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Author(s) :

S. Good, Met Office

N. Rayner, Met Office

T. Block, Brockmann Con-

sult

Chris Merchant, Science Leader, U. of Reading

R. Wilson, Project Manager Space ConneXions Ltd.

Mordet

Accepted:

Checked

Craig Donlon

ESA Technical Officer

Distribution : SST_cci team members

ESA (Craig Donlon)

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



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| 0.11 | | | First complete draft. | | | | |
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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 1991 and continuing to 31 December 2013 (this version of the Product User Guide describes an experimental release, EXP1.2, and includes developments with respect to the previous 'long-term' Version 1 release).
- Data from the series of Along Track Scanning Radiometer (ATSR) sensors (a single orbit per file on a 0.05° regular latitude-longitude grid) and from the series of Advanced Very High Resolution Radiometer (AVHRR) sensors (a single orbit per file on an irregular grid with grid cell spacing about 4 km). These start in August 1991.

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. 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 SST are not available as part of this experimental release of products. However, these are available as part of the Version 1 release (see http://esa-sst-cci.org/). These were obtained by combining orbit data, using optimal interpolation to provide SSTs where there were no measurements (a single file per day; 0.05° regular latitude-longitude grid). These data start in September 1991 and end in December 2010.

During the ESA SST CCI project, use was made of other SST products. Where permission has been granted these are made available with the ESA SST CCI data. A document describing all the data included in this 'climate research data package' (CRDP), including those that are not available from the project webpages, can be found at http://www.esa-sst-cci.org/PUG/documents.htm.

What tools are available for these products?

Tools are provided 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 EXP1.2 data, being an experimental release, are not formally archived. Although intended primarily for internal research and development, they are now available to any interested party, along with the user tool, at http://www.esa-sst-cci.org/PUG/tools.htm. For any queries regarding access or tools, please contact science.leader@esa-SST-cci.org.



Page 3

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 examples of reading the data are given in Section 7. Data arrays in NetCDF files are known as 'variables' and each variable has metadata stored with it. The names of key variables in the long term 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 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_error |
| 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 μ m depth.
- ** 'analysis' is the term used for the combination/interpolation of the SSTs in the orbit files; available only as part of the Version 1 release.
- 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:

- As revealed by the _FillValue attribute, the number inserted into the data array where no SST was available is -32768. Many tools will identify these automatically. It is essential to check for fill values as the quality level in some locations with missing data are incorrectly set to 5.
- 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.
- In the EXP1.2 release, about a third of MetOp-A L2P files contain no data during the period July 2011 to April 2013 (because all values have been masked as cloud). Problems with cloud masking will be addressed in the next reprocessing.



Further information and how to contact us

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

| | CK START GUIDE TO ESA SST CCI PRODUCTS | 3 |
|---|---|----------------------------|
| Wha | at products are available? | 3 |
| Wha | at tools are available for these products? | 3 |
| How | to obtain the data and tools | 3 |
| How | to read the ESA SST CCI data | 4 |
| Furth | her information and how to contact us | 5 |
| 1. D | OOCUMENT PURPOSE AND STRUCTURE | 8 |
| 1.1 | Purpose and scope | 8 |
| 1.2 | Document structure | 8 |
| 2. IN | NTRODUCTION TO THE ESA SST CCI PROJECT | 9 |
| 2.1 | Background | 9 |
| 2.2 | The ESA SST CCI project | 11 |
| 2.3 | The future | 13 |
| 2.3 | | 13 |
| | SETTING STARTED WITH THE ESA SST CCI DATA | |
| | | 14 |
| 3. G | SETTING STARTED WITH THE ESA SST CCI DATA | 14 14 |
| 3. G 3.1 | Which SST product do I need? | 14 14 20 |
| 3. G 3.1 3.2 | Which SST product do I need? How do I get the data? How do I use the ESA SST CCI data? | 14 14 20 |
| 3. G 3.1 3.2 3.3 | Which SST product do I need? How do I get the data? How do I use the ESA SST CCI data? | 14 20 20 23 |
| 3. G 3.1 3.2 3.3 3.4 3.5 | Which SST product do I need? How do I get the data? How do I use the ESA SST CCI data? Contact us | 14 20 20 23 |
| 3. G 3.1 3.2 3.3 3.4 3.5 4. T | Which SST product do I need? How do I get the data? How do I use the ESA SST CCI data? Contact us Frequently asked questions | 14 20 20 23 23 |
| 3. G 3.1 3.2 3.3 3.4 3.5 4. T | Which SST product do I need? How do I get the data? How do I use the ESA SST CCI data? Contact us Frequently asked questions TOOLS THAT CAN BE USED TO WORK WITH THE DATA | 1420232323 |
| 3. G 3.1 3.2 3.3 3.4 3.5 4. T 4.1 4.2 | Which SST product do I need? How do I get the data? How do I use the ESA SST CCI data? Contact us Frequently asked questions TOOLS THAT CAN BE USED TO WORK WITH THE DATA ESA SST CCI tools. | 142023232727 |
| 3. G 3.1 3.2 3.3 3.4 3.5 4. T 4.1 4.2 | Which SST product do I need? How do I get the data? How do I use the ESA SST CCI data? Contact us Frequently asked questions TOOLS THAT CAN BE USED TO WORK WITH THE DATA ESA SST CCI tools. Other tools | 1420232327273133 |



| 5.3 | Analysis - long term product | 38 |
|--|---|----------------|
| 6. U | SING THE DATA FILES | 40 |
| 6.1 | File names | 40 |
| 6.2 | Format of the data files | 41 |
| 6.3 | Tools that can be used to work with the data files | 41 |
| 6.4 | Contents of the data files | 42 |
| 7. W | ORKED EXAMPLES | 54 |
| 7.1 | SNAP | 55 |
| 7.2 | The ESA SST CCI tools | 61 |
| 7.3 | Python | 62 |
| 7.4 | Example of working with the uncertainty information | 70 |
| 8. D | ICTIONARY OF ACRONYMS, ABBREVIATIONS AND JARGON | 73 |
| 9. R | EFERENCES | 75 |
| 10. A | | |
| | PPENDIX 1: SUMMARY OF HOW THE DATA WERE PRODUCED | 79 |
| 10.1 | PPENDIX 1: SUMMARY OF HOW THE DATA WERE PRODUCED Retrieval of SST from satellite measurements | |
| | | 79 |
| 10.2 | Retrieval of SST from satellite measurements | 79 82 |
| 10.2 11. A | Retrieval of SST from satellite measurements Processing of L2 and L3 data to obtain L4 products | 79 82 84 |
| 10.2 11. A 11.1 | Retrieval of SST from satellite measurements Processing of L2 and L3 data to obtain L4 products PPENDIX 2: SAMPLE LISTINGS OF FILE CONTENTS | 79 82 84 |
| 10.2 11. A 11.1 11.2 | Retrieval of SST from satellite measurements Processing of L2 and L3 data to obtain L4 products PPENDIX 2: SAMPLE LISTINGS OF FILE CONTENTS Header from an L2P file | 79 82 84 84 88 |
| 10.2 11. A 11.1 11.2 11.3 | Retrieval of SST from satellite measurements Processing of L2 and L3 data to obtain L4 products PPENDIX 2: SAMPLE LISTINGS OF FILE CONTENTS Header from an L2P file Header from an L3U file | 79 82 84 84 88 |



1. DOCUMENT PURPOSE AND STRUCTURE

1.1 Purpose and scope

This document is the user guide for the data products produced by the ESA SST CCI project in experimental Release 1.2 (EXP1.2). 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 the 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 (note however that the ESA SST CCI project has not used the full swath). 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) views the Earth in the microwave part of the spectrum, allowing it 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).

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) (Figure 1).



Figure 1.The ESA SST CCI project partners.

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 independent of *in situ* observations, 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

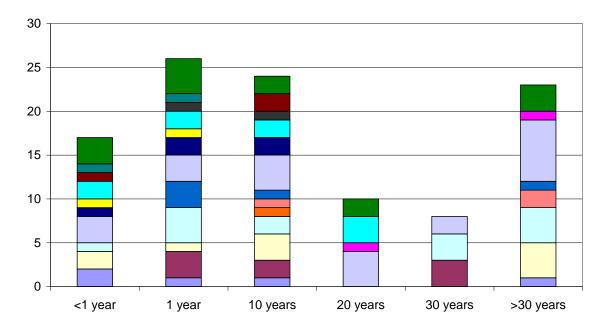
The ESA SST CCI project began in August 2010, the initial phase lasted about three years. Phase 2 started in January 2014. Its scope includes user requirements gathering, algorithm development, algorithm benchmarking, data production and validation, disseminating those data, and obtaining user feedback. 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 Phase 1. 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 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 break their requirements down into 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 people from around the world.





■ Other □ Climate variability Clouds ■ Monitoring of climate ■ Dataset production ■ Detection and attribution of climate change ■ High latitude modelling ■ Decadal forecasting ■ Coastal oceanography ■ Seasonal forecasting □ Ocean biology or chemistry □ Regional modelling ■ Atmospheric reanalysis ■ Climate model evaluation ■ Ocean reanalysis ■ Climate model initialisation

Figure 2. Requirements for temporal coverage of SST data at the point at which the data are usable for an application. The types of applications are given by the colours.

The results were wide ranging and a full description can be found in the ESA SST CCI User Requirements Document with further metrics obtained from the results also available [RD.385; RD.189; available from http://www.esa-sst-cci.org/PUG/documents.htm]. One key result is shown in Figure 2. It shows the requirements that users have for the length of a dataset in order for it to be of any use to them. It demonstrates that the approximately 20 years of ESA SST CCI products are usable for the majority of applications, with types of applications represented by the colours. However, nearly a third of users are looking for datasets covering 30 or more years — highlighting the need to continue to extend the climate-quality satellite record forwards and back in time to lengthen the record.

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 experimental Release 1.2 (EXP1.2) 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 spans mid-1991 through to April 2012 and the end of 2013 respectively. The main objective of these 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

The experimental Release 1.2 (EXP1.2) products produced by the ESA SST CCI project are being made available to users on request. 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]. The intention is to allow the ESA SST CCI algorithms to be implemented operationally, enabling the data to be produced 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 (FAQ) 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 two SST products for experimental Release 1.2 (EXP1.2), each of which consists of sets of data from single satellite instruments (or series of instruments). In brief, the products are:

Stable, low-bias SST data starting during 1991 and continuing through to April 2012 (ATSR) and the end of 2013 (AVHRR) and consisting of:

- data from the ATSR series of sensors (level 2 pre-processed (L2P) data: single orbit of
 data per file on an irregular grid with grid cell spacing about 1 km; and level 3 uncollated
 (L3U) data: a single orbit of data per file on a 0.05° regular latitude-longitude grid see
 Section 3.1.2 for more information about data levels); and
- data from the AVHRR series of sensors (L2P data: single orbit of data per file on an irregular grid with grid cell spacing about 4 km).

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 (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.

[Daily combinations of the orbit data from the Version 1 release in Phase 1, using optimal interpolation to provide SSTs where there were no observations (level 4 (L4) analysis: single file per day on a 0.05° regular latitude-longitude grid) (starts September 1991) are also available (see http://esa-sst-cci.org/), but these have not been recreated from the orbit data from experimental Release 1.2.

These 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.



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. (L3C products are not provided in this release, but an ESA SST CCI tool is available to re-grid the L2P and L3U data as desired. See Section 4.1.)
- 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 3. 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 data are stored on a regular latitude-longitude grid but with large areas unfilled 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.



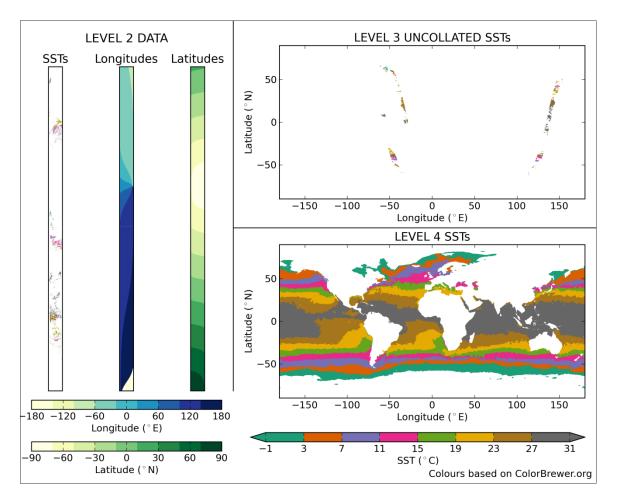


Figure 3. Illustration of how data are stored according to the 'level' of the data, using example ESA SST CCI data from 26 November 2006 from Phase 1. White areas correspond to locations with no SSTs. These occur, for example, due to cloud preventing an SST retrieval or because there was land or ice 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 1. 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 4 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 1, reading down the columns headed A to I yields the list of datasets that fall into those categories.



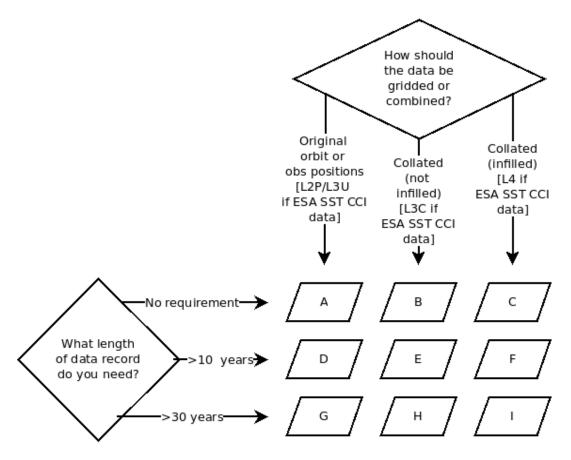


Figure 4. Guide to finding the category of data that you require. Products that meet these requirements are listed in Table 1.

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, there are two avenues to finding further information. First, the footnotes below the table give suggestions on where to go to find out more about it. Second, the ESA SST CCI project has made use of a number of the datasets. Where permission has been granted these have been made available from the same location as the ESA SST CCI data (see Section 3.2). The data are described in the 'climate research data package' (CRDP) documentation [RD.388] which is available at http://www.esa-sst-cci.org/PUG/documents.htm).

Please contact us if any information in Table 1 is inaccurate, or to add a new dataset – see Section 3.4 for contact information.

Table 1. SST data that meet the requirements shown in Figure 4 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 | Туре | Period | More info | Α | В | С | D | Ξ | F | G | Н | I |
|------------------------------------|-----------|---|--------------|---|---|---|---|---|---|---|---|---|
| ICOADS | I | 1800 – present | 1 | Х | Χ | | Χ | Χ | | Х | Х | |
| HadSST3 | I | 1850 – present | 2 | | Χ | | | Χ | | | Х | |
| ERSST v3 | I | 1854 – present | 3 | | | Χ | | | Χ | | | Х |
| Kaplan et al. (1998) | I | 1856 – present | 4 | | | X | | | Х | | | Х |
| HadISST1 | I, S | 1870 – present | 5 | | | Χ | | | Χ | | | Х |
| COBE | I | 1891 – 2008 | 6 | | | Χ | | | Χ | | | Х |
| NOCS daily OI | I | 1973 – 2009 | 7 | | | Х | | | Х | | | Х |
| AVHRR Pathfinder | S (P, IR) | 1981 – 2011 | 8 | | Χ | | | Χ | | | Х | |
| Other AVHRR | S (P, IR) | 1981 – present | 9 | Х | | | Χ | | | Х | | |
| Reynolds et al. daily OI (2007) | I, S | 1981 – present | 10 | | | Х | | | Х | | | Х |
| OSTIA | I, S | 1985 – 2007 (reanalysis; near real time data also available) | 11 | | | Х | | | Х | | | |

¹¹ [RD.239]; http://ghrsst-pp.metoffice.com/pages/latest_analysis/ostia.html; http://www.myocean.eu/



¹ http://icoads.noaa.gov/

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

³ http://www.ncdc.noaa.gov/oa/climate/research/sst/ersstv3.php

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

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

^{6 [}RD.85]

⁷ [RD.99]; http://www.noc.soton.ac.uk/ooc/CLIMATOLOGY/noc2.php

⁸ [RD.205]; http://www.nodc.noaa.gov/SatelliteData/pathfinder4km

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

¹⁰ [RD.76]; http://www.emc.ncep.noaa.gov/research/cmb/sst_analysis/; http://www.ncdc.noaa.gov/oa/climate/research/sst/description.php

| Product | Туре | Period | More info | Α | В | С | D | Е | F | G | Н | 1 |
|--|-------------------|--|--------------|---|---|---|---|---|---|---|---|---|
| ATSR – long term (ESA SST CCI, experimental Re- lease 1.2) | S (P) | 1991 – Apr 2012 | 12 | X | | | X | | | | | |
| AVHRR – long term (ESA SST CCI, experimental Release 1.2) | S (P) | 1991 – 2013 | 13 | X | | | X | | | | | |
| Analysis –long term (ESA SST CCI Version 1 from Phase 1) | S (P) | 1991 – 2010 | 14 | | | X | | | X | | | |
| ATSR series (processed using the 'SADIST' re- trieval method) | S (P, IR) | 1991 – 2012 | 15 | Х | | | Х | | | | | |
| ATSR Reprocessing for Climate (at time of writing, latest version is v1.1.1) | S (P, IR) | 1991 - 2011 | 16 | | X | | | x | | | | |
| TMI | S (O, MW) | 1997 – present | 17 | X | | | Х | | | | | |
| RTG SST | I, S | 2001 – present | 18 | | | Χ | | | Χ | | | |
| AMSR-E | S (P, PMWR) | 2002 – 2011 | 19 | X | | | | | | | | |
| RSS MWOI merged analysis (9 km) | S (P, O, PMWR) | 2002 – present (global cover- age) | 20 | | | х | | | Х | | | |

²⁰ http://www.ssmi.com/sst/microwave_oi_sst_browse.html



¹² See the rest of this document; Table 3 gives a summary of the features of this data product

¹³ See the rest of this document; Table 4 gives a summary of the features of this data product

¹⁴ See the rest of this document; Table 5 gives a summary of the features of this data product

¹⁵http://earth.esa.int/object/index.cfm?fobjectid=4006; http://envisat.esa.int/earth/www/object/index.cfm?fobjectid=3773

¹⁶ [RD.322]; <u>http://badc.nerc.ac.uk/view/neodc.nerc.ac.uk__ATOM__DE_3abf8c96-a7d6-11e0-9cb8-00e081470265</u>

¹⁷ http://trmm.gsfc.nasa.gov/overview_dir/tmi.html

¹⁸ http://polar.ncep.noaa.gov/sst/

¹⁹ http://aqua.nasa.gov/about/instrument_amsr.php

| Product | Туре | Period | More info | Α | В | С | D | Е | F | G | Н | I |
|----------------------------------|--------------------------|----------------|--------------|---|---|---|---|---|---|---|---|---|
| SEVIRI | S (G, IR) | 2005 – present | 21 | Х | | | | | | | | |
| FNMOC 10 km high res analysis | I, S | 2005 – present | 22 | | | Х | | | | | | |
| RAMSSA 9 km | I, S (P, IR, PMWR) | 2008 – present | 23 | | | X | | | | | | |
| ODYSSEA | S (IR, MW, P, G) | 2010 – present | 24 | | Х | Х | | | | | | |

3.2 How do I get the data?

The EXP1.2 data, being an experimental release, are not formally archived. Although intended primarily for internal research and development, they can be made available to any interested parties. Please contact science.leader@esa-SST-cci.org to discuss any interest in access.

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:

20000101000105-ESACCI-L2P_GHRSST-SSTskin-AVHRR15_G-EXP1.2-v02.0-fv1.0.nc

The first part, indicative date, is the date of the data in the form YYYYMMDD (the 1st of January 2000 in the example). The second part, indicative time, is a time within that day in the form

²⁴ http://www.mersea.eu.org/html/information/catalog/products/CERSAT-GLOB-ODYSSEA-SST-NRT-OBS.html



²¹ http://www.eumetsat.int/Home/Main/Satellites/MeteosatSecondGeneration/Instruments/index.htm?l=en; http://www.ghrsst.org

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

²³ [RD.314]; http://www.ghrsst.org

HHMMSS (00 hours, 1 minute and 5 seconds in the example). 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), 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 long term product files is provided in Table 2. The notes below the table highlight some of the key attributes that are attached to the data.

Description of the content of key vari-Names of variables in files Names of variables in files ables in the NetCDF files containing single orbits of containing infilled, comdata bined data Latitudes of the data points Lat lat Longitudes of the data points Lon Ion Sea surface temperature at the skin* sea surface Not applicable temperature Total uncertainty of the sea surface sses standard Not applicable temperature at the skin*# deviation sea_surface_ Sea surface temperature at 20cm analysed_sst** depth and 10.30 am and pm local time temperature depth Total uncertainty of the sea surface sst depth analysis error temperature at 20 cm depth and 10.30 total_uncertainty am and pm local time# mask**** Quality / location type (ocean / sea ice I2p_flags and

Table 2. Summary of the key variables in the NetCDF files.

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

quality_level***

- ** SSTs in the infilled files are combined/interpolated estimates of the daily average SST at 20 cm depth; these have not been updated in experimental Release 1.2
- *** 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:

/ lake etc.) information

- As revealed by the _FillValue attribute, the number inserted into the data array where no SST was available is -32768. Many tools will identify these automatically. It is essential to check for fill values as the quality level in some locations with missing data is incorrectly set to 5.
- 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 7.3.1.

 In the EXP1.2 release, about a third of MetOp-A L2P files contain no data during the period July 2011 to April 2013 (because all values have been masked as cloud). Problems with cloud masking will be addressed in the next reprocessing.

3.3.2 Using the uncertainty estimates

L2P and L3U files contain uncertainties broken down into components from errors that correlate on different spatial and temporal scales:

- 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.

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 7.4.

L4 files (from Phase 1 Version 1) contain a single uncertainty field called analysis_error, 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 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 and L3U files one has been adjusted to a standard time and depth.
- **Don't** forget to use the individual uncertainty components and propagate uncertainty as recommended if averaging the data.
- **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.294].

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.



Page 23

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 form 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 \sim 10 μ m 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/science-and-applications/sst-definitions/.

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 long-term data product provides SSTs covering a 20 year period that are designed to be stable and accurate. The SSTs are retrieved independently of *in situ* measurements and are not blended with *in situ* measurements at level 4 (unlike most satellite and analysis SST datasets). ESA SST CCI products give an independent set of SSTs that can be used to confront the *in situ* record, and 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 long-term product currently starts in during 1991 and terminates in April 2012 (ATSR) and December 2013 (AVHRR), i.e. length is approximately 20 years.

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 long term products for all the data levels is ~2.5 TB). However, it is planned to make data available on a limited selection of coarser grids. Tools will be 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 (from Phase 1) do not have uncertainty correlation scale information embedded.

The best stability and precision are from 1996 onwards, the first ATSR in the series performing less well in these regards than the second and third.

3.5.6.3 Future developments

After the end of Phase 2 of the project (expected to run from 2014-2017), it is planned that the SST algorithms will be applied routinely, with the products extended to present observations after a short delay from the time of satellite observation. A challenge to address will be the lack of an ATSR-class sensor (following the loss of Envisat in 2012) until the Sea and Land Surface Tem-



perature Radiometer (SLSTR) becomes operational. A further challenge will be to extend the ESA SST CCI products back prior to the first ATSR using AVHRRs only, in a way that is consistent and gives good stability. Innovations in retrieval techniques will be required to extend the products with similar quality before 1991 and from 2012 onwards.

In the EXP1.2 release, about a third of MetOp-A L2P files contain no data during the period July 2011 to April 2013 (because all values have been masked as cloud). Problems with cloud masking will be addressed in the next reprocessing.

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.

The journal reference is: Merchant, C. J., Embury, O., Roberts-Jones, J., Fiedler, E., Bulgin, C. E., Corlett, G. K., Good, S., McLaren, A., Rayner, N., Morak-Bozzo, S. and Donlon, C. (2014), Sea surface temperature datasets for climate applications from Phase 1 of the European Space Agency Climate Change Initiative (SST CCI). Geoscience Data Journal, 1: 179–191. doi: 10.1002/gdj3.20



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 courser 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

Visit http://www.esa-sst-cci.org/PUG/tools.htm or 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 downloaded as described in Section 4.1.1, 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 divide 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 uncertainties. 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

uncertainties. The default value is

'./conf/auxdata/x0_space.txt'.

--coverageUncertainty.x0Time <FILE> A txt file that provides lookup table 2/3 for coverage

uncertainties. 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 observations only, dual view, 3 channel retrieval, below aloud agreeing (AD3b) you gould use the

bayes cloud screening (nD3b) you could use the regex 'ATS AVG 3PAARC\\d{8} D nD3b[.]nc[.]qz'.

-h,--help Displays this help.

-I,--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 default 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></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></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></depth> | The SST depth. Must be one of [skin, depth_20, depth_100]. The default value is 'skin'. |
| startDate <date></date> | The start date for the analysis given in the format YYYY-MM-DD. The default value is '1990-01-01'. |
| temporalRes <num></num> | The temporal resolution. Must be one of [daily, weekly7d, weekly5d, monthly, seasonal, annual]. The default value is 'monthly'. |
| totalUncertainty <bool></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'. |

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.

Displays the version of this program and exits.

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]

-v,--version

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 interval 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></dir> | Directory that hosts the products of type 'ARC_L3U'. |
|-------------------------|--|
| -c,config <file></file> | Reads a configuration (key-value pairs) from given FILE. |
| CCI_L2P.dir <dir></dir> | Directory that hosts the products of type 'CCI_L2P'. |
| CCI_L3C.dir <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 'ARC_L3U' type '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 observations only, dual view, 3 channel retrieval, bayes cloud screening (nD3b) you could use the regex 'ATS_AVG_3PAARC\\d{8}_D_nD3b[.]nc[.]gz'.

-h,--help

Displays this help.

-I,--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 table 1. The value 'conf/auxdata/coverage_uncertainty_parameters.nc'.

--lut2File <FILE>

A plain text file that provides lookup table 2. The value '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 region mask in plain text form. The region 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' indicates that the region represented by the cell will be considered in the averaging 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). Network Common data form Description Language (CDL) listings of example output files are given in Appendix 2.

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 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 0 gives some worked examples for how SNAP can be used.



4.2.2 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.

4.2.3 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
 (http://code.google.com/p/netcdf4-python/), numpy (http://www.numpy.org/), matplotlib
 (http://matplotlib.org/) and iris (http://scitools.org.uk/iris/). Refer to Section 7.3 for worked examples.
- IDL (http://www.exelisvis.com/ProductsServices/IDL.aspx).
- Matlab (http://www.mathworks.co.uk/products/matlab/).
- GrADS (http://www.iges.org/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 instrument) used in each of the two ESA SST CCI experimental Release 1.2 (EXP1.2) products and for the Phase 1 Version 1 analyses made by combining data from the different instruments and filling in any gaps.

The format of the table follows the template under development by the GHRSST Climate Data Record Technical Advisory Group described in [RD.317].

A summary of validation statistics are provided below. More details of these can be found in the ESA SST CCI Product Validation and Intercomparison Report [RD.381] and the ESA SST CCI Climate Assessment Report [RD.380], available from http://www.esa-sst-cci.org/PUG/documents.

5.1 ATSR – long term product

Table 3. Information evaluating the ESA SST CCI ATSR EXP1.2 product as a climate record.

| SUMMARY | | | | | | |
|------------------------------------|--|--|--|--|--|--|
| Status of assessment | Dataset producer's information, not yet GHRSST-approved | | | | | |
| Dataset name and version | ESA SST CCI ATSR EXP product version 1.2 | | | | | |
| 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 DESCRIPT | IVE FEATURES | | | | | |
| Period covered | 02-08-1991 to 30-04-2012 | | | | | |
| 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 | Not currently being extended | | | | | |
| Dataset volume | 2.52 TB (L2P) and 640 GB (L3U) | | | | | |
| Valid data fraction | SST from clear-sky observations only, this being ~14% of total data over oceans | | | | | |
| Data level / grid | L2P (1km irregular grid) and L3U (0.05° regular latitude-longitude grid) | | | | | |



| | T | |
|--|--|--|
| Observation technology | The Along-Track Scanning Radiometer (ATSR) series of infrared sensors currently 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 | Skin SST (SST of upper ~10 μm depth). 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 | | |
| Systematic difference Global median difference of satellite minus reference across the full dataset. | 2-channel daytime median difference from drifting buoy reference is: • <-0.05K (2001-2012); • between -0.2K and 0.1K (1991-2000) 3-channel nighttime median difference from drifting buoy reference is: • -0.1K (2001-2012); • -0.15K (1991-2000) | |
| Systematic uncertainty Geographical variation in the difference of satellite minus reference | TBD | |
| Non-systematic uncertainty Uncertainty associated with all effects not included in systematic uncertainty | | |
| Stability 95% confidence interval for the relative multi- year trend between satellite SSTs and the Global Tropical Moored Buoy Array | Daytime (1995-2011) in tropical Pacific: 0.24mK/year < trend < 2.06mK/year Nighttime (1995-2011) in tropical Pacific: 2.62mK/year < trend < 4.64mK/year | |
| Sensitivity to true SST | Approximately 100% | |
| 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 | | |
| AVAILABILITY, DOCUME | NTATION AND FEEDBACK | |
| Data URL / ftp / DOI | http://www.esa-sst-cci.org/ | |
| · | · | |



| Primary peer reviewed reference | Merchant, C. J., O. Embury, N. A. Rayner, D. I. Berry, G. Corlett, K. Lean, K. L. Veal, E. C. Kent, D. Llewellyn-Jones, J. J. Remedios, and R. Saunders (2012), A twenty-year independent record of sea surface temperature for climate from Along Track Scanning Radiometers, J. Geophys. Res., 117, C12013, doi:10.1029/2012JC008400 [RD.296] | |
|---|---|--|
| 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 | Yes – see Merchant, C. J., O. Embury, N. A. Rayner, D. I. Berry, G. Corlett, K. Lean, K. L. Veal, E. C. Kent, D. Llewellyn-Jones, J. J. Remedios, and R. Saunders (2012), A twenty-year independent record of sea surface temperature for climate from Along Track Scanning Radiometers, J. Geophys. Res., 117, C12013, doi:10.1029/2012JC008400 ([RD.296]) and references therein. | |
| 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 – long term product

Table 4. Information evaluating the ESA SST CCI AVHRR Long Term product as a climate record.

| SUMMARY | |
|------------------------------------|---|
| Status of assessment | Dataset producer's information, not yet GHRSST-approved |
| Dataset name and version | ESA SST CCI AVHRR EXP product version 1.2 |
| 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 |
| Principal recommended applications | Climate research particularly applications requiring long-term, stable, low-bias records of SST |



| KEY DESCRIPTIVE FEATURES | |
|--|---|
| Period covered | 16-09-1991 to 31-12-2013 |
| Geographic range | Global |
| | |
| Spatial resolution | 4 km irregular grid |
| Temporal resolution | Twice daily |
| Timeliness of new data | Not currently being extended |
| Dataset volume | 4.3 TB |
| 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) |
| 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) |
| Type(s) of SST | Skin SST (SST of upper ~10 μm depth). 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 |
| QUANTITAT | IVE METRICS |
| Systematic difference Global median difference of satellite minus ref- | 2-channel daytime median difference from drifting buoy reference is: |
| erence across the full dataset. | between -0.2K and -0.35K (2004-2013); |
| | between -0.1K and -0.25K (1995-2003); |
| | • between 0.1K and -0.15K (1991-1994) |
| | 3-channel nighttime median difference from drifting buoy reference is: • -0.15K (2004-2013); • between -0.2K and 0K (1995-2003); • between -0.6K and 0.25K (1991-1994) |
| Systematic uncertainty | 2-channel daytime temporal-mean differences |
| Geographical variation in the difference of satellite minus reference | from drifting buoy reference data are largely (in >50% of geographical locations) between -0.3 |



| Non-systematic uncertainty Uncertainty associated with all effects not included in systematic | and -0.1 K. Differences are more negative (around -0.5 K) than this in the tropical Atlantic, north Indian Ocean and Warm Pool areas. 3-channel night-time temporal-mean differences from drifting buoy reference data are overwhelmingly (in >80% of locations) between -0.3 |
|--|---|
| | and -0.1 K. |
| Stability 95% confidence interval for the relative multi- year trend between satellite SSTs and the Global Tropical Moored Buoy Array | Daytime (1995-2011) in tropical Pacific: - 5.35mK/year < trend < -2.64mK/year Nighttime (1995-2011) in tropical Pacific: - 3.76mK/year < trend < -1.23mK/year |
| Sensitivity to true SST | Approximately 100% |
| 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 | |
| AVAILABILITY, DOCUMEI | NTATION AND FEEDBACK |
| Data URL / ftp / DOI | http://www.esa-sst-cci.org/ |
| Primary peer reviewed reference | Merchant, C. J., Embury, O., Roberts-Jones, J., Fiedler, E., Bulgin, C. E., Corlett, G. K., Good, S., McLaren, A., Rayner, N., Morak-Bozzo, S. and Donlon, C. (2014) "Sea surface temperature datasets for climate applications from Phase 1 of the European Space Agency Climate Change Initiative (SST CCI)." Geoscience Data Journal, 1 (2). pp. 179-191. ISSN 2049-6060 doi: 10.1002/gdj3.20 [RD.386] |
| 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 PRINC | CIPLES (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) SST_CCI-ATBDv2-UOE-001, Issue 1, 17 May 2013.[RD.387] |
| 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 - long term product

Table 5. Information evaluating the ESA SST CCI Analysis Long Term product as a climate record.

| SUMMARY | | |
|------------------------------------|---|--|
| Status of assessment | Dataset producer's information, not yet GHRSST-approved | |
| Dataset name and version | ESA SST CCI Analysis LT product version 1.0 | |
| 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 DESCRIPT | IVE FEATURES | |
| Period covered | 01-09-1991 to 31-12-2010 | |
| 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 400 km – see [RD.294]). | |
| Temporal resolution | Daily | |
| Timeliness of new data | Not currently being extended | |
| Dataset volume | 114 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 reanalysis). 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 | | |



| | T |
|--|--|
| Systematic difference | ~0.05 K, some evidence that analyses are bi- |
| Global median difference of satellite minus reference across the full dataset. | ased towards the day time SST |
| Systematic uncertainty | Robust standard deviation of differences be- |
| Geographical variation in the difference of satellite minus reference | tween analyses and reference is ~0.25 K |
| Non-systematic uncertainty | |
| Uncertainty associated with all effects not included in systematic uncertainty | |
| Stability | For 1991 – 1995: -1.8 < trend < 22.1 (mK year ⁻¹) |
| 95% confidence interval for the relative multi- year trend between satellite SSTs and the Global Tropical Moored Buoy Array | For 1995 – 2010: 0.1 < trend < 3.2 (mK year ⁻¹) |
| Sensitivity to true SST | Variable |
| 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 | |
| AVAILABILITY, DOCUME | NTATION 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 Merchant, C. J., Embury, O., Roberts-Jones, J., |
| | Fiedler, E., Bulgin, C. E., Corlett, G. K., Good, S., McLaren, A., Rayner, N., Morak-Bozzo, S. and Donlon, C. (2014), Sea surface temperature datasets for climate applications from Phase 1 of the European Space Agency Climate Change Initiative (SST CCI). Geoscience Data Journal, 1: 179–191. doi: 10.1002/gdj3.20 |
| 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 PRINC | IPLES (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 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:

20000101000105-ESACCI-L2P_GHRSST-SSTskin-AVHRR15_G-EXP1.2-v02.0-fv1.0.nc

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 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, or L4. See Section 3.1.2 and/or the file contents descriptions for each data level (Sections 6.4.3, 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 $\sim 10 \mu m$, $\sim 1 m m$, 0.2m or $\sim 10 m$). 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 'LT' then the file is a full version release. If this part of the filename is 'EXP', then it is an experimental release. For L4 files, this part of the filename is 'GLOB_LT'. The addition of 'GLOB' prefix denotes that the file contains global data. The additional segregator in the example filename is EXP.

6.1.7 File version

A version number in the form xx.x 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 follow the standards defined by the Climate and Forecasting (CF) conventions [RD.177].

Three 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 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 three 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 6.4.3, L3U in Section 6.4.4 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], 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 6. Most of the contents were adapted from the definitions in the GDS [RD.87].

Table 6. 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 Obsertion 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 <prod string=""> <data level=""></data></prod> | | |
| 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, pro- duced using <algorithm name="">.</algorithm></data></product> | |
| 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 G library v2.1.10 | | |
| comment | Miscellaneous information. | | |



| Name of global attrib- ute | Description | Contents or form of contents | |
|-------------------------------|--|---|--|
| license | How the data are licensed for use. GHRSST protocol describes data use as freand 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-ESAC 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 | |
| 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. | | |
| netcdf_version_id | The version of the NetCDF library used to create the file. | | |
| 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). | | |
| 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. | See date_created for ymmddThhmmssZ, replac- | |
| 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 | | |



| Name of global attribute | Description | Contents or form of contents |
|-------------------------------|---|-----------------------------------|
| 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 cast 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 |
| 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.c | |
| keywords | Standard words that describe the data, taken from the source specified in keywords_vocabulary. Oceans > Ocean Te ture > Sea Surface To perature | |
| keywords_ vocabulary | Defines the source of the text in the keywords attribute; [RD.176]. NASA Global Change ter Directory (GCMD ence Keywords | |
| standard_name_ vocabulary | Defines the source of the standard names for the variables [RD.177]. NetCDF Climate and I cast (CF) Metadata Covention | |
| 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. | |



| Name of global attribute | Description | Contents or form of contents |
|------------------------------------|---|------------------------------------|
| 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 | |
| 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 | |
| geospa- tial_vertical_min | Depth of the deepest SST in the file (the value is negative as the direction is downwards). | |
| geospa- tial_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 product at <institution> as part the ESA SST CCI project partners created the ESA SST CCI project partners created the data file.</institution> | |
| Project | The name of the project. Climate Change Initiative – European Space Agency | |



| Name of global attribute | Description | Contents or form of contents |
|--------------------------|---|--------------------------------|
| 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, 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 7. 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 7. List of attributes that are provided with variables in the NetCDF files.

| Name of variable attrib- ute | 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). | | |
| valid_max | The maximum valid value of the data (before applying scale_factor and add_offset). | | |
| standard_name | A unique descriptive name for the data, taken from the CF conventions ([RD.177]; http://cf-pcmdi.llnl.gov/). Most (but not all va have a correspondi standard name defit the CF conventions) | | |
| comment | Miscellaneous information. Most variables have the attribute. | | |
| source | A list of data sources used for the data in this variable. Geophysical data va | | |
| References | References that provide more information about the data. Applicable to a few variables (see also the gloattribute 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. | |
| 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 contain flags, masks or quality formation. | |
| 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. | |
| Height | Height that wind data corresponds to. Used only for varia containing wind specillary data. | |
| time_offset | Difference between SST reference time and time that wind data correspond to (hours). Used only for variable containing wind speed cillary data. | |
| correlation_ length_scale | Estimated spatial correlation length scale for uncertainties. Only used for some untainty variables. | |
| correlation_ time_scale | Estimated temporal correlation length scale for uncertainties. Only used for some ur tainty variables. | |
| axis | For variables containing coordinates, this indicates the axis that the coordinate corresponds to ('X', 'Y' or 'T' for longitude, latitude or time). | |
| bounds | For coordinate variables, this indicates a variable that contains the bounds of the grid cells. Coordinate variables only indicates a variable variables only indicates. | |

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 8. The data are stored in variables in the NetCDF file with the names given in Table 9.



Table 8. 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 9. 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 8.

| 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. |
| | sst_dtime (timexnjxni) | The time difference of each SST from the base time (see 'time' above). |
| Geophysical variables | sea_surface_ temperature (timexnjxni) | The best available skin SST retrievals with no adjustment to a standard depth or time. |
| | sea_surface_ temperature_depth (timexnjxni) | SSTs adjusted to a standard depth and local time (not available in all products). |
| | wind_speed (timexnjxni) | Wind speed (sourced from the ERA Interim reanalysis). |
| Quality information | quality_level (time×nj×ni) | Only use SSTs for which the value in this variable is 5 and the value in the SST data array is not the fill value (-32768). Other numbers indicate bad quality or missing data. |
| Uncertainty information – | sses_standard_ deviation (timexnjxni) | The total uncertainty in the SSTs in the sea_surface_temperature variable. |
| total uncer- tainty | 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 – | large_scale_correlated_ uncertainty (time×nj×ni) | Component of uncertainty that is correlated over large spatial scales. |
| individual components | synoptically_ correlated_uncertainty (timexnjxni) | Component of uncertainty that is correlated over synoptic (~100 km) spatial scales. |
| | uncorrelated_ uncertainty (timexnjxni) | Component of uncertainty that is uncorrelated between SSTs. |
| | adjustment_uncertainty | Component of uncertainty associated with adjusting |



| Category | Name of data (size of array) | Description | |
|-----------------------|------------------------------|--|--|
| | (time×nj×ni) | SSTs to a standard depth and time; correlated over synoptic (~100 km) spatial scales. | |
| Retrieval information | I2p_flags (timexnjxni) | 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 7 are currently in use. The meanings are: | |
| | | Bit Description Meaning if set to 0 Type of sensor Infrared Microwave Cocan or land Ocean Land Sea ice indicator No sea ice present Lake indicator Not a lake Lake River indicator Not a river River Number of satellite views available Meaning if set to 0 Infrared Microwave Cocan Land No sea ice present Not a lake Lake Not a river River One (na- dir) view views | |
| | | 7 Number of satel- Two Three lite radiance channels avail- able | |
| 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. In the case of the ESA SST CCI data, the grid is a regular latitude longitude grid with 0.05° spacing. The content of L3U files is very similar to L2P files.

The dimensions of the data arrays in the L3U files are defined in Table 10 and the variables found in the files are listed in Table 11.

Table 10. 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. |
| lon | These are the dimensions of the regular latitude-longitude grid on which |
| lat | 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). |
| bnds | Used to define arrays that give the bounds of the latitudes, longitudes and times of the data; always set to 2. |



Table 11. 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 10.

| Category | Name of data (size of array) | Description | | |
|--------------------------------------|---|--|--|--|
| Coordinates | lat (lat) | Central latitude of each grid cell. | | |
| | lat_bnds (bndsxlat) | 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. | | |
| | time_bnds (bnds×time) | The start and end times of the data collection for the data in the file. | | |
| | sst_dtime (timexlatxlon) | The time difference of each SST from the base time (see 'time' above). | | |
| Geophysical variables | sea_surface_ temperature (timexlatxlon) | The best available skin SST retrievals with no adjustment to a standard depth or time. | | |
| | sea_surface_ temperature_depth (timexlatxlon) | SSTs adjusted to a standard depth and local time (not available in all products). | | |
| | wind_speed (timexlatxlon) | Wind speed (sourced from the ERA Interim reanalysis). | | |
| Quality information | quality_level (timexlatxlon) | Only use SSTs for which the value in this variable is 5 and the value in the SST data array is not the fill value (-32768). Other numbers indicate bad quality or missing data. | | |
| Uncertainty information – | sses_standard_ deviation (timexlatxlon) | The total uncertainty in the SSTs in the sea_surface_temperature variable. | | |
| total uncer- tainty | sst_depth_total_ uncertainty (timexlatxlon) | The total uncertainty in the SSTs in the sea_surface_temperature_depth variable (not available in all products). | | |
| Uncertainty information – individual | large_scale_correlated_ uncertainty (timexlatxlon) | Component of uncertainty that is correlated over large spatial scales. | | |
| components | synoptically_ correlated_uncertainty (timexlatxlon) | 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 | Component of uncertainty associated with adjusting SSTs to a standard depth and time; correlated over | | |



| Category | | Name of data (size of array) | Desc | ription | | |
|-----------------------|-----|------------------------------|---|--|-----------------------|---------------------|
| | | (time×lat×lon) | synop | otic (~100 km) spatia | l scales. | |
| Retrieval i formation | in- | I2p_flags (timexlatxlon) | 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 7 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 |
| | | | 3 | Lake indicator | Not a lake | Lake |
| | | | 4 | River indicator | Not a river | River |
| | | | 6 | Number of satel- lite views avail- able | One (na- dir) view | Two (dual) views |
| | | | 7 | Number of satel- lite radiance channels avail- able | Two | Three |
| Other | | sses_bias (timexlatxlon) | data | SA SST CCI data of array (it is filled with files this is used to STs. | h zeros). In d | other GHRSST |

6.4.5 'L4' data format

Level 4 data (from Phase 1, Release 1) 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. In the case of the ESA SST CCI data, the grid is a regular latitude-longitude grid with 0.05° spacing.

The dimensions of the data in an L4 file are described in Table 12 and the variables contained in the files are listed in Table 13.

Table 12. 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 |
| lat | 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). |
| bnds | Used to define arrays that give the bounds of the latitudes, longitudes and times of the data; always set to 2. |



Table 13. 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 12.

| Category | Name of data (size of array) | Description |
|---------------------------|---|---|
| Coordinates | lat (lat) | Central latitude of each grid cell. |
| | lat_bnds (bndsxlat) | 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 (timexlatxlon) | Sea ice concentrations (sourced from OSI-SAF data). |
| Uncertainty information – | analysis_error (time×lat×lon) | Uncertainty in the SSTs (one error standard deviation). |
| total uncer- tainty | sea_ice_fraction_ error (time×lat×lon) | The uncertainty in the sea ice fraction data (one error standard deviation). |
| Location information | mask (timexlatxlon) | 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 on how to obtain and use the data. Three sections are included that demonstrate using the ESA SST CCI data with different tools: SNAP (Section 0), the ESA SST CCI tools (7.2) and Python (7.3). Finally, Section 7.4 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 14.

Table 14. 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 7.3.1. Using the iris Python module to print out a listing of metadata related to a variable is shown in Section 7.3.2. |
| Using the scale_factor and add_offset attributes to unpack data from the NetCDF files | Instructions are given in Section 7.3.1. |
| 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 7.3.2 (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 7.4. |
| 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 7.3.2. 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 7.2.2. An example of how to use L3U uncertainty information is provided in Section 7.4. |
| 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 7.2.1. Python is used to read and plot L4 data in Section 7.3. Use of L4 uncertainty information when averaging is discussed very briefly in Section 7.4. |



| 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 7.3.2. 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 7.3.2. |
| 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 7.4. |
| Regional averaging and time series generation. | Use of the ESA SST CCI tools is recommended – see Section 7.2.2. |
| Working with uncertainties | The ESA SST CCI tools handle uncertainties automatically – see Section 7.2. Propagating uncertainties when averaging data is described in Section 7.4. |

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; a listing of the file contents is then displayed on the left of the screen. 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 5 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 7.3.1 for more information about how to apply these manually).



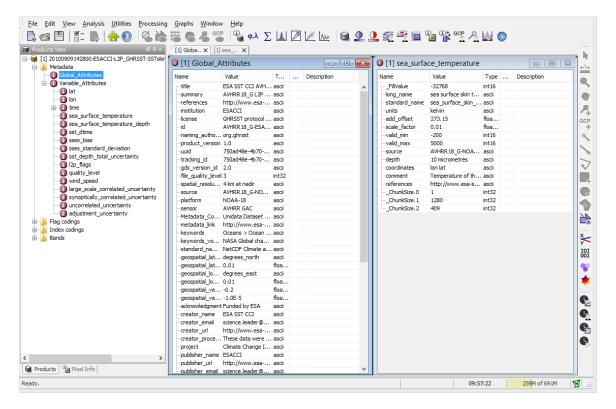


Figure 5. Using SNAP to display metadata about the file and one of the variables stored in the file.

How to display L2P flag metadata and applying this to reveal land and ocean locations is illustrated in Figure 6. The *I2p_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 *I2p_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 7.1.3.

The resulting data are also shown in figure 6. 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).

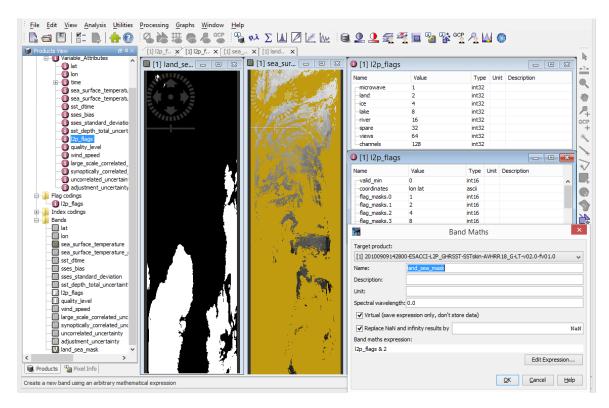


Figure 6. The *I2p_flags* variable attributes and applying the information to show land and ocean locations.

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, 'Create Band by Band Maths' was selected from the Tools 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 7. 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).

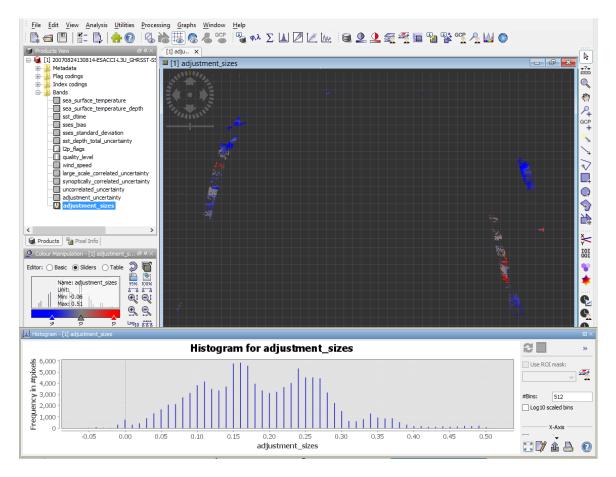


Figure 7. Using VISAT to show the differences between the adjusted and unadjusted SST data in a L3U file. A histogram of the differences is also being displayed

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 8, in which SNAP is being used to display the SST field.



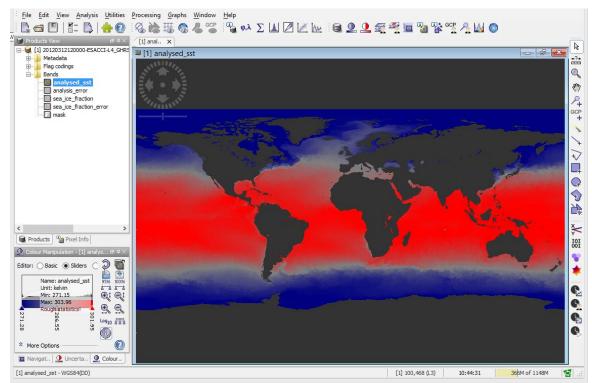


Figure 8. Starting point of the example of filtering with SNAP.

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 'Create Filtered Band' from the Tools 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 9. 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 10.

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 VISAT. This is done by choosing 'Create Band by Band Maths' from the Tools menu. The result is in Figure 11.

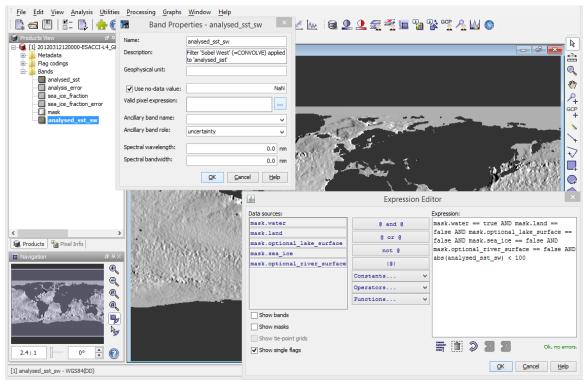


Figure 9. Using the mask to remove data affected by ice etc.

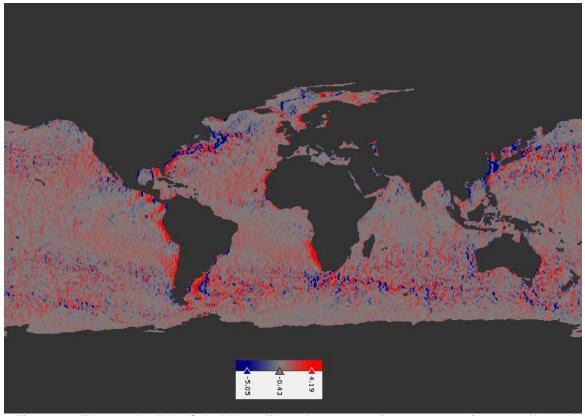


Figure 10. The result of the Sobel West filter after processing to remove ice etc. affected locations.



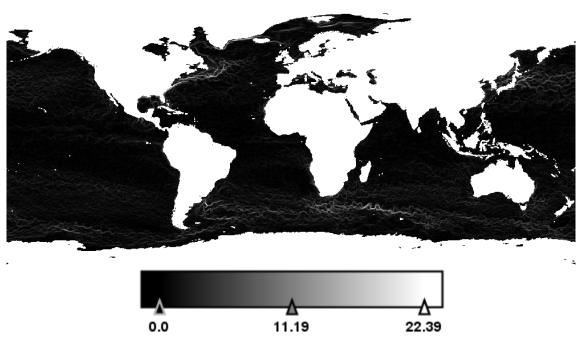


Figure 11. The combined Sobel North and West filters showing regions with high local horizontal gradients.

7.2 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.

7.2.1 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_I4.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_error. 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. A listing of the header of the NetCDF file can be found in the appendix.

7.2.2 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

7.3 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. As some modules we discuss do not yet work with version 3 of Python, 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.

7.3.1 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 12.

```
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'
IonData
          = ncid.variables[var][:]
lonLongName = ncid.variables[var].long_name
```



SST-CCI-Phase-II SST CCI Product User Guide

```
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'
sealceFractionData
                     = ncid.variables[var][0, :, :]
sealceFractionLongName = ncid.variables[var].long_name
ax = plt.subplot(2, 2, 4)
sealcePlot = ax.imshow(sealceFractionData, vmin=0, vmax=1, origin='lower')
ax.set_title('Sea ice fraction data array')
cb = plt.colorbar(sealcePlot, orientation='horizontal')
cb.set_label(sealceFractionLongName)
ncid.close() # Close the NetCDF file.
plt.show() # Show our completed plot.
```



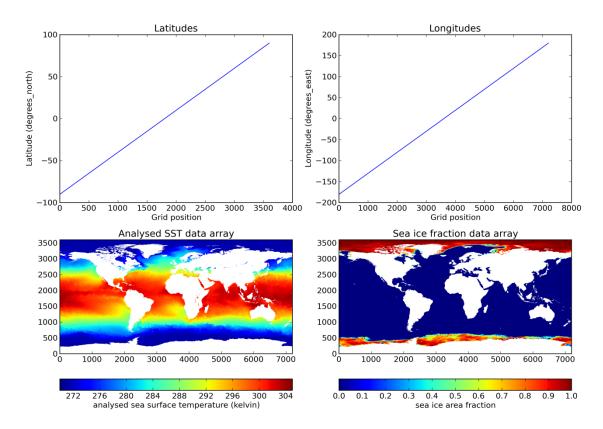


Figure 12. Result of applying the Python code to read and visualise the data.

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.

7.3.2 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 7.3.1 above. The result of running this code is shown in Figure 13.

```
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()
```



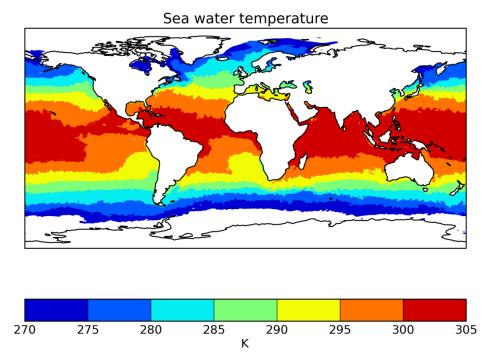


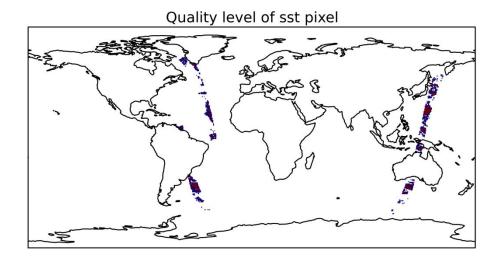
Figure 13. Result of using the iris module to read and plot the analysed SST data.

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 12 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 and L3U data, it is desirable to check the flags and quality level information. Use of the I2p_flags variable was demonstrated in Section Error! Reference source not found. 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. This contains either 0 (no data) or 5 (excellent quality). A plot of this variable from an example Phase 1 Release 1 L3U file is shown in Figure 14, with the code used given below.



import iris



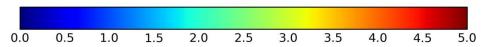


Figure 14. Quick plot of the quality_level variable from a L3U file. Only values of 0 (blue) and 5 (red) are used in the ESA SST CCI files.

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 - 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, produced 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 webpages at http://scitools.org.uk/iris/docs/latest/ index.html for the latest information.

7.4 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. This component is estimated by the ESA SST CCI tools (see Sections 4.1 and 7.2), but is not discussed further here.

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 and L3U 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.



Page 70

Mathematically, this is represented by: $\frac{\sqrt{\sum\limits_{i=1}^{n}\sigma_{i}^{2}}}{n}$ 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
$$\sqrt{\frac{1}{\eta} \frac{\displaystyle \sum_{i=1}^{n} \sigma_{i}^{2}}{n}}$$
 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.

 $\frac{\displaystyle\sum_{i=1}^n \sigma_i}{n}$ The operation can be summarised as $\frac{\displaystyle\sum_{i=1}^n \sigma_i}{n}$ 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

| ltem | 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 grid- ded historical surface temperature anomalies version 4. |
| HadSST2 and HadSST3 | The Met Office Hadley Centre dataset of gridded <i>in situ</i> 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 observa- tions | 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 |
| 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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| RD.189 | CCI Phase 1 (SST): Technical note on product metrics derived from the user requirements document. |



| RD.205 | Kilpatrick, K. A., et al. (2001), Overview of the NOAA/NASA advanced very high resolution radiometer Pathfinder algorithm for sea surface temperature and associated matchup database, Journal of Geophysical Research-Oceans, 106(C5), 9179-9197. |
|--------|--|
| RD.210 | Kennedy J.J., Rayner, N.A., Smith, R.O., Saunby, M. and Parker, D.E. (2011). Reassessing biases and other uncertainties in sea-surface temperature observations since 1850 part 1: measurement and sampling errors. J. Geophys. Res., 116, D14103, doi:10.1029/2010JD015218. |
| RD.211 | Kennedy J.J., Rayner, N.A., Smith, R.O., Saunby, M. and Parker, D.E. (2011). Reassessing biases and other uncertainties in sea-surface temperature observations since 1850 part 2: biases and homogenisation. J. Geophys. Res., 116, D14104, doi:10.1029/2010JD015220. |
| RD.213 | Donlon, C. J., et al. (2012), The Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA) system, Remote Sensing of Environment, 116, 140-158. |
| RD.216 | Casey, K.S., T.B. Brandon, P. Cornillon, and R. Evans (2010). "The Past, Present and Future of the AVHRR Pathfinder SST Program", in Oceanography from Space: Revisited, eds. V. Barale, J.F.R. Gower, and L. Alberotanza, Springer. DOI: 10.1007/978-90-481-8681-5_16. |
| RD.218 | SST_CCI Round Robin Protocol, SST_CCI-RRP-UoL-001 |
| RD.226 | MacCallum and Merchant (2012), ESA SST CCI Algorithm Selection Report, http://www.esa-sst-cci.org/. |
| RD.227 | Fairall, C., E. Bradley, J. Godfrey, G. Wick, J. Edson, and G. Young (1996), Cool-skin and warm-layer effects on sea surface temperature, J. Geophys. Res., 101(C1), 1295-1308. |
| RD.239 | 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.246 | O'Carroll, A.G., J.R. Eyre and R.W. Saunders, 2008: Three-way error analysis between AATSR, AMSR-E, and in situ sea surface temperature observations, J. Atmos. Ocean. Tech., 25, 1197-1207, doi: 10.1175/2007JTECHO542.1 |
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| RD.259 | SST_CCI System Specification Document, SST_CCI-SSD-BC-001 |
| RD.263 | Kantha L.H., and Clayson C.A., An improved mixed layer model for geophysical applications. J. Geophys. Res. Vol. 99 (C12), 25235-25266, 1994. |
| RD.294 | Jonah Roberts-Jones, Emma Fiedler, Matthew Martin, Alison McLaren, Improvements to the Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA) system, UKMO Tech Document. SST_CCI_TN_UKMO_002 |



| RD.296 | Merchant, C. J., O. Embury, N. A. Rayner, D. I. Berry, G. Corlett, K. Lean, K. L. Veal, E. C. Kent, D. Llewellyn-Jones, J. J. Remedios, and R. Saunders (2012), A twenty-year independent record of sea surface temperature for climate from Along Track Scanning Radiometers, J. Geophys. Res., 117, C12013, doi:10.1029/2012JC008400. |
|--------|---|
| RD.310 | Thomas S M, Heidinger, A K, Pavolonis M J, Comparison of NOAA's Operational AVHRR-Derived Cloud Amount to Other Satellite-Derived Cloud Climatologies, Journal of Climate, American Meteorological Society, Volume 17, pages 4805-4822, 2004 |
| RD.311 | Heidinger A. K., Evan A. T., Foster, M. J. and Walther, A. A Naïve Bayesian Cloud-Detection Scheme Derived from CALIPSO and Applied within PATMOS-x, Journal of Applied Meteorology and Climatology, Volume 51, Pages 1129-1144, 2012. |
| RD.313 | Morice, C. P., J. J. Kennedy, N. A. Rayner, and P. D. Jones (2012), Quantifying uncertainties in global and regional temperature change using an ensemble of observational estimates: The HadCRUT4 dataset, J. Geophys. Res., 117, D08101, doi:10.1029/2011JD017187. |
| RD.314 | Beggs, H. (2007), A high-resolution blended sea surface temperature analysis over the Australian region, BMRC Research Report No. 130, Bureau of Meteorology Research Centre, Australia. |
| RD.315 | Compo, G. P., Whitaker, J. S., Sardeshmukh, P. D., Matsui, N., Allan, R. J., Yin, X., Gleason, B. E., Vose, R. S., Rutledge, G., Bessemoulin, P., Brönnimann, S., Brunet, M., Crouthamel, R. I., Grant, A. N., Groisman, P. Y., Jones, P. D., Kruk, M., Kruger, A. C., Marshall, G. J., Maugeri, M., Mok, H. Y., Nordli, Ø., Ross, T. F., Trigo, R. M., Wang, X. L., Woodruff, S. D., and Worley, S. J. (2011), The Twentieth Century Reanalysis Project. Quarterly J. Roy. Meteorol. Soc., 137, 1-28. DOI: 10.1002/qj.776. |
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| RD.317 | Merchant, C. J., Mittaz, J. and Corlett, G. K. (2013), Climate data evaluation framework, GHRSST document reference CDR-TAG_CDEF/Version 1.0. |
| RD.322 | Embury, O; Merchant, C; ARC (AATSR Reprocessing for Climate) data; 2011; NERC Earth Observation Data Centre; available from http://badc.nerc.ac.uk/view/neodc.nerc.ac.uk ATOM DE 3abf8c96-a7d6-11e0-9cb8-00e081470265. |
| RD.323 | Hunter, J. D. (2007), Matplotlib: A 2D graphics environment, Computing In Science & Engineering, 9, 3, 90-95, IEEE COMPUTER SOC |
| RD.324 | Met Office (2010-2013), Iris: A Python library for analysing and visualising meteorological and oceanographic data sets, v1.3, http://scitools.org.uk/ |
| RD.372 | Bulgin, C.E., Merchant, C.J. and Donlon, C. (2-15). Sampling uncertainty in global area coverage (GAC) and gridded sea surface temperature retrievals. Remote Sensing of Environment. |



| RD.375 | SST_cci Phase II MMS Implementation Plan v1-u2 |
|--------|--|
| RD.376 | SST_CCI Phase II Multi-sensor Match-up Dataset Specification, SST_CCI-TN-UoL-201 |
| RD.380 | ESA SST_CCI Phase II Climate Assessment Report (CAR), SST_CCI-CAR-UKMO-201 |
| RD.381 | ESA SST_CCI Phase II Product Validation and Intercomparison Report (PVIR), SST_CCI-PVIR-UOL-201 |
| RD.383 | SST_CCI Phase II Product Specification Document (PSD), SST_CCI-PSD-UKMO-201 |
| RD.385 | SST_CCI Phase II User Requirements Document (URD), SST_CCI-URD-UKMO-201 |
| RD.386 | Merchant, C. J., Embury, O., Roberts-Jones, J., Fiedler, E., Bulgin, C. E., Corlett, G. K., Good, S., McLaren, A., Rayner, N., Morak-Bozzo, S. and Donlon, C. (2014) Sea surface temperature datasets for climate applications from Phase 1 of the European Space Agency Climate Change Initiative (SST CCI). Geoscience Data Journal, 1 (2). pp. 179-191. ISSN 2049-6060 doi: 10.1002/gdj3.20 |
| RD.387 | CCI-SST Algorithm Theoretical Basis Document (ATBD) SST_CCI-ATBDv2-UOE-001, Issue 1, 17 May 2013. |
| RD.388 | CCI-SST Climate Research Data Pack (CRDP) SST_CCI-CRDP-UKMO-001, Issue 1, 30 September 2013. |



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

This appendix summarises the algorithms used within the ESA SST CCI project; detailed in the Algorithm Theoretical Basis Document (ATBD; [RD.387]). References for external algorithms are given in the relevant sections.

10.1 Retrieval of SST from satellite measurements

Within 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.387.

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 15. 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.

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.181; RD.387].

The Bayesian scheme simulates brightness temperatures under clear sky conditions using a fast radiative transfer model with inputs from numerical weather predication data. Cloudy sky probabilities are represented using probability density functions and this background information is used in conjunction with the observations and their relative errors to calculate a probability of clear sky. For AVHRR, the CLAVR-x naive Bayesian method is used [RD.310; RD.311]. This combines six cloud classifiers to give a probability of clear-sky which is then used to classify a pixel as clear, partially clear, cloud or partial cloud. For AVHRR cloud detection at high latitudes uses an additional Bayesian calculation which further classifies each location as ocean, cloud or ice.

In the EXP1.2 release, about a third of MetOp-A L2P files contain no data during the period July 2011 to April 2013 (because all values have been masked as cloud). Problems with cloud masking will be addressed in the next reprocessing.

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.



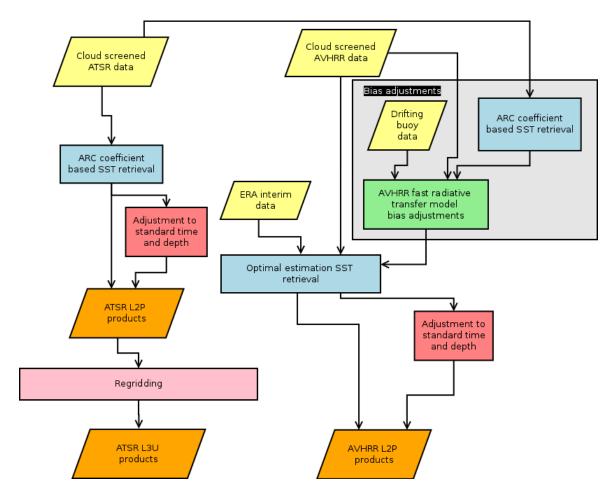


Figure 15. Overview of the processing of ATSR- and AVHRR-series data to produce the output data files for the long term ESA SST CCI products. ATSR SSTs are retrieved using a coefficient based approach; AVHRR series SSTs are retrieved using optimal estimation. The optimal estimation approach requires 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' 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]. 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 fast radiative transfer model outputs.

A bias correction for the fast radiative transfer model is calculated using the results of the coefficient based retrievals applied to ATSR-2 and AATSR data, which can be viewed as unbiased. The approach conveniently also compensates for any sensor calibration drift. The radiative transfer model is used to simulate the signal at the satellite given atmospheric profiles taken from reanalysis data and the SST calculated from the coefficient based retrieval. The difference between the simulated signal and that provided by the sensor gives an estimate of the bias. This is calculated for different times, locations and varying atmospheric conditions.

For the ATSR series of sensors, biases are parameterised in an equation that includes components for the drift in calibration over time and errors in the radiative transfer calculation. Coefficients that define the relative size of these components are obtained by regression against the bias estimates. For AVHRR data, a similar approach is taken but the calibration drift is replaced by a term that is related to the sensor temperature.

The ATSR SSTs that are required to simulate the signal received by the AVHRR sensor are not available at the same time and location as the AVHRR measurements. Drifting buoy data are used to estimate the change in SST between the times of the two satellite overpasses and adjust the ATSR SSTs accordingly. This method ties the AVHRR data to the ATSRs data, resulting in a data product that has the accuracy of the ATSRs and the coverage of the AVHRRs.

Within the ESA SST CCI processing, coefficient based retrievals are used for two purposes. First, they are used to retrieve SSTs from ATSR data. After an algorithm selection competition in Phase 1, the optimal estimation method was chosen in preference to the coefficient based and other methods to calculate SSTs for AVHRR data; optimal estimation was also used in Phase 1 to retrieve SST for ATSR-2 and AATSR data, but is not in experimental Release 1.2 (EXP1.2) products as it provides no added benefit. The optimal estimation approach used has been updated for EXP1.2 products to reduce the impact of instrument (radiometric) noise (see ATBD, RD.387 for details).

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 corre-



lated between 0.05° grid cells. This uncertainty component is new for experimental Release 1.2 products and 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 the temperature at approximately 10µm 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 10.30 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 10.30 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

For ATSR data 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.

10.2 Processing of L2 and L3 data to obtain L4 products

10.2.1 OSTIA processing system

An implementation of the Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA) processing system was used in Phase 1 to create L4 data products from the L2 and L3 SSTs. It is described in [RD.239 and RD.294]. In brief, the analysis system uses an iterative method to solve the optimal interpolation equations. 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 L4 products have not been updated in experimental Release 1.2.

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 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 second order autoregressive functions. The two



length scales were re-estimated for the ESA SST CCI project. The new length scales are anisotropic and vary with latitude. Background error variances were improved to be seasonally variable.

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 all 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 \20000101000105-ESACCI-L2P GHRSST-SSTskin-AVHRR15 G-EXP1.2-v02.0-fv1.0 {
dimensions:
    ni = 409
    nj = 13380;
    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 projection";
    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 projection";
    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 temperature";
         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_uncertainty^2+uncorrelated_u
ncertainty^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 temperature 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 uncertainty^2+uncorrelated u
ncertainty^2+adjustment uncertainty^2)";
         sea surface temperature depth:references = "http://www.esa-sst-cci.org";
         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";
    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 contained in the
variables large_scale_correlated_uncertainty, synoptically_correlated_uncertainty,
uncorrelated uncertainty and adjustment 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 I2p flags(time, nj, ni);
         l2p_flags:_FillValue = -32768s;
         l2p_flags:long_name = "L2P flags" ;
         l2p_flags:valid_min = 0s ;
         I2p_flags:valid_max = 255s ;
         I2p flags:flag meanings = "microwave land ice lake river spare views channels";
         I2p_flags:flag_masks = 1s, 2s, 4s, 8s, 16s, 32s, 64s, 128s;
         12p_flags:comment = "These flags are important to properly use the data";
         I2p flags:coordinates = "Ion 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.";
         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 uncertainty 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 uncertainty 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 unlikely to be correlated
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 estimates 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 uncertainty";
         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";
// 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 v2.1.10";
         :license = "GHRSST protocol describes data use as free and open";
         :id = "AVHRR15 G-ESACCI-L2P-EXP-v1.2";
         :naming_authority = "org.ghrsst";
         :product_version = "1.2";
         :uuid = "bb36812c-f02a-11e4-8721-8b949b596394";
         :tracking id = "bb36812c-f02a-11e4-8721-8b949b596394";
         :gds version_id = "2.0";
         :netcdf_version_id = "4.3.2 of Jul 22 2014 16:21:31";
         :date_created = "20150501T185144+0100";
         :file_quality_level = 3;
         :spatial_resolution = "4 km at nadir";
         :start_time = "20000101T000105Z";
```



```
:time_coverage_start = "20000101T000105Z";
         :stop_time = "20000101T015234Z";
         :time_coverage_end = "20000101T015234Z"
         :time_coverage_duration = "P0DT01H51M29S";
         :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 Temperature";
         :keywords_vocabulary = "NASA Global change Master Directory (GCMD) Science
Keywords";
         :standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata
Convention";
         :geospatial_lat_units = "degrees_north";
         :geospatial_lat_resolution = 0.01f;
         :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 max = 90.f;
         :geospatial lat min = -90.f;
         : geospatial lon max = -180.f:
         :geospatial_lon_min = 180.f;
         :processing level = "L2P";
         :cdm_data_type = "swath" :
         :source_file = "20000101000100-ESACCI-L1C-AVHRR15_G-fv01.0.nc";
}
```

11.2 Header from an L3U file

 $\label{eq:control_control_control_control} \begin{subarray}{l} netcdf $$ \20000102155711-ESACCI-L3U_GHRSST-SSTskin-ATSR2-EXP1.2-v02.0-fv1.0 \{ dimensions: \\ lat = $3600 ; \\ lon = 7200 ; \\ time = UNLIMITED ; // (1 currently) \\ bnds = 2 ; \\ variables: \\ float lat(lat) ; \end{subarray}$



```
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 projection";
         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 projection";
    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 projection";
         Ion: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 projection" ;
    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 temperature";
         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_uncertainty^2+uncorrelated_u
ncertainty^2)";
         sea surface temperature:references = "http://www.esa-sst-cci.org";
```



```
sea surface temperature:source = "ATSR2-ESA-L1-v2.1";
         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 temperature 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_uncertainty^2+uncorrelated_u
ncertainty^2+adjustment_uncertainty^2)";
         sea_surface_temperature_depth:references = "http://www.esa-sst-cci.org";
         sea_surface_temperature_depth:source = "ATSR2-ESA-L1-v2.1";
         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";
    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 contained in the
variables large_scale_correlated_uncertainty, synoptically_correlated_uncertainty,
uncorrelated uncertainty and adjustment 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 I2p_flags(time, lat, lon);
         I2p_flags:_FillValue = -32768s;
         l2p_flags:long_name = "L2P flags" ;
         I2p_flags:valid_min = 0s ;
         I2p_flags:valid_max = 255s ;
         l2p_flags:flag_meanings = "microwave land ice lake river spare views channels";
         12p flags:flag masks = 1s, 2s, 4s, 8s, 16s, 32s, 64s, 128s;
         12p_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.";
         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 uncertainty 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 uncertainty 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 unlikely to be correlated
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 estimates 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 uncertainty";
         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";
// 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, produced using ARC
algorithm.";
         :references = "http://www.esa-sst-cci.org";
         :institution = "ESACCI";
         :history = "Created using GBCS library v2.1.10";
         :license = "GHRSST protocol describes data use as free and open";
         :id = "ATSR2-ESACCI-L3U-EXP-v1.2";
         :naming_authority = "org.ghrsst";
         :product_version = "1.2";
         :uuid = "d6558c96-f05c-11e4-8d1b-f7fc9e8270fa";
         :tracking_id = "d6558c96-f05c-11e4-8d1b-f7fc9e8270fa";
         :gds version id = "2.0";
         :netcdf_version_id = "4.3.2 of Jul 22 2014 16:21:31";
         :date_created = "20150502T005025+0100";
         :file quality level = 3;
         :spatial resolution = "1 km at nadir";
         :start_time = "20000102T155711Z";
         :time_coverage_start = "20000102T155711Z";
         :stop_time = "20000102T171906Z";
         :time_coverage_end = "20000102T171906Z";
         :time_coverage_duration = "P0DT01H21M55S";
         :time coverage resolution = "P0DT1H40M00S";
```



```
:source = "ATSR2-ESA-L1-v2.1, 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 Temperature";
         :keywords_vocabulary = "NASA Global change Master Directory (GCMD) Science
Keywords":
         :standard name vocabulary = "NetCDF Climate and Forecast (CF) Metadata
Convention":
         :geospatial_lat_units = "degrees_north";
         :geospatial lat resolution = 0.05f;
         :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_max = 90.f;
         :geospatial_lat_min = -90.f;
         :geospatial_lon_max = -180.f;
         :geospatial lon min = 180.f;
         :processing_level = "L3U";
         :cdm data type = "grid";
         :source file =
"AT2_TOA_1PURAL20000102_155711_000000001049_00182_24585_0000.E2";
```

11.3 Header from an L4 file from Phase 1 Release 1.0

```
netcdf \20000101120000-ESACCI-L4_GHRSST-SSTdepth-OSTIA-GLOB_LT-v02.0-fv01.0 {
    dimensions:
        time = UNLIMITED ; // (1 currently)
        bnds = 2 ;
        lat = 3600 ;
        lon = 7200 ;
    variables:
        float time_bnds(time, bnds) ;
            time_bnds:comment = "Contains the start and end times for the time period the data
represent" ;
        time_bnds:long_name = "Time cell boundaries" ;
        time bnds:units = "seconds since 1981-01-01 00:00:00";
```



```
int time(time);
         time:units = "seconds since 1981-01-01 00:00:00";
         time:standard name = "time";
         time:axis = "T";
         time:calendar = "gregorian";
         time:bounds = "time_bnds";
         time:comment = "";
         time:long_name = "reference time of sst file";
    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:reference_datum = "geographical coordinates, WGS84 projection";
         lat:bounds = "lat_bnds";
         lat:comment = ""
    float lat bnds(lat, bnds);
         lat bnds:units = "degrees north";
         lat_bnds:long_name = "Latitude cell boundaries" ;
         lat_bnds:valid_min = -90.f;
         lat bnds:valid max = 90.f;
         lat_bnds:reference_datum = "geographical coordinates, WGS84 projection" ;
         lat_bnds:comment = "Contains the northern and southern boundaries of the grid cells.";
    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:reference_datum = "geographical coordinates, WGS84 projection" ;
         lon:bounds = "lon_bnds" ;
         lon:comment = "";
    float lon bnds(lon, bnds);
         lon_bnds:units = "degrees_east" ;
         lon bnds:long name = "Longitude cell boundaries";
         lon bnds:valid min = -180.f;
         lon bnds:valid max = 180.f;
         lon_bnds:reference_datum = "geographical coordinates, WGS84 projection";
         lon bnds:comment = "Contains the eastern and western boundaries of the grid cells.";
    short analysed_sst(time, lat, lon);
         analysed_sst:_FillValue = -32768s;
         analysed_sst:units = "kelvin";
         analysed_sst:scale_factor = 0.01f;
         analysed_sst:add_offset = 273.15f;
         analysed_sst:long_name = "analysed sea surface temperature" ;
         analysed_sst:valid_min = -300s;
         analysed sst:valid max = 4500s;
         analysed sst:standard name = "sea water temperature";
         analysed_sst:depth = "20 cm";
         analysed_sst:source = "ATSR<1,2>-ESACCI-L3U-v1.0, AATSR-ESACCI-L3U-v1.0,
AVHRR<12,14,15,16,17,18>_G-ESACCI-L2P-v1.0, AVHRRMTA-ESACCI-L2P-v1.0";
         analysed_sst:comment = "SST analysis produced for ESA SST CCI project using the
OSTIA system in reanalysis mode.";
    short analysis error(time, lat, lon);
```



```
analysis error: FillValue = -32768s:
         analysis_error:units = "kelvin";
         analysis error:scale factor = 0.01f;
         analysis_error:add_offset = 0.f;
         analysis_error:long_name = "estimated error standard deviation of analysed_sst";
         analysis_error:valid_min = 0s;
         analysis_error:valid_max = 32767s;
         analysis_error:comment = "SST analysis standard error produced for ESA SST CCI
project using the OSTIA system in reanalysis mode.";
         analysis_error:standard_name = "sea_water_temperature standard_error";
    byte sea_ice_fraction(time, lat, lon);
         sea ice fraction: FillValue = -128b;
         sea_ice_fraction:units = "1";
         sea_ice_fraction:scale_factor = 0.01f;
         sea_ice_fraction:add_offset = 0.f;
         sea_ice_fraction:long_name = "sea ice area fraction" ;
         sea_ice_fraction:valid_min = 0b;
         sea ice fraction:valid max = 100b;
         sea ice fraction:standard name = "sea ice area fraction";
         sea_ice_fraction:source = "EUMETSAT_OSI-SAF-ICE-v1.1, EUMETSAT_OSI-SAF-
ICE-v2.2";
         sea_ice_fraction:comment = "Sea ice fraction field regridded from EUMETSAT OSI-SAF
product.";
    byte sea_ice_fraction_error(time, lat, lon);
         sea_ice_fraction_error:_FillValue = -128b;
         sea_ice_fraction_error:units = "1";
         sea_ice_fraction_error:scale_factor = 0.01f ;
         sea_ice_fraction_error:add_offset = 0.f;
         sea_ice_fraction_error:long_name = "sea ice area fraction error estimate";
         sea ice fraction error:valid min = 0b;
         sea_ice_fraction_error:valid_max = 100b;
         sea_ice_fraction_error:source = "EUMETSAT_OSI-SAF-ICE-v1.1";
         sea_ice_fraction_error:comment = "Estimated error standard deviation of sea ice
fraction";
         sea_ice_fraction_error:standard_name = "sea_ice_area_fraction standard_error";
    byte mask(time, lat, lon);
         mask: FillValue = -128b;
         mask:long name = "sea/land/lake/ice field composite mask";
         mask:valid min = 1b;
         mask:valid max = 31b;
         mask: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 = "b0: 1=grid cell is open sea water, b1: 1=grid cell is land, b2: 1=grid
cell is lake surface, b3: 1=grid cell is sea ice, b4-b7: reserved for future grid mask data";
// global attributes:
         :title = "ESA SST CCI OSTIA L4 product";
         :summary = "OSTIA L4 product from the ESA SST CCI project, produced using OSTIA
reanalysis system v2.0";
         :references = "http://www.esa-sst-cci.org";
         :institution = "ESACCI";
         :history = "Created using OSTIA reanalysis system v2.0";
         :license = "GHRSST protocol describes data use as free and open";
         :id = "OSTIA-ESACCI-L4-v01.0";
```



```
:naming authority = "org.ghrsst";
         :product version = "1.0";
         :uuid = "19b1f7a4-d8d1-44eb-9cfa-37cc33c4c2c1";
         :tracking_id = "19b1f7a4-d8d1-44eb-9cfa-37cc33c4c2c1";
         :gds_version_id = "2.0"
         :netcdf version id = "4.1.3";
         :file_quality_level = 3;
         :spatial_resolution = "0.05 degree";
         :date created = "20130305T135622Z";
         :start_time = "20000101T000000Z";
         :time_coverage_start = "20000101T000000Z";
         :stop_time = "20000101T235959Z";
         :time_coverage_end = "20000101T235959Z";
         :time_coverage_duration = "P1D";
         :time_coverage_resolution = "P1D" ;
         :metadata_link = "http://www.esa-cci.org";
         :keywords = "Oceans > Ocean Temperature > Sea Surface Temperature";
         :keywords vocabulary = "NASA Global Change Master Directory (GCMD) Science
Kevwords":
         :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 = -0.2f;
         :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";
         :project = "Climate Change Initiative - European Space Agency";
         :creator_processing_institution = "These data were produced at the Met Office as part of
the ESA SST CCI project.";
         :publisher_name = "ESACCI";
         :publisher url = "http://www.esa-sst-cci.org";
         :publisher_email = "science.leader@esa-sst-cci.org";
         :comment = "WARNING Some applications are unable to properly handle signed byte
values. If values are encountered > 127, please subtract 256 from this reported value";
         :westernmost longitude = -180.f;
         :easternmost_longitude = 180.f;
         :southernmost latitude = -90.f;
         :northernmost_latitude = 90.f;
         :geospatial_lat_max = 90.f;
         :geospatial_lat_min = -90.f;
         :geospatial_lon_max = 180.f;
         :geospatial_lon_min = -180.f;
         :processing_level = "L4";
         :cdm_data_type = "grid";
         :Metadata Conventions = "Unidata Dataset Discovery v1.0";
         :Conventions = "CF-1.5, Unidata Observation Dataset v1.0";
         :source = "ATSR<1,2>-ESACCI-L3U-v1.0, AATSR-ESACCI-L3U-v1.0,
AVHRR<12,14,15,16,17,18>_G-ESACCI-L2P-v1.0, AVHRRMTA-ESACCI-L2P-v1.0,
EUMETSAT_OSI-SAF-ICE-v1.1, EUMETSAT_OSI-SAF-ICE-v2.2";
         :platform = "ERS-<1,2>, Envisat, NOAA-<12,14,15,16,17,18>, MetOpA";
         :sensor = "ATSR, AATSR, AVHRR_GAC";
}
```



11.4 Header from output of ESA SST CCI tool 'regrid'

```
netcdf \20000101-20000201-Global-ESACCI-L3U_GHRSST-SST_depth_20-regridded5.0-LT-
v2.0-fv1.1 {
dimensions:
    lat = 36;
    lon = 72;
    time = 1;
    bnds = 2;
variables:
    float lat(lat);
         lat:units = "degrees north";
         lat:long_name = "latitude" ;
         lat:bounds = "lat bnds";
    float lon(lon);
         lon:units = "degrees east";
         lon:long name = "longitude";
         lon:bounds = "lon bnds";
    float lat bnds(lat, bnds);
         lat_bnds:units = "degrees_north";
         lat_bnds:long_name = "latitude cell boundaries" ;
    float lon_bnds(lon, bnds);
         lon_bnds:units = "degrees_east" ;
         lon_bnds:long_name = "longitude cell boundaries" ;
    float sst_depth_20(time, lat, lon);
         sst_depth_20:units = "kelvin";
         sst_depth_20:long_name = "mean of sst depth_20 in kelvin";
         sst_depth_20:_FillValue = NaNf;
    float sst depth 20 anomaly(time, lat, lon);
         sst depth 20 anomaly:units = "kelvin";
         sst_depth_20_anomaly:long_name = "mean of sst depth_20 anomaly in kelvin";
         sst_depth_20_anomaly:_FillValue = NaNf;
    float coverage_uncertainty(time, lat, lon);
         coverage_uncertainty:units = "kelvin";
         coverage uncertainty:long name = "coverage uncertainty";
         coverage uncertainty: FillValue = NaNf;
    float uncorrelated uncertainty(time, lat, lon);
         uncorrelated uncertainty:units = "kelvin";
         uncorrelated_uncertainty:long_name = "uncorrelated uncertainty in kelvin";
         uncorrelated_uncertainty:_FillValue = NaNf;
    float large_scale_correlated_uncertainty(time, lat, lon);
         large_scale_correlated_uncertainty:units = "kelvin";
         large_scale_correlated_uncertainty:long_name = "large scale correlated uncertainty in
kelvin";
         large_scale_correlated_uncertainty:_FillValue = NaNf;
    float synoptically_correlated_uncertainty(time, lat, lon);
         synoptically correlated uncertainty:units = "kelvin";
         synoptically_correlated_uncertainty:long_name = "synoptically correlated uncertainty in
kelvin":
         synoptically correlated uncertainty: FillValue = NaNf;
    float adjustment_uncertainty(time, lat, lon);
         adjustment_uncertainty:units = "kelvin";
         adjustment_uncertainty:long_name = "adjustment uncertainty in kelvin";
         adjustment_uncertainty:_FillValue = NaNf;
// global attributes:
         :title = "Re-gridded CCI_L3U SST";
```



```
:institution = "IAES, University of Edinburgh";
         :contact = "c.merchant@ed.ac.uk";
         :fileFormatVersion = "1.1";
         :toolName = "regrid";
         :toolVersion = "2.0";
         :generated_at = "2013-05-31T13:35:34";
         :product_type = "CCI_L3U";
         :sst_depth = "depth_20";
         :start date = "2000-01-01T00:00:00";
         :end date = "2000-02-01T00:00:00";
         :temporal_resolution = "monthly";
         :geospatial_lon_resolution = 5.;
         :geospatial_lat_resolution = 5.;
         :region_name = "Global";
         :source_filename_regex = ".*ESACCI-L3U.*nc";
}
```

11.5 Header from output of ESA SST CCI tool 'regavg'

```
netcdf \19911101-20101231-Global_average-ESACCI-L3U_GHRSST-SST_depth_20_average-
PS-DM-v1.2-fv1.1 {
dimensions:
    time = 230;
variables:
    float start_time(time);
         start time:units = "seconds";
         start_time:long_name = "reference start time of averaging period in seconds until 1981-
01-01T00:00:00";
    float end time(time);
         end_time:units = "seconds";
         end_time:long_name = "reference end time of averaging period in seconds until 1981-
01-01T00:00:00";
    float sst depth 20(time);
         sst depth 20:units = "kelvin";
         sst depth 20:long name = "mean of sst depth 20 in kelvin";
         sst depth 20: FillValue = NaNf;
    float sst_depth_20_anomaly(time);
         sst_depth_20_anomaly:units = "kelvin";
         sst_depth_20_anomaly:long_name = "mean of sst depth_20 anomaly in kelvin";
         sst_depth_20_anomaly:_FillValue = NaNf;
    float coverage_uncertainty(time);
         coverage_uncertainty:units = "1";
         coverage_uncertainty:long_name = "mean of sampling/coverage uncertainty";
         coverage_uncertainty:_FillValue = NaNf;
    float uncorrelated_uncertainty(time);
         uncorrelated_uncertainty:units = "kelvin";
         uncorrelated uncertainty:long name = "mean of uncorrelated uncertainty in kelvin";
         uncorrelated_uncertainty:_FillValue = NaNf;
    float large_scale_correlated_uncertainty(time);
         large_scale_correlated_uncertainty:units = "kelvin";
         large_scale_correlated_uncertainty:long_name = "mean of large scale correlated
uncertainty in kelvin";
         large scale correlated uncertainty: FillValue = NaNf;
    float synoptically_correlated_uncertainty(time);
         synoptically correlated uncertainty:units = "kelvin";
```



```
synoptically correlated uncertainty:long name = "mean of synoptically correlated
uncertainty in kelvin";
                                      synoptically_correlated_uncertainty:_FillValue = NaNf;
                  float adjustment_uncertainty(time);
                                     adjustment_uncertainty:units = "kelvin";
                                     adjustment_uncertainty:long_name = "mean of adjustment uncertainty in kelvin";
                                     adjustment_uncertainty:_FillValue = NaNf;
// global attributes:
                                     :title = "CCI_L3U SST_depth_20 anomalies";
                                     :institution = "IAES, University of Edinburgh";
                                     :contact = "c.merchant@ed.ac.uk";
                                     :file_format_version = "1.1";
                                     :tool_name = "regavg";
                                     :tool_version = "1.2";
                                     :generated_at = "2013-03-10T09:30:02";
                                     :product_type = "CCI_L3U";
                                     :sst depth = "depth 20";
                                     :start_date = "1991-11-01T00:00:00";
                                     :end_date = "2010-12-31T00:00:00";
                                     :temporal_resolution = "monthly";
                                     :region_name = "Global" ;
                                     :filename_regex = "\\d{14}-ESACCI-L3[CU]{1}_GHRSST-
SST((skin)|(subskin)|(depth)|(fnd))[-
|((ATSR1)|(ATSR2)|(AATSR)|(AMSRE)|(SEVIRI_SST)|(TMI))[-]((LT)|(DM))-v \cdot (1,2) \cdot (1,2
fv\\d{1,2}\\.\\d{1}.nc";
```

