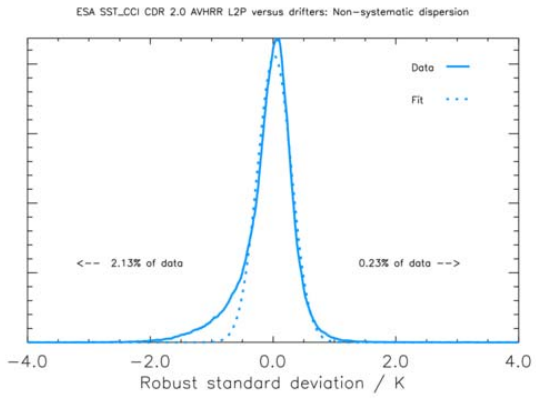
Sensitivity to true SST *Average weight of the satellite observations in determining SSTs in the dataset, the difference from 100% representing the weight of prior information in the SSTs*	Approximately 100%
AVAILABILITY, DOCUMENTATION AND FEEDBACK	
Data URL / ftp / DOI	http://www.esa-sst-cci.org/
Primary peer reviewed reference	C.J. Merchant et al (2019) Satellite-based time-series of sea-surface temperature since 1981 for climate applications, in prep for Nature Science Data [RD.414]
Source of technical documents	http://www.esa-sst-cci.org/
Dataset restrictions	None, free and open access
Facility for user feedback	science.leader@esa-sst-cci.org
Other documentation	Product User Guide (see http://www.esa-sst-cci.org/)
OTHER PRINCIPLES (GCOS)	
2. and 12. Overlaps between sensors exist and are exploited	A stable record is achieved by exploiting overlaps between sensors and using a combination of channels which is available for all three sensors.
3. Detailed history of methods/algorithms is available	CCI-SST Algorithm Theoretical Basis Document (ATBD) 2019 [RD.415]
11. Constant sampling within diurnal cycle	SSTs are provided that are adjusted to represent a standard point in the diurnal cycle (10.30 local time, morning or evening)

5.2 AVHRR

Table 5. Information evaluating the ESA SST CCI AVHRR Version 2 product as a climate record.

SUMMARY	
Status of assessment	Dataset producer's information
Dataset name and version	ESA SST CCI AVHRR product version 2
Lead Investigator and/or Agency	Chris Merchant, University of Reading
Principal strengths of data set	Consistently processed data spanning multiple AVHRR sensors, adjusted using ATSR series data as a reference (1991-2012) and using overlaps between sensors and tuning to *in situ* data to achieve stability prior to 1991.
Principal recommended applications	Climate research particularly applications requiring long–term, stable, low-bias records of SST
KEY DESCRIPTIVE FEATURES	
Period covered	24-08-1981 to 31-12-2016

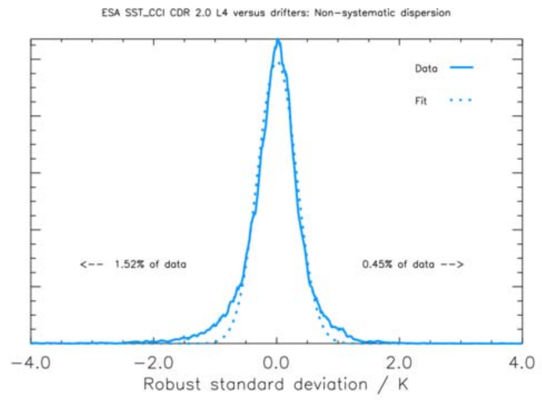
Geographic range	Global
Spatial resolution	4 km irregular grid
Temporal resolution	Twice daily
Timeliness of new data	Will be extended by the Copernicus Climate Change Service
Dataset volume	6.6 TB (L2P), 3.6TB (L3U) and 2.2TB (L3C)
Valid data fraction	SST from clear-sky observations only, this being ~14% of total
Data level / grid	L2P (irregular latitude-longitude grid with 4 km spacing at nadir to the satellite) and L3U/L3C (0.05° regular latitude-longitude grid)
Observation technology	The Advanced Very-High Resolution Radiometer (AVHRR) series of infrared sensors on the NOAA and MetOp-A satellites
Dependence on other data	Numerical weather prediction fields (ERA Interim re-analysis), ATSR and *in situ* measurements
Type(s) of SST	1. Skin SST (SST of upper ~10 μm depth). 2. SST at 0.2 m (standardised with respect to diurnal cycle). Diurnal variability modelling is used to estimate SST_{20cm} from SST_{skin}.
Traceability	Not yet established
Uncertainty info in product	Provided for each SST is total uncertainty and components of uncertainty from effects with different spatiotemporal correlation scales
QUANTITATIVE METRICS	
Difference relative to drifting buoys *Global median difference of satellite minus drifting buoy SST, across full dataset.*	-0.01 K
Geographical variation in difference relative to drifting buoys *Geographical variation in the difference, as described by the standard deviation of median satellite minus drifting buoy SST differences on space scales of ~1000 km, across the full dataset*	0.06 K

Dispersion relative to drifting buoys *Spread of differences associated with non-systematic effects as quantified by a robust standard deviation of differences of satellite and drifting buoy data, after removing the geographical variations in differences quantified above*	0.31 K 
Stability *95% confidence interval for the relative multi-year trend between satellite SSTs and the Global Tropical Moored Buoy Array*	Daytime (1991-2010) in tropical Pacific: 3.6 mK/year < trend < 15.5 mK/year Nighttime (1991-2010) in tropical Pacific: -2.1 mK/year < trend < 9.8 mK/year
Sensitivity to true SST *Average weight of the satellite observations in determining SSTs in the dataset, the difference from 100% representing the weight of prior information in the SSTs*	Approximately 100%
AVAILABILITY, DOCUMENTATION AND FEEDBACK	
Data URL / ftp / DOI	http://www.esa-sst-cci.org/
Primary peer reviewed reference	C.J. Merchant et al (2019) Satellite-based time-series of sea-surface temperature since 1981 for climate applications, in prep for Nature Science Data [RD.414]
Source of technical documents	http://www.esa-sst-cci.org/
Dataset restrictions	None, free and open access
Facility for user feedback	science.leader@esa-sst-cci.org
Other documentation	Product User Guide (see http://www.esa-sst-cci.org/)
OTHER PRINCIPLES (GCOS)	
2. and 12. Overlaps between sensors exist and are exploited	A stable record is achieved by exploiting overlaps between sensors.
3. Detailed history of methods/algorithms is available	CCI-SST Algorithm Theoretical Basis Document (ATBD) 2019 [RD.415]
11. Constant sampling within diurnal cycle	SSTs are provided that are adjusted to represent a standard point in the diurnal cycle (10.30 local time, morning or evening)

5.3 Analysis

Table 6. Information evaluating the ESA SST CCI Analysis Version 2 product as a climate record.

SUMMARY	
Status of assessment	Dataset producer's information
Dataset name and version	ESA SST CCI Analysis product version 2
Lead Investigator and/or Agency	Chris Merchant, University of Reading
Principal strengths of data set	Statistically infilled combination of data from the ATSR and AVHRR series of sensors
Principal recommended applications	Climate research particularly applications requiring long–term, stable, low-bias records of SST
KEY DESCRIPTIVE FEATURES	
Period covered	01-09-1981 to 31-12-2016
Geographic range	Global
Spatial resolution	0.05° regular latitude-longitude grid; actual resolution is not necessarily this fine (length scales governing the spreading of observation information range between 15 km and 300 km – see [RD.407].
Temporal resolution	Daily
Timeliness of new data	Will be extended by the Copernicus Climate Change Service
Dataset volume	228 GB
Valid data fraction	100% of the ocean (any locations with no SST observations are filled in)
Data level / grid	L4 (0.05° regular latitude-longitude grid)
Observation technology	The Along-Track Scanning Radiometer (ATSR) series and the Advanced Very-High Resolution Radiometer (AVHRR) series of infrared sensors
Dependence on other data	SSTs input to the analysis use numerical weather prediction fields (ERA Interim re-analysis). Sea ice information is also used (EUMETSAT OSI SAF).
Type(s) of SST	SSTdepth (SST at 0.2 m)
Traceability	Not yet established
Uncertainty info in product	Provided for each SST is an estimate of total uncertainty
QUANTITATIVE METRICS	
Difference relative to drifting buoys *Global median difference of satellite minus drifting buoy SST, across full dataset.*	-0.04 K (1991 – 2012)

Geographical variation in difference relative to drifting buoys *Geographical variation in the difference, as described by the standard deviation of median satellite minus drifting buoy SST differences on space scales of ~1000 km, across the full dataset*	0.05 K (1991 – 2012)
Dispersion relative to drifting buoys *Spread of differences associated with non-systematic effects as quantified by a robust standard deviation of differences of satellite and drifting buoy data, after removing the geographical variations in differences quantified above*	0.34 K (1991 – 2012) 
Stability *95% confidence interval for the relative multi-year trend between analysis SSTs and the Global Tropical Moored Buoy Array*	In Tropical Pacific (1991 – 2012): -1.51 mK/year < trend < -0.05 mK/year
Sensitivity to true SST *Average weight of the satellite observations in determining SSTs in the dataset, the difference from 100% representing the weight of prior information in the SSTs*	Variable
AVAILABILITY, DOCUMENTATION AND FEEDBACK	
Data URL / ftp / DOI	http://www.esa-sst-cci.org/
Primary peer reviewed reference	Roberts-Jones, J., E. Fiedler and M. Martin, 2012: Daily, global, high-resolution SST and sea-ice reanalysis for 1985-2007 using the OSTIA system, J. Climate, 25, 6215-6232, doi:10.1175/JCLI-D-11-00648.1 [RD.239] and ESA SST CCI Technical Note [RD.294] and C.J. Merchant et al (2019) Satellite-based time-series of sea-surface temperature since 1981 for climate applications, in prep for Nature Science Data [RD.414]
Source of technical documents	http://www.esa-sst-cci.org/
Dataset restrictions	None, free and open access
Facility for user feedback	science.leader@esa-SST-cci.org
Other documentation	Product User Guide (see http://www.esa-sst-cci.org/)

OTHER PRINCIPLES (GCOS)	
2. and 12. Overlaps between sensors exist and are exploited	Yes (see information about the input datasets)
3. Detailed history of methods/algorithms is available	Yes (see references above)
11. Constant sampling within diurnal cycle	SSTs are representative of daily averages.

6. USING THE DATA FILES

The data files for the ESA SST CCI products are described in this section. The file naming convention is discussed in Section 6.1. The format of the files is described in Section 6.2 and the structure of the data within the files is given in Section 6.4.

6.1 File names

The format of the ESA SST CCI filenames is:

```
<Indicative date><Indicative time>-ESACCI-<Processing level>_GHRSST-<SST
Type>-<Product string>-<Additional segregator>-v02.0-fv<File version>.nc
```

For example:

20000101000206-ESACCI-L2P_GHRSST-SSTskin-AVHRR15_G-CDR2.0-v02.0-fv01.0nc

The components of the file names denoted in <> are described in the sections below.

6.1.1 Indicative date

A date in the form YYYYMMDD, where YYYY is the year, MM is the month and DD is the day. This is the date that best represents the observation date of the data in the file. In the example the date is 01 January 2000.

6.1.2 Indicative time

An identifying time (in the coordinated universal time (UTC) standard) for the data in the form HHMMSS, where HH is the hour, MM is the minute and SS are the seconds. For files containing single orbits of data (i.e. L2P and L3U files) it represents the beginning of the orbit; for collated (L3C) or analysed data (L4) it is the central time of the collation window or the nominal time of the analysis respectively. In the example filename the time is 00 hours, 1 minute and 5 seconds.

6.1.3 Processing level

The 'level' of the data; either L2P, L3U, L3C or L4. See Section 3.1.2 and/or the file contents descriptions for each data level (Sections 0, 6.4.4 and 6.4.5) for explanations of these. The processing level in the example filename is L2P.

6.1.4 SST type

This is the depth of the SST provided in the file. For the ESA SST CCI products it might be SSTskin, SSTsubskin, SSTdepth or SSTfnd (corresponding to ~10μm, ~1mm, 0.2m or ~10m). See Section 3.1.2 for more details. When there are two SST types in a file, the file name contains the type of SST retrieved directly from the satellite measurements, and not the type of SST after adjustment to a standard depth and time. SST type in the example is SSTskin.

6.1.5 Product string

This section of the filename provides information about the satellite sensor or the analysis system used for the data in the file. The product string shown in the example is AVHRR15_G (the AVHRR sensor flown on the NOAA-15 satellite).

6.1.6 Additional segregator

The additional segregator is used to distinguish between two classes of ESA SST CCI product. If this part of the filename contains ‘CDR’ the file is a full version release. If this part of the filename is ‘EXP’, it is an experimental release. For L4 files, this part of the filename is ‘GLOB_CDR’. The addition of ‘GLOB’ prefix denotes that the file contains global data. The additional segregator in the example filename is CDR.

6.1.7 File version

A version number in the form xx.x that is incremented when new versions of the file become available. The file version in the example is 01.0.

6.2 Format of the data files

All data are contained in Network Common Data Format (NetCDF) files. This format allows multiple data arrays and metadata to be stored together in one file. Examples of reading data from NetCDF files are provided in Section 7.

More specifically, the data format of the files is NetCDF-4. This means that the files cannot be read by versions of the NetCDF software library earlier than version 4. Data within the files are compressed. The NetCDF software automatically handles the decompression of the data. Although the data compression slows down data access, it significantly reduces the file size. If access speed is a concern, the command below can be used in Linux to remove internal compression of data (similar commands are available for other operating systems). The program used, nccopy, is provided as part of the NetCDF library.

nccopy -d 0 <NetCDF4 file name> <Name for uncompressed version of file>

The ESA SST CCI data files use the ‘classic’ NetCDF-4 data model.

For more information about NetCDF, see http://www.unidata.ucar.edu/software/netcdf/.

6.3 Tools that can be used to work with the data files

As NetCDF is a commonly used format, there are many tools available to view and work on the data within the files. For example see http://www.unidata.ucar.edu/software/netcdf/software.html and the tools listed in Section 4.

6.4 Contents of the data files

Each ESA SST CCI data file contains metadata describing the file and its contents (in NetCDF, these are referred to as global attributes), multiple data arrays (which are referred to as variables) and metadata specific to each variable (variable attributes). The names and form of the variables and attributes follow international standards. In particular, the files are consistent with the GHRSST Data Specification version 2.0 (GDS 2.0, [RD.87]), which is a file specification defined for use of SST data made available through the GHRSST project. The files also include metadata required by the CCI Data Standards v2.0 and follow the standards defined by the Climate and Forecasting (CF) conventions [RD.177].

Four different file formats are used for the ESA SST CCI data products. The specification chosen for each product depends on the ‘level’ of SST data contained within them (L2P, L3U, L3C or L4 – see Section 3.1.2 for definitions of these). To find the file format for a given dataset, refer to the directory of ESA SST CCI products in Section 4. The description of each data product includes the data level and therefore which file format description to read.

In the sections below each of the four file formats are described. First, the global attributes that are common to all the files are listed. Then, attributes that apply to variables are given. Finally, the variables that are contained in the files are listed for each data level in turn (L2P format in Section 0, L3U in Section 6.4.4, L3C in Section 6.4.5 and L4 in Section 6.4.5). A sample listing of the structure of each type of file is given in Appendix 2.

For a complete, technical description of the file format see the ESA SST CCI Product Specification Document [RD.383 (for L2 and L3 v2 products); RD.409 (for L4 v2 products)] which can be downloaded from http://www.esa-sst-cci.org/.

6.4.1 Global attributes

The global attributes common to all the ESA SST CCI product files are described in Table 7. Most of the contents were adapted from the definitions in the GDS [RD.87].

Table 7. List of global attributes found in all ESA SST CCI product files.

Name of global attribute	Description	Contents or form of contents
Conventions	Describes the conventions followed when defining the contents of the file.	CF-1.5, Unidata Observation Dataset v1.0
title	A descriptive name for the data. Includes product string (see Section 6.1.5) and the data level of the product.	ESA SST CCI <Product String> <Data Level> product
summary	A description of the data. Includes product string (see Section 6.1.5), the data level of the product and the name of the algorithm used to produce the data (see Appendix 1).	<Product String> <Data Level> product from the ESA SST CCI project, produced using <algorithm name>.
references	References that provide more information about the data.	
institution	A standardised name for the creators of the data file.	ESACCI
history	Used to detail the history of the data compilation.	e.g. Created using GBCS library v2.1.10
comment	Miscellaneous information.	
license	How the data are licensed for use.	GHRSST protocol describes data use as free and open.
id	This contains a name for the dataset that uniquely identifies it from other data provided through the GHRSST project.	e.g. AVHRR15_G-ESACCI-L2P-EXP-v1.2
naming_authority	Together with the id, this provides a unique identifier for the dataset.	org.ghrsst
product_version	The version of the product updated during reprocessing.	Product version example: 1.2

Name of global attribute	Description	Contents or form of contents
uuid	A Universally Unique Identifier for the file. For example see http://www.ossp.org/pkg/lib/uuid/.	
tracking_id	Contains the same value as uuid above.	
gds_version_id	The version of the GDS [RD.87] that was followed when creating the file.	2.0
netcdf_version_id	The version of the NetCDF library used to create the file.	Format example: 4.3.2
date_created	File creation date in format shown in next column, where T is used to delimit the date and time information and Z indicates that the time is Coordinated Universal Time (UTC).	Format: yyyymmddThhmmssZ
file_quality_level	A number that gives an indication of the quality of data in the file.	0: unknown quality; 1: extremely suspect; 2: suspect; 3: no known problems.
spatial_resolution	An indication of the spatial resolution of data in the file.	
start_time	Defines the time of the first measurement contained in the file. See date_created for explanation of the format.	Format: yyyymmddThhmmssZ, replacing the lower case letters with the appropriate numbers
time_coverage_start	Identical to start_time.	See start_time
stop_time	As start_time but the time of the last measurement.	See start_time
time_coverage_end	Identical to stop_time.	See start_time
time_coverage_duration	Difference between stop_time and start_time in the form PdDThHmMsS. In this format, P indicates that it is a duration, DT delimits the number of days from the time, with H, M and S marking the hours, minutes and seconds.	Format: PdDThHmMsS, replacing the lower case letters with the appropriate numbers
time_coverage_resolution	Temporal resolution of data in the file i.e. the orbit repeat period or the frequency of L3/L4 data.	See time_coverage_duration

Name of global attribute	Description	Contents or form of contents
source	List of all source data used for the file.	
platform	List of satellites on which the sensors used to generate the data were mounted.	
sensor	List of sensors used for the data in this file.	
Metadata_Conventions	The name of metadata conventions followed.	Unidata Dataset Discovery v1.0
metadata_link	Link to metadata record.	http://www.esa-cci.org
keywords	Standard words that describe the data, taken from the source specified in keywords_vocabulary.	Oceans > Ocean Temperature > Sea Surface Temperature
keywords_vocabulary	Defines the source of the text in the keywords attribute; [RD.176].	NASA Global Change Master Directory (GCMD) Science Keywords
standard_name_vocabulary	Defines the source of the standard names for the variables [RD.177].	NetCDF Climate and Forecast (CF) Metadata Convention
geospatial_lat_units	Units of geospatial_lat_resolution.	degrees_north
geospatial_lat_resolution	Latitude resolution.	
geospatial_lon_units	Units of the geospatial_lon_resolution.	degrees_east
geospatial_lon_resolution	Longitude resolution.	
northernmost_latitude	Northern extent of the data.	
geospatial_lat_max	Identical to northernmost_latitude.	
southernmost_latitude	Southern extent of the data.	
geospatial_lat_min	Identical to southernmost_latitude	

Name of global attribute	Description	Contents or form of contents
easternmost_ longitude	Eastern extent of the data.	
geospatial_lon_max	Identical to easternmost_ longitude	
westernmost_ longitude	Western extent of the data.	
geospatial_lon_min	Identical to westernmost_ longitude	
geospatial_vertical_min	Depth of the deepest SST in the file (the value is negative as the direction is downwards).	
geospatial_vertical_max	Depth of the shallowest SST in the file (value is negative as the direction is downwards).	
acknowledgment	Funding source.	Funded by ESA
creator_name	Description of data creators.	ESA SST CCI
creator_email		science.leader@esa-sst-cci.org
creator_url		http://www.esa-sst-cci.org/
creator_processing_ institution	Additional information about the creators of the data – used to signify which of the ESA SST CCI project partners created the data file.	These data were produced at <institution> as part of the ESA SST CCI project.
Project	The name of the project.	Climate Change Initiative – European Space Agency
publisher_name	Information about the data publisher.	ESACCI
publisher_url		http://www.esa-sst-cci.org
publisher_email		science.leader@esa-sst-cci.org
processing_level	Data level (L2P, L3U, L3C, or L4).	
cdm_data_type	Describes the form of the data (“swath” or “grid”).	

6.4.2 Variable attributes

The attributes that contain the metadata associated with particular variables are listed in Table 8. Note that each variable will only have a subset of these attributes. The final column shows the variables to which each attribute is applicable.

Table 8. List of attributes that are provided with variables in the NetCDF files.

Name of variable attribute	Description	Applicable to which variables?
_FillValue	The number put into the data arrays where there are no valid data (before applying the scale_factor and add_offset attributes).	Most variables but not applicable to latitude, longitude, time and flag fields.
Units	The units of the data after applying the scale_factor and add_offset conversion.	Most variables have this attribute.
scale_factor	Multiply the data stored in the NetCDF file by this number.	Most variables but not applicable to latitude, longitude, time and flag fields.
add_offset	After applying scale_factor above, add this to obtain the data in the units specified in the units attribute.	Most variables but not applicable to latitude, longitude, time and flag fields.
long_name	A descriptive name for the data.	All
valid_min	The minimum valid value of the data (before applying scale_factor and add_offset).	All
valid_max	The maximum valid value of the data (before applying scale_factor and add_offset).	All
standard_name	A unique descriptive name for the data, taken from the CF conventions ([RD.177]; https://cf-trac.llnl.gov/trac).	Most (but not all variables have a corresponding standard name defined in the CF conventions)
comment	Miscellaneous information.	Most variables have this attribute.
source	A list of data sources used for the data in this variable.	Geophysical data variable.
References	References that provide more information about the data.	Applicable to a few variables (see also the global attribute with the same name).
Depth	Effective depth for SST data.	SST variables.
Coordinates	Identifies coordinate variables associated with a data array.	Variables in L2P files.
reference_datum	Information about the coordinates.	Latitude and longitude variables only.

Name of variable attribute	Description	Applicable to which variables?
Calendar	Information about the calendar used for the time coordinate.	Time variable only.
flag_meanings	List of descriptions of the meanings of flags, masks etc.	Only variables containing flags, masks or quality information.
flag_values	Mutually exclusive values that correspond to the meanings in flag_meanings e.g. 1, 2, 3, 4, 5. The variable will contain one of these numbers in each location.	Only variables containing flags, masks or quality information.
flag_masks	Values that can be set in combination corresponding to the meanings in flag_meanings e.g. 1, 2, 4, 8, 16. The variable will contain in each location the sum of all the flags that are set e.g. if the first three flags are set the variable will contain 1+2+4=7.	Only variables containing flags, masks or quality information.
Height	Height that wind data corresponds to.	Used only for variables containing wind speed ancillary data.
time_offset	Difference between SST reference time and time that wind data correspond to (hours).	Used only for variables containing wind speed ancillary data.
correlation_ length_scale	Estimated spatial correlation length scale for uncertainties.	Only used for some uncertainty variables.
correlation_ time_scale	Estimated temporal correlation length scale for uncertainties.	Only used for some uncertainty variables.
axis	For variables containing coordinates, this indicates the axis that the coordinate corresponds to (‘X’, ‘Y’ or ‘T’ for longitude, latitude or time).	Coordinate variables only.
bounds	For coordinate variables, this indicates a variable that contains the bounds of the grid cells.	Coordinate variables only.

6.4.3 ‘L2P’ data format

Level 2 pre-processed (L2P) data files contain SSTs from a single orbit of a satellite instrument. The SSTs are stored as a data strip corresponding to the section of the Earth viewed by the satellite as it travelled through its orbit.

The dimensions of the data in the file are described in Table 9. The data are stored in variables in the NetCDF file with the names given in Table 10.

Table 9. The dimensions of the data in a L2P file.

Dimension name	Description
time	This is always 1 because there is only one orbit of data per file.
ni	Data array dimension corresponding to the direction perpendicular to the track of the instrument.
nj	Data array dimension corresponding to the direction along the track of the instrument.

Table 10. Data arrays stored in L2P data files. The dimensions of the arrays are given in parenthesis after the name of the variable in the NetCDF file. The dimensions are defined in Table 9.

Category	Name of data (size of array)	Description
Coordinates	lat (nj×ni)	Central latitude of each point in the data arrays.
	lon (nj×ni)	Central longitude of each point in the data arrays.
	time (time)	A base time from which the time of each SST value is referenced. Here it refers to the start time of the granule. In order to determine the exact time of a specific pixel or grid cell variables, sst_dtime and sst_depth_dtime are provided (see below). These provide the difference in seconds between the pixel observation time and the reference time for the file.
	sst_dtime (time×nj×ni)	The time difference in seconds between the pixel observation time and the reference time for the file (see 'time' above).
	sst_depth_dtime (time×nj×ni)	The time difference in seconds between the pixel observation time adjusted to a standard local time and the reference time for the file (not available in all products).
Geophysical variables	sea_surface_temperature (time×nj×ni)	The best available skin SST retrievals with no adjustment to a standard depth or time.
	sea_surface_temperature_depth (time×nj×ni)	SSTs adjusted to a standard depth and local time (not available in all products).
	wind_speed (time×nj×ni)	Wind speed (sourced from the ERA Interim reanalysis).
Quality information	quality_level (time×nj×ni)	Indicates the general quality of that pixel – higher values being better. Quantitative analyses should use the higher quality levels (4 or 5). Quality levels 2 and 3 may be useful for qualitative analyses, but the pixels have an increased chance of being cloud contaminated. Quality level of the SST: 0 no data 1 bad data

Category	Name of data (size of array)	Description
		2 worst usable data 3 low quality 4 good quality 5 best quality
Uncertainty information – total uncertainty	sses_standard_ deviation (time×nj×ni)	The total uncertainty in the SSTs in the sea_surface_temperature variable.
	sst_depth_total_ uncertainty (time×nj×ni)	The total uncertainty in the SSTs in the sea_surface_temperature_depth variable (not available in all products).
Uncertainty information – individual components	large_scale_correlated_ uncertainty (time×nj×ni)	Component of uncertainty that is correlated over large spatial scales.
	synoptically_ correlated_uncertainty (time×nj×ni)	Component of uncertainty that is correlated over synoptic (~100 km) spatial scales.
	uncorrelated_ uncertainty (time×nj×ni)	Component of uncertainty that is uncorrelated between SSTs.
	adjustment_uncertainty (time×nj×ni)	Component of uncertainty associated with adjusting SSTs to a standard depth and time; correlated over synoptic (~100 km) spatial scales.
Retrieval information	l2p_flags (time×nj×ni)	Indicates the type of pixel and what kind of SST retrieval was applied. Pixel type information includes: land, ice, lake, or river. Pixels in the Level 2 products may have these flags set but will not contain any SST data (other than the Caspian Sea). The dual-view bit (6) will be set for retrievals from one of the dual-view sensors (ATSR or SLSTR). The three-channel bit (7) indicates that the more accurate three-channel retrieval has been used. Although the three-channel retrieval can only be used at night, the use of the two-channel retrieval is not a guarantee that the pixel corresponds to a daytime observation (the retrieval may have switched to two-channel due to an instrument failure); therefore, there is a separate daytime flag (8) which indicates if the solar zenith angle was < 90° when the pixel was observed. When written in binary format, each digit of each number provides information about the retrieval in each location. The least significant digit is called bit 0 and there are 16 bits in total, although only 8 are currently in use. The meanings are: **Bit / Description / Meaning if set to 0 / Meaning if set to 1** 0 / Type of sensor / Infrared / Microwave 1 / Ocean or land / Ocean / Land 2 / Sea ice indicator / No sea ice / Sea ice present

Category	Name of data (size of array)	Description
		3 Lake indicator — Not a lake — Lake 4 River indicator — Not a river — River 6 Number of satellite views available — One (nadir) view — Two (dual) views 7 Number of satellite radiance channels available — Two — Three 8 Day/night — Night time — Day time (solar zenith angle < 90°)
Other	sses_bias (time×nj×ni)	For ESA SST CCI data **only** it is safe to ignore this data array (it is filled with zeros). In other GHRSST data files this is used to give an indication of bias in the SSTs.

6.4.4 'L3U' data format

Level 3 uncollated (L3U) data files contain regridded SSTs from a single orbit file. The content of L3U files is very similar to L2P files.

Level 3 files are stored on a global regular latitude/longitude grid and variables have the following dimensions:

time: UNLIMITED (1)

lat: Number of latitude points (3600)

lon: Number of longitude points (7200)

The resolution used for the products is 0.05° hence the full size of the arrays is 7200x3600. The time dimension is specified as **unlimited**, allowing standard netCDF tools to easily concatenate and manipulate multiple files, but each L3 file contains a single time slice (corresponding to a day).

The dimensions of the data arrays in the L3U files are defined in Table 11 and the variables found in the files are listed in

Table 12.

Table 11. The dimensions of the data in a L3U file.

Dimension name	Description
time	This is always 1 because there is only one orbit of data per file.

Dimension name	Description
lon	These are the dimensions of the regular latitude-longitude grid on which the data are stored. For ESA SST CCI data these dimensions are 7200 and 3600 for lon and lat respectively (i.e., a global 0.05° x 0.05° grid).
lat	
bnds	Used to define arrays that give the bounds of the latitudes, longitudes and times of the data; always set to 2.

Table 12. Data arrays stored in L3U data files. The dimensions of the arrays are given in parenthesis after the name of the variable in the NetCDF file. These are defined in Table 11.

Category	Name of data (size of array)	Description
Coordinates	lat (lat)	Central latitude of each grid cell.
	lat_bnds (bnds×lat)	The latitudes of the edges of each grid cell.
	lon (lon)	Central longitude of each grid cell.
	lon_bnds (bnds×lon)	The longitudes of the edges of each grid cell.
	time (time)	A base time from which the time of each SST value is referenced. Here it refers to the start time of the granule. In order to determine the exact time of a specific pixel or grid cell variables, sst_dtime and sst_depth_dtime are provided (see below). These provide the difference in seconds between the pixel observation time and the reference time for the file.
	time_bnds (bnds×time)	The start and end times of the data collection for the data in the file.
	sst_dtime (time×lat×lon)	The time difference in seconds between the pixel observation time and the reference time for the file (see 'time' above).
	sst_depth_dtime (time×nj×ni)	The time difference in seconds between the pixel observation time adjusted to a standard local time and the reference time for the file (not available in all products).
Geophysical variables	sea_surface_ temperature (time×lat×lon)	The best available skin SST retrievals with no adjustment to a standard depth or time.
	sea_surface_ temperature_depth (time×lat×lon)	SSTs adjusted to a standard depth and local time (not available in all products).
	wind_speed (time×lat×lon)	Wind speed (sourced from the ERA Interim reanalysis).
Quality information	quality_level (time×lat×lon)	Indicates the general quality of that pixel – higher values being better. Quantitative analyses should use the higher quality levels (4 or 5). Quality lev-

Category	Name of data (size of array)	Description
		els 2 and 3 may be useful for qualitative analyses, but the pixels have an increased chance of being cloud contaminated. Quality level of the SST: 0 no data 1 bad data 2 worst usable data 3 low quality 4 good quality 5 best quality
Uncertainty information – total uncertainty	sses_standard_deviation (time×lat×lon)	The total uncertainty in the SSTs in the sea_surface_temperature variable.
	sst_depth_total_uncertainty (time×lat×lon)	The total uncertainty in the SSTs in the sea_surface_temperature_depth variable (not available in all products).
Uncertainty information – individual components	large_scale_correlated_uncertainty (time×lat×lon)	Component of uncertainty that is correlated over large spatial scales.
	synoptically_correlated_uncertainty (time×lat×lon)	Component of uncertainty that is correlated over synoptic (~100 km) spatial scales.
	uncorrelated_uncertainty (time×lat×lon)	Component of uncertainty that is uncorrelated between SSTs. A new uncertainty component arising from under-sampling of 0.05° grid cells due to their partial obscuration by cloud has been estimated for the experimental Release 1.2 L3U products and added to the component arising from instrument noise.
	adjustment_uncertainty (time×lat×lon)	Component of uncertainty associated with adjusting SSTs to a standard depth and time; correlated over synoptic (~100 km) spatial scales.
Retrieval information	l2p_flags (time×lat×lon)	Indicates the type of pixel and what kind of SST retrieval was applied. Pixel type information includes: land, ice, lake, or river. Pixels in the Level 2 products may have these flags set but will not contain any SST data (other than the Caspian Sea). The dual-view bit (6) will be set for retrievals from one of the dual-view sensors (ATSR or SLSTR). The three-channel bit (7) indicates that the more accurate three-channel retrieval has been used. Although the three-channel retrieval can only be used at night, the use of the two-channel retrieval is not a guarantee that the pixel corresponds to a daytime observation (the retrieval may have switched to two-channel due to an instrument failure); therefore, there is a separate daytime flag (8) which indicates if the solar zenith angle

<table>
<tr><th>Category</th><th>Name of data (size of array)</th><th>Description</th></tr>
<tr><td></td><td></td><td>was < 90° when the pixel was observed.
When written in binary format, each digit of each number provides information about the retrieval in each location. The least significant digit is called bit 0 and there are 16 bits in total, although only 8 are currently in use. The meanings are:
<table>
<tr><th>Bit</th><th>Description</th><th>Meaning if set to 0</th><th>Meaning if set to 1</th></tr>
<tr><td>0</td><td>Type of sensor</td><td>Infrared</td><td>Microwave</td></tr>
<tr><td>1</td><td>Ocean or land</td><td>Ocean</td><td>Land</td></tr>
<tr><td>2</td><td>Sea ice indicator</td><td>No sea ice</td><td>Sea ice present</td></tr>
<tr><td>3</td><td>Lake indicator</td><td>Not a lake</td><td>Lake</td></tr>
<tr><td>4</td><td>River indicator</td><td>Not a river</td><td>River</td></tr>
<tr><td>6</td><td>Number of satellite views available</td><td>One (nadir) view</td><td>Two (dual) views</td></tr>
<tr><td>7</td><td>Number of satellite radiance channels available</td><td>Two</td><td>Three</td></tr>
<tr><td>8</td><td>Day/night</td><td>Night time</td><td>Day time (solar zenith angle < 90°)</td></tr>
</table></td></tr>
<tr><td>Other</td><td>sses_bias (time×lat×lon)</td><td>For ESA SST CCI data only it is safe to ignore this data array (it is filled with zeros). In other GHRSST data files this is used to give an indication of bias in the SSTs.</td></tr>
</table>

6.4.5 'L3C' data format

Level 3 collated (L3C) data files contain regridded SSTs from all orbits in a particular day, separated out into day and night files. The content of L3C files is very similar to L3U files.

Level 3 files are stored on a global regular latitude/longitude grid and variables have the following dimensions:

time: UNLIMITED (1)

lat: Number of latitude points (3600)

lon: Number of longitude points (7200)

The resolution used for the products is 0.05° hence the full size of the arrays is 7200x3600. The time dimension is specified as **unlimited**, allowing standard netCDF tools to easily concatenate and manipulate multiple files, but each L3 file contains a single time slice (corresponding to a day).

The dimensions of the data arrays in the L3C files are defined in Table 13 and the variables found in the files are listed in Table 14.

Table 13. The dimensions of the data in a L3C file.

Dimension name	Description
time	This is always 1 because there is only one orbit of data per file.
lon	These are the dimensions of the regular latitude-longitude grid on which the data are stored. For ESA SST CCI data these dimensions are 7200 and 3600 for lon and lat respectively (i.e., a global 0.05° x 0.05° grid).
lat	
bnds	Used to define arrays that give the bounds of the latitudes, longitudes and times of the data; always set to 2.

Table 14. Data arrays stored in L3C data files. The dimensions of the arrays are given in parenthesis after the name of the variable in the NetCDF file. These are defined in Table 13.

Category	Name of data (size of array)	Description
Coordinates	lat (lat)	Central latitude of each grid cell.
	lat_bnds (bnds×lat)	The latitudes of the edges of each grid cell.
	lon (lon)	Central longitude of each grid cell.
	lon_bnds (bnds×lon)	The longitudes of the edges of each grid cell.
	time (time)	A base time from which the time of each SST value is referenced. Here it refers to the centre time of collation window (midday for daily files). sst_dtime and sst_depth_dtime are provided (see below). These provide the difference in seconds between the pixel observation time and the reference time for the file.
	time_bnds (bnds×time)	The start and end times of the data collection for the data in the file.
	sst_dtime (time×lat×lon)	The time difference in seconds between the pixel observation time and the reference time for the file (see 'time' above).
	sst_depth_dtime (time×nj×ni)	The time difference in seconds between the pixel observation time adjusted to a standard local time and the reference time for the file (not available in all products).
Geophysical variables	sea_surface_ temperature (time×lat×lon)	The best available skin SST retrievals with no adjustment to a standard depth or time.
	sea_surface_ temperature_depth (time×lat×lon)	SSTs adjusted to a standard depth and local time (not available in all products).

Category	Name of data (size of array)	Description
	wind_speed (time×lat×lon)	Wind speed (sourced from the ERA Interim reanalysis).
Quality information	quality_level (time×lat×lon)	Indicates the general quality of that pixel – higher values being better. Quantitative analyses should use the higher quality levels (4 or 5). Quality levels 2 and 3 may be useful for qualitative analyses, but the pixels have an increased chance of being cloud contaminated. Quality level of the SST: 0 no data 1 bad data 2 worst usable data 3 low quality 4 good quality 5 best quality
Uncertainty information – total uncertainty	sses_standard_ deviation (time×lat×lon)	The total uncertainty in the SSTs in the sea_surface_temperature variable.
	sst_depth_total_ uncertainty (time×lat×lon)	The total uncertainty in the SSTs in the sea_surface_temperature_depth variable (not available in all products).
Uncertainty information – individual components	large_scale_correlated_ uncertainty (time×lat×lon)	Component of uncertainty that is correlated over large spatial scales.
	synoptically_ correlated_uncertainty (time×lat×lon)	Component of uncertainty that is correlated over synoptic (~100 km) spatial scales.
	uncorrelated_ uncertainty (time×lat×lon)	Component of uncertainty that is uncorrelated between SSTs. A new uncertainty component arising from under-sampling of 0.05° grid cells due to their partial obscuration by cloud has been estimated for the experimental Release 1.2 L3U products and added to the component arising from instrument noise.
	adjustment_uncertainty (time×lat×lon)	Component of uncertainty associated with adjusting SSTs to a standard depth and time; correlated over synoptic (~100 km) spatial scales.
Retrieval information	l2p_flags (time×lat×lon)	Indicates the type of pixel and what kind of SST retrieval was applied. Pixel type information includes: land, ice, lake, or river. Pixels in the Level 2 products may have these flags set but will not contain any SST data (other than the Caspian Sea). The dual-view bit (6) will be set for retrievals from one of the dual-view sensors (ATSR or SLSTR). The three-channel bit (7) indicates that the more accurate three-channel retrieval has been used. Although the three-channel retrieval can only be

<table>
<tr><th>Category</th><th>Name of data (size of array)</th><th>Description</th></tr>
<tr><td></td><td></td><td>used at night, the use of the two-channel retrieval is not a guarantee that the pixel corresponds to a daytime observation (the retrieval may have switched to two-channel due to an instrument failure); therefore, there is a separate daytime flag (8) which indicates if the solar zenith angle was < 90° when the pixel was observed.

When written in binary format, each digit of each number provides information about the retrieval in each location. The least significant digit is called bit 0 and there are 16 bits in total, although only 8 are currently in use. The meanings are:
<table>
<tr><th>Bit</th><th>Description</th><th>Meaning if set to 0</th><th>Meaning if set to 1</th></tr>
<tr><td>0</td><td>Type of sensor</td><td>Infrared</td><td>Microwave</td></tr>
<tr><td>1</td><td>Ocean or land</td><td>Ocean</td><td>Land</td></tr>
<tr><td>2</td><td>Sea ice indicator</td><td>No sea ice</td><td>Sea ice present</td></tr>
<tr><td>3</td><td>Lake indicator</td><td>Not a lake</td><td>Lake</td></tr>
<tr><td>4</td><td>River indicator</td><td>Not a river</td><td>River</td></tr>
<tr><td>6</td><td>Number of satellite views available</td><td>One (nadir) view</td><td>Two (dual) views</td></tr>
<tr><td>7</td><td>Number of satellite radiance channels available</td><td>Two</td><td>Three</td></tr>
<tr><td>8</td><td>Day/night</td><td>Night time</td><td>Day time (solar zenith angle < 90°)</td></tr>
</table></td></tr>
<tr><td>Other</td><td>sses_bias (time×lat×lon)</td><td>For ESA SST CCI data only it is safe to ignore this data array (it is filled with zeros). In other GHRSST data files this is used to give an indication of bias in the SSTs.</td></tr>
</table>

6.4.6 'L4' data format

Level 4 data contain SSTs constructed from multiple orbits of an instrument and/or multiple instruments that have been collated and regridded. Statistical methods are used to combine data and infill areas of the ocean where no observations are available.

Level 4 files are stored on a global regular latitude/longitude grid and variables have the following dimensions:

time: UNLIMITED (1)

lat: Number of latitude points (3600)

lon: Number of longitude points (7200)

The resolution used for the products is 0.05° hence the full size of the arrays is 7200x3600. The time dimension is specified as **unlimited**, allowing standard netCDF tools to easily concatenate and manipulate multiple files, but each L4 file contains a single time slice (corresponding to a day).

The dimensions of the data in an L4 file are described in Table 15 and the variables contained in the files are listed in Table 16.

Table 15. The dimensions of the data in an L4 file.

Dimension name	Description
time	This is always 1 because there is only one orbit of data per file.
lon	These are the dimensions of the regular latitude-longitude grid on which the data are stored. For ESA SST CCI data these dimensions are 7200 and 3600 for lon and lat respectively (i.e., a global 0.05° x 0.05° grid).
lat	
bnds	Used to define arrays that give the bounds of the latitudes, longitudes and times of the data; always set to 2.

Table 16. Data arrays stored in L4 data files. The dimensions of the arrays are given in parenthesis after the name of the variable in the NetCDF file. These are defined in Table 15.

Category	Name of data (size of array)	Description
Coordinates	lat (lat)	Central latitude of each grid cell.
	lat_bnds (bnds×lat)	The latitudes of the edges of each grid cell.
	lon (lon)	Central longitude of each grid cell.
	lon_bnds (bnds×lon)	The longitudes of the edges of each grid cell.
	time (time)	The time (middle of the day) that the data represent.
	time_bnds (bnds×time)	The start and end time of the day that the data represent.
Geophysical variables	analysed_sst (time×lat×lon)	SST at each location. Note that this may be either the temperature at a depth of 20 cm or the foundation temperature (look for either SSTdepth or SSTfnd in the file names – see Section 3.5.3 for details of what these are), depending on the product. It is also important to examine the mask variable (see below), as this gives information such as whether a location is covered by sea ice.
	sea_ice_fraction (time×lat×lon)	Sea ice concentrations. These were produced by analysing input data sourced from the OSI SAF (OSI SAF: EUMETSAT Ocean and Sea Ice Satellite Application Facility. Global sea ice concentration continuous reprocessing offline product (2017 onwards), [Online]. Norwegian and Danish Meteorological Institutes. Available from

		http://osisaf.met.no).
Uncertainty information – total uncertainty	analysis_uncertainty (time×lat×lon)	Uncertainty in the SSTs (one error standard deviation).
Location information	mask (time×lat×lon)	When written in binary format, each digit of each number provides information about whether there is ocean, land, sea ice in each location. The least significant digit is called bit 0 and there are 8 bits in total, although only 5 are currently in use. The meanings are: **Bit** **Meaning if set to 1** 0 Water 1 Land 2 Lake 3 Sea ice 4 River

7. WORKED EXAMPLES

In this section, some examples are provided of how to obtain and use the data. Three sections are included that demonstrate using the ESA SST CCI data with different tools: SNAP (Section 7.1), the ESA SST CCI tools (7.2) and Python (7.4). Finally, Section 7.5 gives an example of how to work with the uncertainty information. To find a particular aspect of working with the data within these sections, please use the information provided in Table 17.

Table 17. Index of examples provided.

Topic	Examples provided
Examining file contents and metadata	• Use of SNAP to do this is covered in Section 7.1.1. • Extracting data and metadata using Python is described in Section 7.4.1. • Using the iris Python module to print out a listing of metadata related to a variable is shown in Section 7.4.2.
Using the scale_factor and add_offset attributes to unpack data from the NetCDF files	• Instructions are given in Section 7.4.1.
Working with L2P data	• Use of SNAP for examining L2P metadata is described in Section 7.1.1. • Application of the flag information is also described in Section 7.1.1. • The quality flag is illustrated in Section 7.4.2 (the example uses L3U data but is also applicable to L2P data). • An example of how to use L2P uncertainty information is given in Section 7.5.
Working with L3U data	• Application of the flag information is described in Section 7.1.1 (the example shows L2P data, but the method is also applicable to L3U data). • The quality flag information is illustrated in Section 7.4.2. • Use of SNAP to illustrate the effect of time and depth adjustments on L3U data is shown in Section 7.1.2. • The ESA SST CCI tools are used to produce a time series from L3U data in Section 7.3.2. • An example of how to use L3U uncertainty information is provided in Section 7.5.
Working with L4 data	• An application of SNAP to L4 data (including the application of the mask to the data) is given in Section 7.1.3. • The ESA SST CCI tools are used to regrid L4 data in Section 7.3.1. • Python is used to read and plot L4 data in Section 7.4. • Use of L4 uncertainty information when averaging is discussed very briefly in Section 7.5.

Topic	Examples provided
Using masks and flags	• Applying the L2P and L3U flag information is shown in Section 7.1.1. • The L2P and L3U quality flags are discussed in Section 7.4.2. • Using SNAP to find locations with ocean SSTs in L4 data is described in Section 7.1.3. • Applying the L4 masks to find ocean SSTs using Python is shown in Section 7.4.2.
Regridding data	• Use of the ESA SST CCI tools is recommended – see Section 7.2. • The propagation of uncertainties when regridding is described in Section 7.5.
Regional averaging and time series generation.	• Use of the ESA SST CCI tools is recommended – see Section 7.3.2.
Working with uncertainties	• The ESA SST CCI tools handle uncertainties automatically – see Section 7.2. • Propagating uncertainties when averaging data is described in Section 7.5.

7.1 SNAP

The free Sentinel Application Platform software SNAP allows the visualisation and analysis of earth observation datasets including the ESA SST CCI products. It can be obtained from http://step.esa.int/main/toolboxes/snap/. In this section some example uses of SNAP are provided. Each example makes use of the SNAP-Desktop application, a tool for displaying and analysing satellite data with an easy to use graphical user interface. Uses of the SNAP extend far beyond the examples shown here; users are encouraged to experiment with the software themselves.

7.1.1 Examining the contents of the ESA SST CCI products

SNAP can be used to open any of the ESA SST CCI product files using ‘Open Product’ in the file menu and a listing of the file contents is then displayed on the left of the screen. Please use the option “NetCDF following CF conventions” when asked to select a NetCDF format. Clicking on the items brings up additional windows that show the metadata associated with the file or variables, or an image view of the data. Figure 3 shows a screenshot of SNAP being used to display metadata from an ESA SST CCI Phase 1 Release 1.0 L2P file. An interesting attribute is the *file_quality_level* global attribute. In this example, this is set to 3, which means that there are no known problems with the data. In the attributes for *sea_surface_temperature_depth* the *_FillValue* is given along with the *add_offset* and *scale_factor* attributes that must be used to convert the data in the NetCDF file to the units described in the metadata (note that SNAP does this automatically; see Section 7.4.1 for more information about how to apply these manually).

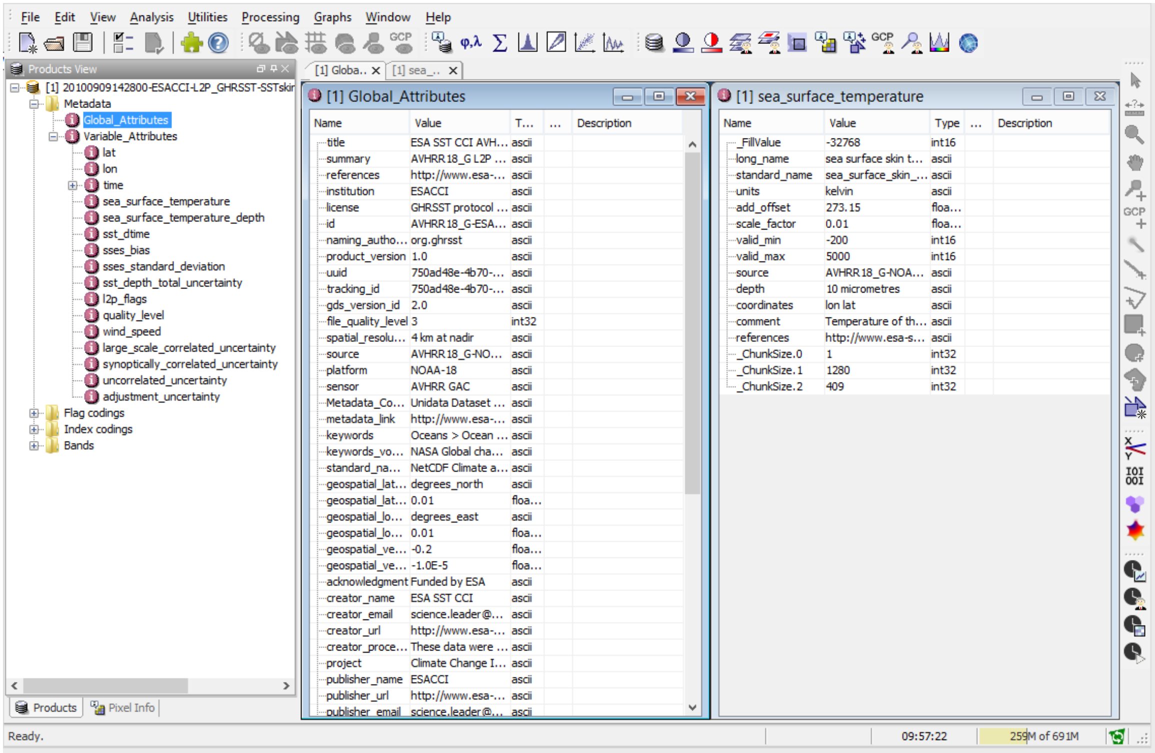


Figure 3. Using SNAP to display metadata about the file and one of the variables stored in the file.

How to display L2P flag metadata and applying this to reveal land and ocean locations is illustrated in Figure 4. The *l2p_flags* variable within the NetCDF file has attributes that describe how to interpret the flags. These attributes are shown at the top right of the figure. The *flag_mask* and *flag_meaning* attributes need to be used together. For example if the *l2p_flags* variable is masked using the value 2, locations that are land are revealed. When using SNAP, this information can be presented in a more readable form by displaying the information in the flag codings section at the left of the screen. This brings up the window shown in the mid-right of the figure.

The process of performing the masking is shown in the bottom right of the figure. The data in the *l2p_flags* variable has had a bitwise AND operation applied with the number 2, which corresponds to land ('l2p_flags AND 2'). Note that SNAP has the facility to create expressions that apply masks which are easier to read – an example of this is given in Section 7.1.1.

The resulting data are also shown in the figure. The image displayed on the right is the SST data (greys) with a missing data overlay (yellow) to show the shape of the data array. In the image on the left is the result of applying the land sea mask operation. The result of the operation is that the value used for masking (2 in this case) is shown in white (land locations) and other data with a value of zero are shown in black (ocean locations).

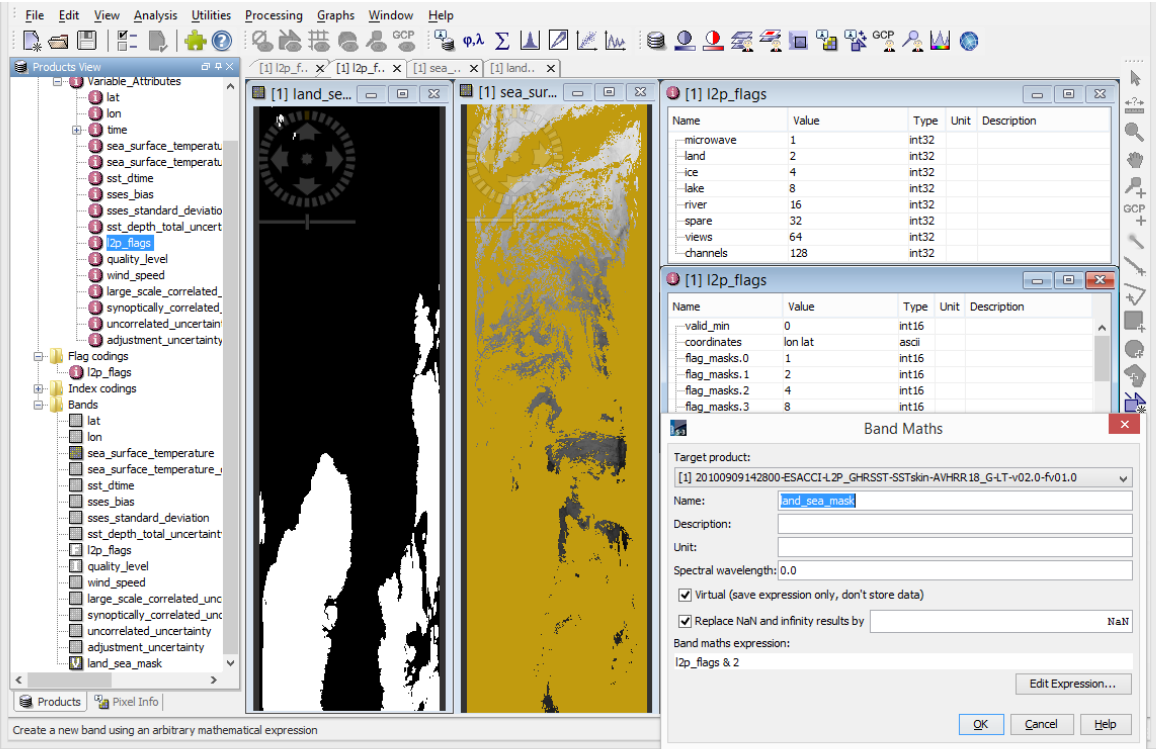


Figure 4. The *l2p_flags* variable attributes and applying the information to show land and ocean locations.

This method of interrogating the flag information is also applicable to L3U and L3C files.

7.1.2 Examining the effect of the time and depth adjustments to the SSTs

SNAP can perform mathematical operations on the satellite data quickly and easily. In this example, SNAP is used to show the effect of adjusting the SST data to represent a standard time of day and depth in the ocean.

To obtain the difference between the adjusted SSTs and the non-adjusted SSTs, 'Band Maths' was selected from the Raster menu. Then, 'Edit expression' was selected from the window that pops up, which provides an expression editor for defining the mathematics that are required (in this case 'sea_surface_temperature_depth minus sea_surface_temperature'). The resulting data are shown in Figure 5. A graticule overlay was also added (showing a 5° grid) and a histogram of the differences calculated (which can be done using the option in the Analysis menu). The colour scale was changed to show reds and blues rather than grey scale using the colour manipulation tool and then output by right clicking on the image view and choosing the appropriate option. Using the Statistics tool in the Analysis menu, the adjustments applied are displayed (the data ranged between -0.06°C and 0.51°C and the median was 0.1799°C).

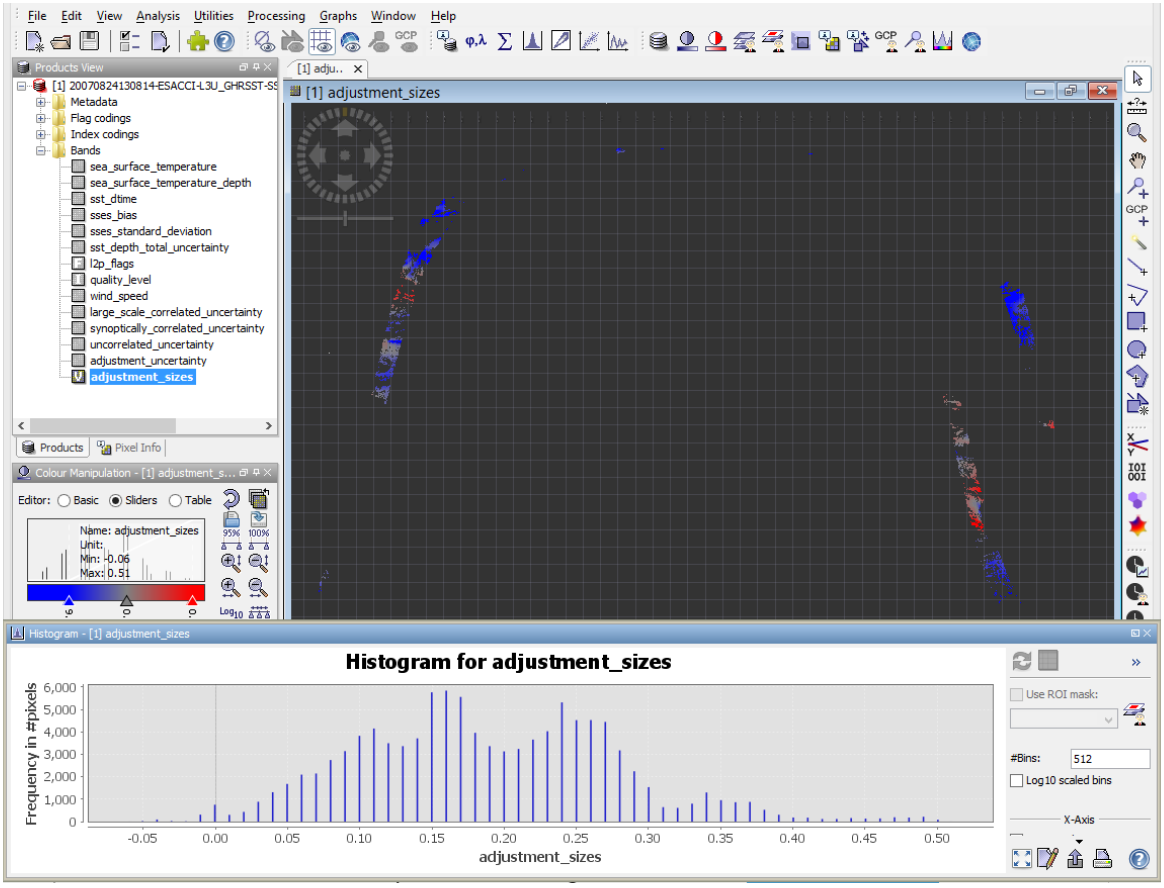


Figure 5. Using SNAP to show the differences between the adjusted and unadjusted SST data in a L3U file. A histogram of the differences is also being displayed

7.1.3 Detailed example of working with L4 data with SNAP

This subsection shows the process of filtering the data from a Phase 1 Release 1 L4 file to find the local gradients in the SSTs.

The original data are shown in Figure 6, in which SNAP is being used to display the SST field.

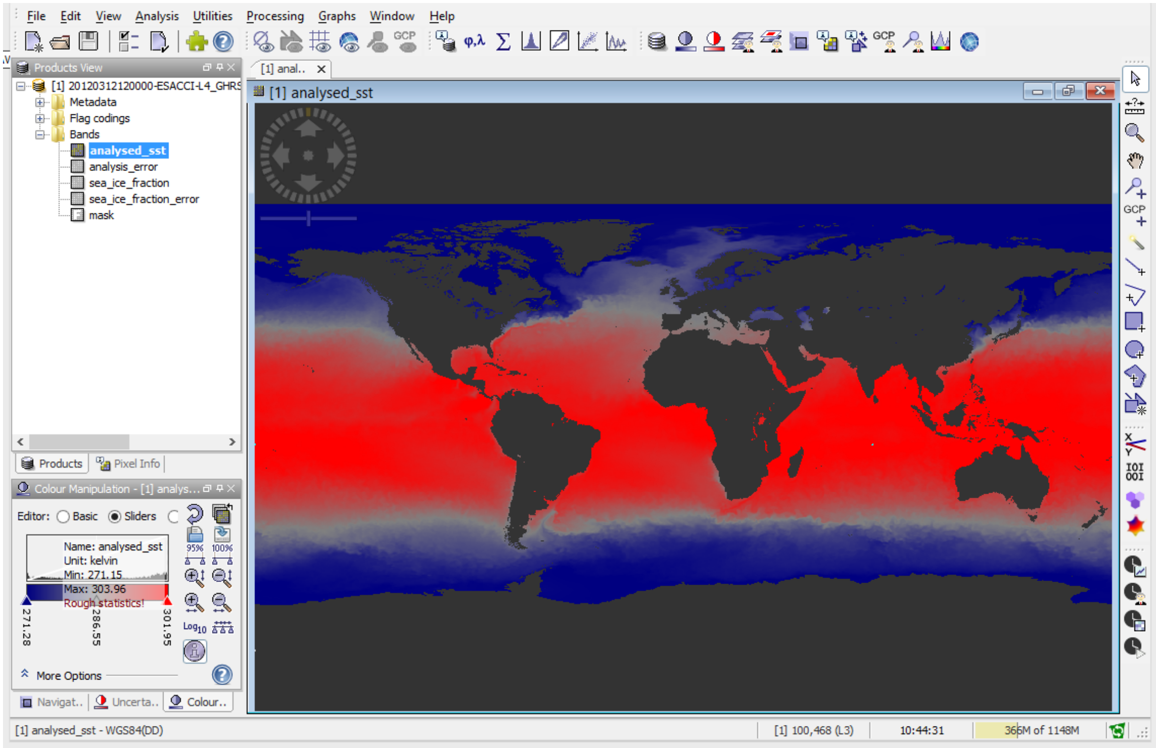


Figure 6. Starting point of the example of filtering with SNAP.

The first step of the processing was to apply a Sobel West filter, which approximates the local zonal gradients in the SST field. This is done very simply by selecting 'Filtered Band …' from the Raster menu. The mask variable is also used, to determine where there are valid ocean SSTs. To do this, right clicking on the filtered data band in the list to left of the screen brings up the 'properties' menu. The button marked '…' to the right of the valid pixel expression box brings up an expression editor which allows the user to define valid data. This process is shown in Figure 7. After applying the mask it was necessary to adjust the colour scale. This was achieved using the Colour Manipulation tool that can be displayed using an icon at the top of the screen. The '95%' button was clicked to ensure that the colour scale spanned the range encompassing 95% of the data. The results are in Figure 7.

The same process was then used to apply a Sobel North filter. The range of gradients displayed are much larger meridionally than zonally.

Finally, the results of the Sobel West and Sobel North filtering were combined using the band mathematics capability of SNAP. This is done by choosing 'Band Maths' from the Raster menu. The result is in Figure 8.

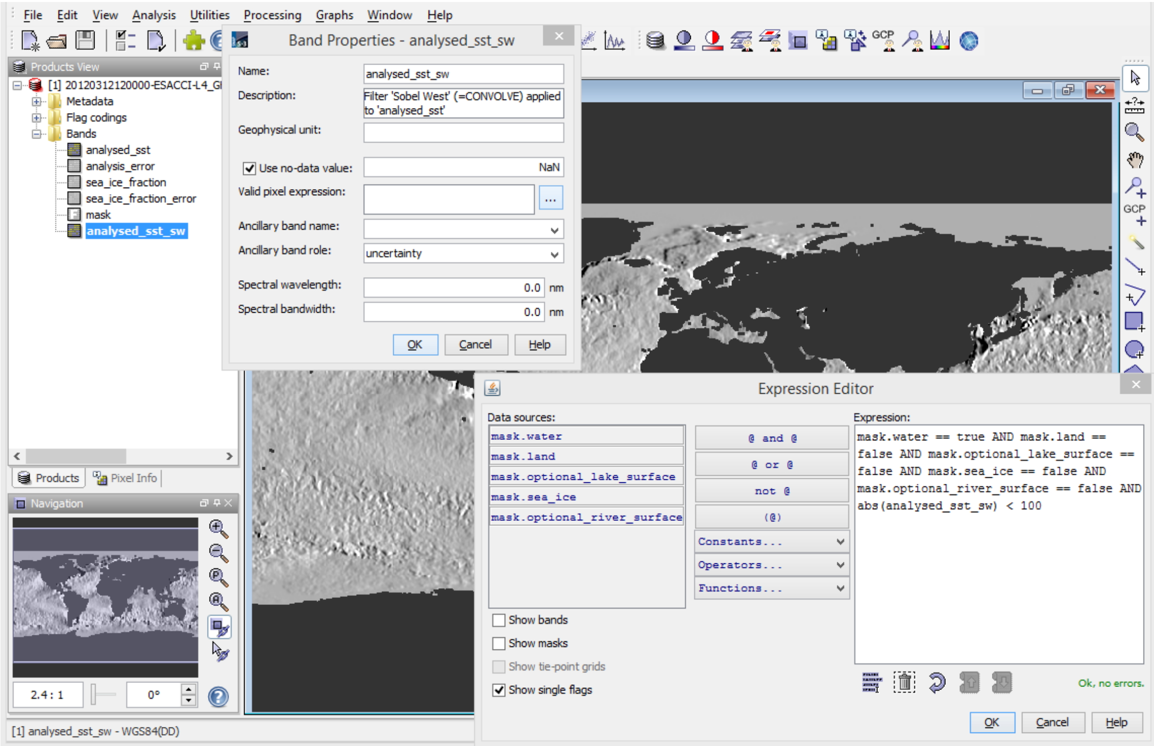


Figure 7. Using the mask to remove data affected by ice etc.

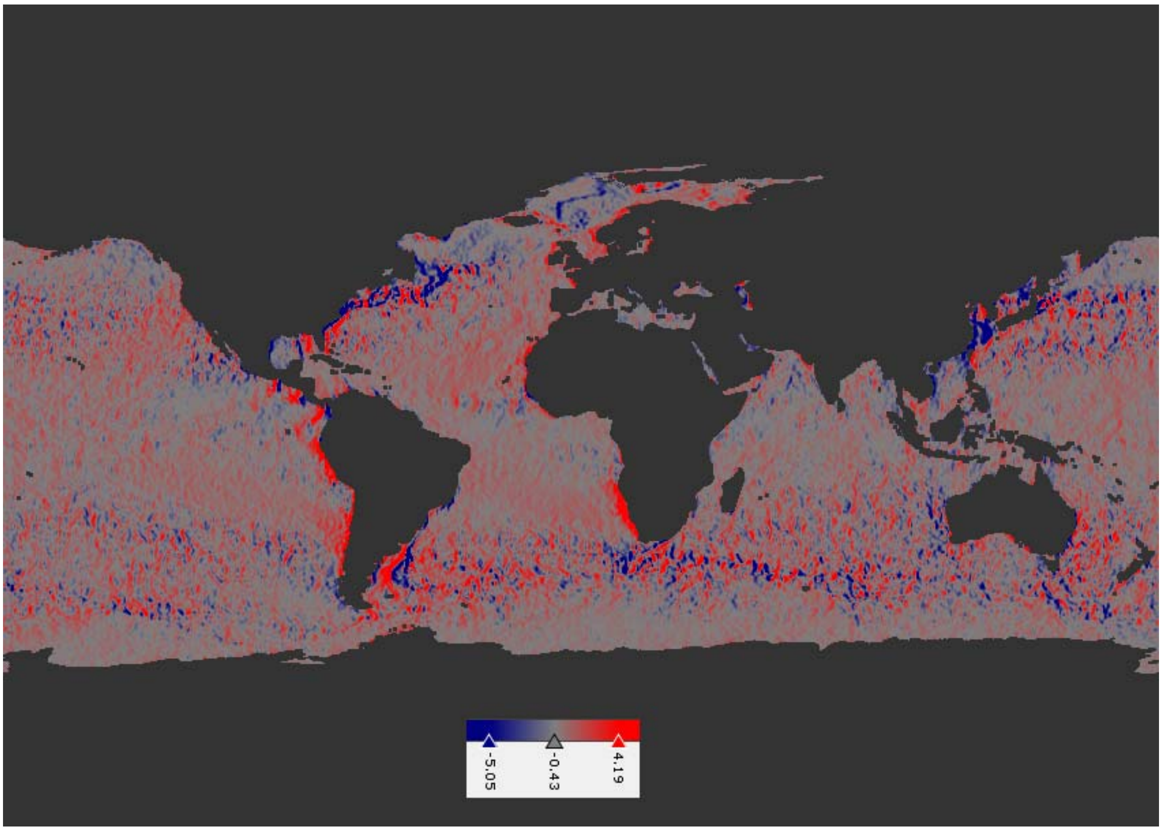


Figure 8. The result of the Sobel West filter after processing to remove ice etc. affected locations.

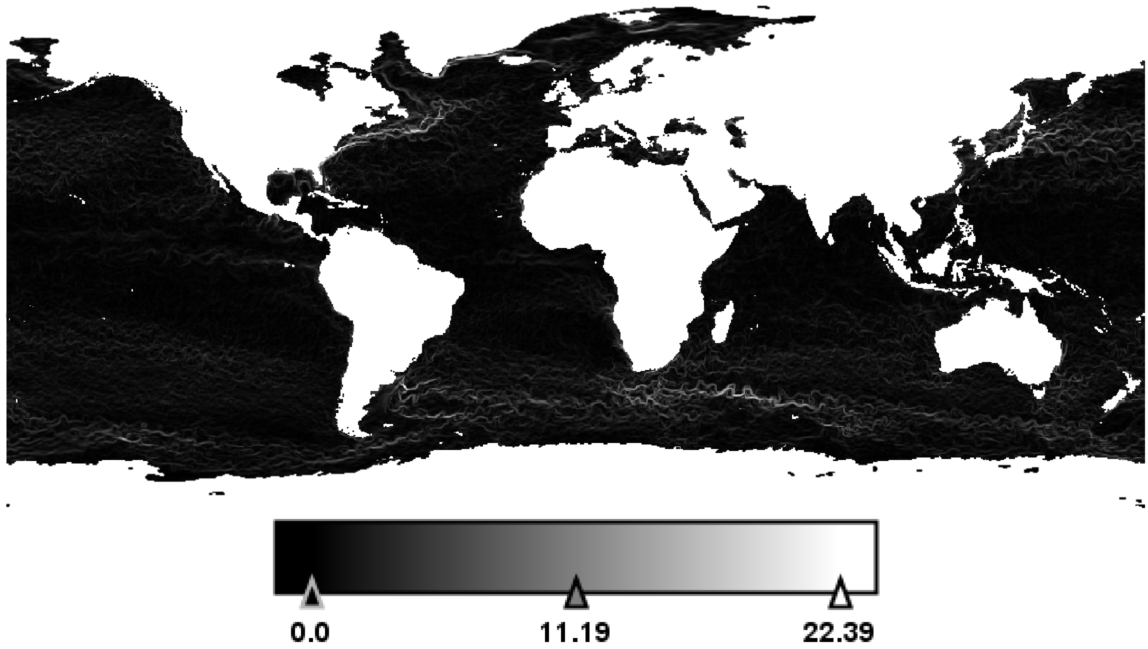


Figure 9. The combined Sobel North and West filters showing regions with high local horizontal gradients.

7.2 The ESA CCI Toolbox

The open source Climate Analysis Toolbox of the ESA Climate Change Initiative (CCI toolbox) allows users to ingest, analyse and visualize about 122TBytes of ESA's global satellite-derived climate observations including the ESA SST CCI products. The CCI-toolbox is developed with the end-user in mind and suitable for scientists, students as well as non-programmers who wish to manipulate climate data for research. The toolbox is available for Windows, Linux or Mac operating systems and can be obtained from http://www.climatetoolbox.io.

First-time users are advised to watch the quick-start tutorial video on the fundamentals of using the CCI-toolbox at:

https://www.youtube.com/watch?v=w0ZEK4aIC9I&feature=youtu.be.

The video illustrates how to use the CCI-toolbox to ingest, perform operations and visualize data.

7.2.1 SST Data Ingestion and Visualization with the CCI Toolbox

All ESA SST CCI products available on the ESA CCI Open Data Portal can be ingested directly into the CCI Toolbox for visualization and/or manipulation. One interesting capability of the CCI Toolbox is the ability to view concise information on filtered products, select desired variables as well as optionally subset data, both spatially and temporally. The ingested dataset can further be delimited for a prefered region(s) by drawing a polygon(s) on the data and using the ***subset_spatial*** operator to generate a data subset for the desired region. This makes the CCI Toolbox easy to use and user-friendly.

To use the Open Data Portal to ingest data directly from ESA, select the product from the data store and click on the ‘download and/open remote dataset’ icon to specify your region constraints (Figure 10).

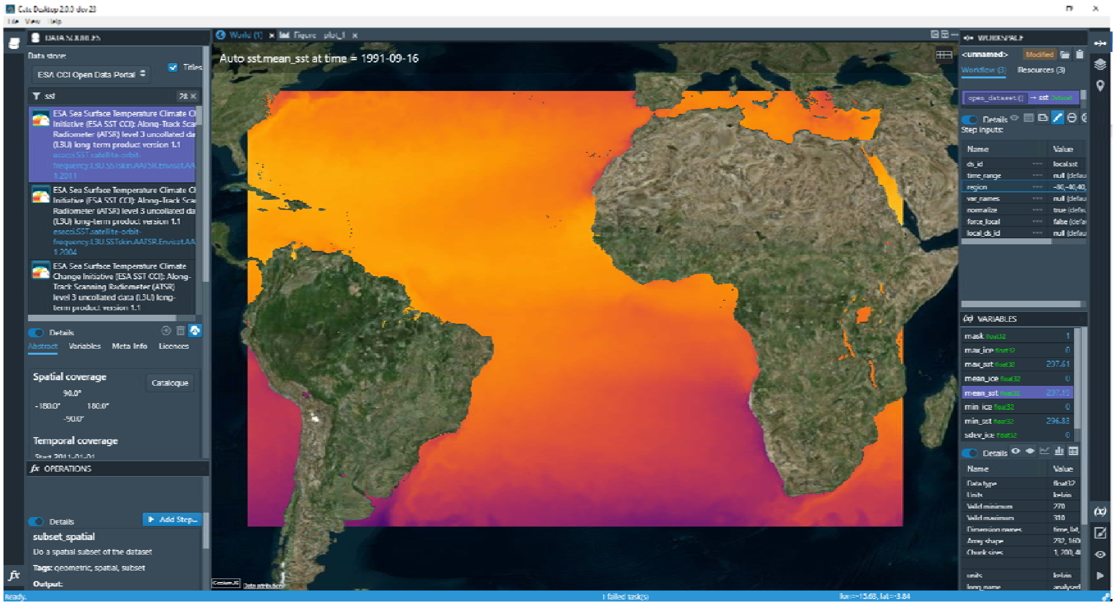


Figure 10. Example of ingested ESA CCI SST product with the CCI Toolbox

7.2.2 SST Data Analysis with the CCI Toolbox

All ESA SST CCI products ingested into the CCI Toolbox can be manipulated and analysed using several operators available in the CCI Toolbox. Resources generated from data ingested or from data manipulations using operators such as ***coregister*** (for data co-registration/remapping), ***tseries_mean*** (for extraction of spatial time series) and ***plot_map*** (for map composition) can be saved to local sources in different formats.

Example:

In this example the CCI Toolbox is used to compute and plot a spatial average of the SST time-series mean for the West African Coast.

In the CCI Toolbox it is possible to import and use polygon geodata (e.g in shapefiles format) or to draw polygons on top of the visualization layer to subset data for a specific region of interest. The vertices of the selected area can be invoked to spatially subset the SST data (Figure 11). The ***tseries_mean*** operator can be used to extract the spatial mean time-series of the mean SST variable and to generate a resource for the spatial averaging. This generated SST time series for the West African coast can be plotted using the ***plot_line*** operator in the CCI Toolbox (Figure 12).

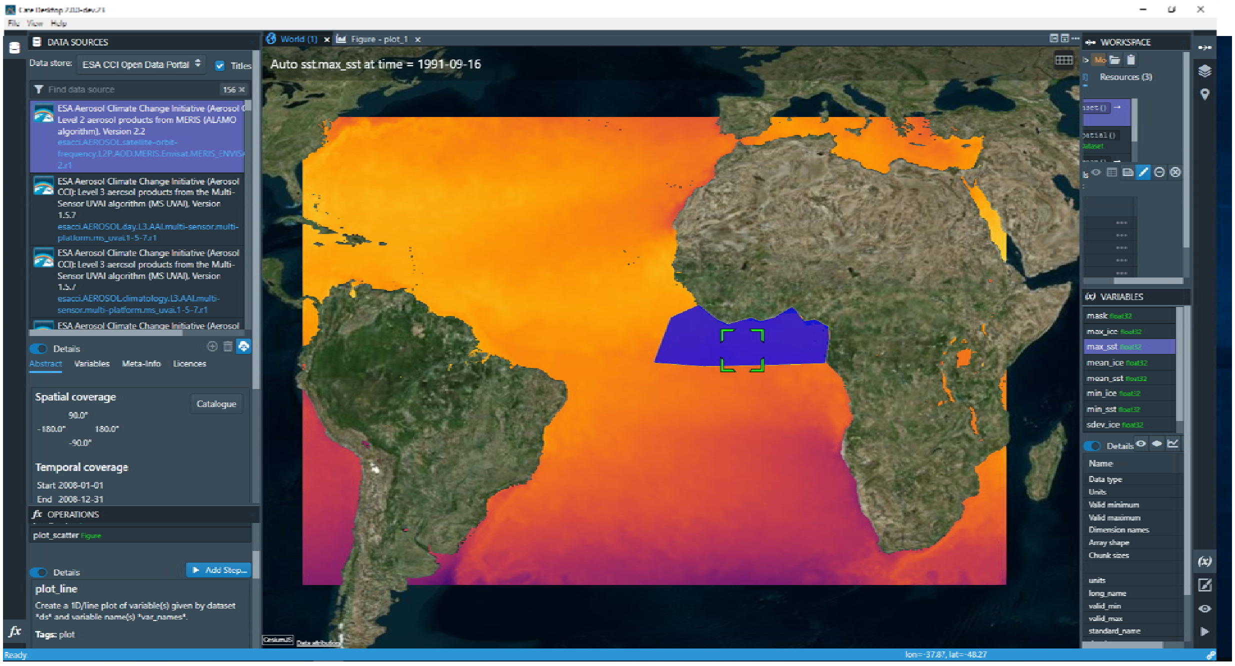


Figure 11. Example of using a "place" function to draw a polygon

Figure 12. Using the "subset_spatial" operator to spatially subset the data and generate a new resource from the result

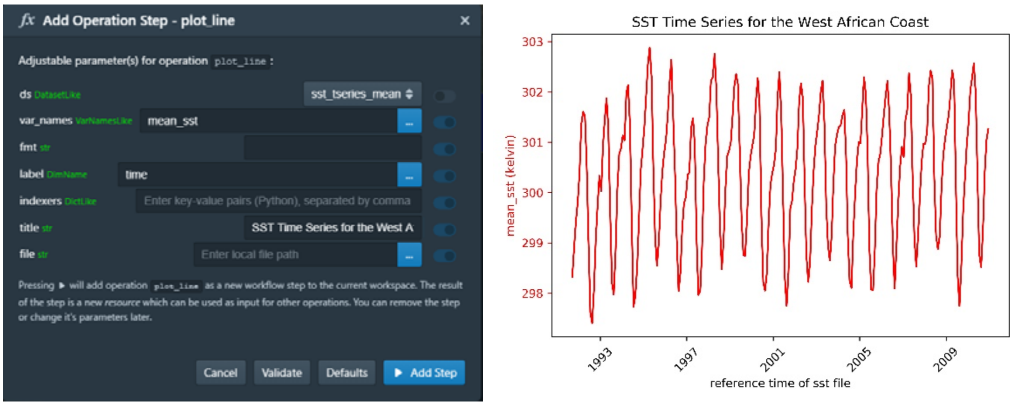


Figure 13. Plotting the time-series of the mean SST for the region selected

7.3 The ESA SST CCI tools

The ESA SST CCI project has developed two tools for regridding and averaging its products. These were described in Section 4.1. Here, an example of the use of each of the tools is provided.

7.3.1 Regridding data

In this example a Phase1 Release 1 level 4 output file is regridded onto a 5° regular latitude-longitude grid. A configuration file, called ‘regrid_l4.properties’, was created with the following contents:

```
CCI_L4.dir                = .
climatologyDir            = SST_CCI/climatology
startDate                 = 2006-11-26
endDate                   = 2006-11-26
outputDir                 = SST_CCI/output
productType               = CCI_L4
spatialRes                = 5.0
temporalRes               = daily
sstDepth                  = depth_20
region                    = Global=-180,90,180,-90
```

This defines various options including where the data are and where the output should be saved. The meaning of the options and additional options that can be set were described previously in Section 4.1.3 or can be obtained by running the regrid executable with the –h option set.

To run the regridder using the above options, the command is (assuming the executable and the properties file are in the current directory):

```
regrid –c regrid_l4.properties
```

The result of this operation was an output file (in the output directory defined in the properties file) called 20061126-20061127-Global-ESACCI-L4_GHRSST-SST_depth_20_regridded-PS-DM-v0.1-fv1.1.nc. The regridded data in the file are stored in variables called sst_depth_20, sst_depth_20_anomaly, sea_ice_fraction, coverage_uncertainty and analysis_uncertainty. The coverage uncertainty variable is an additional uncertainty component produced during the regridding process to account for the uncertainty from missing data e.g. due to cloud.

7.3.2 Regional averaging and generation of time series

This example demonstrates how to use the ESA SST CCI regional averaging tool to calculate global monthly average temperature anomaly time series from the ATSR and AVHRR series data individually.

To generate the ATSR series the following configuration file was created:

```
CCI_L3U.dir     = SST_CCI/data
startDate       = 1991-10-01
endDate         = 2010-12-31
outputDir       = SST_CCI/output
productType     = CCI_L3U
temporalRes     = monthly
sstDepth        = depth_20
```

Section 4.1.4 provides details on the specified options. The regional averaging tool was run using the command **regavg**. Note that if the configuration file is called regavg.properties it will be read automatically. Otherwise the –c option can be used to set the name of the configuration file, or command line options can be used if wished.

The result from the tool is written to a NetCDF file containing the time series and uncertainty information. The tool was also applied to the AVHRR data using the following configuration:

```
CCI_L2P.dir     = SST_CCI/data
startDate       = 1991-10-01
endDate         = 2010-12-31
outputDir       = SST_CCI/output
productType     = CCI_L2P
temporalRes     = monthly
sstDepth        = depth_20
```

7.4 Python

Python (http://www.python.org) is a free, general purpose programming language that is available on multiple operating systems including Linux, Windows and Mac OS. The core package can be extended using extra modules to increase its functionality. Modules are freely available that allow the use of Python for scientific data analysis and plotting and it is necessary to install these to try the examples shown in this section.

Explicit use is made of the following modules:

- netCDF4 – for reading and writing NetCDF files; see http://code.google.com/p/netcdf4-python.
- matplotlib – for scientific plotting; see http://matplotlib.org [RD.323].
- iris – tools for analysing and plotting geophysical data; see http://scitools.org.uk [RD.324].

However, there are dependences on other modules (for example use of the numpy module, http://www.numpy.org) that will need to be installed. Python version 2.7 is used for these examples.

Python in combination with Matplotlib, Iris etc. was used in the code that produced many of the plots in this user guide. This section contains some code snippets that give a flavour of how these were produced. An example of how to do a basic read and plot of a level 4 data file is provided first. Then, the iris module is demonstrated, which is designed specifically for the purpose of reading, analysing and plotting geophysical data.

7.4.1 Basic reading and plotting example

The following code demonstrates how data can be read in from a file and plotted using Python; this example uses a file from Phase 1 Release 1. Copying it directly into the Python command line will run the code. Sections of text with a # symbol at the beginning are comments. The result is shown in Figure 14.

```
from netCDF4 import Dataset
import matplotlib.pyplot as plt

# Open the ESA SST CCI file.
ncid = Dataset(
  '20061126120000-ESACCI-L4_GHRSST-SSTdepth-OSTIA-GLOB_LT-v02.0-
fv01.0.nc')

# Set up a large plotting window.
plt.figure(figsize=(14, 10))

# Do a line plot of the latitude coordinate
# in the upper left part of the plotting window.
# Metadata stored in the NetCDF file are used
# to define the y axis label.
var = 'lat'
latData     = ncid.variables[var][:]
latLongName = ncid.variables[var].long_name
latUnits    = ncid.variables[var].units

ax = plt.subplot(2, 2, 1)
ax.plot(latData)
ax.set_xlabel('Grid position')
ax.set_ylabel(latLongName + ' (' + latUnits + ')')
ax.set_title('Latitudes')

# Do a line plot of the longitude coordinate
# in the upper right part of the plotting window.
# (This is a replica of the code above except
# replacing latitude with longitude and changing
# the plot position).
var = 'lon'
lonData     = ncid.variables[var][:]
lonLongName = ncid.variables[var].long_name
lonUnits    = ncid.variables[var].units

ax = plt.subplot(2, 2, 2)
ax.plot(lonData)
ax.set_xlabel('Grid position')
ax.set_ylabel(lonLongName + ' (' + lonUnits + ')')
ax.set_title('Longitudes')

# Do a plot of the SST data array at
# the bottom left of the screen.
var = 'analysed_sst'
analysedSSTData     = ncid.variables[var][0, :, :]
analysedSSTLongName = ncid.variables[var].long_name
```

```
analysedSSTUnits    = ncid.variables[var].units

ax = plt.subplot(2, 2, 3)
sstPlot = ax.imshow(analysedSSTData, vmin=270, vmax=305, origin='lower')
ax.set_title('Analysed SST data array')
cb = plt.colorbar(sstPlot, orientation='horizontal')
cb.set_label(analysedSSTLongName + ' (' + analysedSSTUnits + ')')

# Do a plot of the sea ice concentration data array.
var = 'sea_ice_fraction'
seaIceFractionData     = ncid.variables[var][0, :, :]
seaIceFractionLongName = ncid.variables[var].long_name

ax = plt.subplot(2, 2, 4)
seaIcePlot   =   ax.imshow(seaIceFractionData,   vmin=0,   vmax=1,   ori-
gin='lower')
ax.set_title('Sea ice fraction data array')
cb = plt.colorbar(seaIcePlot, orientation='horizontal')
cb.set_label(seaIceFractionLongName)

ncid.close() # Close the NetCDF file.
plt.show() # Show our completed plot.
```

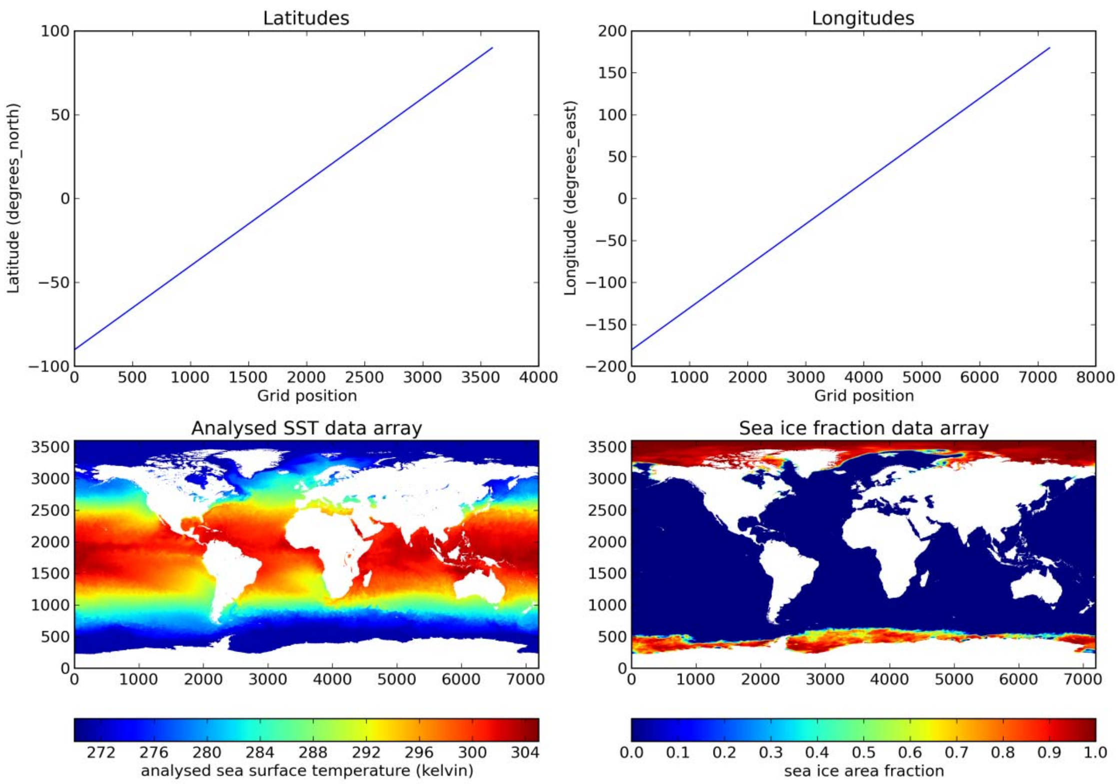


Figure 14. Result of applying the Python code to read and visualise the data.

As described in the file format sections of this document, some of the data arrays stored in the NetCDF files need a scale factor and offset to be applied to convert them into the correct units. The netCDF4 module used in this example has done this automatically. However, the manual procedure is described below:

1. Open the NetCDF file.
2. Read the variable of interest from the NetCDF file.
3. Read the add_offset, scale_factor and _FillValue variable attributes (if present – some variables such as those containing the latitude and longitude points do not have these and do not require conversion).
4. For all data points that do not contain the number from the _FillValue attribute calculate: converted_data = original_data × scale_factor + add_offset.
5. Read the units attribute to determine the units post conversion.
6. Repeat 2-5 for other variables in the file.
7. Close the NetCDF file.

Two other points to notice are:

- The SST data array has SST values where there is a high sea ice concentration and where there are lakes. To only use SSTs from ocean locations it is necessary to check the 'mask' variable in the data files.
- The coordinates and data arrays are not associated with each other in this simple example, for example the x and y axes in the SST plot show the position in the data arrays rather than longitude and latitude.

The next example will demonstrate ways to do both of these things.

7.4.2 Using 'iris' to read, analyse and plot ESA SST CCI data

The iris Python module is being developed at the Met Office for the purpose of analysing and visualising geophysical data. The first example below demonstrates the use of iris to read and plot the Phase 1 Release 1 SST data shown in Section 7.4.1 above. The result of running this code is shown in Figure 15.

```
import iris
import iris.quickplot as qplt
import matplotlib.pyplot as plt

# Load the analysed_sst variable data array into
# an iris structure known as a 'cube'. Note that
# the standard name for the data (from the CF
# conventions) is used to select the data to read.
# A slice operation [0, :, :] is used to remove the
# time dimension of the data array.
file   =  '20061126120000-ESACCI-L4_GHRSST-SSTdepth-OSTIA-GLOB_LT-v02.0-fv01.0.nc'
SSTCube = iris.load_cube(file,
                         'sea_water_temperature')[0, :, :]

# Also read the 'mask' data array so that ice and
# lake areas can be excluded from the plot. This
# variable does not have a standard name so the
# name of the variable is used instead.
maskCube = iris.load_cube(file,
```

```
    iris.Constraint(cube_func=lambda    cube:    cube.var_name    ==
'mask'))[0, :, :]

# Find the non ocean SST values and mask them
# in the SST data array. This is any point
# where the mask is not equal to 1.
SSTCube.data.mask[maskCube.data != 1] = True

# Do a quick plot of the data. In this case
# a contour plot is done; qplt.pcolormesh could
# be used instead to do a block plot.
qplt.contourf(SSTCube, vmin=270, vmax=305)
plt.gca().coastlines()
plt.show()
```

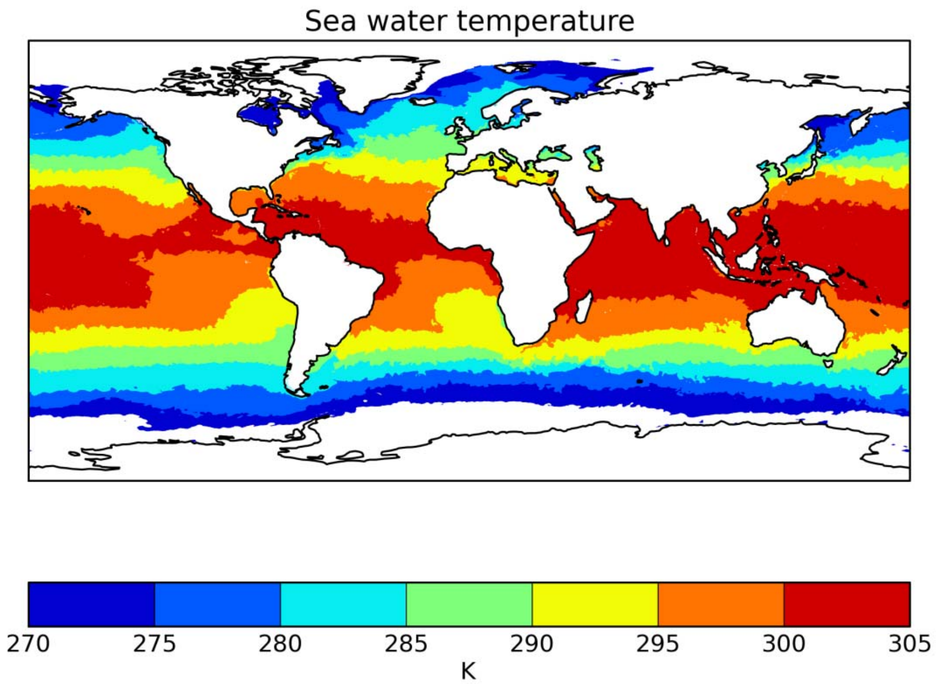


Figure 15. Result of using the iris module to read and plot the analysed SST data.

Iris provides a plot of the data with a colour bar and titles taken from the metadata in the NetCDF file. All parts of the plot are adjustable if required (for example the colours used can be changed, as can the latitude and longitude ranges displayed). Note that the areas displayed in Figure 14 where there are high sea ice concentrations or lakes are not shown in this version. This is due to using the information in the mask variable to find only those locations where there are ocean SSTs available.

Similarly, when using L2P, L3U and L3C data, it is desirable to check the flags and quality level information. Use of the l2p_flags variable was demonstrated in Section 7.1.1. This provides information about the type of SST retrieval and whether a location is over the land, ice, lake or rivers. Also available, in the quality_level variable, is a rating of the quality of each SST. A plot of this variable from an example Phase 1 Release 1 L3U file is shown in Figure 16, with the code used given below. Note that there are more quality levels in version 2 products.

```
import iris
import iris.quickplot as qplt
```

```
import matplotlib.pyplot as plt

# Variable is selected using the long_name attribute because there is no
# standard_name attribute for this.
cube = iris.load_cube(
   '20061126000044-ESACCI-L3U_GHRSST-SSTskin-AATSR-LT-v02.0-fv01.0.nc',
                     'quality level of SST pixel')
qplt.pcolormesh(cube[0, :, :])
plt.gca().coastlines()
plt.show()
```

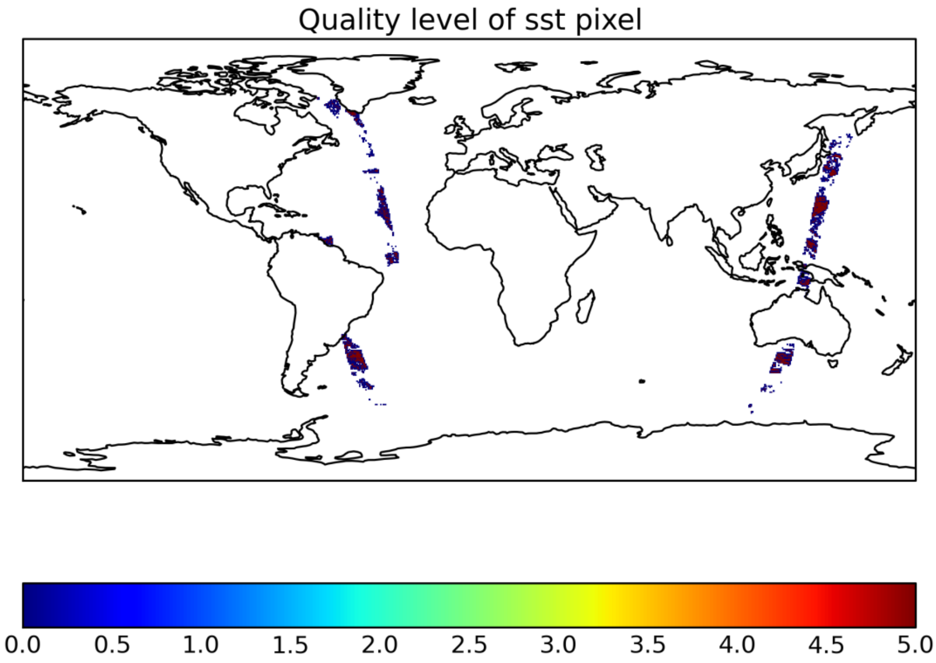


Figure 16. Quick plot of the quality_level variable from a L3U file.

It is also possible view metadata about the variable using iris. Printing the SSTCube variable gives this information, which is automatically read by the software.

```
print SSTCube
```

The result of this is:

```
sea_water_temperature / kelvin      (latitude: 3600; longitude: 7200)
     Dimension coordinates:
          latitude                           x                -
          longitude                          -                x
     Scalar coordinates:
          time: 2006-11-26 12:00:00
     Attributes:
          Conventions: CF-1.5, Unidata Observation dataset v1.0
          Metadata_Conventions: Unidata Observation Dataset v1.0
          acknowledgment: Funded by ESA
```

cdm_data_type: grid
comment: SST analysis produced for ESA SST CCI project using the OSTIA system in...
creator_email: science.leader@esa-sst-cci.org
creator_name: ESA SST CCI
creator_processing_institution: These data were produced at the Met Office as part of the ESA SST CCI ...
creator_url: http://www.esa-sst-cci.org
date_created: 20130206T015243Z
depth: 20 cm
easternmost_longitude: 180.0
file_quality_level: 3
gds_version_id: 2.0
geospatial_lat_max: 90.0
geospatial_lat_min: -90.0
geospatial_lat_resolution: 0.05
geospatial_lat_units: degrees_north
geospatial_lon_max: 180.0
geospatial_lon_min: -180.0
geospatial_lon_resolution: 0.05
geospatial_lon_units: degrees_east
geospatial_vertical_max: -0.2
geospatial_vertical_min: -0.2
history: Created using OSTIA reanalysis system v2.0
id: OSTIA-ESACCI-L4-v01.0
institution: ESACCI
keywords: Oceans > Ocean Temperature > Sea Surface Temperature
keywords_vocabulary: NASA Global Change Master Directory (GCMD) Science Keywords
license: GHRSST protocol describes data use as free and open
metadata_link: http://www.esa-cci.org
naming_authority: org.ghrsst
netcdf_version_id: 4.1.3
northernmost_latitude: 90.0
platform: ENVISAT, NOAA-<12,14,15,16,17,18>, MetOpA
processing_level: L4
product_version: 1.0
project: Climate Change Initiative - European Space Agency
publisher_email: science.leader@esa-sst-cci.org
publisher_name: ESACCI
publisher_url: http://www.esa-sst-cci.org
references: http://www.esa-sst-cci.org
sensor: AATSR, AVHRR
source: AATSR_ESACCI_L3U-v1.0, ATSR<1,2>_ESACCI_L3U-v1.0, AVHRR<12,14,15,16,17...
southernmost_latitude: -90.0
spatial_resolution: 0.05 degree

```
          standard_name_vocabulary:  NetCDF  Climate  and  Forecast  (CF)
Metadata Convention
          start_time: 20061126T000000Z
          stop_time: 20061126T235959Z
          summary: OSTIA L4 product from the ESA SST CCI project, pro-
duced using OSTIA reanalysis...
          time_coverage_duration: P1D
          time_coverage_end: 20061126T235959Z
          time_coverage_resolution: P1D
          time_coverage_start: 20061126T000000Z
          title: ESA SST CCI OSTIA L4 product
          tracking_id: 19b1f7a4-d8d1-44eb-9cfa-37cc33c4c2c1
          uuid: 19b1f7a4-d8d1-44eb-9cfa-37cc33c4c2c1
          westernmost_longitude: -180.0
```

It is simple to perform other operations and analysis on the data. For example to find the SST at 0° longitude, 0° latitude the command would be (assuming that the previous code has already been run):

```
print(iris.analysis.interpolate.linear(SSTCube,
                     [('latitude', 0), ('longitude', 0)]).data)
```

The answer that is returned is:

```
300.217468262
```

Iris includes many other functions – aggregation of data, mathematical operations etc. – and is constantly being improved with new functionality. It is recommended that users visit the iris web-pages at http://scitools.org.uk/iris/docs/latest/index.html for the latest information.

7.5 Example of working with the uncertainty information

The ESA SST CCI project provides detailed uncertainty information within the SST data files. Here, proper use of this uncertainty information is discussed for the example of calculating an average over a particular region. Note that there can be additional uncertainty associated with this operation through incomplete sampling of the area being averaged.

More detailed information about uncertainty information for the SST CCI products can be found in material presented at a user workshop on uncertainties (http://www.esa-sst-cci.org/PUG/workshop.htm). As well as material from presentations on the uncertainties, practical exercises on using the uncertainties can also be found there.

L2P, L3U and L3C data are provided with multiple uncertainty components: uncorrelated uncertainty (due to effects that are random between locations), synoptically correlated uncertainty (due to effects that are correlated over scales of approximately 100 km and 1 day), large scale correlated uncertainty (due to effects that are highly correlated over large scales) and adjustment uncertainty (for SSTs that have been adjusted to a standard time and depth, correlated as synoptically correlated uncertainty). When averaging the data the recommended way to deal with the uncertainties is as follows:

1. Random uncertainty components should be aggregated by:

a. Square the random uncertainty numbers that correspond to the SSTs to be averaged.

b. Sum the values obtained in a.

c. Calculate the square root of the result of b.

d. Divide result of c by the number of SST values being averaged.

Mathematically this is represented by: $\frac{\sqrt{\sum_{i=1}^{n}\sigma_i^2}}{n}$ where n is the number of SSTs being averaged and σ_i is the random uncertainty associated with SST value i.

2. For each synoptically correlated uncertainty component in turn aggregate as follows:

   a. Combine uncertainty numbers:

      (i) Square the synoptically correlated uncertainty numbers that correspond to the SSTs to be averaged.

      (ii) Sum the values obtained in a(i).

      (iii) Divide a(ii) by the number of SSTs.

   b. Calculate the effective number of synoptic areas in the grid box:

      (i) Find the mean spatial separation of the SSTs that are being averaged (in km) and divide the result by the spatial correlation length scale of the uncertainties (100 km).

      (ii) Find the mean temporal separation of the SSTs that are being averaged (in days) and divide the result by the temporal correlation length scale (1 day).

      (iii) Calculate the reciprocal of the exponent of the average of b(i) and b(ii).

      (iv) Calculate the result of b(iii) multiplied by the number of SSTs being averaged minus one, and then add one to the result.

      (v) The effective number of synoptic areas is the number of SSTs being averaged divided by the result of b(iv).

   c. Divide the result of a by the result of b and calculate the square root.

Mathematically, this is $\sqrt{\frac{1}{\eta}\frac{\sum_{i=1}^{n}\sigma_i^2}{n}}$ where η is given by $\frac{n}{1+\exp\left[-\frac{1}{2}\left(\frac{d_{xy}}{100}+d_t\right)\right](n-1)}$,

d_{xy} is the mean spatial separation of the SSTs to be averaged (in km), d_t is the mean temporal separation, n is the number of SSTs being averaged and σ_i is the synoptically correlated uncertainty associated with SST value i.

3. Large scale correlated uncertainties should be aggregated by:

    a. Sum the large scale correlated uncertainty values that correspond to the SSTs to be averaged.

    b. Divide the result of a by the number of SSTs being averaged.

    The operation can be summarised as $\frac{\sum_{i=1}^{n}\sigma_i}{n}$ where n is the number of SSTs being averaged and σ_i is the large scale correlated uncertainty associated with SST value i.

Uncertainty components can then be summed in quadrature to give an overall uncertainty value.

L4 data are provided with only one uncertainty component. In the ESA SST CCI tools this component is assumed to be uncorrelated between locations (i.e. it is used as described above for the random uncertainty).

8. DICTIONARY OF ACRONYMS, ABBREVIATIONS AND JARGON

Item	Definition
ARC	ATSR Reprocessing for Climate
(A)ATSR	(Advanced) Along Track Scanning Radiometer
AVHRR	Advanced Very High Resolution Radiometer
AMSR-E	Advanced Microwave Scanning Radiometer – Earth Observing System
BT	Brightness Temperature
CCI	Climate Change Initiative
CDL	Network Common data form Description Language
COBE	Centennial *in situ* observation based estimates
CF	Climate Forecast
CRDP	Climate research data package
DMI	Danmarks Meteorologiske Institut (Danish Meteorological Institute)
ECV	Essential Climate Variable
Envisat	Environment Satellite; an ESA satellite
ERSST v3	Extended Reconstruction SST version 3
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
EXP	Experimental product release
FNMOC	Fleet Numerical Meteorology and Oceanographic Center, USA
GCOS	Global Climate Observing System
GDS	GHRSST Data Processing Specification
GHRSST	Group for High-Resolution SST
HadCRUT4	The Met Office Hadley Centre and University of East Anglia dataset of gridded historical surface temperature anomalies version 4.
HadSST2 and HadSST3	The Met Office Hadley Centre dataset of gridded *in situ* temperature anomalies, versions 2 and 3.
HadISST1	The Met Office Hadley Centre sea ice and sea surface temperature dataset version 1.
ICOADS	International Comprehensive Ocean-Atmosphere Data Set
IR	Infrared
in situ observations	Observations made by an instrument at the position of the thing being measured.
L2P	Level 2 Preprocessed data; see Section 3.1.2
L3U	Level 3 Uncollated data; see Section 3.1.2
L3C	Level 3 Collated data; see Section 3.1.2
L4	Level 4 data; see Section 3.1.2
LT	Long term (refers to the ESA SST CCI long term product).
MERSEA	Marine Environment and Security for the European Area
MetOp	Meteorological Operational (EUMETSAT satellite)
MSG	Meteosat Second Generation

Item	Definition
NetCDF	Network Common Data Format
NOAA	National Oceanic and Atmospheric Administration
NOCS	National Oceanographic Centre Southampton
ODYSSEA	Ocean Data analYsis System for merSEA
OE	Optimal Estimation
OI	Optimal Interpolation
OS	Operating System
OSTIA	Operational Sea Surface Temperature and Sea Ice Analysis
PMWR	Passive Microwave Radiometers
RAMSSA	Regional Australian Multi-Sensor SST Analysis
Retrieval	A term used for the process of calculating SST from the measurements made by a satellite instrument.
RSS MWOI	Remote Sensing Systems Microwave Optimally Interpolated SSTs
RTG	Real Time Global
SADIST	Synthesis of ATSR data into sea surface temperatures
SEVIRI	Spinning Enhanced Visible and Infrared Imager
SNAP	Sentinel Application Platform software
SST	Sea Surface Temperature
TMI	Tropical Rainfall Measuring Mission (TRMM) Microwave Imager
UNFCCC	United Nations Framework Convention on Climate Change

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10. APPENDIX 1: SUMMARY OF HOW THE DATA WERE PRODUCED

This appendix summarises the algorithms used within Phase 2 of the ESA SST CCI project; detailed in the Algorithm Theoretical Basis Document (ATBD; [RD.415]). References for external algorithms are given in the relevant sections.

10.1 Retrieval of SST from satellite measurements

Within Phase 2 of the ESA SST CCI project, SST retrievals are made for data from two instruments: the Along-Track Scanning Radiometers (ATSRs) and the Advanced Very-High Resolution Radiometers (AVHRRs). In this section we briefly describe the methods used and highlight the strengths and weaknesses of these. For a complete description please refer to RD.415.

10.1.1 Data processing for the ATSRs and AVHRRs

The SST retrieval process for the ATSR and AVHRR instruments is illustrated by the flow diagram in Figure 19. The individual components of the retrieval are summarised below.

Input data

The ATSR and AVHRR-series instruments make observations in a number of channels across the infrared part of the electromagnetic spectrum. The observed radiances are calibrated and converted into equivalent brightness temperatures (BTs), defined as the temperature of a black body emitting the observed amount of radiation.

The ATSRs instruments are well calibrated, dual-view radiometers intended to produce long-term, consistent SST observations. Three ATSR instruments have flown on board ESA's two European Remote Sensing (ERS) satellites and Envisat satellite. All three satellites were in stable sun-synchronous orbits with near-constant equatorial crossing times – the ERS-1 and ERS-2 platforms crossed at 10:30 and Envisat had a crossing time of 10:00 all of which were maintained within a few minutes.

Unlike the AVHRR instruments, the ATSRs were designed specifically for climate applications with significant improvements to calibration, characterization and stability. One feature unique to the ATSRs was the introductions of the dual-view capability using a single telescope with a conical scanning pattern. Having two views of the Earth's surface allows the instrument to gather more information and more effectively separate surface and atmospheric effects; i.e. the SST retrieval can be made more robust to atmospheric conditions, including water vapour and stratospheric aerosol. However, it also means the ATSR instruments have a much narrower swath – only 512 km wide compared to the 2800 km for AVHRRs. As a result it takes ~3 days for an ATSR instrument to collect global observations.

The AVHRRs are a series of multipurpose imaging instruments carried onboard the National Oceanic and Atmospheric Administration (NOAA) Polar Operational Environmental Satellites (POES) and EUMETSAT Polar System (EPS) MetOp satellites. The first AVHRR instrument was carried onboard the TIROS-N satellite launched in October 1978. The equator crossing times of the various satellites as shown in Figure 17. The NOAA satellites are all in drifting orbits, meaning that the equator crossing times are slowly changing; which will affect the SST skin retrieval. The EUMETSAT MetOp satellites are in controlled orbits with equator crossing times of 9:30.

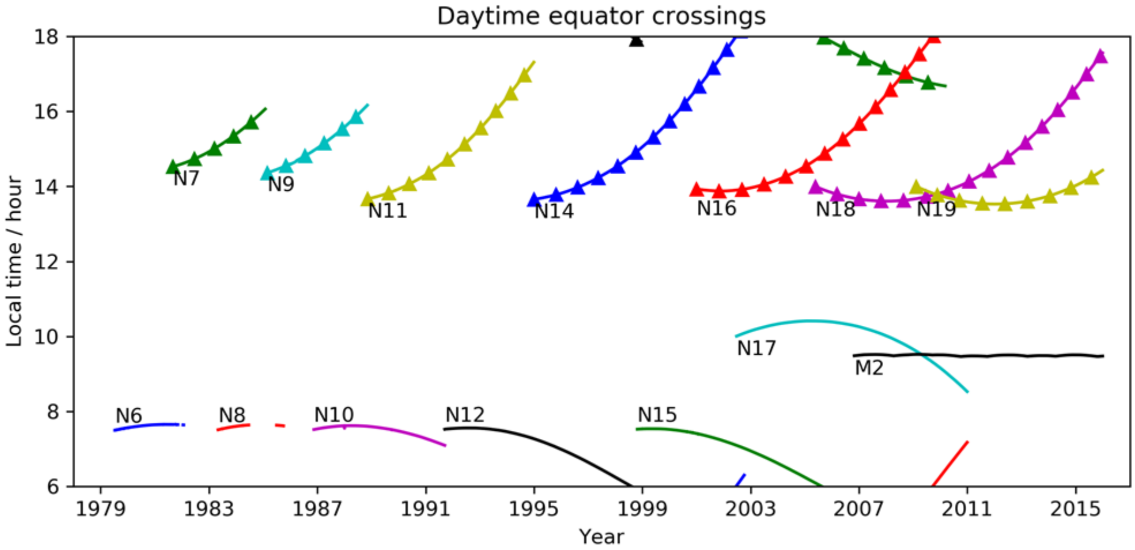

Figure 17. AVHRR equator crossing times. Solid lines indicate descending node crossings, lines with triangles indicate ascending node crossings. N6 denotes the AVHRR onboard the NOAA-6 satellite, etc. M2 denotes the AVHRR onboard MetOP-A. NOTE – this diagram shows periods when AVHRR Level-1 data exists; it does not imply that the data is of sufficient quality to generate corresponding SST data.

The AVHRR instruments were not designed for climate monitoring of SST and are not as well calibrated as the ATSR instruments. However; they have been operational and recording data for far longer, they have a wider swath and multiple satellites are in orbit meaning they produce much more complete coverage than the other instruments. The AVHRR swath is approximately 2800 km on the Earth's surface and the satellite completes approximately 14 orbits each day so a single satellite could potentially achieve global daily coverage. However, usable data is restricted to cloud-free regions and the data quality degrades towards the edge of the satellite swath due to the larger viewing angles.

Daytime uncertainties are much higher than the night-time estimates – especially towards the edge of the satellite swath and in the tropics. Under night-time conditions the retrieval can use three of the sensor channels: 3.7, 11, and 12 µm; which allows the most accurate and sensitive SST estimate to be produced. However, during the day the 3.7 µm channel is affected by reflected solar radiance and cannot be used for the retrieval. With only the 11 and 12 µm channels (both of which are much more sensitive to atmospheric water vapour) in use, the daytime estimate is generally less accurate.

Selected portions of the record from AVHRR instruments on several satellites were used, in order to maximise data quality. Table 18 below details the data used from each instrument.

Table 18. Period of data used in SST CCI Phase 2 CDR2.0 products from AVHRR instruments on different satellites.

Satellite name	Period of data used
NOAA-7	24/08/1981-18/02/1985
NOAA-9	04/01/1985-07/11/1988, 12/12/1991-06/01/1992
NOAA-11	12/10/1988-13/09/1994

NOAA-12	16/09/1991-14/12/1998
NOAA-14	19/01/1995-31/12/1999
NOAA-15	24/09/1998-09/03/2010, plus other single days during April-July 2010
NOAA-16	01/06/2003-31/12/2006
NOAA-17	10/07/2002-31/12/2009
NOAA-18	05/06/2005-31/12/2009
NOAA-19	22/02/2009-31/12/2016
MetOp-A	21/11/2006-31/12/2016

The spatial resolution of the AVHRR instruments is approximately 1.1 km at nadir (directly below the satellite). However, due to hardware limitations when the instruments were originally designed it was not possible to record a complete orbit of full resolution data for transmission to the ground station. Therefore, the on-board processor samples the real-time data to produce reduced resolution Global Area Coverage (GAC) data with a nominal resolution of ~4 km. This is achieved by averaging four pixels out of five in every third scanline as illustrated in Figure 18.

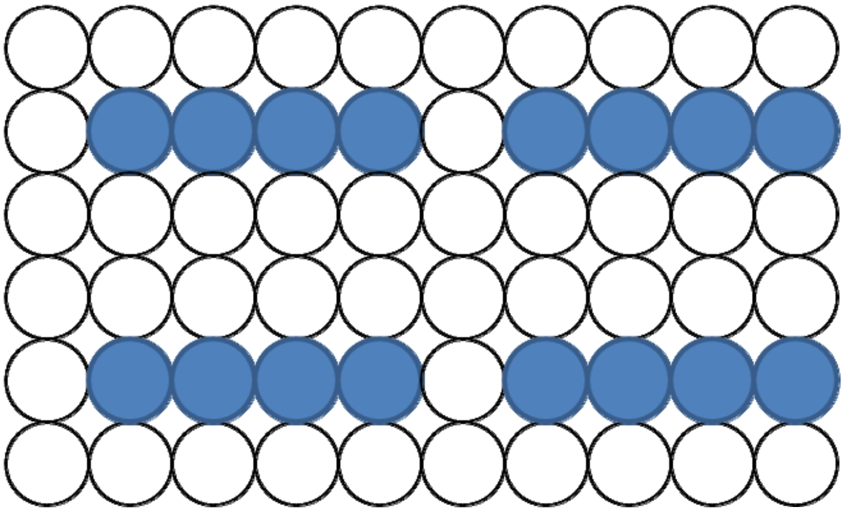

Figure 18. Schematic of GAC pixels (blue) which are the average of four full resolution pixels (circles). White circles indicate full resolutions pixels which are not included in the averaging.

AVHRR calibration corrections

A key development in Phase 2 of the ESA SST CCI project has been to extend the products back to the early 1980s. This relies on the early AVHRR instruments. In order to use these instruments, improvement of the instrument calibration was required.

Calibration biases were reduced by: filtering outliers; using a consistent fundamental calibration [RD.411] for all instruments, rather than the inconsistent calibration used operationally; and modelling the impact of four sources of error not captured by the fundamental calibration (solar contamination of the calibration target for the 3.7micron channel, stray light effects combined with orbital drift, errors in estimating the internal calibration targets radiant temperature due to strong thermal gradients, and a scene temperature dependent bias).

Cloud and sea ice detection

Cloud in the instrument's field of view will contaminate the surface signal and is therefore screened prior to SST retrieval using a Bayesian cloud detection scheme [RD.180; RD.410].

The Bayesian scheme simulates brightness temperatures under clear sky conditions using a fast radiative transfer model with inputs from numerical weather prediction data. Cloudy sky probabilities are represented using probability density functions and this background information is used in conjunction with the observations and their relative uncertainties to calculate a probability of clear sky. In version 2 products, this Bayesian scheme has also been adapted for application to AVHRR by better modelling of surface reflectance and changes needed to better address the problem in areas affected by sunglint and in areas of shallow water. The Bayesian scheme is an improvement on the CLAVR-X scheme used in version 1 products (for retrievals on GAC resolution) and on the operational approach used at EUMETSAT (for retrievals on FRAC resolution). Cloud detection at high latitudes uses an additional Bayesian calculation which further classifies each location as ocean, cloud or ice.

SST retrievals

The SST retrieval exploits data in the different channels and views to retrieve surface temperature, correcting for the atmosphere's impact on the signal.

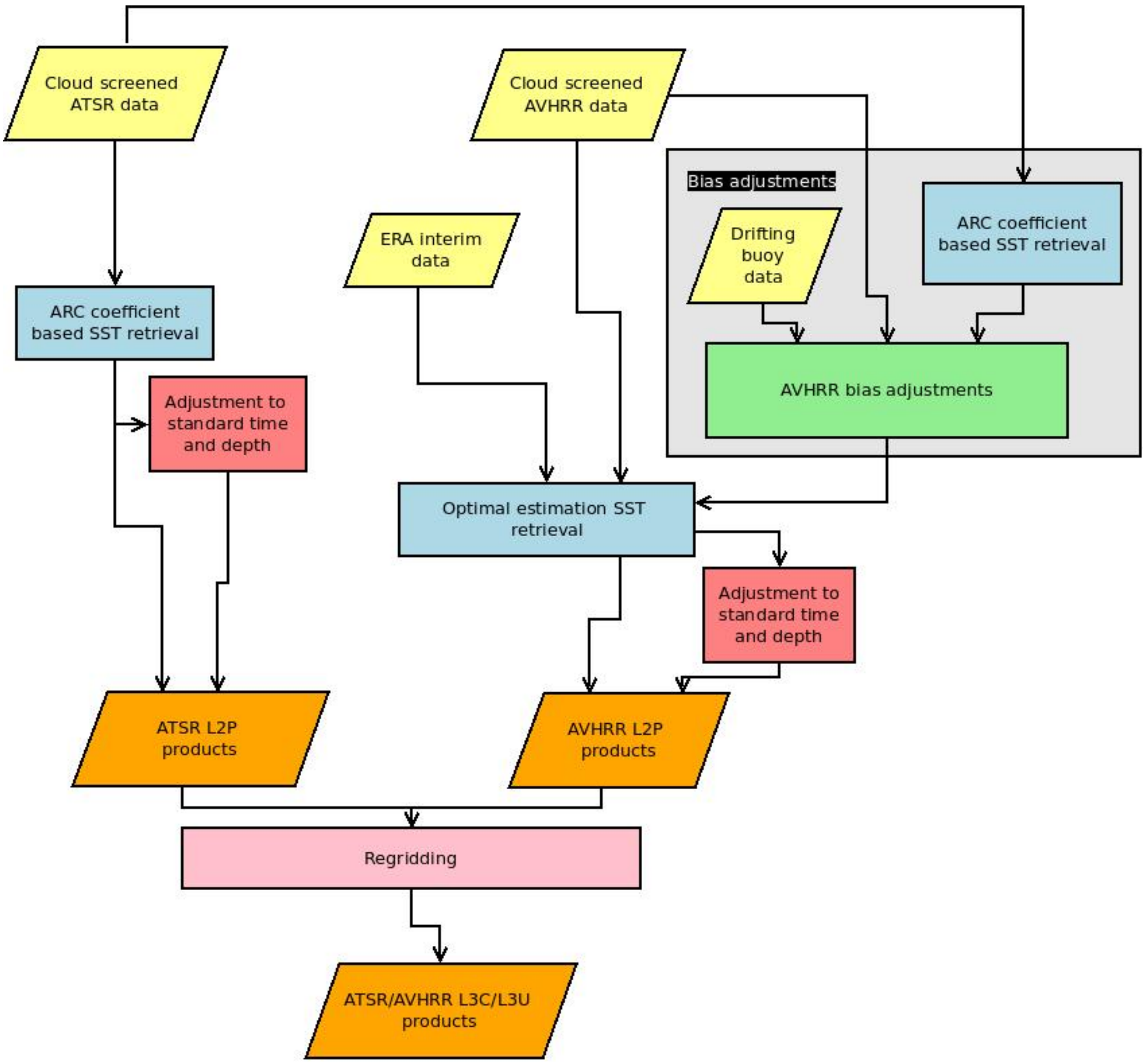

Figure 19. Overview of the processing of ATSR- and AVHRR-series data to produce the output data files for the ESA SST CCI version 2 products. ATSR SSTs are retrieved using a coefficient based approach; AVHRR series SSTs are retrieved using optimal estimation. The optimal estimation approach requires bias corrections for the fast radiative transfer model that is used; these are calculated using ATSR-2 and AATSR SSTs. Yellow boxes denote input data; blue shows SST retrieval steps; green are bias adjustment calculations; red indicates adjustment of SSTs to standard time and depth using a diurnal variability model; pink is used where the full resolution ATSR series data are regridded; orange are the output ESA SST CCI products.

Two types of SST retrieval are used in the data processing. One is a 'coefficient based' method and the other an 'optimal estimation' (OE) method. The coefficient based retrievals calculate SST from a linear combination of the BTs, with each weighted by a coefficient. The coefficients were developed during the ATSR Reanalysis for Climate (ARC) project [RD.296] and updated in Phase II of the ESA CCI SST project. An accurate radiative transfer model was used to simulate the signal seen at the satellite under a range of realistic atmospheric conditions (as obtained from a reanalysis). The resulting BTs were regressed against the SSTs used in the simulations, yielding the coefficients.

In the optimal estimation retrievals the SST and the total column water vapour are estimated at the same time. A fast radiative transfer model is used to simulate the signal sensed by the satellite given a first guess SST and atmospheric conditions obtained from reanalysis. Using knowledge of how the satellite BTs change with variation in SST and total column water vapour, along with estimates of the uncertainties associated with the observations, reanalysis and radiative transfer model, the SST and total column water vapour can be calculated. By defining the first guess SST as very uncertain, the SST that is retrieved has low dependence on that first guess. Consequently the SST that is retrieved using this method is fully sensitive to the surface temperature, which is not true of all retrieval algorithms. An issue with this method is that the fast radiative transfer model is biased. However, use of a more accurate 'line by line' radiative transfer model is prohibited by the amount of time it takes to run. Therefore bias corrections are calculated and applied to the OE SST outputs.

A bias correction for the OE SST is calculated using the results of the coefficient based retrievals applied to ATSR-2 and AATSR data, which can be viewed as unbiased, and comparing them against the OE retrieval applied to AVHRR data. The approach conveniently also compensates for any sensor calibration drift. To account for the different time of observation of ATSR2/AATSR and AVHRR sensors the change in SST is estimated using the Kantha Clayson model [RD.263] (also see adjustments for time and depth below). This method ties the AVHRR data to the ATSRs data, resulting in a data product that has the coverage of the AVHRRs, but zero overall bias relative to ATSR. For AVHRR data in the 1980, before the launch of the first ATSR, we use *in situ* data as the reference SST instead.

ATSR SST retrievals can be made robust to the impact of stratospheric aerosols, due to the dual view capability of the instrument. AVHRR instruments have only a single view, so there is insufficient information in the measurements from AVHRR alone to retrieve SST accurately when stratospheric aerosols are present. Since major volcanic eruptions have occurred in the period since the early 1980s, the associated infrared aerosol optical depth of these eruptions has been estimated using additional information available from the HIRS instrument. This additional information is used in the SST retrieval and taken account of in the radiative transfer model to reduce the bias in the retrievals associated with the presence of the additional aerosol.

The retrieval algorithms are optimised to produce a climate-quality SST – i.e. minimum systematic errors, maximum sensitivity to true SST changes and minimum sensitivity to prior SST (i.e. independence from *in situ*). Meeting these requirements can mean the retrieval has a high sensitivity to radiometric noise resulting in larger uncorrelated uncertainties. For the gridded (L3/L4) products uncorrelated errors will be reduced by the averaging process and become negligible over large spatial / temporal scales. However, they can remain significant for full resolution SST products. Noise in the full resolution SST products can be reduced by noting that the water vapour in the atmosphere varies smoothing on few-km scales. Over these distances the "atmospheric correction" or difference between the SST and top-of-atmosphere BT can be assumed to be constant. The noise reduction is only applied to the full-resolution (L2P) products.

Uncertainty estimation

As part of the retrievals, estimates are generated for four uncertainty components:

- uncorrelated_uncertainty – uncertainty from effects that are not correlated from location to location (such as random noise in the satellite sensors).

- synoptically_correlated_uncertainty – uncertainty from effects that are assumed (provisionally) to be correlated over distances of 100 km and 1 day (related to atmospheric conditions).

- large_scale_correlated_uncertainty – uncertainty from effects that can be assumed to be correlated everywhere and long time scales (such as over all calibration of the satellite sensor).

- adjustment_uncertainty – only applicable if using SSTs that have been adjusted to the standard time (10.30/22.30 h) and depth (20 cm); (provisionally) assumed to be correlated over 100 km and 1 day.

A further uncertainty component arising from under-sampling of 0.05° grid cells due to their partial obscuration by cloud is then estimated for the L3U products. This should be treated as not correlated between 0.05° grid cells. This uncertainty component is contained within the uncorrelated uncertainty variable in the L3U files.

Adjustments for time and depth

SSTs retrieved from ATSR and AVHRR data are skin SSTs i.e. they are temperature at approximately 10 µm depth. This depth is not always the most useful for product users [RD.385]. Observation times of different sensors can also be inconsistent and may drift through the lifetime of the satellite mission.

To compensate for these effects, the ESA SST CCI project provides an adjusted SST for each retrieved skin SST. The adjusted SSTs are representative of the temperature at 20 cm depth and at 1030 local time in the morning or evening.

The adjustments are performed in two stages. First, the skin SST is adjusted to be a subskin SST (representative of the temperature in the top 1 mm of the water). The temperature in this layer is affected by interactions with the atmosphere and the loss of heat as radiation. The effect of this is estimated using a model of this skin effect called the Fairall model [RD.227], which is driven by information from the ERA-Interim reanalysis [RD.40]. Uncertainty in this adjustment is also estimated.

The second stage of the adjustment is to convert from subskin SST to 20 cm depth SST and from the measurement time to 1030 local time. The Kantha Clayson model [RD.263] is used for this, which is a diffusion model of the mixed layer of the ocean. As with the Fairall model, it is driven by ERA-Interim data. The model integrates forward in time, calculating temperature at different depth points (including 20 cm) for each 10 minute time step. Uncertainties are estimated using drifting buoy data to assess the performance of the model.

Generating L3U data from the retrieved SSTs

The retrieved SSTs are averaged onto a 0.05° regular latitude-longitude grid. Uncertainty estimates are also averaged. However, for the first component of uncertainty listed above, errors are uncorrelated and are therefore reduced by a factor $1/\sqrt{n}$ where n is the number of clear sky pixels. An estimate of the sampling uncertainty associated with incomplete sampling of the grid box due to cloud and other factors is also estimated and combined with the other uncorrelated uncertainty.

Generating L3C data

L3C data are aggregated from L3U, collecting separately the daytime and nighttime parts of each orbits into separate day and night files, based on the solar zenith angle applicable to each value.

10.2 Processing of L2 and L3 data to obtain L4 products

10.2.1 OSTIA processing system

A new implementation of the Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA) processing system was used in Phase 2 to create L4 data products from the L2 and L3 SSTs. In brief, the analysis system uses the NEMOVAR variational assimilation scheme [RD.283;

RD.284] rather than the iterative method used to solve optimal interpolation equations in Phase I. In addition to the SSTs, inputs to the system are a ‘background’ SST field and information about the covariance of errors in that background and the observations.

The background SSTs are calculated by persisting the previous day’s analysis forward to the present, with some relaxation to climatological values. Observation errors are assumed to be uncorrelated with each other. The background error covariance information has been improved in Phase 2 to be “flow dependent” and is parameterised as a set of background error variances at the analysis grid points with correlations between background errors from location to location specified by two length scales. The flow dependence varies the ratio of the two length scales according to the characteristics of the SST field in a particular location. Background error variances are seasonally variable. The shorter background error length scale has been further shortened for Phase 2 to improve the effective resolution of the analysis [RD.407].

Also included with the SST analyses are sea ice concentrations. These were produced by analysing input data sourced from the OSI SAF CDR v2 product (OSI-450, http://osisaf.met.no/p/ice/), followed by the OSI SAF continuous reprocessing (OSI SAF: EUMETSAT Ocean and Sea Ice Satellite Application Facility. Global sea ice concentration continuous reprocessing offline product (2017 onwards), [Online]. Norwegian and Danish Meteorological Institutes. Available from http://osisaf.met.no).

10.2.2 Uncertainty estimation

In the OSTIA processing system, uncertainties are calculated using a special analysis in which observation values are set to have a value of one and background values are set to be zero with other system settings identical to those used when performing the SST analysis. The resulting analysis has values that are zero or close to zero where observations had little influence on the resulting SST, but has values close to one where observations have strongly influenced the SST. The assumption is made that this analysis is linearly related to the analysis error variance. The background error variance data are used to relate the values from the special analysis to the analysis error variance. The result is that the analysis error variance is 4.5 times the background error variance if no observations influenced the analysis and 0.5 times the background error variance if the analysis was fully determined by observations. See [RD.213] for more details.

11. APPENDIX 2: SAMPLE LISTINGS OF FILE CONTENTS

This appendix contains listings of the headers of NetCDF files for examples of the ESA SST CCI data products and the output of tools. The listings were produced using the ncdump tool that is provided with the NetCDF library. The format of the listings is 'network Common data form Description Language' (CDL), which is described at http://www.unidata.ucar.edu/software/netcdf/docs/netcdf/CDL-Syntax.html.

11.1 Header from an L2P file

```
netcdf \20000101000206-ESACCI-L2P_GHRSST-SSTskin-AVHRR15_G-CDR2.0-v02.0-
fv01.0 {
dimensions:
    ni = 409 ;
    nj = 13022 ;
    time = 1 ;
variables:
    float lat(nj, ni) ;
        lat:long_name = "Latitude coordinates" ;
        lat:standard_name = "latitude" ;
        lat:units = "degrees_north" ;
        lat:valid_min = -90.f ;
        lat:valid_max = 90.f ;
        lat:reference_datum = "geographical coordinates, WGS84 projec-
tion" ;
    float lon(nj, ni) ;
        lon:long_name = "Longitude coordinates" ;
        lon:standard_name = "longitude" ;
        lon:units = "degrees_east" ;
        lon:valid_min = -180.f ;
        lon:valid_max = 180.f ;
        lon:reference_datum = "geographical coordinates, WGS84 projec-
tion" ;
    int time(time) ;
        time:long_name = "reference time of sst file" ;
        time:standard_name = "time" ;
        time:units = "seconds since 1981-01-01 00:00:00" ;
        time:calendar = "gregorian" ;
    short sea_surface_temperature(time, nj, ni) ;
        sea_surface_temperature:_FillValue = -32768s ;
        sea_surface_temperature:long_name = "sea surface skin tempera-
ture" ;
        sea_surface_temperature:standard_name =
"sea_surface_skin_temperature" ;
        sea_surface_temperature:units = "kelvin" ;
        sea_surface_temperature:add_offset = 273.15f ;
        sea_surface_temperature:scale_factor = 0.01f ;
        sea_surface_temperature:valid_min = -200s ;
        sea_surface_temperature:valid_max = 5000s ;
        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:references = "http://www.esa-sst-cci.org"
;
        sea_surface_temperature:source = "AVHRR15_G-ESACCI-L1C-v1" ;
        sea_surface_temperature:depth = "10 micrometres" ;
```

```
        sea_surface_temperature:coordinates = "lon lat" ;
    short sea_surface_temperature_depth(time, nj, ni) ;
        sea_surface_temperature_depth:_FillValue = -32768s ;
        sea_surface_temperature_depth:long_name = "sea surface tempera-
ture at 0.2 m" ;
        sea_surface_temperature_depth:standard_name =
"sea_water_temperature" ;
        sea_surface_temperature_depth:units = "kelvin" ;
        sea_surface_temperature_depth:add_offset = 273.15f ;
        sea_surface_temperature_depth:scale_factor = 0.01f ;
        sea_surface_temperature_depth:valid_min = -200s ;
        sea_surface_temperature_depth:valid_max = 5000s ;
        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:references = "http://www.esa-sst-
cci.org" ;
        sea_surface_temperature_depth:source = "AVHRR15_G-ESACCI-L1C-v1"
;
        sea_surface_temperature_depth:depth = "0.2 metre" ;
        sea_surface_temperature_depth:coordinates = "lon lat" ;
    short sst_dtime(time, nj, ni) ;
        sst_dtime:_FillValue = -32768s ;
        sst_dtime:long_name = "time difference from reference time" ;
        sst_dtime:units = "seconds" ;
        sst_dtime:add_offset = 0.f ;
        sst_dtime:scale_factor = 1.f ;
        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" ;
    short sst_depth_dtime(time, nj, ni) ;
        sst_depth_dtime:_FillValue = -32768s ;
        sst_depth_dtime:long_name = "time difference from reference time"
;
        sst_depth_dtime:units = "seconds" ;
        sst_depth_dtime:add_offset = 0.f ;
        sst_depth_dtime:scale_factor = 1.f ;
        sst_depth_dtime:valid_min = -32767s ;
        sst_depth_dtime:valid_max = 32767s ;
        sst_depth_dtime:comment = "time plus sst_depth_dtime gives sec-
onds after 1981-01-01 00:00:00" ;
        sst_depth_dtime:coordinates = "lon lat" ;
    byte sses_bias(time, nj, ni) ;
        sses_bias:_FillValue = -128b ;
        sses_bias:long_name = "SSES bias estimate" ;
        sses_bias:units = "kelvin" ;
        sses_bias:add_offset = 0.f ;
        sses_bias:scale_factor = 0.01f ;
        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:long_name = "SSES standard deviation" ;
```

```
        sses_standard_deviation:units = "kelvin" ;
        sses_standard_deviation:add_offset = 1.27f ;
        sses_standard_deviation:scale_factor = 0.01f ;
        sses_standard_deviation:valid_min = -127b ;
        sses_standard_deviation:valid_max = 127b ;
        sses_standard_deviation:comment = "Uncertainty data are also con-
tained in the variables large_scale_correlated_uncertainty, synopti-
cally_correlated_uncertainty, uncorrelated_uncertainty and adjust-
ment_uncertainty" ;
        sses_standard_deviation:coordinates = "lon lat" ;
    short sst_depth_total_uncertainty(time, nj, ni) ;
        sst_depth_total_uncertainty:_FillValue = -32768s ;
        sst_depth_total_uncertainty:long_name = "Total uncertainty in
sea_surface_temperature_depth" ;
        sst_depth_total_uncertainty:units = "kelvin" ;
        sst_depth_total_uncertainty:add_offset = 0.f ;
        sst_depth_total_uncertainty:scale_factor = 0.001f ;
        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" ;
    short l2p_flags(time, nj, ni) ;
        l2p_flags:_FillValue = -32768s ;
        l2p_flags:long_name = "L2P flags" ;
        l2p_flags:valid_min = 0s ;
        l2p_flags:valid_max = 255s ;
        l2p_flags:flag_meanings = "microwave land ice lake river spare
views channels" ;
        l2p_flags:flag_masks = 1s, 2s, 4s, 8s, 16s, 32s, 64s, 128s ;
        l2p_flags:comment = "These flags are important to properly use
the data" ;
        l2p_flags:coordinates = "lon lat" ;
    byte quality_level(time, nj, ni) ;
        quality_level:_FillValue = 0b ;
        quality_level:long_name = "quality level of SST pixel" ;
        quality_level:valid_min = 0b ;
        quality_level:valid_max = 5b ;
        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 ;
        quality_level:comment = "These are overall quality indicators and
are used for all GHRSST SSTs" ;
        quality_level:coordinates = "lon lat" ;
    byte wind_speed(time, nj, ni) ;
        wind_speed:_FillValue = -128b ;
        wind_speed:long_name = "10m wind speed" ;
        wind_speed:standard_name = "wind_speed" ;
        wind_speed:units = "m s-1" ;
        wind_speed:add_offset = 12.7f ;
        wind_speed:scale_factor = 0.1f ;
        wind_speed:valid_min = -127b ;
        wind_speed:valid_max = 127b ;
        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:references = "http://www.esa-sst-cci.org" ;
        wind_speed:source = "ERA_INTERIM-ECMWF-WSP-v1.0" ;
        wind_speed:time_offset = 0.f ;
```

```
        wind_speed:height = "10 m" ;
        wind_speed:coordinates = "lon lat" ;
    short large_scale_correlated_uncertainty(time, nj, ni) ;
        large_scale_correlated_uncertainty:_FillValue = -32768s ;
        large_scale_correlated_uncertainty:long_name = "Uncertainty from
errors likely to be correlated over large scales" ;
        large_scale_correlated_uncertainty:units = "kelvin" ;
        large_scale_correlated_uncertainty:add_offset = 0.f ;
        large_scale_correlated_uncertainty:scale_factor = 0.001f ;
        large_scale_correlated_uncertainty:valid_min = 0s ;
        large_scale_correlated_uncertainty:valid_max = 5000s ;
        large_scale_correlated_uncertainty:comment = "Component of uncer-
tainty that is correlated over large scales; can be combined with other
uncertainty estimates to form a total uncertainty" ;
        large_scale_correlated_uncertainty:references = "http://www.esa-
sst-cci.org" ;
        large_scale_correlated_uncertainty:coordinates = "lon lat" ;
    short synoptically_correlated_uncertainty(time, nj, ni) ;
        synoptically_correlated_uncertainty:_FillValue = -32768s ;
        synoptically_correlated_uncertainty:long_name = "Uncertainty from
errors likely to be correlated over synoptic scales" ;
        synoptically_correlated_uncertainty:units = "kelvin" ;
        synoptically_correlated_uncertainty:add_offset = 0.f ;
        synoptically_correlated_uncertainty:scale_factor = 0.001f ;
        synoptically_correlated_uncertainty:valid_min = 0s ;
        synoptically_correlated_uncertainty:valid_max = 5000s ;
        synoptically_correlated_uncertainty:comment = "Component of un-
certainty that is correlated over synoptic scales; can be combined with
other uncertainty estimates to form a total uncertainty" ;
        synoptically_correlated_uncertainty:correlation_length_scale =
"100 km" ;
        synoptically_correlated_uncertainty:correlation_time_scale = "1
day" ;
        synoptically_correlated_uncertainty:references = "http://www.esa-
sst-cci.org" ;
        synoptically_correlated_uncertainty:coordinates = "lon lat" ;
    short uncorrelated_uncertainty(time, nj, ni) ;
        uncorrelated_uncertainty:_FillValue = -32768s ;
        uncorrelated_uncertainty:long_name = "Uncertainty from errors
likely to be uncorrelated between SSTs" ;
        uncorrelated_uncertainty:units = "kelvin" ;
        uncorrelated_uncertainty:add_offset = 0.f ;
        uncorrelated_uncertainty:scale_factor = 0.001f ;
        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 es-
timates to form a total uncertainty" ;
        uncorrelated_uncertainty:references = "http://www.esa-sst-
cci.org" ;
        uncorrelated_uncertainty:coordinates = "lon lat" ;
    short adjustment_uncertainty(time, nj, ni) ;
        adjustment_uncertainty:_FillValue = -32768s ;
        adjustment_uncertainty:long_name = "Time and depth adjustment un-
certainty" ;
        adjustment_uncertainty:units = "kelvin" ;
        adjustment_uncertainty:add_offset = 0.f ;
        adjustment_uncertainty:scale_factor = 0.001f ;
```

```
        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 = "http://www.esa-sst-cci.org"
;
        adjustment_uncertainty:coordinates = "lon lat" ;
        adjustment_uncertainty:correlation_length_scale = "100 km" ;
        adjustment_uncertainty:correlation_time_scale = "1 day" ;
    byte aerosol_dynamic_indicator(time, nj, ni) ;
        aerosol_dynamic_indicator:_FillValue = -128b ;
        aerosol_dynamic_indicator:long_name = "aerosol dynamic indicator"
;
        aerosol_dynamic_indicator:units = "" ;
        aerosol_dynamic_indicator:add_offset = 0.f ;
        aerosol_dynamic_indicator:scale_factor = 0.01f ;
        aerosol_dynamic_indicator:valid_min = -127b ;
        aerosol_dynamic_indicator:valid_max = 127b ;
        aerosol_dynamic_indicator:coordinates = "lon lat" ;
        aerosol_dynamic_indicator:time_offset = 0.f ;
        aerosol_dynamic_indicator:source = "ATSR SDI" ;
        aerosol_dynamic_indicator:comment = "ATSR Saharan Dust Index" ;
        aerosol_dynamic_indicator:references = "Good, E.J., Kong, X., Em-
bury, O., Merchant, C.J., Remedios, J.J. (2012). An infrared desert dust
index for the Along-Track Scanning Radiometers, Remote Sensing of Envi-
ronment, 116(15), DOI:10.1016/j.rse.2010.06.016" ;
    byte probability_clear(time, nj, ni) ;
        probability_clear:_FillValue = -128b ;
        probability_clear:long_name = "Probability of pixel being clear"
;
        probability_clear:units = "" ;
        probability_clear:add_offset = 0.f ;
        probability_clear:scale_factor = 0.01f ;
        probability_clear:valid_min = 0b ;
        probability_clear:valid_max = 100b ;
        probability_clear:coordinates = "lon lat" ;
        probability_clear:comment = "Probability of pixel being clear as
estimated by Bayesian cloud detection" ;
    byte sensitivity(time, nj, ni) ;
        sensitivity:_FillValue = -128b ;
        sensitivity:long_name = "Sensitivity to SST" ;
        sensitivity:units = "K/K" ;
        sensitivity:add_offset = 1.f ;
        sensitivity:scale_factor = 0.01f ;
        sensitivity:valid_min = -100b ;
        sensitivity:valid_max = 100b ;
        sensitivity:coordinates = "lon lat" ;
        sensitivity:comment = "Sensitivity of retrieved SST to true
changes in SST" ;

// global attributes:
        :Conventions = "CF-1.5, Unidata Observation Dataset v1.0" ;
        :title = "ESA SST CCI AVHRR15_G L2P product" ;
        :summary = "AVHRR15_G L2P product from the ESA SST CCI project,
produced using smoothed OE algorithm." ;
        :references = "http://www.esa-sst-cci.org" ;
        :institution = "ESACCI" ;
        :history = "Created using GBCS library v2.5.0" ;
```

```
        :license = "GHRSST protocol describes data use as free and open"
;
        :id = "AVHRR15_G-ESACCI-L2P-CDR2.0-v2.0" ;
        :naming_authority = "org.ghrsst" ;
        :product_version = "2.0" ;
        :uuid = "cb6f5dc4-c427-11e7-9943-ff3bb971b542" ;
        :tracking_id = "cb6f5dc4-c427-11e7-9943-ff3bb971b542" ;
        :gds_version_id = "2.0" ;
        :netcdf_version_id = "4.3.2 of Jul 22 2014 16:21:31" ;
        :date_created = "20171108T015445Z" ;
        :file_quality_level = 3 ;
        :spatial_resolution = "4.0 km at nadir" ;
        :start_time = "20000101T000206Z" ;
        :time_coverage_start = "20000101T000206Z" ;
        :stop_time = "20000101T015036Z" ;
        :time_coverage_end = "20000101T015036Z" ;
        :time_coverage_duration = "P0DT01H48M29S" ;
        :time_coverage_resolution = "P0DT1H40M00S" ;
        :source = "AVHRR15_G-ESACCI-L1C-v1, ERA_INTERIM-ECMWF-WSP-v1.0" ;
        :platform = "NOAA-15" ;
        :sensor = "AVHRR_GAC" ;
        :Metadata_Conventions = "Unidata Dataset Discovery v1.0" ;
        :metadata_link = "http://www.esa-cci.org" ;
        :keywords = "Oceans > Ocean Temperature > Sea Surface Tempera-
ture" ;
        :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 = 0.01f ;
        :geospatial_lon_units = "degrees_east" ;
        :geospatial_lon_resolution = 0.01f ;
        :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
the STFC CEMS as part of the ESA SST CCI project" ;
        :project = "Climate Change Initiative - European Space Agency" ;
        :publisher_name = "ESACCI" ;
        :publisher_url = "http://www.esa-sst-cci.org" ;
        :publisher_email = "science.leader@esa-SST-cci.org" ;
        :comment = "For information about uncertainty estimates see the
comment attributes to the sea_surface_temperature and
sea_surface_temperature_depth variables" ;
        :northernmost_latitude = 90. ;
        :southernmost_latitude = -90. ;
        :easternmost_longitude = 180. ;
        :westernmost_longitude = -180. ;
        :geospatial_lat_min = -90.f ;
        :geospatial_lat_max = 90.f ;
        :geospatial_lon_min = -180.f ;
        :geospatial_lon_max = 180.f ;
        :processing_level = "L2P" ;
        :cdm_data_type = "swath" ;
```

```
        :source_file = "20000101000206-ESACCI-L1C-AVHRR15_G-fv01.0.nc" ;
        :product_specification_version  =  "SST_CCI-PSD-UKMO-201-Issue-1-
signed" ;
}
```

11.2 Header from an L3U file

```
netcdf     \20000102155711-ESACCI-L3U_GHRSST-SSTskin-ATSR2-CDR2.0-v02.0-
fv01.0 {
dimensions:
    lat = 3600 ;
    lon = 7200 ;
    time = UNLIMITED ; // (1 currently)
    bnds = 2 ;
variables:
    float lat(lat) ;
        lat:long_name = "Latitude" ;
        lat:standard_name = "latitude" ;
        lat:units = "degrees_north" ;
        lat:valid_min = -90.f ;
        lat:valid_max = 90.f ;
        lat:reference_datum  =  "geographical  coordinates,  WGS84  projec-
tion" ;
        lat:axis = "Y" ;
        lat:bounds = "lat_bnds" ;
    float lat_bnds(lat, bnds) ;
        lat_bnds:long_name = "Latitude cell boundaries" ;
        lat_bnds:units = "degrees_north" ;
        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 pro-
jection" ;
    float lon(lon) ;
        lon:long_name = "Longitude" ;
        lon:standard_name = "longitude" ;
        lon:units = "degrees_east" ;
        lon:valid_min = -180.f ;
        lon:valid_max = 180.f ;
        lon:reference_datum  =  "geographical  coordinates,  WGS84  projec-
tion" ;
        lon:axis = "X" ;
        lon:bounds = "lon_bnds" ;
    float lon_bnds(lon, bnds) ;
        lon_bnds:long_name = "Longitude cell boundaries" ;
        lon_bnds:units = "degrees_east" ;
        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 pro-
jection" ;
    int time(time) ;
        time:long_name = "reference time of sst file" ;
        time:standard_name = "time" ;
        time:units = "seconds since 1981-01-01 00:00:00" ;
        time:calendar = "gregorian" ;
```

```
        time:axis = "T" ;
        time:bounds = "time_bnds" ;
    int time_bnds(time, bnds) ;
        time_bnds:long_name = "Time cell boundaries" ;
        time_bnds:units = "seconds since 1981-01-01 00:00:00" ;
        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:long_name = "sea surface skin tempera-
ture" ;
        sea_surface_temperature:standard_name =
"sea_surface_skin_temperature" ;
        sea_surface_temperature:units = "kelvin" ;
        sea_surface_temperature:add_offset = 273.15f ;
        sea_surface_temperature:scale_factor = 0.01f ;
        sea_surface_temperature:valid_min = -200s ;
        sea_surface_temperature:valid_max = 5000s ;
        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:references = "http://www.esa-sst-cci.org"
;
        sea_surface_temperature:source = "ATSR2-ESA-L1-v3" ;
        sea_surface_temperature:depth = "10 micrometres" ;
    short sea_surface_temperature_depth(time, lat, lon) ;
        sea_surface_temperature_depth:_FillValue = -32768s ;
        sea_surface_temperature_depth:long_name = "sea surface tempera-
ture at 0.2 m" ;
        sea_surface_temperature_depth:standard_name =
"sea_water_temperature" ;
        sea_surface_temperature_depth:units = "kelvin" ;
        sea_surface_temperature_depth:add_offset = 273.15f ;
        sea_surface_temperature_depth:scale_factor = 0.01f ;
        sea_surface_temperature_depth:valid_min = -200s ;
        sea_surface_temperature_depth:valid_max = 5000s ;
        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:references = "http://www.esa-sst-
cci.org" ;
        sea_surface_temperature_depth:source = "ATSR2-ESA-L1-v3" ;
        sea_surface_temperature_depth:depth = "0.2 metre" ;
    int sst_dtime(time, lat, lon) ;
        sst_dtime:_FillValue = -2147483648 ;
        sst_dtime:long_name = "time difference from reference time" ;
        sst_dtime:units = "seconds" ;
        sst_dtime:add_offset = 0.f ;
        sst_dtime:scale_factor = 1.f ;
        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" ;
    int sst_depth_dtime(time, lat, lon) ;
        sst_depth_dtime:_FillValue = -2147483648 ;
```

```
        sst_depth_dtime:long_name = "time difference from reference time"
;
        sst_depth_dtime:units = "seconds" ;
        sst_depth_dtime:add_offset = 0.f ;
        sst_depth_dtime:scale_factor = 1.f ;
        sst_depth_dtime:valid_min = -43200 ;
        sst_depth_dtime:valid_max = 43200 ;
        sst_depth_dtime:comment = "time plus sst_depth_dtime gives sec-
onds after 1981-01-01 00:00:00" ;
    byte sses_bias(time, lat, lon) ;
        sses_bias:_FillValue = -128b ;
        sses_bias:long_name = "SSES bias estimate" ;
        sses_bias:units = "kelvin" ;
        sses_bias:add_offset = 0.f ;
        sses_bias:scale_factor = 0.01f ;
        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:long_name = "SSES standard deviation" ;
        sses_standard_deviation:units = "kelvin" ;
        sses_standard_deviation:add_offset = 1.27f ;
        sses_standard_deviation:scale_factor = 0.01f ;
        sses_standard_deviation:valid_min = -127b ;
        sses_standard_deviation:valid_max = 127b ;
        sses_standard_deviation:comment = "Uncertainty data are also con-
tained in the variables large_scale_correlated_uncertainty, synopti-
cally_correlated_uncertainty, uncorrelated_uncertainty and adjust-
ment_uncertainty" ;
    short sst_depth_total_uncertainty(time, lat, lon) ;
        sst_depth_total_uncertainty:_FillValue = -32768s ;
        sst_depth_total_uncertainty:long_name = "Total uncertainty in
sea_surface_temperature_depth" ;
        sst_depth_total_uncertainty:units = "kelvin" ;
        sst_depth_total_uncertainty:add_offset = 0.f ;
        sst_depth_total_uncertainty:scale_factor = 0.001f ;
        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" ;
    short l2p_flags(time, lat, lon) ;
        l2p_flags:_FillValue = -32768s ;
        l2p_flags:long_name = "L2P flags" ;
        l2p_flags:valid_min = 0s ;
        l2p_flags:valid_max = 255s ;
        l2p_flags:flag_meanings = "microwave land ice lake river spare
views channels" ;
        l2p_flags:flag_masks = 1s, 2s, 4s, 8s, 16s, 32s, 64s, 128s ;
        l2p_flags:comment = "These flags are important to properly use
the data" ;
    byte quality_level(time, lat, lon) ;
        quality_level:_FillValue = 0b ;
        quality_level:long_name = "quality level of SST pixel" ;
        quality_level:valid_min = 0b ;
        quality_level:valid_max = 5b ;
        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 ;
        quality_level:comment = "These are overall quality indicators and
are used for all GHRSST SSTs" ;
    byte wind_speed(time, lat, lon) ;
        wind_speed:_FillValue = -128b ;
        wind_speed:long_name = "10m wind speed" ;
        wind_speed:standard_name = "wind_speed" ;
        wind_speed:units = "m s-1" ;
        wind_speed:add_offset = 12.7f ;
        wind_speed:scale_factor = 0.1f ;
        wind_speed:valid_min = -127b ;
        wind_speed:valid_max = 127b ;
        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:references = "http://www.esa-sst-cci.org" ;
        wind_speed:source = "ERA_INTERIM-ECMWF-WSP-v1.0" ;
        wind_speed:time_offset = 0.f ;
        wind_speed:height = "10 m" ;
    short large_scale_correlated_uncertainty(time, lat, lon) ;
        large_scale_correlated_uncertainty:_FillValue = -32768s ;
        large_scale_correlated_uncertainty:long_name = "Uncertainty from
errors likely to be correlated over large scales" ;
        large_scale_correlated_uncertainty:units = "kelvin" ;
        large_scale_correlated_uncertainty:add_offset = 0.f ;
        large_scale_correlated_uncertainty:scale_factor = 0.001f ;
        large_scale_correlated_uncertainty:valid_min = 0s ;
        large_scale_correlated_uncertainty:valid_max = 5000s ;
        large_scale_correlated_uncertainty:comment = "Component of uncer-
tainty that is correlated over large scales; can be combined with other
uncertainty estimates to form a total uncertainty" ;
        large_scale_correlated_uncertainty:references = "http://www.esa-
sst-cci.org" ;
    short synoptically_correlated_uncertainty(time, lat, lon) ;
        synoptically_correlated_uncertainty:_FillValue = -32768s ;
        synoptically_correlated_uncertainty:long_name = "Uncertainty from
errors likely to be correlated over synoptic scales" ;
        synoptically_correlated_uncertainty:units = "kelvin" ;
        synoptically_correlated_uncertainty:add_offset = 0.f ;
        synoptically_correlated_uncertainty:scale_factor = 0.001f ;
        synoptically_correlated_uncertainty:valid_min = 0s ;
        synoptically_correlated_uncertainty:valid_max = 5000s ;
        synoptically_correlated_uncertainty:comment = "Component of un-
certainty that is correlated over synoptic scales; can be combined with
other uncertainty estimates to form a total uncertainty" ;
        synoptically_correlated_uncertainty:references = "http://www.esa-
sst-cci.org" ;
        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:long_name  =  "Uncertainty  from  errors
likely to be uncorrelated between SSTs" ;
        uncorrelated_uncertainty:units = "kelvin" ;
        uncorrelated_uncertainty:add_offset = 0.f ;
        uncorrelated_uncertainty:scale_factor = 0.001f ;
        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 es-
timates to form a total uncertainty" ;
        uncorrelated_uncertainty:references     =     "http://www.esa-sst-
cci.org" ;
    short adjustment_uncertainty(time, lat, lon) ;
        adjustment_uncertainty:_FillValue = -32768s ;
        adjustment_uncertainty:long_name = "Time and depth adjustment un-
certainty" ;
        adjustment_uncertainty:units = "kelvin" ;
        adjustment_uncertainty:add_offset = 0.f ;
        adjustment_uncertainty:scale_factor = 0.001f ;
        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 = "http://www.esa-sst-cci.org"
;
        adjustment_uncertainty:correlation_length_scale = "100 km" ;
        adjustment_uncertainty:correlation_time_scale = "1 day" ;
    byte aerosol_dynamic_indicator(time, lat, lon) ;
        aerosol_dynamic_indicator:_FillValue = -128b ;
        aerosol_dynamic_indicator:long_name = "aerosol dynamic indicator"
;
        aerosol_dynamic_indicator:units = "" ;
        aerosol_dynamic_indicator:add_offset = 0.f ;
        aerosol_dynamic_indicator:scale_factor = 0.01f ;
        aerosol_dynamic_indicator:valid_min = -127b ;
        aerosol_dynamic_indicator:valid_max = 127b ;
        aerosol_dynamic_indicator:coordinates = "lon lat" ;
        aerosol_dynamic_indicator:time_offset = 0.f ;
        aerosol_dynamic_indicator:source = "ATSR SDI" ;
        aerosol_dynamic_indicator:comment = "ATSR Saharan Dust Index" ;
        aerosol_dynamic_indicator:references = "Good, E.J., Kong, X., Em-
bury, O., Merchant, C.J., Remedios, J.J. (2012). An infrared desert dust
index for the Along-Track Scanning Radiometers, Remote Sensing of Envi-
ronment, 116(15), DOI:10.1016/j.rse.2010.06.016" ;
    byte sensitivity(time, lat, lon) ;
        sensitivity:_FillValue = -128b ;
        sensitivity:long_name = "Sensitivity to SST" ;
        sensitivity:units = "K/K" ;
        sensitivity:add_offset = 1.f ;
        sensitivity:scale_factor = 0.01f ;
        sensitivity:valid_min = -100b ;
        sensitivity:valid_max = 100b ;
        sensitivity:coordinates = "lon lat" ;
        sensitivity:comment  =  "Sensitivity  of  retrieved  SST  to  true
changes in SST" ;

// global attributes:
        :Conventions = "CF-1.5, Unidata Observation Dataset v1.0" ;
        :title = "ESA SST CCI ATSR2 L3U product" ;
        :summary = "ATSR2 L3U product from the ESA SST CCI project, pro-
duced using ARC algorithm." ;
        :references = "http://www.esa-sst-cci.org" ;
        :institution = "ESACCI" ;
        :history = "Created using GBCS library v2.5.0" ;
```

```
        :license = "GHRSST protocol describes data use as free and open"
;
        :id = "ATSR2-ESACCI-L3U-CDR2.0-v2.0" ;
        :naming_authority = "org.ghrsst" ;
        :product_version = "2.0" ;
        :uuid = "eafb613e-c354-11e7-b1cb-5bae94248e7f" ;
        :tracking_id = "eafb613e-c354-11e7-b1cb-5bae94248e7f" ;
        :gds_version_id = "2.0" ;
        :netcdf_version_id = "4.3.2 of Jul 22 2014 16:21:31" ;
        :date_created = "20171107T004514Z" ;
        :file_quality_level = 3 ;
        :start_time = "20000102T155711Z" ;
        :time_coverage_start = "20000102T155711Z" ;
        :stop_time = "20000102T171905Z" ;
        :time_coverage_end = "20000102T171905Z" ;
        :time_coverage_duration = "P0DT01H21M54S" ;
        :time_coverage_resolution = "P0DT1H40M00S" ;
        :Metadata_Conventions = "Unidata Dataset Discovery v1.0" ;
        :metadata_link = "http://www.esa-cci.org" ;
        :keywords = "Oceans > Ocean Temperature > Sea Surface Tempera-
ture" ;
        :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 = 0.05f ;
        :geospatial_lon_units = "degrees_east" ;
        :geospatial_lon_resolution = 0.05f ;
        :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
the STFC CEMS as part of the ESA SST CCI project" ;
        :project = "Climate Change Initiative - European Space Agency" ;
        :publisher_name = "ESACCI" ;
        :publisher_url = "http://www.esa-sst-cci.org" ;
        :publisher_email = "science.leader@esa-SST-cci.org" ;
        :comment = "For information about uncertainty estimates see the
comment attributes to the sea_surface_temperature and
sea_surface_temperature_depth variables" ;
        :northernmost_latitude = 90. ;
        :southernmost_latitude = -90. ;
        :easternmost_longitude = 180. ;
        :westernmost_longitude = -180. ;
        :geospatial_lat_min = -90.f ;
        :geospatial_lat_max = 90.f ;
        :geospatial_lon_min = -180.f ;
        :geospatial_lon_max = 180.f ;
        :processing_level = "L3U" ;
        :cdm_data_type = "grid" ;
        :source_file =
"AT2_TOA_1PURAL20000102_155711_000000001049_00182_24585_0000.E2" ;
        :product_specification_version = "SST_CCI-PSD-UKMO-201-Issue-1-
signed" ;
```

```
        :spatial_resolution = "0.05 degree" ;
        :source = "ATSR2-ESA-L1-v3" ;
        :platform = "ERS-2" ;
        :sensor = "ATSR" ;
}
```

11.3 Header from an L3C file

```
netcdf       \20000102120000-ESACCI-L3C_GHRSST-SSTskin-ATSR2-CDR2.0_day-
v02.0-fv01.0 {
dimensions:
    lat = 3600 ;
    lon = 7200 ;
    time = UNLIMITED ; // (1 currently)
    bnds = 2 ;
variables:
    float lat(lat) ;
        lat:long_name = "Latitude" ;
        lat:standard_name = "latitude" ;
        lat:units = "degrees_north" ;
        lat:valid_min = -90.f ;
        lat:valid_max = 90.f ;
        lat:reference_datum = "geographical coordinates, WGS84 projec-
tion" ;
        lat:axis = "Y" ;
        lat:bounds = "lat_bnds" ;
    float lat_bnds(lat, bnds) ;
        lat_bnds:long_name = "Latitude cell boundaries" ;
        lat_bnds:units = "degrees_north" ;
        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 pro-
jection" ;
    float lon(lon) ;
        lon:long_name = "Longitude" ;
        lon:standard_name = "longitude" ;
        lon:units = "degrees_east" ;
        lon:valid_min = -180.f ;
        lon:valid_max = 180.f ;
        lon:reference_datum = "geographical coordinates, WGS84 projec-
tion" ;
        lon:axis = "X" ;
        lon:bounds = "lon_bnds" ;
    float lon_bnds(lon, bnds) ;
        lon_bnds:long_name = "Longitude cell boundaries" ;
        lon_bnds:units = "degrees_east" ;
        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 pro-
jection" ;
    int time(time) ;
        time:long_name = "reference time of sst file" ;
        time:standard_name = "time" ;
        time:units = "seconds since 1981-01-01 00:00:00" ;
```

```
        time:calendar = "gregorian" ;
        time:axis = "T" ;
        time:bounds = "time_bnds" ;
    int time_bnds(time, bnds) ;
        time_bnds:long_name = "Time cell boundaries" ;
        time_bnds:units = "seconds since 1981-01-01 00:00:00" ;
        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:long_name = "sea surface skin tempera-
ture" ;
        sea_surface_temperature:standard_name =
"sea_surface_skin_temperature" ;
        sea_surface_temperature:units = "kelvin" ;
        sea_surface_temperature:add_offset = 273.15f ;
        sea_surface_temperature:scale_factor = 0.01f ;
        sea_surface_temperature:valid_min = -200s ;
        sea_surface_temperature:valid_max = 5000s ;
        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:references = "http://www.esa-sst-cci.org"
;
        sea_surface_temperature:source = "ATSR2-ESA-L1-v3" ;
        sea_surface_temperature:depth = "10 micrometres" ;
    short sea_surface_temperature_depth(time, lat, lon) ;
        sea_surface_temperature_depth:_FillValue = -32768s ;
        sea_surface_temperature_depth:long_name = "sea surface tempera-
ture at 0.2 m" ;
        sea_surface_temperature_depth:standard_name =
"sea_water_temperature" ;
        sea_surface_temperature_depth:units = "kelvin" ;
        sea_surface_temperature_depth:add_offset = 273.15f ;
        sea_surface_temperature_depth:scale_factor = 0.01f ;
        sea_surface_temperature_depth:valid_min = -200s ;
        sea_surface_temperature_depth:valid_max = 5000s ;
        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:references = "http://www.esa-sst-
cci.org" ;
        sea_surface_temperature_depth:source = "ATSR2-ESA-L1-v3" ;
        sea_surface_temperature_depth:depth = "0.2 metre" ;
    int sst_dtime(time, lat, lon) ;
        sst_dtime:_FillValue = -2147483648 ;
        sst_dtime:long_name = "time difference from reference time" ;
        sst_dtime:units = "seconds" ;
        sst_dtime:add_offset = 0.f ;
        sst_dtime:scale_factor = 1.f ;
        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" ;
    int sst_depth_dtime(time, lat, lon) ;
        sst_depth_dtime:_FillValue = -2147483648 ;
```

```
        sst_depth_dtime:long_name = "time difference from reference time"
;
        sst_depth_dtime:units = "seconds" ;
        sst_depth_dtime:add_offset = 0.f ;
        sst_depth_dtime:scale_factor = 1.f ;
        sst_depth_dtime:valid_min = -43200 ;
        sst_depth_dtime:valid_max = 43200 ;
        sst_depth_dtime:comment = "time plus sst_depth_dtime gives sec-
onds after 1981-01-01 00:00:00" ;
    byte sses_bias(time, lat, lon) ;
        sses_bias:_FillValue = -128b ;
        sses_bias:long_name = "SSES bias estimate" ;
        sses_bias:units = "kelvin" ;
        sses_bias:add_offset = 0.f ;
        sses_bias:scale_factor = 0.01f ;
        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:long_name = "SSES standard deviation" ;
        sses_standard_deviation:units = "kelvin" ;
        sses_standard_deviation:add_offset = 1.27f ;
        sses_standard_deviation:scale_factor = 0.01f ;
        sses_standard_deviation:valid_min = -127b ;
        sses_standard_deviation:valid_max = 127b ;
        sses_standard_deviation:comment = "Uncertainty data are also con-
tained in the variables large_scale_correlated_uncertainty, synopti-
cally_correlated_uncertainty, uncorrelated_uncertainty and adjust-
ment_uncertainty" ;
    short sst_depth_total_uncertainty(time, lat, lon) ;
        sst_depth_total_uncertainty:_FillValue = -32768s ;
        sst_depth_total_uncertainty:long_name = "Total uncertainty in
sea_surface_temperature_depth" ;
        sst_depth_total_uncertainty:units = "kelvin" ;
        sst_depth_total_uncertainty:add_offset = 0.f ;
        sst_depth_total_uncertainty:scale_factor = 0.001f ;
        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" ;
    short l2p_flags(time, lat, lon) ;
        l2p_flags:_FillValue = -32768s ;
        l2p_flags:long_name = "L2P flags" ;
        l2p_flags:valid_min = 0s ;
        l2p_flags:valid_max = 511s ;
        l2p_flags:flag_meanings = "microwave land ice lake river spare
views channels day" ;
        l2p_flags:flag_masks = 1s, 2s, 4s, 8s, 16s, 32s, 64s, 128s, 256s
;
        l2p_flags:comment = "These flags are important to properly use
the data" ;
    byte quality_level(time, lat, lon) ;
        quality_level:_FillValue = 0b ;
        quality_level:long_name = "quality level of SST pixel" ;
        quality_level:valid_min = 0b ;
        quality_level:valid_max = 5b ;
```

```
        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 ;
        quality_level:comment = "These are overall quality indicators and
are used for all GHRSST SSTs" ;
    byte wind_speed(time, lat, lon) ;
        wind_speed:_FillValue = -128b ;
        wind_speed:long_name = "10m wind speed" ;
        wind_speed:standard_name = "wind_speed" ;
        wind_speed:units = "m s-1" ;
        wind_speed:add_offset = 12.7f ;
        wind_speed:scale_factor = 0.1f ;
        wind_speed:valid_min = -127b ;
        wind_speed:valid_max = 127b ;
        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:references = "http://www.esa-sst-cci.org" ;
        wind_speed:source = "ERA_INTERIM-ECMWF-WSP-v1.0" ;
        wind_speed:time_offset = 0.f ;
        wind_speed:height = "10 m" ;
    short large_scale_correlated_uncertainty(time, lat, lon) ;
        large_scale_correlated_uncertainty:_FillValue = -32768s ;
        large_scale_correlated_uncertainty:long_name = "Uncertainty from
errors likely to be correlated over large scales" ;
        large_scale_correlated_uncertainty:units = "kelvin" ;
        large_scale_correlated_uncertainty:add_offset = 0.f ;
        large_scale_correlated_uncertainty:scale_factor = 0.001f ;
        large_scale_correlated_uncertainty:valid_min = 0s ;
        large_scale_correlated_uncertainty:valid_max = 5000s ;
        large_scale_correlated_uncertainty:comment = "Component of uncer-
tainty that is correlated over large scales; can be combined with other
uncertainty estimates to form a total uncertainty" ;
        large_scale_correlated_uncertainty:references = "http://www.esa-
sst-cci.org" ;
    short synoptically_correlated_uncertainty(time, lat, lon) ;
        synoptically_correlated_uncertainty:_FillValue = -32768s ;
        synoptically_correlated_uncertainty:long_name = "Uncertainty from
errors likely to be correlated over synoptic scales" ;
        synoptically_correlated_uncertainty:units = "kelvin" ;
        synoptically_correlated_uncertainty:add_offset = 0.f ;
        synoptically_correlated_uncertainty:scale_factor = 0.001f ;
        synoptically_correlated_uncertainty:valid_min = 0s ;
        synoptically_correlated_uncertainty:valid_max = 5000s ;
        synoptically_correlated_uncertainty:comment = "Component of un-
certainty that is correlated over synoptic scales; can be combined with
other uncertainty estimates to form a total uncertainty" ;
        synoptically_correlated_uncertainty:references = "http://www.esa-
sst-cci.org" ;
        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:long_name = "Uncertainty from errors
likely to be uncorrelated between SSTs" ;
        uncorrelated_uncertainty:units = "kelvin" ;
        uncorrelated_uncertainty:add_offset = 0.f ;
```

```
        uncorrelated_uncertainty:scale_factor = 0.001f ;
        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 es-
timates to form a total uncertainty" ;
        uncorrelated_uncertainty:references     =     "http://www.esa-sst-
cci.org" ;
    short adjustment_uncertainty(time, lat, lon) ;
        adjustment_uncertainty:_FillValue = -32768s ;
        adjustment_uncertainty:long_name = "Time and depth adjustment un-
certainty" ;
        adjustment_uncertainty:units = "kelvin" ;
        adjustment_uncertainty:add_offset = 0.f ;
        adjustment_uncertainty:scale_factor = 0.001f ;
        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 = "http://www.esa-sst-cci.org"
;
        adjustment_uncertainty:correlation_length_scale = "100 km" ;
        adjustment_uncertainty:correlation_time_scale = "1 day" ;
    byte aerosol_dynamic_indicator(time, lat, lon) ;
        aerosol_dynamic_indicator:_FillValue = -128b ;
        aerosol_dynamic_indicator:long_name = "aerosol dynamic indicator"
;
        aerosol_dynamic_indicator:units = "" ;
        aerosol_dynamic_indicator:add_offset = 0.f ;
        aerosol_dynamic_indicator:scale_factor = 0.01f ;
        aerosol_dynamic_indicator:valid_min = -127b ;
        aerosol_dynamic_indicator:valid_max = 127b ;
        aerosol_dynamic_indicator:coordinates = "lon lat" ;
        aerosol_dynamic_indicator:time_offset = 0.f ;
        aerosol_dynamic_indicator:source = "ATSR SDI" ;
        aerosol_dynamic_indicator:comment = "ATSR Saharan Dust Index" ;
        aerosol_dynamic_indicator:references = "Good, E.J., Kong, X., Em-
bury, O., Merchant, C.J., Remedios, J.J. (2012). An infrared desert dust
index for the Along-Track Scanning Radiometers, Remote Sensing of Envi-
ronment, 116(15), DOI:10.1016/j.rse.2010.06.016" ;
    byte sensitivity(time, lat, lon) ;
        sensitivity:_FillValue = -128b ;
        sensitivity:long_name = "Sensitivity to SST" ;
        sensitivity:units = "K/K" ;
        sensitivity:add_offset = 1.f ;
        sensitivity:scale_factor = 0.01f ;
        sensitivity:valid_min = -100b ;
        sensitivity:valid_max = 100b ;
        sensitivity:coordinates = "lon lat" ;
        sensitivity:comment = "Sensitivity of retrieved SST to true
changes in SST" ;

// global attributes:
        :_NCProperties                    =                    "ver-
sion=1|netcdflibversion=4.4.1.1|hdf5libversion=1.10.1" ;
        :Conventions = "CF-1.5, Unidata Observation Dataset v1.0" ;
        :title = "ESA SST CCI ATSR2 L3C product" ;
```

```
        :summary = "ATSR2 L3C product from the ESA SST CCI project, pro-
duced using ARC algorithm." ;
        :references = "http://www.esa-sst-cci.org" ;
        :institution = "ESACCI" ;
        :history = "created with collate_l3.py" ;
        :license = "Creative Commons Licence by attribution
(http://creativecommons.org/licenses/by/4.0/)" ;
        :id = "ATSR2-ESACCI-L3C-CDR-v2.0" ;
        :naming_authority = "org.ghrsst" ;
        :product_version = "2.0" ;
        :uuid = "d932c877-62dd-4093-be3c-3c4cb716911c" ;
        :tracking_id = "d932c877-62dd-4093-be3c-3c4cb716911c" ;
        :gds_version_id = "2.0" ;
        :netcdf_version_id = "4.4.1.1" ;
        :date_created = "20180726T120522Z" ;
        :file_quality_level = 3 ;
        :start_time = "20000102T000000Z" ;
        :time_coverage_start = "20000102T000000Z" ;
        :stop_time = "20000103T000000Z" ;
        :time_coverage_end = "20000103T000000Z" ;
        :time_coverage_duration = "P1DT0H00M00S" ;
        :time_coverage_resolution = "P1DT0H00M00S" ;
        :source = "ATSR2-ESA-L1-v3, ERA_INTERIM-ECMWF-WSP-v1.0" ;
        :platform = "ERS-2" ;
        :sensor = "ATSR" ;
        :Metadata_Conventions = "Unidata Dataset Discovery v1.0" ;
        :metadata_link = "http://www.esa-cci.org" ;
        :keywords = "Oceans > Ocean Temperature > Sea Surface Tempera-
ture" ;
        :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 = 0.05f ;
        :geospatial_lon_units = "degrees_east" ;
        :geospatial_lon_resolution = 0.05f ;
        :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 on
the JASMIN infrastructure at STFC as part of the ESA SST CCI project" ;
        :project = "Climate Change Initiative - European Space Agency" ;
        :publisher_name = "ESACCI" ;
        :publisher_url = "http://www.esa-sst-cci.org" ;
        :publisher_email = "science.leader@esa-SST-cci.org" ;
        :comment = "For information about uncertainty estimates see the
comment attributes to the sea_surface_temperature and
sea_surface_temperature_depth variables" ;
        :northernmost_latitude = 90. ;
        :southernmost_latitude = -90. ;
        :easternmost_longitude = 180. ;
        :westernmost_longitude = -180. ;
        :geospatial_lat_min = -90.f ;
        :geospatial_lat_max = 90.f ;
```

```
        :geospatial_lon_min = -180.f ;
        :geospatial_lon_max = 180.f ;
        :processing_level = "L3C" ;
        :cdm_data_type = "grid" ;
        :source_file  =  "20000102155711-ESACCI-L3U_GHRSST-SSTskin-ATSR2-
CDR2.0-v02.0-fv01.0.nc,  20000102171905-ESACCI-L3U_GHRSST-SSTskin-ATSR2-
CDR2.0-v02.0-fv01.0.nc,  20000102185941-ESACCI-L3U_GHRSST-SSTskin-ATSR2-
CDR2.0-v02.0-fv01.0.nc,  20000102204017-ESACCI-L3U_GHRSST-SSTskin-ATSR2-
CDR2.0-v02.0-fv01.0.nc,  20000102222053-ESACCI-L3U_GHRSST-SSTskin-ATSR2-
CDR2.0-v02.0-fv01.0.nc" ;
        :product_specification_version  =  "SST_CCI-PSD-UKMO-201-Issue-1-
signed" ;
        :spatial_resolution = "0.05 degree" ;
        :creation_date = "2018-07-26T12:05:22Z" ;
}
```

11.4 Header from an L4 file

```
netcdf      \20000111120000-ESACCI-L4_GHRSST-SSTdepth-OSTIA-GLOB_CDR2.0-
v02.0-fv01.0 {
dimensions:
    time = 1 ;
    lat = 3600 ;
    lon = 7200 ;
variables:
    int time(time) ;
        time:long_name = "reference time of sst field" ;
        time:standard_name = "time" ;
        time:axis = "T" ;
        time:units = "seconds since 1981-01-01 00:00:00" ;
        time:comment = "" ;
    float lat(lat) ;
        lat:standard_name = "latitude" ;
        lat:long_name = "latitude" ;
        lat:units = "degrees_north" ;
        lat:valid_min = -90.f ;
        lat:valid_max = 90.f ;
        lat:axis = "Y" ;
        lat:comment  =  "  Latitude  geographical  coordinates,WGS84  projec-
tion" ;
    float lon(lon) ;
        lon:standard_name = "longitude" ;
        lon:long_name = "longitude" ;
        lon:units = "degrees_east" ;
        lon:valid_min = -180.f ;
        lon:valid_max = 180.f ;
        lon:axis = "X" ;
        lon:comment  =  "  Longitude  geographical  coordinates,WGS84  projec-
tion" ;
    short analysed_sst(time, lat, lon) ;
        analysed_sst:long_name = "analysed sea surface temperature" ;
        analysed_sst:standard_name = "sea_water_temperature" ;
        analysed_sst:units = "kelvin" ;
        analysed_sst:coordinates = "lon lat" ;
        analysed_sst:_FillValue = -32768s ;
        analysed_sst:add_offset = 273.15f ;
        analysed_sst:scale_factor = 0.01f ;
        analysed_sst:valid_min = -300s ;
```

```
        analysed_sst:valid_max = 4500s ;
        analysed_sst:source = "ATSR<1,2>-ESACCI-L3U-v2.0, AATSR-ESACCI-L3U-v2.0, AVHRR<06,07,08,09,10,11,12,14,15,16,17,18,19>_G-ESACCI-L2P-v2.0, AVHRRMTA-ESACCI-L2P-v2.0" ;
    short analysis_uncertainty(time, lat, lon) ;
        analysis_uncertainty:long_name = "estimated error standard deviation of analysed_sst" ;
        analysis_uncertainty:standard_name = "sea_water_temperature standard_error" ;
        analysis_uncertainty:units = "kelvin" ;
        analysis_uncertainty:coordinates = "lon lat" ;
        analysis_uncertainty:_FillValue = -32768s ;
        analysis_uncertainty:add_offset = 0.f ;
        analysis_uncertainty:scale_factor = 0.01f ;
        analysis_uncertainty:valid_min = 0s ;
        analysis_uncertainty:valid_max = 32767s ;
    byte sea_ice_fraction(time, lat, lon) ;
        sea_ice_fraction:long_name = "sea ice area fraction" ;
        sea_ice_fraction:standard_name = "sea_ice_area_fraction" ;
        sea_ice_fraction:units = "1" ;
        sea_ice_fraction:coordinates = "lon lat" ;
        sea_ice_fraction:_FillValue = -128b ;
        sea_ice_fraction:add_offset = 0.f ;
        sea_ice_fraction:scale_factor = 0.01f ;
        sea_ice_fraction:valid_min = 0b ;
        sea_ice_fraction:valid_max = 100b ;
        sea_ice_fraction:source = "ESA Sea Ice CCI" ;
        sea_ice_fraction:comment = " Sea ice area fraction" ;
    byte mask(time, lat, lon) ;
        mask:long_name = "land sea ice lake bit mask" ;
        mask:coordinates = "lon lat" ;
        mask:_FillValue = -128b ;
        mask:valid_min = 1b ;
        mask:valid_max = 31b ;
        mask:flag_masks = 1b, 2b, 4b, 8b, 16b ;
        mask:flag_meanings = "water land optional_lake_surface sea_ice optional_river_surface" ;
        mask:source = "NAVOCEANO_landmask_v1.0 EUMETSAT_OSI-SAF_icemask ARCLake_lakemask" ;
        mask:comment = " Land/ open ocean/ sea ice /lake mask" ;

// 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 OSTIA reanalysis sytem v3.0" ;
        :references = "http://www.esa-sst-cci.org" ;
        :institution = "ESACCI" ;
        :history = "Created using OSTIA reanalysis system v3.0" ;
        :comment = "These data were produced at the Met Office as part of the ESA SST CCI project. WARNING Some applications are unable to properly handle signed byte values. If values are encountered > 127, please subtract 256 from this reported value" ;
        :license = "Creative Commons Licence by attribution (https://creativecommons.org/licenses/by/4.0/)" ;
        :id = "OSTIA-ESACCI-L4-GLOB-v2.0" ;
        :naming_authority = "org.ghrsst" ;
        :product_version = "2.0" ;
```

```
        :uuid = "7fdf2639-26e5-4d4f-a60e-0bcfc9744204" ;
        :tracking_id = "7fdf2639-26e5-4d4f-a60e-0bcfc9744204" ;
        :gds_version_id = "2.0" ;
        :netcdf_version_id = "4.2.1.1 of Oct 19 2012 14:25:16" ;
        :date_created = "20180622T003536Z" ;
        :file_quality_level = 3 ;
        :spatial_resolution = "0.05 degree" ;
        :start_time = "20000111T000000Z" ;
        :time_coverage_start = "20000111T000000Z" ;
        :stop_time = "20000112T000000Z" ;
        :time_coverage_end = "20000112T000000Z" ;
        :time_coverage_duration = "P1D" ;
        :time_coverage_resolution = "P1D" ;
        :northernmost_latitude = 90.f ;
        :geospatial_lat_max = 90.f ;
        :southernmost_latitude = -90.f ;
        :gepspatial_lat_min = -90.f ;
        :easternmost_longitude = 180.f ;
        :geospatial_lon_max = 180.f ;
        :westernmost_longitude = -180.f ;
        :geospatial_lon_min = -180.f ;
        :geospatial_vertical_min = -0.2f ;
        :geospatial_vertical_max = -0.2f ;
        :source = "ATSR<1,2>-ESACCI-L3U-v2.0, AATSR-ESACCI-L3U-v2.0,
AVHRR<06,07,08,09,10,11,12,14,15,16,17,18,19>_G-ESACCI-L2P-v2.0,
AVHRRMTA-ESACCI-L2P-v2.0, ESACCI-ICE-v2" ;
        :platform = "ERS-<1,2>, Envisat, NOAA-
<06,07,08,09,10,11,12,14,15,16,17,18,19>, MetOpA" ;
        :sensor = "ATSR, AATSR, AVHRR_GAC" ;
        :Metadata_Conventions = "Unidata Dataset Discovery v1.0" ;
        :metadata_link = "http://www.esa-cci.org" ;
        :keywords = "Oceans > Ocean Temperature > Sea Surface Tempera-
ture" ;
        :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 = 0.05f ;
        :geospatial_lon_units = "degrees_east" ;
        :geospatial_lon_resolution = 0.05f ;
        :acknowledgment = "Funded by ESA" ;
        :creator_name = "SST_cci" ;
        :creator_email = "science.leader@esa-sst-cci.org" ;
        :creator_processing_institution = "These data were produced at
the Met Office as part of the ESA SST CCI project." ;
        :creator_url = "http://www.esa-sst-cci.org" ;
        :project = "Climate Change Initiative - European Space Agency" ;
        :publisher_name = "ESACCI" ;
        :publisher_url = "http://www.esa-sst-cci.org" ;
        :publisher_email = "science.leader@esa-SST-cci.org" ;
        :processing_level = "L4" ;
        :cdm_data_type = "grid" ;
        :product_specification_version = "SST_CCI-PSD-UKMO-201-Issue-H" ;
}
```