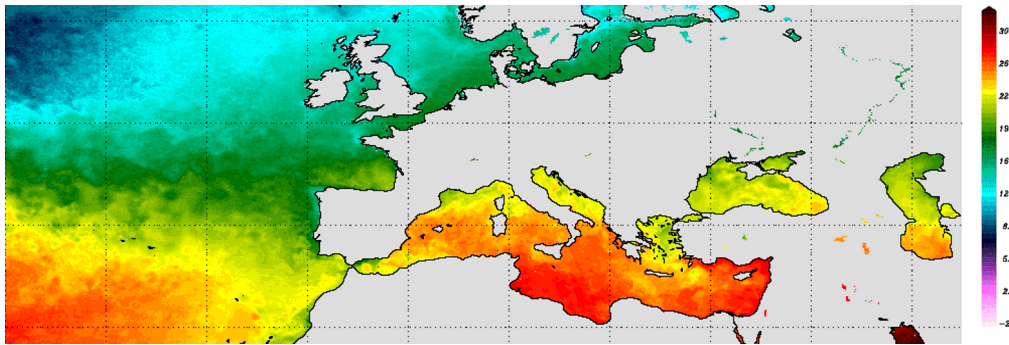


ESA CCI Phase 3 Sea Surface Temperature (SST)



Product User Guide D4.2 v1.1

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QUICK START GUIDE TO ESA SST CCI PRODUCTS

What products are available?

The SST-CCI Climate Data Record (CDR) provides global SST in the period 1980 through 2021 derived from three series of thermal infra-red sensors: the Advanced Very High Resolution Radiometers (AVHRRs), the Along-Track Scanning Radiometers (ATSRs), and the Sea and Land Surface Temperature Radiometers (SLSTRs); and two microwave sensors: the Advanced Microwave Scanning Radiometers (AMSR). The data have been extended since 2022 in the form of an Interim CDR (ICDR) providing an ongoing extension at short delay (approximately 2 weeks behind present). The ICDR was funded by the Copernicus Climate Change Service (C3S) for 2022 and is now funded by the UK Earth Observation Climate Information Service (EOCIS) and UK Marine and Climate Advisory Service (UKMCAS) for 2023 onwards. The temporal coverage for each sensor is shown in Figure 1.

The following data products are available: single-sensor products at their native resolution (Level 2P), single-sensor products remapped to a 0.05° regular latitude-longitude grid (Level 3U), single-sensor products collated into daily files (Level 3C), and a daily gap-free product which combines data from all sensors (Level 4). Data from the infra-red sensors are provided in all three single-sensor levels (Level 2P, Level 3U, and Level 3C), while the microwave AMSR products are only available at level 2P as the native resolution of the AMSR sensors is lower than the 0.05° grid used for Level 3.

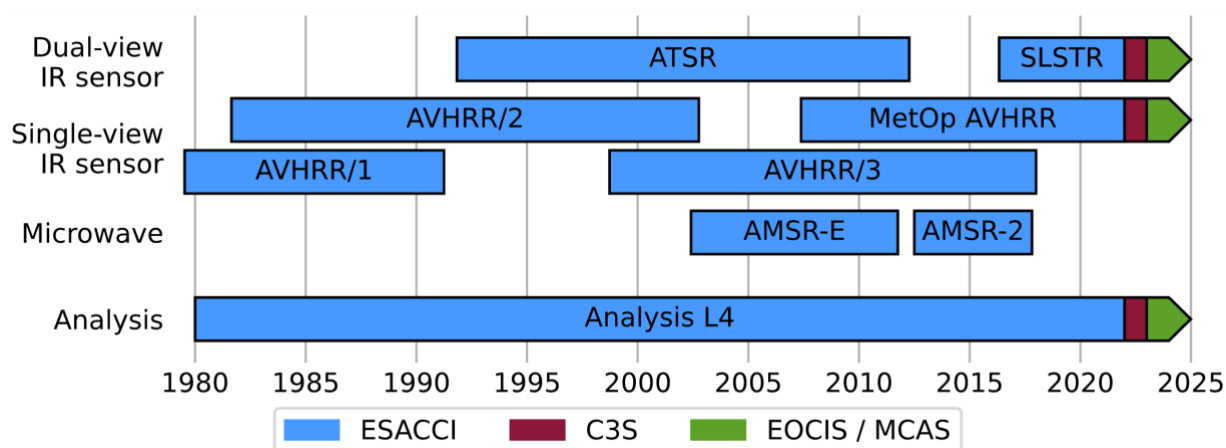


Figure 1: Overview of products included in SST-CCI CDR v3.0. Data from 2022 onwards are Interim-CDR (ICDR) funded by C3S (2022) and EOCIS / MCAS (2023 onwards).

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

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Daily, spatially complete fields of estimated daily mean SST are also available. These were obtained by combining orbit data, using a variational data assimilation technique to provide SSTs where there were no measurements (a single file per day; 0.05° regular latitude-longitude grid). These data start in January 1980 and continue to present; data from 2022 onwards are the ICDR funded by C3S and EOCIS / UKMCAS.

What tools are available for these products?

The ESA Climate Toolbox is a Python package currently under development for the ESA Climate Change Initiative. It will allow easy access to climate data from the Open Data Portal for analysis, processing, and visualisation. For further details see:

<https://climate.esa.int/en/explore/analyse-climate-data/>

The Sentinel Toolboxes are designed for viewing, interpreting, and analysing satellite imagery. The toolboxes support many ESA CCI data in addition to Sentinel 1/2/3 missions and a range of other satellite missions. They are available from: <https://step.esa.int/>

How to obtain the data

The SST-CCI data may be obtained from:

- The ESA CCI Open Data Portal: <https://climate.esa.int/en/odp>
- The CEDA archive (version 3 data):
 - <https://catalogue.ceda.ac.uk/uuid/debfbf49823f4eb99ab0a578f8b25136>
 - Direct access: https://data.ceda.ac.uk/neodc/eocis/data/global_and_regional/sea_surface_temperature/CDR_v3/
- The CEDA archive (all versions):
 - <https://catalogue.ceda.ac.uk/uuid/1dc189bbf94209b48ed446c0e9a078af>
 - Direct access: <http://data.ceda.ac.uk/neodc/esacci/sst/data/>
- Flexible user-defined access to data in the forms of re-gridded data, local time-series, and regional subsets of the Level 4 data may also be obtained using online tools at: <https://surftemp.net/>

How to read the ESA SST CCI data

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

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Table 1: Main data variables present in single-sensor Level 2 and 3 products.

Variable	Description
sea surface temperature	SST as measured by the satellite sensor (Retrieved SST). For infrared radiometers this is the skin temperature, corresponding to a depth of approximately 10 μm . For microwave radiometers this is the sub-skin at approximately 1 mm depth.
sea surface temperature total uncertainty	Total estimated uncertainty in sea surface temperature variable.
sea surface temperature depth	SST adjusted to a standard depth of 20 cm and 10:30 local time (equivalent to daily average).
sea surface temperature depth total uncertainty	Total estimated uncertainty in SST _{0.2m}
sea surface temperature depth anomaly	Difference between SST _{0.2m} and a daily climatology.

- Quality information is provided in the `quality_level` variable. For most purposes users should only consider good quality SSTs where `quality_level` is 4 or 5. The lower levels are provided for expert users.
- The variable `l2p_flags` contains bit flags providing pixel-level information on land/sea mask and the retrieval type.

Table 2: Main data variables present in blended, gap-free, Level 4 products.

Variable	Description
<code>analysed_sst</code>	Daily mean estimate of SST at 0.2m depth as produced by the analysis system used to combine and interpolate the single-sensor data.
<code>analysed_sst_uncertainty</code>	Estimated uncertainty in the analysed SST.
<code>sea_ice_fraction</code>	Amount of sea-ice as a fraction from 0 to 1

- The auxiliary variable `mask` provides bit-mask information. Ice-free ocean SST locations will have `mask = 1`.

Important

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

Further information and how to contact us

Table 3 gives the full SST CCI product names, a basic description to include in any written work carried out using the products and acceptable short forms of the names to include once the full name and description have been included early in the article or technical report. The first reference to the dataset should include the full title and/or full name, including the version number, which unambiguously identifies the dataset. Subsequent references may use the shorted forms e.g. “using the SST CCI SLSTR products” or “features in the CCI analysis SSTs were clearer”.

Full citation information is provided in the catalogue entries in the Open Data Portal and CEDA. DOIs are listed in the tables in Section 5, and also recorded in the file metadata so you may easily find the catalogue entry from the files you are using.

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Table 3: List of SST CCI products and data volumes. The full name including level and version should be used on first use in reports or articles. * The Short Product and Short SST names may be used once the full name has been included earlier in the article or technical report.

Title	ESA SST CCI ATSR L2P v2.1 [link]	ESA SST CCI ATSR L3U v2.1 [link]	ESA SST CCI ATSR L3C v2.1 [link]
Full name	European Space Agency Sea Surface Temperature Climate Change Initiative: Along-Track Scanning Radiometer		
	level-2 pre-processed product version 2.1	level-3 uncollated product version 2.1	level-3 collated product version 2.1
Basic description (quotable when citing data)	global sea surface temperatures from Along Track Scanning Radiometers,		
	presented on the native geometry of observation, and spanning 1991 to 2012	presented on a 0.05° latitude-longitude grid, and spanning 1991 to 2012	daily collations on a 0.05° latitude-longitude grid, and spanning 1991 to 2012
Data volume	2.6 T	270 G	246 G
Short Product*	SST CCI ATSR	Gridded SST CCI ATSR	Gridded daily SST CCI ATSR
Short SST*	CCI ATSR SST	CCI gridded ATSR SST	CCI gridded daily ATSR SST
Title	ESA SST CCI SLSTR L2P v3.0 [link]	ESA SST CCI SLSTR L3U v3.0 [link]	ESA SST CCI SLSTR L3C v3.0 [link]
Full name	European Space Agency Sea Surface Temperature Climate Change Initiative: Sea and Land Surface Temperature Radiometer		
	level-2 pre-processed product version 3.0	level-3 uncollated product version 3.0	level-3 collated product version 3.0
Basic description (quotable when citing data)	global sea surface temperatures from Sea and Land Surface Temperature Radiometers,		
	presented on the native geometry of observation, and spanning 2016 to 2021	presented on a 0.05° latitude-longitude grid, and spanning 2016 to 2021	daily collations on a 0.05° latitude-longitude grid, and spanning 2016 to 2021
Data volume	5.0 T	915 G	175 G
Short Product*	SST CCI SLSTR	Gridded SST CCI SLSTR	Gridded daily SST CCI SLSTR
Short SST*	CCI SLSTR SST	CCI gridded SLSTR SST	CCI gridded daily SLSTR SST
Title	ESA SST CCI AVHRR L2P v3.0 [link]	ESA SST CCI AVHRR L3U v3.0 [link]	ESA SST CCI AVHRR L3C v3.0 [link]
Full name	European Space Agency Sea Surface Temperature Climate Change Initiative: Advanced Very High Resolution Radiometer		
	level-2 pre-processed product version 3.0	level-3 uncollated product version 3.0	level-3 collated product version 3.0
Basic description (quotable when citing data)	global sea surface temperatures from Advanced Very High Resolution Radiometers,		
	presented on the native geometry of observation, and spanning 1980 to 2021	presented on a 0.05° latitude-longitude grid, and spanning 1980 to 2021	daily collations on a 0.05° latitude-longitude grid, and spanning 1980 to 2021
Data volume	28 T (23 MetOp)	5.2 T (1.9 MetOp)	4.3 T (1.4 MetOp)
Short Product*	SST CCI AVHRR	Gridded SST CCI AVHRR	Gridded daily SST CCI AVHRR
Short SST*	CCI AVHRR SST	CCI gridded AVHRR SST	CCI gridded daily AVHRR SST
Title	ESA SST CCI AMSR L2P v3.0 [link]		
Full name	European Space Agency Sea Surface Temperature Climate Change Initiative: Advanced Microwave Scanning Radiometer level-2 pre-processed product version 3.0		
Basic description	global sea surface temperatures from Advanced Microwave Scanning Radiometers, presented on the native geometry of observation, and spanning 2002 to 2017		
Data volume	391 G		
Short Product*	SST CCI AMSR		
Short SST*	CCI AMSR SST		
Title	ESA SST CCI Analysis v3.0 [link]		
Full name	European Space Agency Sea Surface Temperature Climate Change Initiative: Analysis product version 3.0		
Basic description	global daily-mean sea surface temperatures, presented on a 0.05° latitude-longitude grid, with gaps between available daily observations filled by statistical means, spanning 1980 to 2021		
Data volume	230 G		
Short Product*	SST CCI analysis		
Short SST*	CCI analysis SST		

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When citing this dataset please also cite the associated data paper:

Embury, O., Merchant, C.J., Good, S.A., Rayner, N.A., Høyer, J.L., Atkinson, C., Block, T., Alerskans, E., Pearson, K.J., Worsfold, M., McCarroll, N., Donlon, C. (2024). Satellite-based time-series of sea-surface temperature since 1980 for climate applications. *Sci Data* 11, 326. doi:[10.1038/s41597-024-03147-w](https://doi.org/10.1038/s41597-024-03147-w)

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, contact us via the website <https://climate.esa.int/en/projects/sea-surface-temperature/contacts/> or email o.embury@reading.ac.uk. We also welcome any feed-back about the data to this address.

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1. INTRODUCTION

1.1 Purpose and Scope

This document is the user guide for the Version 3 data products produced by the ESA SST CCI project. A number of worked examples are provided to demonstrate how to get started with the data.

The main aim of the document is to aid a user in selecting a data product they require (including understanding its features and limitations) and to then enable them to read and use the data.

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	Description of tools that can be used to work on the data products.
Section 5	A detailed description of the ESA SST CCI data files.
Section 6	Data usage information including file naming and data format.
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.

1.3 Reference Documents

All ESA SSI CCI documentation can be found at:

<https://climate.esa.int/en/projects/sea-surface-temperature/SST-key-documents/>

Reference	Document
ATBD	SST CCI Phase 3 (2023). Algorithm Theoretical Basis Document. SST_CCI_D2.1_ATBD_v3.1
CAR	SST CCI Phase 3 (2023). Climate Assessment Report. SST_CCI_D5.1_CAR_v1
PSD	SST CCI Phase 2 (2017). Product Specification Document. SST_CCI-PSD-UKMO-201
PVIR	SST CCI Phase 3 (2023). Product Validation and Intercomparison Report. SST_CCI_D4.1_PVIR_v2.1
UCR	SST CCI Phase 2 (2018). Uncertainty Characterisation Report. SST_CCI-UCR-UOR-201
URD	SST CCI Phase 2 (2017). User Requirements Document. SST_CCI-URD-UKMO-201

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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’ (Morice et al., 2012), 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 40+ years. The longest record comes from a series of instruments known as the Advanced Very High Resolution Radiometers (AVHRRs). These are based on polar orbiting platforms (the series of National Oceanic and Atmospheric Administration (NOAA) satellites and more recently on MetOp, which is operated by the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT)), which orbit the Earth about every 100 minutes, passing almost over the poles and viewing a narrow (~2500 km) strip of the surface each time. A second long-term record is provided by the Along Track Scanning Radiometer (ATSR) series of three instruments, which started in 1991 and ended in 2012, and later the Sea and Land Surface Temperature Radiometer (SLSTR) from 2016. These sensors were also housed on polar orbiting platforms. Relative to AVHRRs, they gave more accurate data (Merchant et al., 2009, 2012) but with less coverage (~500 km wide strips for ATSR). 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 (AMSR) views the Earth in the microwave part of the spectrum, allowing them to ‘see’ through the majority of clouds providing greatly improved spatial coverage. However, spatial resolution is much lower: ~50 km compared to 1 to 4 km for the infrared instruments. There are also data from sensors on geostationary satellites – which perform one orbit per day and stay over the same spot on the Earth all the time – such as the Spinning Enhanced Visible and Infrared Imager (SEVIRI) on Meteosat Second Generation (MSG), but these are not used here.

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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 (Kilpatrick et al., 2001; Casey et al., 2010) and the ATSR Reprocessing for Climate (ARC) data for the ATSR series (Merchant et al., 2012). 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] data-bases 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 original project team comprised the University of Reading (UK) as prime contractor, and partners in the Met Office (UK), the University of Leicester (UK), Météo France (France), Danmarks Meteorologiske Institut (Danish Meteorological Institute; DMI) (Denmark), the Norwegian Meteorological Institute (Norway), Brockmann Consult (Germany), National Oceanography Centre (UK) and Space ConneXions (UK).

A very significant outcome of the project is the bringing together of two long term series of satellite data (from ATSRs and AVHRRs) to produce an SST record that is maximally independent of in situ observations for the period since ATSRs have been available, and combines the strengths of each series while minimising their weaknesses. Since the original data release, two further series of sensors (AMSR and SLSTR) have been added to the Climate Data Record (CDR).

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, and the current phase in July 2019. Its scope includes user requirements gathering, algorithm development, algorithm benchmarking, data production

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and validation, disseminating those data, and obtaining user feedback. One of its major aims is to produce a system for refining and continuing data products into the future.

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

2.2.1 User requirements gathering

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

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

The results were wide ranging and a full description can be found in the ESA SST CCI User Requirements Document (URD) available from <https://climate.esa.int/en/projects/sea-surface-temperature/SST-key-documents/>.

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 2 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.

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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 algorithms to retrieve SST from the measurements made by the satellite instruments. The main objective of the SST-CCI project is to provide stable, accurate, and unbiased estimates of SST. Therefore, the algorithm development has focussed on techniques which can be applied across the long-term sensors in a consistent manner. The main algorithms used in SST-CCI can be grouped in five to broad topics. First, harmonisation between different sensors to account for differences in calibration and characterisation as even sensors of the same design will not produce identical results. Second, cloud detection or image classification to identify areas corresponding to “clear-sky” observations as the sensors cannot see through clouds (or rain in the case of microwave instruments). Third, SST retrieval – the process of converting the satellite measurement of radiances into an estimate of the temperature of the sea surface. Fourth, a Diurnal Variability (DV) model is needed to account for the different times of observation. Finally, an analysis system is used to combine observations from multiple sensors and fill in the gaps due to cloud cover.

Algorithms used have been evolved from those employed in Phase 2 and are documented in the Algorithm Theoretical Basis Document (ATBD). The main evolutions since CDR v2 are:

- Updated radiative transfer model supporting variable CO₂ and tropospheric aerosol simulations. This allows the SST retrieval to be corrected for desert-dust, and removes the associated dust biases seen in version 2 products.
- New bias-aware optimal estimation retrieval for the single-view AVHRR sensors reduces systematic biases.
- Addition of early AVHRR/1 data in the 1980s, and improved AVHRR processing to reduce data gaps in the 1980s.
- Addition of dual-view SLSTR data from 2016 onwards.
- Use of full-resolution MetOp AVHRR data (the version 2 CDR used lower resolution “global area coverage”)
- Inclusion of L2P passive microwave AMSR data.

Early Level 4 data (pre-1997) are adjusted relative to HadSST4 to reduce impact of intermittent periods of anomalous satellite calibration.

2.2.4 The ESA SST CCI products

The ESA SST CCI project produces the long-term climate data record products. This includes single-sensor Level 2 and 3 products from ATSR, SLSTR, AVHRR, and AMSR, and a Level 4 analysis product which combines the data from all sensors to produce a daily gap-free SST. With the version 3 release the CDR now covers 42 years for the period 1980 through end-2021.

In addition, there is an ongoing extension of the CDR in the form of an Interim-CDR produced using the SST-CCI software and systems. Production of the ICDR was funded by the Copernicus Climate Change Service (C3S) for 2022 and by the UK Earth Observation Climate Information Service (EOCIS) and Marine Climate Advisory Service (MCAS) for 2023 onwards.

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2.2.5 Data dissemination

The current SST-CCI products are available from the ESA CCI Open Data Portal. An archive of all versions (including the latest) is available in the CEDA catalogue.

- <https://climate.esa.int/en/odp>
- <https://catalogue.ceda.ac.uk/uuid/1dc189bbf94209b48ed446c0e9a078af>

Feedback from users is strongly encouraged to ensure that future refinements of the products meet users' needs. Contact us via the SST website <https://climate.esa.int/en/projects/sea-surface-temperature/contacts/> or email o.embury@reading.ac.uk.

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. This has enabled the ESA SST CCI algorithms to be implemented operationally, enabling the data to be extended in time routinely with the ICDR. In the future, new sensors will be first addressed via the ICDR. The ESA SST CCI focus will be the long-term CDR, further improvements to the 1980s/90s data, and investigation of additional historical sensors not yet included in the ESA SST CCI products.

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

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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 4-8. Here, an extended introduction to the data is provided including, in Section 3.1 a general overview of the terminology and sensors used in satellite remote sensing of SST. Section 3.2 provides a brief overview of the available ESA SST CCI products; Section 3.3 contains links to the data archives; Section 3.4 is an overview of the data format; Section 3.5 lists our contact details; and Section 3.6, a frequently asked questions section. This includes explanations for some of the terms that might be encountered when reading through this chapter and the other parts of this document. See also Section 8, which contains explanations of acronyms, abbreviations, and jargon.

3.1 General Information

3.1.1 SST Types

The term “SST” is used variously to refer to the temperature of water anywhere from the interface with 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 large diurnal cycle, but not the SST in the same location at 10 m. Therefore, there are several types of SST that are sometimes referred to. The ESA SST CCI products use the definitions from the Group for High Resolution Sea Surface Temperature (GHRSSST) Science Team as shown in Figure 2:

- **The interface temperature (SST_{int})** is a hypothetical temperature at the exact air-sea interface.
- **The skin sea surface temperature (SST_{skin})** is defined as the temperature measured by an infrared radiometer, typically operating at wavelengths of 3.7-12 μm . This corresponds to a depth of $\sim 10\text{-}20 \mu\text{m}$. The skin temperature is typically $\sim 0.2 \text{ K}$ cooler than in situ SST measurements, though the exact value is strongly dependent on wind speed.
- **The sub-skin sea surface temperature (SST_{subskin})** represents the temperature at the base of the conductive laminar sub-layer of the ocean surface. For practical purposes the sub skin can be approximated as the temperature observed by a microwave radiometer.
- **The surface temperature at depth (SST_{depth})** is any measurement of the water temperature made below the surface. The majority of in situ measurements including drifting buoys, moorings, profiling floats, and ships are all SST depth measurements. All such measurements should be qualified by the measurement depth in meters e.g. SST_{0.2m}.
- **The foundation temperature (SST_{fund})** is defined as the SST free of diurnal temperature variability, i.e. the starting point of the diurnal cycle that will develop over a day, or the point at which heat gain from solar radiation exceeds the heat loss at the surface. This type of SST is not used for ESA SST CCI products.

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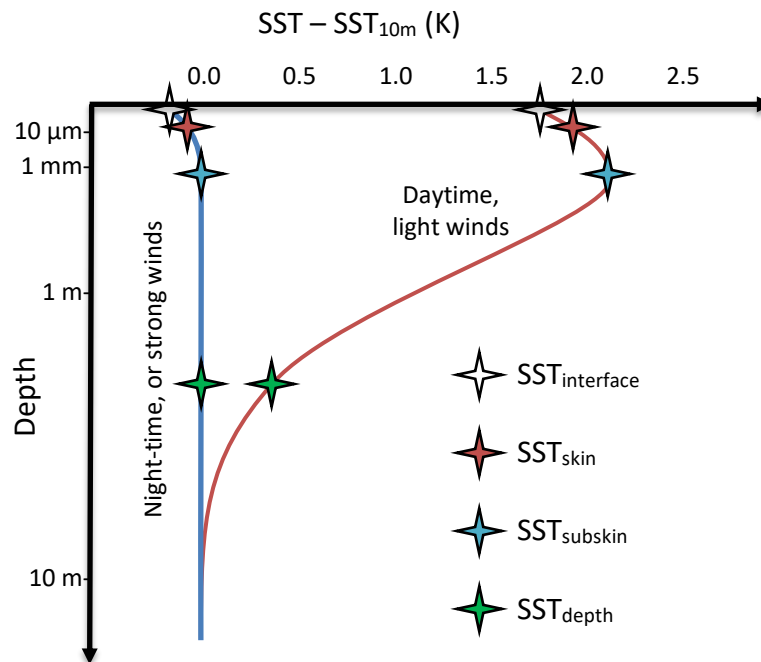


Figure 2: GHRSSST SST types and idealized upper ocean thermal structure for two simplified cases: night-time with a well-mixed surface layer, and a day-time case of near-surface warming under low wind speeds.

3.1.2 Diurnal Variability

There can be large changes in SST throughout the day as the upper layer of the ocean is warmed by solar radiation during the day and cools again at night. The thickness of the warm layer will depend on the wind speed – with higher windspeeds causing the surface to mix so the temperature change will be smaller but reaching to greater depths below the surface. Typically, the daily change in temperature will be 0.1 to 0.5 K, but under low-wind, strong-sun conditions, the change in the satellite-observed skin temperature can be over 5 K. Figure 3 shows the global mean diurnal cycle as estimated from drifting buoys (approx. 20 cm depth), the diurnal cycle in SST_{skin} will be much larger at lower windspeeds as near-surface mixing is reduced.

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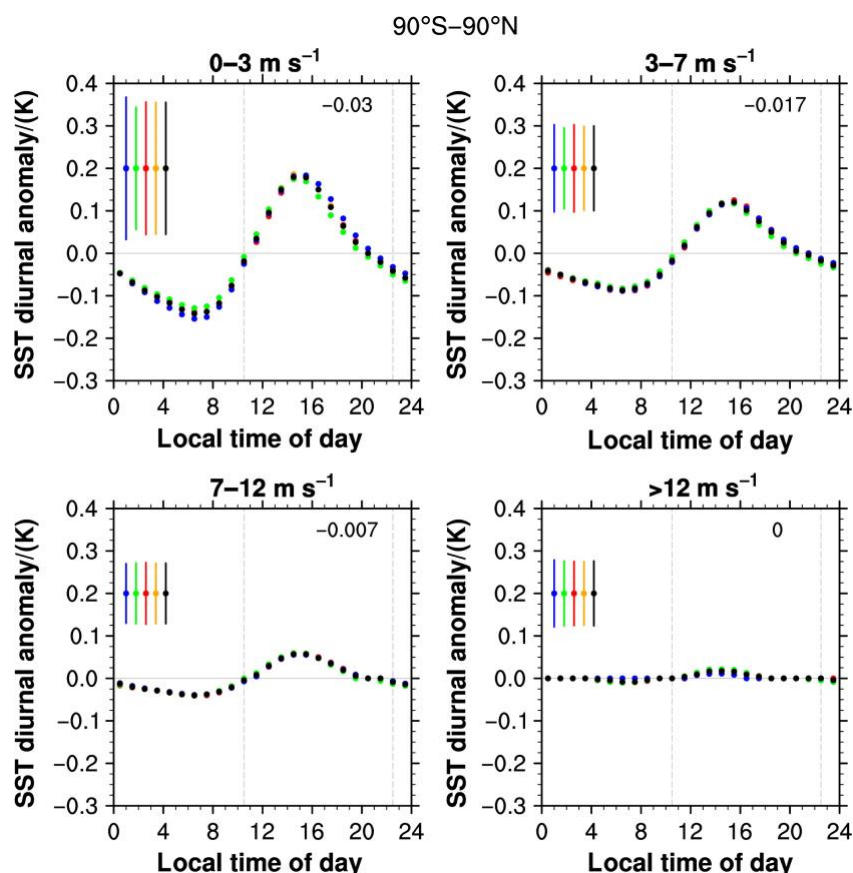


Figure 3: Global mean diurnal cycle of daily SST anomalies from drifting buoys for different wind speeds. The annual mean diurnal cycle is displayed in black, Northern Hemisphere winter (DJF) in blue, spring (MAM) in green, summer (JJA) in red and autumn (SON) in orange. The bars in the top left corner show the associated uncertainties. Reproduced from Morak-Bozzo et al. 2016.

As different satellites will be observing the Earth at different local times of day it is important to consider how the local time of observation will interact with the diurnal cycle. For instance, AVHRR sensors in the “afternoon orbit” will typically launch with an overpass time around 14:00 local time near the peak of the diurnal cycle; however, during their operation they gradually drift to later times and by end of life may be observing the SST around 18:00 local time. For this reason, all SST CCI products also include an adjustment to a standard time of observation – chosen as the nearest of 10:30 or 22:30 local time. This is when the diurnal anomaly is closest to zero (see Figure 3) and the SST is a good approximation to the daily average SST.

3.1.3 Processing Levels

When dealing with satellite data it is common to encounter references to ‘data levels’ or ‘processing 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:

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- **Level 2 Pre-processed (L2P)** – SSTs from a single input (level 1) file, still arranged in the way that the satellite ‘saw’ them. Depending on the source instrument the file may correspond to a single orbit (approx. 100 minutes), or a shorter data granule (typically 3 or 5 minutes).
- **Level 3 Uncollated (L3U)** – contain the same data as a single L2P except the SSTs have been re-gridded and/or averaged spatially. L3U files will typically appear as a single narrow swath around the orbit, with much of the Earth surface unobserved.
- **Level 3 Collated (L3C)** – combine multiple L3U files from a single sensor collected over a short period of time. Typically these are used to produce daily Level 3 files containing all the SSTs observed in a single UTC day.
- **Level 4 (L4)** – SSTs (typically from multiple orbits and sensors) that have been combined and any gaps filled in using statistical techniques.

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

Further details on the file format and contents used for the different processing levels are given in Section 6.

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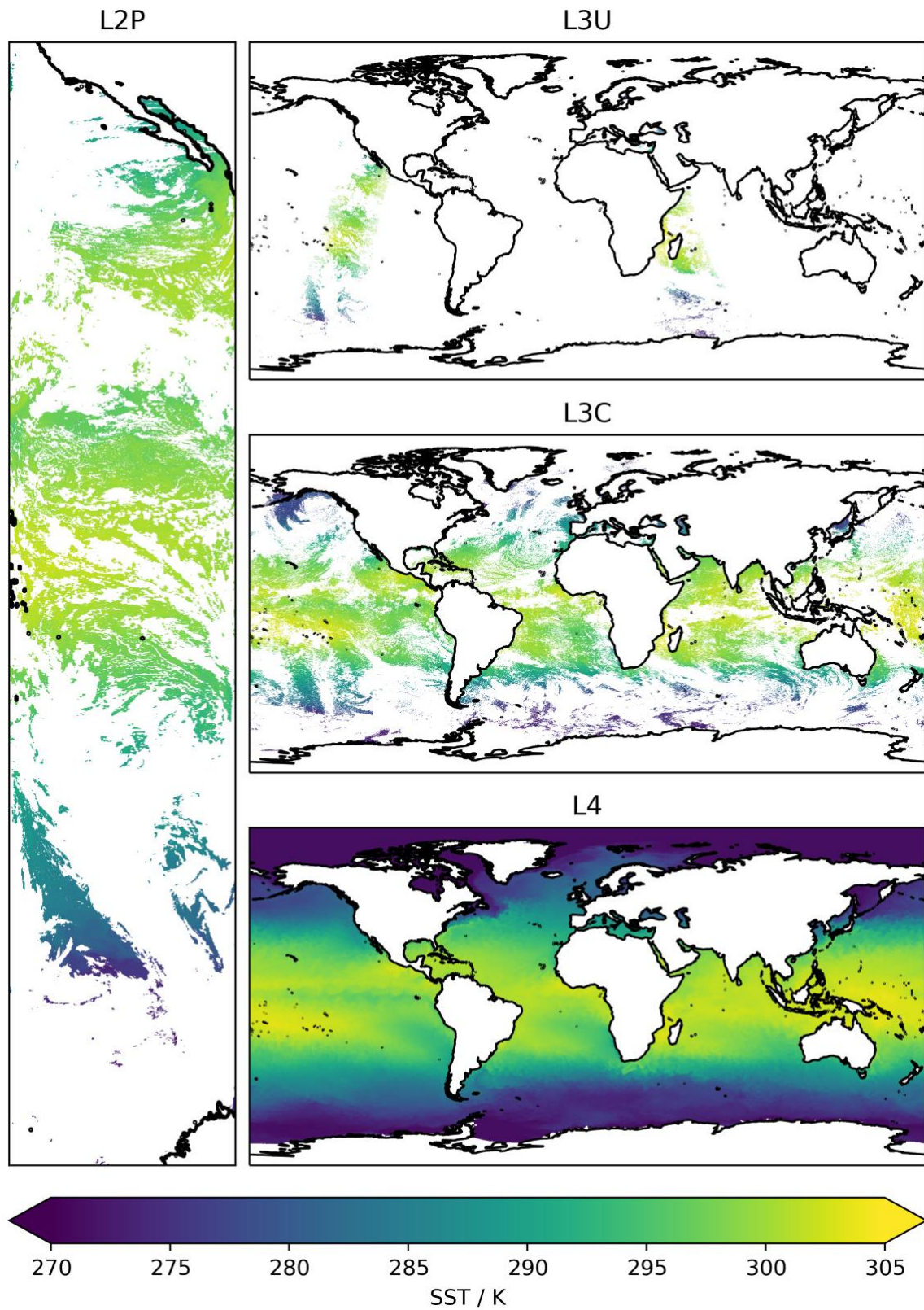


Figure 4: Illustration of how data are stored according to the 'level' of the data, using example ESA SST CCI data from one day. White areas correspond to locations with no SSTs. These occur, for example, due to cloud preventing an SST retrieval or because there was land or ice in the field of view of the instrument.

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3.1.4 Sensors

3.1.4.1 AVHRR

The AVHRRs are a series of multipurpose imaging instruments carried onboard the National Oceanic and Atmospheric Administration (NOAA) Polar Operational Environmental Satellites (POES) and EUMETSAT Polar System (EPS) MetOp satellites. The first AVHRR instrument was carried onboard the TIROS-N satellite launched in October 1978 and the final onboard MetOp-C in November 2018. The equator crossing times of the various satellites are shown in Figure 5. The NOAA satellites are all in drifting orbits, meaning that the equator crossing times are slowly changing. The EUMETSAT MetOp satellites are in controlled orbits with equator crossing times of 9:30. Global full resolution data are available for MetOp AVHRRs, whereas for NOAA AVHRRs, global data are available only at the reduced resolution referred to as “global area coverage” (GAC).

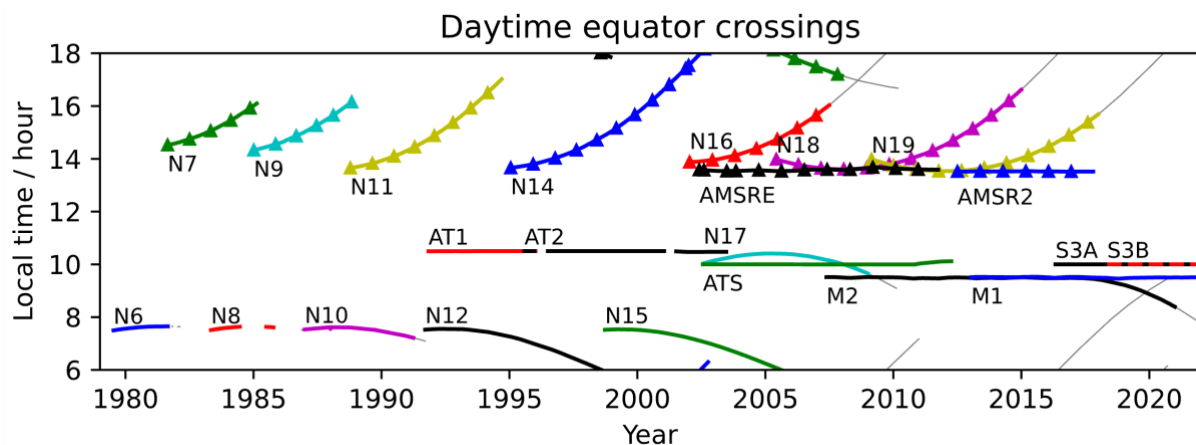


Figure 5: Satellite equator crossing times. Solid lines indicate descending node crossings; lines with triangles indicate ascending node crossings; thin grey lines indicate data were not used in CDR v3.

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

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

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every third scanline as illustrated in Figure 6. The more recent MetOp satellites do not have this limitation and record full orbit data at native resolution of 1.1 km at nadir.

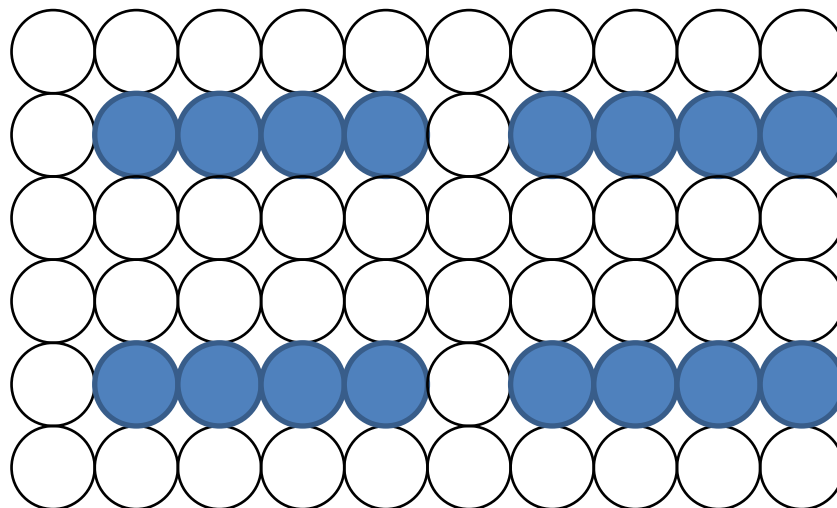


Figure 6: schematic of GAC pixels (blue) which are the average of four full resolution pixels (circles). White circles indicate full resolutions pixels which are not included in the GAC averaging, so data is not available.

3.1.4.2 ATSR and SLSTR

The ATSR and SLSTR instruments are both well calibrated, dual-view radiometers designed to produce long-term consistent SST observations. Three ATSRs were flown on board ESA's European Remote Sensing (ERS) satellite and Envisat between 1991 and 2012; the first SLSTR instrument was carried onboard the Sentinel-3A satellite launched in 2016, and there are currently two SLSTRs in operation. All ATSR and SLSTR sensors have been in stable sun-synchronous orbits with near-constant equatorial crossing times (10:30 for the two ERS satellites, and 10:00 for Envisat and the Sentinel-3 platforms).

Unlike the AVHRR instruments, the ATSRs and SLSTRs were designed specifically for climate applications with significant improvements to calibration, characterization and stability. One feature unique to these sensors is the introduction of a dual-view capability using a single telescope with a conical scanning pattern. Having two views of the Earth's surface allows the instrument to gather more information and more effectively separate surface and atmospheric effects; i.e. the SST retrieval can be made more robust to atmospheric conditions, including water vapour and stratospheric aerosol. However, it also means the instruments have a much narrower swath – the ATSR swath is only 512 km wide compared to the 2800 km for AVHRRs. As a result, it takes ~3 days for an ATSR instrument to collect global observations. The newer SLSTR instrument has a wider swath with ~740 km of dual-view coverage.

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3.1.4.3 AMSR

Advanced Microwave Scanning Radiometers (AMSR) instruments have been used on three satellites: ADEOS II, EOS Aqua, and GCOM-W1. ADEOS II only operated for 10 months before suffering from solar panel failure so it not suitable for use in the CDR. The EOS-Aqua AMSR (known as AMSR-E) was launched in May 2002 and operated for over nine years before failing in October 2011. The GCOM-W1 satellite launched in May 2012 carrying the AMSR2 instrument. Both the AMSR-E and AMSR2 sensors are in early afternoon orbits (1:30 LECT; see Figure 5).

Passive microwave SSTs, as measured by AMSR, are at a lower resolution (approximately 50 km) and lower accuracy than infrared SST measurements. Furthermore, they are affected by Radio Frequency Interference and cannot be used within ~100 km of land or sea-ice due to side-lobe contamination (Alerskans et al., 2020). However, they also have two advantages over infrared observations:

- Microwave radiometers can retrieve SST through clouds, allowing SST to be measured in all conditions except rain.
- Microwave retrievals of SST are not affected by aerosols and the vertical distribution of water vapour in the same way as infrared retrievals are.

Due to the lower resolution of AMSR retrievals, products are only available in L2P format. Figure 7 shows the AMSR scanning geometry, the antenna rotates with a fixed satellite zenith angle of 55 degrees so each scanline is a curved path on the Earth's surface, and the footprint or pixel is elliptical aligned along the direction of view.

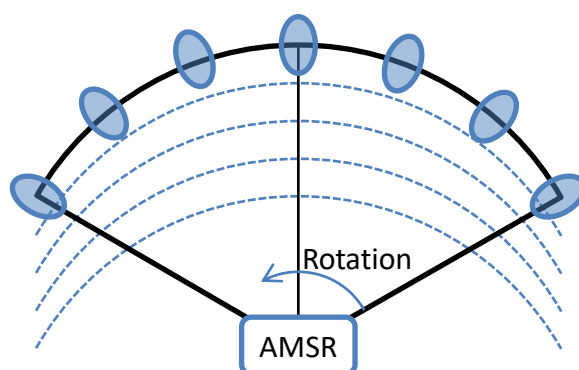


Figure 7: AMSR scanning geometry. Satellite zenith angle of 55° results in an elliptical footprint aligned along the direction of view as the antenna rotates.

3.2 Which SST product do I need?

The ESA SST CCI project has produced a Climate Data Record of SST the period 1980 though 2021 derived from three series of thermal infra-red sensors: the Advanced Very High Resolution Radiometers (AVHRRs), the Along-Track Scanning Radiometers (ATSRs), and the Sea and Land Surface Temperature Radiometers (SLSTRs); and two microwave sensors: the Advanced Microwave Scanning Radiometers (AMSR). Data are provided as both single-sensor

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SSTs (L2P, L3U, L3C) and a blended, gap-filled, daily analysis SST (L4). An overview of the periods covered by each sensor is shown in Figure 8. Further details on the different processing levels are given in Section 3.1.3 and the different sensors in Section 3.1.4.

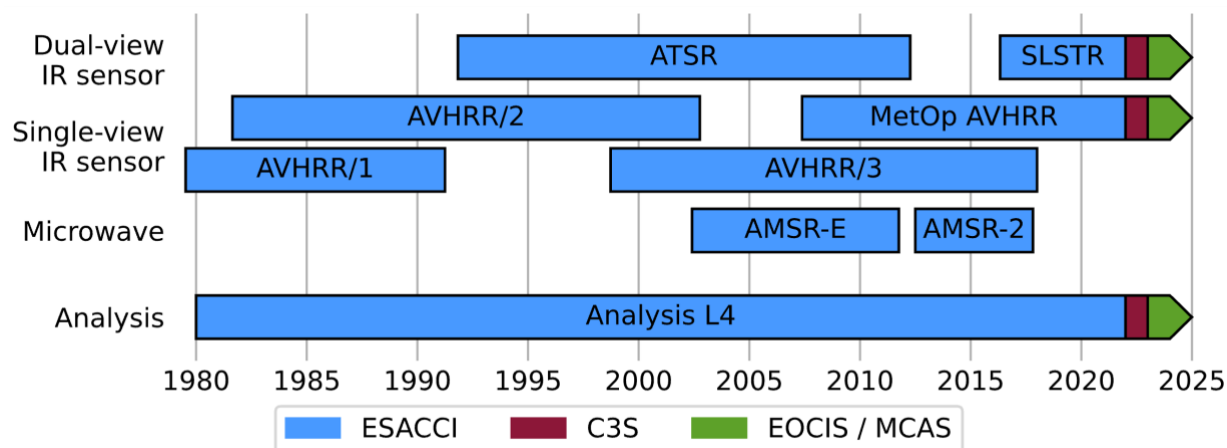


Figure 8: Overview of products included in SST-CCI CDR v3.0. Data from 2022 onwards are Interim-CDR (ICDR) funded by C3S (2022) and EOCIS / MCAS (2023 onwards).

Each file of three of the above four products (the L2P, L3U and L3C) contains two sets of SSTs. The first set provides a measure of the temperature of the skin of the water at the time it was observed; the second set are estimates of the temperature at 20 cm depth and at either 1030 h or 2230 h local time (provision of data at 20 cm depth was one of the requirements revealed by the user requirements gathering exercise [URD]). They have uncertainty estimates that have been broken down into different components and a total uncertainty for each SST value. The SST data are suitable for many uses, such as the study of temporal and spatial variability and comparison to or initialisation of numerical models. Owing to the orbital drift of some satellites, the 20 cm SSTs are better suited to the study of long-term SST change than the skin SSTs as they have been adjusted so that they all represent the same point in the diurnal cycle.

The combined, globally-complete Level 4 analysis for January 1980 to December 2021 provides daily combinations of the orbit data from the Version 3 release, using a variational data assimilation system (run without use of a dynamical ocean model in this case) to provide SSTs where there were no observations. This results in a single file per day on a 0.05° regular latitude-longitude grid). These Level 4 SSTs correspond approximately to the daily average of the temperature of the water at 20 cm depth. Uncertainty estimates are provided. An example use of these data is as a boundary condition for a numerical model.

Most users will want the **Level 4** SST CCI analysis product as it provides an easy-to-use, globally-complete, combination of all available sensors, which can be used as a daily average SST at 20 cm depth. However, some users may want the lower level data for various reasons including:

- The analysis only includes the daily average SST_{20cm}. Use the lower-level data for SST_{skin} or at the observation time.

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- The analysis fills in data gaps using statistical techniques to estimate the SST for nearby observations (both spatially and temporally, with the analysis uncertainty reflecting the uncertainty in this gap-filling process. Use the lower-level data to access direct observations of SST.
- The analysis process used to fill in the data gaps spreads information from observed locations/times into the gaps. This has the effect of slightly smoothing the data such that the “feature resolution” of the analysis is 20-40 km – lower than the grid spacing (0.05° or ~5 km).
- The analysis only uses the best quality Level 2/3 input data – i.e. SST retrievals of the highest quality and most likely to be clear-sky observations. Use the lower-level data to access all observations.
- The analysis includes a single “analysis uncertainty” estimate, while the lower level data has a more detailed breakdown of the different contributions.

Level 3C – provides single-sensor data in an easy-to-use format. These collate all data observed in a single day into two files: one for day-time observations and one for night-time. The data are presented on a global 0.05° grid; they contain both the SST_{skin} and time adjusted SST_{20cm} as detailed above.

Level 2P – provide the single-sensor data in the native sensor resolution. These are for users who require the data at maximum resolution on the original sensor swath.

Level 3U – are only recommended for specialist users who require gridded data without it being collated to daily files.

ATSR / SLSTR – the dual-view sensors provide the most accurate and stable SSTs, which the highest degree of independence from in situ measurements. However, the coverage is limited compared to the AVHRRs and the dual-view sensors have not been available for the full timeseries.

AVHRR – provide the longest timeseries with data from July 1979 onwards. Data quality is lower for these single-view sensors, especially in the 1980s and early 90s, and the NOAA AVHRR retrievals were cross-referenced against in situ observations to improve stability. MetOp AVHRR data are cross-referenced to ATSR/SLSTR and remain maximum independence from in situ.

AMSR – the microwave sensors are not affected by cloud, allowing SST to be measured in all weather conditions except rain. However, retrievals are at lower spatial resolution (~50 km) and lower accuracy than infrared measurements. Furthermore, they are affected by RFI and are not usable within ~100 km of land or sea-ice.

Detailed descriptions of the products can be found in Section 5.

Please use the product names and descriptions found in Table 3 when documenting your work with the ESA SST CCI products.

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3.3 How do I get the data?

The SST-CCI data may be obtained from:

- The ESA CCI Open Data Portal: <https://climate.esa.int/en/odp>
- The CEDA archive:
 - <https://catalogue.ceda.ac.uk/uuid/1dc189bbf94209b48ed446c0e9a078af>
 - Direct access: <http://data.ceda.ac.uk/neodc/esacci/sst/data/>
- Re-gridded, time-series, and regional subsets of the Level 4 data may also be obtained from: <https://surftemp.net/>

3.4 How do I use the ESA SST CCI data?

3.4.1 The data files

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

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

For example:

20000101000206-ESACCI-L2P_GHRSSST-SSTskin-AVHRR15_G-CDR2.0-v02.0-fv01.0.nc

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

L2P: start time of granule.

L3U: start time of granule.

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

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

Finally, the processing level of the data is given. This could be L2P (individual orbits of data, satellite projection; this is the type of data in the example filename), L3U (individual orbits of data, gridded), L3C (contain multiple L3U files from a single sensor combined into a longer time period), or L4 (combined, gridded and infilled data). See Section 3.1.3 for more details on data levels.

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

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Table 4: Summary of the key variables in the netCDF files.

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

* Skin SST is the temperature of the radiating surface layer of the water, which is of 10 μ m depth at wavelengths around the peak of the emission spectrum for typical SSTs.

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

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

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

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

Important

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 7.2.1.

3.4.2 Using the uncertainty estimates

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

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

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- `uncertainty_correlated` – uncertainty from effects that are assumed (provisionally) to be correlated over distances of 100 km and 1 day (related to atmospheric conditions).
- `uncertainty_systematic` – uncertainty from effects that can be assumed to be correlated everywhere and over long time scales (such as over all calibration of the satellite sensor).
- `uncertainty_correlated_time_and_depth_adjustment` – 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 `sea_surface_temperature_total_uncertainty` in the NetCDF files. For adjusted SSTs, the corresponding variable is called `sea_surface_temperature_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 7.3.

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

3.4.3 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 Python, 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/>).

More information about tools is available in Section 4.

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

- Do** make sure the data read from the files are scaled to be in the correct units.
- Do** check for fill values in the data arrays and the quality information and/or data quality flags that say which locations contain usable SSTs.
- Do** make use of the uncertainty information.
- Do** make use of all the appropriate metadata and ancillary data (such as wind speed and sea ice) available in the files.

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- Do** tell us what you think of the data!
- Don't** use the wrong SST and uncertainty fields. Remember there are two sets in the L2P, L3U and L3C files – one has been adjusted to a standard time and depth.
- Don't** forget, if averaging the data, to use the individual uncertainty components and propagate uncertainty as recommended.
- Don't** assume that because the grid spacing of the L4 products is 0.05° that SST features that fine are necessarily resolved. Observational information is spread spatially and temporally (to fill in gaps) during the processing. The length scales that govern this spreading of information are described in Fiedler et al. (2019).

3.5 Contact us

Contact us via the website <https://climate.esa.int/en/projects/sea-surface-temperature/> or email o.embury@reading.ac.uk

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

3.6 Frequently asked questions

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

3.6.1 What types of in situ SST measurements are there?

Kennedy et al. (2011) discusses many of the types of instruments that have been used to measure temperature by in situ instruments.

3.6.2 How do satellites measure SST?

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

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3.6.3 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:

SSTskin – the skin SST is the temperature in the top ~10 μm of water; this is nominally the layer of water that an instrument sensing in the infrared part of the electromagnetic spectrum would be sensitive to.

SSTsubskin – the sub-skin SST is the temperature at a depth ~1 mm of water; nominally the mean depth that microwave sensing instruments are sensitive to.

SSTdepth (SST_{0.2m}) – the SST at a specified depth of 20 cm for ESA SST CCI data, which is the depth often associated with drifting buoy measurements (on average). All 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) in addition to the primary retrieval (skin or subskin).

The foundation temperature is defined as the SST free of diurnal variability (for instance the pre-dawn minimum) but is not used in the SST CCI products. Instead, SST CCI products provide SST_{0.2m} adjusted to 10:30 or 22:30 local time. This is when the diurnal anomaly is closest to zero (see Figure 3) and the SST is a good approximation to the daily average SST.

Section 3.1.1 gives details on the different types of SST (also see Figure 2), and section 3.1.2 discusses diurnal variability. For more information about definitions of SST readers are encouraged to consult the Group for High Resolution SST (GHRSSST) webpages at <https://www.ghrsst.org/ghrsst-data-services/products/>.

3.6.4 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 GHRSSST (<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 (Rayner et al., 2003) [<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 (Compo et al., 2011); https://psl.noaa.gov/data/20thC_Rean/). An example of a satellite-only product is that produced by the Pathfinder project from data from the AVHRR series of instruments (Casey et al., 2010) [<https://www.ncei.noaa.gov/products/avhrr-pathfinder-sst>], which has found many applications (e.g. Good et al., 2007).

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A selection of reports from users of the ESA SST CCI data can be found in Section 5 of the Climate Assessment Report [CAR] available from:

<https://climate.esa.int/en/projects/sea-surface-temperature/SST-key-documents/>.

3.6.5 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 the Algorithm Theoretical Basis Document [ATBD] available from:

<https://climate.esa.int/en/projects/sea-surface-temperature/SST-key-documents/>.

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

3.6.6.1 Key features of ESA SST CCI data

The ESA SST CCI data product provides SSTs covering a 42-year period that are designed to be stable and accurate. The ATSR, SLSTR, and MetOp AVHRR SSTs are retrieved largely independently of in situ measurements. However, in situ measurements are used to tune the NOAA AVHRR and AMSR retrievals. ESA SST CCI data are not blended with in situ measurements at level 4 (unlike most satellite and analysis SST datasets).

Satellite estimates of SST are sensitive to the skin SST (infrared instruments) or sub-skin SST (microwave instruments) which can differ from the depth SST by a few tenths of kelvin. Furthermore, the different (and sometimes drifting) satellite overpass times can result the in diurnal cycle being aliased into the long-term record. The ESA SST CCI products address these issues by providing an estimate of SST at 20 cm depth (nominally corresponding to typical drifter measurements) and adjusted to 10:30 local time (corresponding to the daily average in diurnal SST).

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

3.6.6.2 Limitations

The Level 4 Analysis product starts in January 1980 and runs to end of December 2021, spanning 42 years. The AVHRR data starts earlier, in July 1979, but initial data are very sparse before mid-January 1980 and for some other intervals during 1980 and 1981. The gap-filled products are highly interpolated and less accurate during these intervals. Other sensors cover shorter periods: 1991-2012 for ATSR; 2002-2017 for AMSR; and 2016-onwards for SLSTR. Updates to the data are available in the form of an Interim CDR (ICDR) extension providing an ongoing extension at short delay (approximately 2 weeks behind present). The ICDR was funded by the Copernicus Climate Change Service (C3S) for 2022 and is now funded by the UK Earth Observation Climate Information Service (EOCIS) and Marine Climate Advisory Service (MCAS) for 2023 onwards.

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The ESA SST CCI data are on very fine grids, which is an advantage for some applications but also means that the file sizes are large (total size of the products for all the data levels is ~48 TB). However, data are provided separately with different levels of processing and individual files are provided for each day, so users can select the subset of data that is relevant to them. Alternatively, users may also download data at coarser resolutions, or for specific regions, via the <https://surftemp.net/> website.

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

The best stability and precision data are from 1996 onwards. The first ATSR in the series performed less well in these regards than the second and third, but nonetheless helped stabilize the record from 1991 onwards in the aftermath of major volcanic eruptions.

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

A challenge to address has been the extension of the ESA SST CCI products back prior to the first ATSR using AVHRRs only, in a way that is consistent and gives good stability. It was necessary to cross-reference the NOAA AVHRRs with in situ data. The MetOp AVHRRs are cross-referenced to ATSR / SLSTR and remain fully independent from in situ.

Known issues with the version 3.0 products:

- Data from January 1980 to September 1981 should be treated with caution. These data are based on a single AVHRR sensor (NOAA-06) which returned sparse, and less accurate, data than the later instruments.
- Data between 01/10/1982 and 30/09/1983 should be treated with caution. Throughout this period, the AVHRR data are noisy. Embedded within this period are periods of a month or more where large calibration errors (a few tenths K) are apparent. These biases are reduced compared to version 2.0, but may still impact the SST CCI analysis product, as it relies on the AVHRR retrievals at this time.
- Daytime AVHRR uncertainty estimates are overestimated and are too large in comparison to the validation data – i.e. the retrievals are actually more accurate than the uncertainty estimates suggest.
- The ATSR1 3.7 μm channel failed in May 1992 so subsequent night-time data are produced using 2-channel retrieval (lessening consistency with the night-time data of later ATSRs).
- The ATSR2 scan mirror failed between December 1995 and July 1996 resulting in no ATSR2 data during a period when the available ATSR1 was degrading significantly.
- Data between January 2001 and June 2001 should be treated with caution. This corresponds to the ATSR2 gyroscope failure which means that the SST CCI analysis product must rely just AVHRR data from NOAA-14 and -15, both of which were of lower quality in this period.

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3.6.7 How to cite the data

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

The dataset citation should reference the "ESA SST CCI" project, and from where the data were obtained. Accurate product descriptions and names to use in publications are given in Table 3 and should be used to avoid confusion and enable traceability. Full dataset citations are provided in the catalogue entries of the Open Data Portal and CEDA archive. DOIs are recorded in the file metadata so you may easily find the catalogue entry from the files you are using.

The journal reference is:

Embury, O., Merchant, C.J., Good, S.A., Rayner, N.A., Høyer, J.L., Atkinson, C., Block, T., Alerskans, E., Pearson, K.J., Worsfold, M., McCarroll, N., Donlon, C. (2024). Satellite-based time-series of sea-surface temperature since 1980 for climate applications. *Sci Data* 11, 326. doi:[10.1038/s41597-024-03147-w](https://doi.org/10.1038/s41597-024-03147-w)

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

4.1 ESA Climate Toolbox

The ESA Climate Toolbox is an open source Python package currently under development for the ESA Climate Change Initiative. It will allow easy access to climate data from the Open Data Portal for analysis, processing, and visualisation. For further details see:

<https://climate.esa.int/en/explore/analyse-climate-data/>

4.2 SNAP

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

4.3 Generic NetCDF tools

Generic tools available for viewing and manipulating NetCDF files include:

- `ncdump`: provided with the NetCDF library, this produces a human readable version of the contents of a NetCDF file. More details can be found at <https://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 <https://nco.sourceforge.net/>.
- `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>.

4.4 Data analysis/programming languages

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

- Python (<http://www.python.org/>) with add on modules such as netCDF4 (<https://github.com/Unidata/netcdf4-python>), numpy (<http://www.numpy.org/>), matplotlib (<http://matplotlib.org/>) and iris (<https://scitools.org.uk/iris/docs/latest/>). Refer to Section 7.2 for worked examples.

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- Matlab (<http://www.mathworks.co.uk/products/matlab/>).
- GrADS (<http://cola.gmu.edu/grads/>).
- NCL (<http://www.ncl.ucar.edu/>).

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5. ESA SST CCI PRODUCT FACT SHEETS

In this section, the key features of the ESA SST CCI data are listed. A table of features is provided for each instrument (or series of instruments) used in each of the ESA SST CCI Version 3 products.

The format of the table follows the template from the GHRSSST Climate Data Record Technical Advisory Group described in (Merchant et al., 2014). The tables include comments related to four of the GCOS monitoring principles (<https://gcos.wmo.int/en/essential-climate-variables/about/gcos-monitoring-principles>) which can apply to producers of SST datasets:

2. A suitable period of overlap for new and old observing systems is required.
3. The details and history of local conditions, instruments, operating procedures, data processing algorithms and other factors pertinent to interpreting data (i.e., metadata) should be documented and treated with the same care as the data themselves.
11. Constant sampling within the diurnal cycle (minimizing the effects of orbital decay and orbit drift) should be maintained.
12. A suitable period of overlap for new and old satellite systems should be ensured for a period adequate to determine inter-satellite biases and maintain the homogeneity and consistency of time-series observations.

A summary of validation statistics is provided below. More details of these can be found in the ESA SST CCI Product Validation and Intercomparison Report (PVIR) and the ESA SST CCI Climate Assessment Report (CAR), available from <https://climate.esa.int/en/projects/sea-surface-temperature/SST-key-documents/>

Data from January 1980 to September 1981 should be treated with caution. These data are based on a single AVHRR sensor (NOAA-06) which returned sparse, and less accurate, data than the later instruments.

Data between 01/10/1982 and 30/09/1983 should be treated with caution. Throughout this period, the AVHRR data are noisy. Embedded within this period are periods of a month or more where large calibration errors (a few tenths K) are apparent. These biases are reduced compared to version 2.0, but may still impact the SST CCI analysis product, as it relies on the AVHRR retrievals at this time.

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5.1 AVHRR

Summary	
Status of assessment	Dataset producer's information
Dataset name and version	ESA SST CCI AVHRR product version 3
Lead Investigator and/or Agency	Chris Merchant, University of Reading
Principal strengths of data set	Consistently processed data spanning multiple AVHRR sensors from July 1979 to present. Adjusted using ATSR series data as a reference (MetOp AVHRR) or overlaps between sensors and tuning to in situ data (NOAA AVHRR) to achieve stability.
Principal recommended applications	Climate research particularly applications requiring long-term, stable, low-bias records of SST

Key Descriptive Features	
Period covered	1979-07-13 to 2021-12-31
Geographic range	Global
Spatial resolution	Approx. 4 km at nadir (NOAA AVHRR), 1 km at nadir (MetOp)
Temporal resolution	Global coverage ~twice per day (subject to cloud cover etc.)
Timeliness of new data	Extended by ICDR available at ~14 days latency
Dataset volume	28 TB (L2P), 5.2 TB (L3U), 4.3 TB (L3C)
Valid data fraction	SST from clear-sky observations only, this being ~14% of total
Data level / grid	L2P (swath grid with ~4 km at nadir – NOAA AVHRR) L2P (swath grid with ~1 km at nadir – MetOp AVHRR) L3U/L3C (0.05° regular latitude-longitude grid)
Observation technology	The Advanced Very-High Resolution Radiometer (AVHRR) series of infrared sensors on the NOAA and MetOp satellites
Dependence on other data	Numerical weather prediction fields (ERA Interim / ERA5) ATSR and in situ measurements
Type(s) of SST	<ol style="list-style-type: none"> 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

Availability, Documentation and Feedback	
Data URL / ftp / DOI	https://climate.esa.int/en/odp/#/dashboard L2P: https://doi.org/10.5285/ec659b31a8ca40918e58ec6d03af07a6 L3U: https://doi.org/10.5285/c1d393f990fb4b6688b048222833d92f L3C: https://doi.org/10.5285/be418645dfa542df86165a7caad24284
Primary peer reviewed reference	Embury, O., et al. (2024). Satellite-based time-series of sea-surface temperature since 1980 for climate applications. <i>Sci Data</i> 11, 326. doi: 10.1038/s41597-024-03147-w
Source of technical documents	https://climate.esa.int/en/projects/sea-surface-temperature
Dataset restrictions	None, free and open access
Facility for user feedback	https://climate.esa.int/en/projects/sea-surface-temperature

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Other documentation	Algorithm Theoretical Basis Document (ATBD) Product Validation and Intercomparison Report (PVIR) Climate Assessment Report (CAR) Product Specification Document (PSD) User Requirements Document (URD) Uncertainty Characterisation Report (UCR)
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Other Principles (GCOS)	
2. and 12. Overlaps between sensors exist and are exploited	A stable record is achieved by exploiting overlaps between sensors, and harmonisation against in situ (NOAA AVHRR) or ATSR/SLSTR (MetOp AHVRR)
3. Detailed history of methods/algorithms is available	Algorithm Theoretical Basis Document (ATBD)
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 ATSR

Summary	
Status of assessment	Dataset producer's information
Dataset name and version	ESA SST CCI ATSR product version 2.1
Lead Investigator and/or Agency	Chris Merchant, University of Reading
Principal strengths of data set	Consistently processed data spanning all three ATSR sensors
Principal recommended applications	Climate research particularly applications requiring long-term, stable, low-bias records of SST

Key Descriptive Features	
Period covered	1991-11-01 to 2012-04-08
Geographic range	Global
Spatial resolution	1 km irregular grid and 0.05° regular latitude-longitude grid
Temporal resolution	Global coverage every ~3 days (subject to cloud cover etc.)
Timeliness of new data	Data end in April 2012
Dataset volume	2.6 TB (L2P), 270 GB (L3U), 246 GB (L3C)
Valid data fraction	SST from clear-sky observations only, this being ~14% of total data over oceans
Data level / grid	L2P (swath grid with 1 km at nadir) L3U/L3C (0.05° regular latitude-longitude grid)
Observation technology	The Along-Track Scanning Radiometer (ATSR) series of infrared sensors comprises three instruments: <ul style="list-style-type: none"> • ATSR-1 on the ERS-1 platform (1991-1995) • ATSR-2 on ERS-2 (1995-2001) • Advanced (A)ATSR on Envisat (2002-2012)
Dependence on other data	Numerical weather prediction fields (ERA Interim)
Type(s) of SST	<ol style="list-style-type: none"> 1. Skin SST (SST of upper ~10 µm depth). 2. SST at 0.2 m (standardised with respect to diurnal cycle). Diurnal variability modelling is used to estimate SST_{20cm} from SST_{skin}.
Traceability	Not yet established
Uncertainty info in product	Provided for each SST is total uncertainty and components of uncertainty from effects with different spatiotemporal correlation scales

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Availability, Documentation and Feedback	
Data URL / ftp / DOI	https://climate.esa.int/en/odp/#/dashboard L2P: https://doi.org/10.5285/916b93aaf1474ce793171a33ca4c5026 L3U: https://doi.org/10.5285/2282b4aeb9f24bc3a1e0961e4d545427 L3C: https://doi.org/10.5285/5db2099606b94e63879d841c87e654ae
Primary peer reviewed reference	Merchant, C.J., et al. (2019). Satellite-based time-series of sea-surface temperature since 1981 for climate applications. <i>Sci Data</i> 6, 223. doi: 10.1038/s41597-019-0236-x
Source of technical documents	https://climate.esa.int/en/projects/sea-surface-temperature
Dataset restrictions	None, free and open access
Facility for user feedback	https://climate.esa.int/en/projects/sea-surface-temperature
Other documentation	Algorithm Theoretical Basis Document (ATBD) Product Validation and Intercomparison Report (PVIR) Climate Assessment Report (CAR) Product Specification Document (PSD) User Requirements Document (URD) Uncertainty Characterisation Report (UCR)

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	Algorithm Theoretical Basis Document (ATBD)
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 SLSTR

Summary	
Status of assessment	Dataset producer's information
Dataset name and version	ESA SST CCI SLSTR product version 3
Lead Investigator and/or Agency	Chris Merchant, University of Reading
Principal strengths of data set	Accurate dual-view retrieval consistent with ATSR-series
Principal recommended applications	Climate research particularly applications requiring long-term, stable, low-bias records of SST

Key Descriptive Features	
Period covered	2016-06-01 to 2021-12-31
Geographic range	Global
Spatial resolution	1 km irregular grid and 0.05° regular latitude-longitude grid
Temporal resolution	Global coverage every ~2 days (subject to cloud cover etc.)
Timeliness of new data	Extended by ICDR available at ~14 days latency
Dataset volume	5.0 TB (L2P), 915 GB (L3U), 175 GB (L3C)
Valid data fraction	SST from clear-sky observations only, this being ~14% of total data over oceans
Data level / grid	L2P (swath grid with 1 km at nadir) L3U/L3C (0.05° regular latitude-longitude grid)

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Observation technology	The Sea and Land Surface Temperature Radiometer (SLSTR) series of instruments.
Dependence on other data	Numerical weather prediction fields (ERA5)
Type(s) of SST	<ol style="list-style-type: none"> 1. Skin SST (SST of upper ~10 µm depth). 2. SST at 0.2 m (standardised with respect to diurnal cycle). Diurnal variability modelling is used to estimate SST20cm from SSTskin.
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

Availability, Documentation and Feedback	
Data URL / ftp / DOI	https://climate.esa.int/en/odp/#/dashboard L2P: https://doi.org/10.5285/f4151599eb7b491c9f4ce75489eb8b1e L3U: https://doi.org/10.5285/61b7a51d72b54692890d45818307d72f L3C: https://doi.org/10.5285/a104ed92bddd4c56b11127d4cc49b8d4
Primary peer reviewed reference	Embury, O., et al. (2024). Satellite-based time-series of sea-surface temperature since 1980 for climate applications. <i>Sci Data</i> 11, 326. doi: 10.1038/s41597-024-03147-w
Source of technical documents	https://climate.esa.int/en/projects/sea-surface-temperature
Dataset restrictions	None, free and open access
Facility for user feedback	https://climate.esa.int/en/projects/sea-surface-temperature
Other documentation	Algorithm Theoretical Basis Document (ATBD) Product Validation and Intercomparison Report (PVIR) Climate Assessment Report (CAR) Product Specification Document (PSD) User Requirements Document (URD) Uncertainty Characterisation Report (UCR)

Other Principles (GCOS)	
2. and 12. Overlaps between sensors exist and are exploited	Overlap between SLSTR-A and -B is used. There is no direct overlap with the previous dual-view ATSR instruments.
3. Detailed history of methods/algorithms is available	Algorithm Theoretical Basis Document (ATBD)
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)

5.4 AMSR

Summary	
Status of assessment	Dataset producer's information
Dataset name and version	ESA SST CCI AMSR product version 3
Lead Investigator and/or Agency	Chris Merchant, University of Reading
Principal strengths of data set	Provides SST observations in the presence of clouds. Microwave retrievals are not affected by water vapour and aerosols in the same way as infrared instruments.
Principal recommended applications	Climate research particularly applications requiring long-term, stable, low-bias records of SST

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Key Descriptive Features	
Period covered	2002-06-1 to 2017-10-26
Geographic range	Global
Spatial resolution	Approximately 50 km
Temporal resolution	Global coverage ~twice per day (subject to rain, RFI etc.)
Timeliness of new data	Data end in October 2017
Dataset volume	780 GB (L2P)
Valid data fraction	
Data level / grid	L2P (swath grid with ~50 km resolution)
Observation technology	Advanced Microwave Scanning Radiometers (AMSR) instruments on EOS-Aqua and GCOM-W1
Dependence on other data	Numerical weather prediction fields (ERA-interim)
Type(s) of SST	<ol style="list-style-type: none"> Subskin SST (SST of upper ~1 mm depth). SST at 0.2 m (standardised with respect to diurnal cycle). Diurnal variability modelling is used to estimate SST20cm from SSTskin.
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

Availability, Documentation and Feedback	
Data URL / ftp / DOI	https://climate.esa.int/en/odp/#/dashboard L2P: https://doi.org/10.5285/15a170dad3064fefa8936bd50877a93e
Primary peer reviewed reference	Embury, O., et al. (2024). Satellite-based time-series of sea-surface temperature since 1980 for climate applications. <i>Sci Data</i> 11, 326. doi: 10.1038/s41597-024-03147-w
Source of technical documents	https://climate.esa.int/en/projects/sea-surface-temperature
Dataset restrictions	None, free and open access
Facility for user feedback	https://climate.esa.int/en/projects/sea-surface-temperature
Other documentation	Algorithm Theoretical Basis Document (ATBD) Product Validation and Intercomparison Report (PVIR) Climate Assessment Report (CAR) Product Specification Document (PSD) User Requirements Document (URD) Uncertainty Characterisation Report (UCR)

Other Principles (GCOS)	
2. and 12. Overlaps between sensors exist and are exploited	No
3. Detailed history of methods/algorithms is available	Algorithm Theoretical Basis Document (ATBD)
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)

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5.5 Analysis

Summary	
Status of assessment	Dataset producer's information
Dataset name and version	ESA SST CCI Analysis product version 3
Lead Investigator and/or Agency	Chris Merchant, University of Reading
Principal strengths of data set	Statistically infilled combination of data from the ATSR, SLSTR, AVHRR, and AMSR series of sensors
Principal recommended applications	Climate research particularly applications requiring long-term, stable, low-bias records of SST

Key Descriptive Features	
Period covered	1980-01-01 to 2021-12-31
Geographic range	Global
Spatial resolution	0.05° regular latitude-longitude grid; actual resolution is not necessarily this fine (length scales governing the spreading of observation information range between 15 km and 300 km – see Fiedler et al. (2019)).
Temporal resolution	Daily
Timeliness of new data	Extended by ICDR available at ~14 days latency
Dataset volume	350 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)
Observation technology	AVHRR, ATSR, SLSTR, and AMSR sensors (see information above about individual sensors)
Dependence on other data	Single-sensor SST inputs to the analysis use numerical weather prediction fields (ERA Interim / ERA5). Analysis also uses sea-ice information (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

Availability, Documentation and Feedback	
Data URL / ftp / DOI	https://climate.esa.int/en/odp/#/dashboard https://doi.org/10.5285/4a9654136a7148e39b7feb56f8bb02d2
Primary peer reviewed reference	Embury, O., et al. (2024). Satellite-based time-series of sea-surface temperature since 1980 for climate applications. <i>Sci Data</i> 11, 326. doi: 10.1038/s41597-024-03147-w
Source of technical documents	https://climate.esa.int/en/projects/sea-surface-temperature
Dataset restrictions	None, free and open access
Facility for user feedback	https://climate.esa.int/en/projects/sea-surface-temperature
Other documentation	Algorithm Theoretical Basis Document (ATBD) Product Validation and Intercomparison Report (PVIR) Climate Assessment Report (CAR) Product Specification Document (PSD) User Requirements Document (URD) Uncertainty Characterisation Report (UCR)

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Other Principles (GCOS)	
2. and 12. Overlaps between sensors exist and are exploited	Yes (see information about the input datasets)
3. Detailed history of methods/algorithms is available	Algorithm Theoretical Basis Document (ATBD)
11. Constant sampling within diurnal cycle	SSTs are representative of daily averages.

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6. USING THE DATA FILES

The data files for the ESA SST CCI products are described in this section. ESA SST CCI files follow the GHRSSST Data Specification (GDS) version 2.0 (GHRSSST Science Team, 2012) and the ESA SST CCI Product Specification Document v2.1 (PSD). 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:

```
< Date>< Time>-ESACCI-< Level>_GHRSSST-<SST Type>-<Product>-<Dataset>_<Extra>-v02.0-fv<File version>.nc
```

For example:

```
20000101000206-ESACCI-L2P_GHRSSST-SSTskin-AVHRR15_G-CDR3.0-v02.0-fv01.0nc
```

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

6.1.1 Date

The identifying date for this file using ISO8601 basic format: 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 Time

An identifying time in the Coordinated Universal Time (UTC) using ISO8601 basic format: HHMMSS, where HH is the hour, MM is the minute and SS are the seconds. The time used depends on the level of the dataset:

- L2P** start time of file / granule.
- L3U** start time of file / granule.
- L3C** central time of collation window (120000 for daily files).
- L4** nominal time of analysis (120000 for daily files).

In the example filename the time is 00 hours, 1 minute and 5 seconds.

6.1.3 Level

The GHRSSST processing 'level' of the data; either L2P, L3U, L3C or L4. See Section 3.1.3 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, or SSTdepth (corresponding to ~10 μ m, ~1mm, 0.2m or ~10m). See Section 3.1.1 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.

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6.1.5 Product

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).

Table 5: Product codes used for ESA SST CCI products.

Product	Description
AATSR	Advanced Along Track Scanning Radiometer (AATSR) on Envisat satellite
ATSR<X>	Along Track Scanning Radiometer (ATSR) on ERS-1 or -2
AVHRR<X>_G	Advanced Very High Resolution Radiometer (AVHRR) on NOAA-<X> satellite (reduced "GAC" resolution)
AVHRRMT<X>	Advanced Very High Resolution Radiometer (AVHRR) on MetOp-<X> satellite (full resolution)
SLSTR<X>	Sea and Land Surface Temperature Radiometer (SLSTR) on Sentinel 3<X> satellite
AMSR<X>	Advanced Microwave Scanning Radiometer: AMSRE on EOS Aqua or AMSR2 on GCOM-W1 satellite
OSTIA	Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA)

6.1.6 Dataset

Shows which version of the CDR (or ICDR) this file belongs to. For the version 3 files this will be one of:

- CDR3.0
- ICDR3.0
- GLOB_CDR3.0
- GLOB_ICDR3.0

The 'GLOB' prefix is used for Level 4 files to maintain the conventions used for other files produced with the OSTIA system. The addition of 'GLOB' prefix denotes that the file contains global data.

6.1.7 Extra

Optional extra test used to distinguish between files with the same <Product> strings. This is used in in the case of L3C files to indicate if the file contains collated daytime or nighttime observations.

Note

The <Dataset> and <Extra> elements correspond to the GHRSSST <Additional Segregator> component, which is why they are separated by an underscore ("_") rather than a dash ("-").

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6.1.8 File version

A file version number in the form `xx.x` that is incremented when new versions of the file become available. The file version is separate to the product or dataset version (see section 6.1.6) and will only be used when it is necessary to replace files within a given dataset.

This is not expected to be used for CDR files, which are extensively tested before release. However, the short-delay ICDR files may need to be replaced, in which case an updated file version will be used.

6.2 Format of the data files

All data are contained in Network Common Data Format (netCDF; Unidata, 1989) files following Climate and Forecast (CF; Hassell et al., 2017) conventions and GDS2.0 (GHR SST Science Team, 2012). The netCDF format allows multiple data arrays and metadata to be stored together in one file. The CF-conventions are the de facto standard for netCDF formatting and metadata to ensure the files are flexible, self-describing, and interoperable across different communities. GDS2.0 is the international standard used for satellite-based SST data products. 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>
```

Or converted to netCDF-3 format using:

```
nccopy -3 <NetCDF4 file name> <netCDF3 file name>
```

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 GHR SST Data Specification version 2.0 (GHR SST Science Team, 2012),

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which is a file specification defined for use of SST data made available through the GHR SST project. The files also include metadata required by the CCI Data Standards v2.0 and follow the standards defined by the CF conventions (Hassell et al., 2017): <https://cfconventions.org/>.

Four different file formats are used for the ESA SST CCI data products. The specification chosen for each product depends on the 'level' of SST data contained within them (L2P, L3U, L3C or L4 – see Section 3.1.3 for definitions of these).

In the sections below each of the four file formats are described. First, the global attributes that are common to all the files are listed. Then, attributes that apply to variables are given. Finally, the variables that are contained in the files are listed for each data level in turn: L2P format in Section 6.4.3, L3U in Section 6.4.4, L3C in Section 6.4.5 and L4 in Section 6.4.6.

For a complete, technical description of the file format see the ESA SST CCI Product Specification Document (PSD) which can be downloaded from <https://climate.esa.int/en/projects/sea-surface-temperature/SST-key-documents/>.

6.4.1 Global attributes

The global attributes common to all the ESA SST CCI product files are described in Table 6 below. Most of the contents were adapted from the definitions in the GDS2.0 (GHR SST Science Team, 2012).

Table 6: Global attributes common to all SST CCI products.

Name of global attribute	Description	Contents or form of contents
Conventions	Describes the conventions followed when defining the contents of the file.	CF-1.5, Unidata Observation Dataset v1.0
title	A descriptive name for the data. Includes product string (see Section 6.1.5) and the data level of the product.	ESA SST CCI <Product String> <Data Level> product
summary	A description of the data. Includes product string (see Section 6.1.5), the data level of the product and the name of the algorithm used to produce the data (see ATBD).	<Product String> <Data Level> product from the ESA SST CCI project, produced using <algorithm name>.
references	References that provide more information about the data.	Embury, O. et al., 2024...
institution	A standardised name for the creators of the data file.	ESACCI
history	Used to detail the history of the data compilation.	e.g. Created using GBCS library v3.4.2
comment	Miscellaneous information.	
license	How the data are licensed for use.	Creative Commons Licence by attribution (https://creativecommons.org/licenses/by/4.0/)
id	This contains a name for the dataset that uniquely identifies it from other data provided through the GHR SST project.	e.g. AVHRR15_G-ESACCI-L2P-CDR-v3.0

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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.	e.g. 3.0
uuid	A Universally Unique Identifier for the file. For example see: http://www.ossf.org/pkg/lib/uuid/ .	e.g.: 088352d0-38ee-11ec-8566-1c34da4bed2e
tracking_id	Contains the same value as uuid above.	
gds_version_id	The version of the GDS [RD.87] that was followed when creating the file.	2.0
netcdf_version_id	The version of the NetCDF library used to create the file.	e.g. 4.3.2
date_created	File creation date in format shown in next column, where T is used to delimit the date and time information and Z indicates that the time is Coordinated Universal Time (UTC).	Format: yyyyymmddThhmmssZ
file_quality_level	A number that gives an indication of the quality of data in the file.	0: unknown quality; 1: extremely suspect; 2: suspect; 3: no known problems.
spatial_resolution	An indication of the spatial resolution of data in the file.	
start_time	Defines the time of the first measurement contained in the file. See date_created for explanation of the format.	Format: yyyyymmddThhmmssZ, replacing the lower case letters with the appropriate numbers
time_coverage_start	Identical to start_time.	See start_time
stop_time	As start_time but the time of the last measurement.	See start_time
time_coverage_end	Identical to stop_time.	See start_time
time_coverage_duration	Difference between stop_time and start_time in the form PdDThHmMsS. In this format, P indicates that it is a duration, DT delimits the number of days from the time, with H, M and S marking the hours, minutes and seconds.	Format: PdDThHmMsS, replacing the lower case letters with the appropriate numbers
time_coverage_resolution	Temporal resolution of data in the file i.e. the orbit repeat period or the frequency of L3/L4 data.	See time_coverage_duration
source	List of all source data used for the file.	e.g. AVHRR15_G-ESACCI-L1C-v1.7
platform	List of satellites on which the sensors used to generate the data were mounted.	e.g. NOAA-15
sensor	List of sensors used for the data in this file.	e.g. AVHRR_GAC
Metadata_Conventions	The name of metadata conventions followed.	Unidata Dataset Discovery v1.0
metadata_link	Link to metadata record.	https://doi.org/10.5285/ec659b31a8ca40918e58ec6d03af07a6
keywords	Standard words that describe the data, taken from the source specified in keywords_vocabulary.	Oceans > Ocean Temperature > Sea Surface Temperature

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keywords_vocabulary	Defines the source of the text in the keywords attribute; [RD.176].	NASA Global Change Master Directory (GCMD) Science Keywords
standard_name_vocabulary	Defines the source of the standard names for the variables [RD.177].	NetCDF Climate and Forecast (CF) Metadata Convention
geospatial_lat_units	Units of geospatial_lat_resolution.	degrees_north
geospatial_lat_resolution	Latitude resolution.	
geospatial_lon_units	Units of the geospatial_lon_resolution.	degrees_east
geospatial_lon_resolution	Longitude resolution.	
northernmost_latitude	Northern extent of the data.	
geospatial_lat_max	Identical to northernmost_latitude.	
southernmost_latitude	Southern extent of the data.	
geospatial_lat_min	Identical to southernmost_latitude	
easternmost_longitude	Eastern extent of the data.	
geospatial_lon_max	Identical to easternmost_longitude	
westernmost_longitude	Western extent of the data.	
geospatial_lon_min	Identical to westernmost_longitude	
geospatial_vertical_min	Depth of the deepest SST in the file (the value is negative as the direction is downwards).	
geospatial_vertical_max	Depth of the shallowest SST in the file (value is negative as the direction is downwards).	
acknowledgment	Funding source.	Funded by ESA
creator_name	Description of data creators.	Owen Embury
creator_email		o.embury@reading.ac.uk
creator_url		https://climate.esa.int/en/projects/sea-surface-temperature
creator_institution		University of Reading
Project	The name of the project.	Climate Change Initiative – European Space Agency
contributor_name	Additional institutions that contributed to the creation of this data.	JASMIN
contributor_role		This work used JASMIN, the UK's collaborative data analysis environment (https://jasmin.ac.uk)
publisher_name	Information about the data publisher.	NERC EDS Centre for Environmental Data Analysis
publisher_url		https://www.ceda.ac.uk
publisher_email		support@ceda.ac.uk
processing_level	Data level (L2P, L3U, L3C, or L4).	
cdm_data_type	Describes the form of the data (“swath” or “grid”).	
contact		https://climate.esa.int/en/projects/sea-surface-temperature

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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: Variable attributes used across SST CCI products.

Name of variable attribute	Description	Applicable to which variables?
_FillValue	The number put into the data arrays where there are no valid data (before applying the scale_factor and add_offset attributes).	Most variables but not applicable to latitude, longitude, time and flag fields.
Units	The units of the data after applying the scale_factor and add_offset conversion.	Most variables have this attribute.
scale_factor	Multiply the data stored in the NetCDF file by this number.	Most variables but not applicable to latitude, longitude, time and flag fields.
add_offset	After applying scale_factor above, add this to obtain the data in the units specified in the units attribute.	Most variables but not applicable to latitude, longitude, time and flag fields.
long_name	A descriptive name for the data.	All
valid_min	The minimum valid value of the data (before applying scale_factor and add_offset).	All
valid_max	The maximum valid value of the data (before applying scale_factor and add_offset).	All
standard_name	A unique descriptive name for the data, taken from the CF conventions (Hassell et al., 2017 http://cfconventions.org/)	Most (but not all variables have a corresponding standard name defined in the CF conventions)
comment	Miscellaneous information.	Most variables have this attribute.
source	A list of data sources used for the data in this variable.	Geophysical data variable.
References	References that provide more information about the data.	Applicable to a few variables (see also the global attribute with the same name).
Depth	Effective depth for SST data.	SST variables.
Coordinates	Identifies coordinate variables associated with a data array.	Variables in L2P files.
reference_datum	Information about the coordinates.	Latitude and longitude variables only.
Calendar	Information about the calendar used for the time coordinate.	Time variable only.
flag_meanings	List of descriptions of the meanings of flags, masks etc.	Only variables containing flags, masks or quality information.
flag_values	Mutually exclusive values that correspond to the meanings in flag_meanings e.g. 1, 2, 3, 4, 5. The variable will contain one of these numbers in each location.	Only variables containing flags, masks or quality information.

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flag_masks	Values that can be set in combination corresponding to the meanings in flag_meanings e.g. 1, 2, 4, 8, 16. The variable will contain in each location the sum of all the flags that are set e.g. if the first three flags are set the variable will contain 1+2+4=7.	Only variables containing flags, masks or quality information.
Height	Height that wind data corresponds to.	Used only for variables containing wind speed ancillary data.
time_offset	Difference between SST reference time and time that wind data correspond to (hours).	Used only for variables containing wind speed ancillary data.
correlation_length_scale	Estimated spatial correlation length scale for uncertainties.	Only used for some uncertainty variables.
correlation_time_scale	Estimated temporal correlation length scale for uncertainties.	Only used for some uncertainty variables.
axis	For variables containing coordinates, this indicates the axis that the coordinate corresponds to ('X', 'Y' or 'T' for longitude, latitude or time).	Coordinate variables only.
bounds	For coordinate variables, this indicates a variable that contains the bounds of the grid cells.	Coordinate variables only.

6.4.3 'L2P' data format

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

The dimensions of the data in the file are described in Table 8. The data are stored in variables in the netCDF file with the names given in Table 9.

Table 8: L2P netCDF dimensions.

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: List of variables found in L2P netCDF files. All variables have dimensions [time × nj × ni] unless specified (applies to lat, lon, and time).

Variable name	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.

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time [time]	A base time from which the time of each SST value is referenced. Here it refers to the start time of the granule. In order to determine the exact time of a specific pixel or grid cell variables, sst_dtime and sst_depth_dtime are provided (see below). These provide the difference in seconds between the pixel observation time and the reference time for the file.
sst_dtime	The time difference in seconds between the pixel observation time and the reference time for the file (see 'time' above).
sst_depth_dtime	The time difference in seconds between the pixel observation time adjusted to a standard local time and the reference time for the file (not available in all products).
Geophysical variables	
sea_surface_temperature	The best available skin (or sub-skin) SST retrievals with no adjustment to a standard depth or time.
sea_surface_temperature_depth	SSTs adjusted to a standard depth and local time.
sea_surface_temperature_depth_anomaly	SST anomaly difference between SST0.2m and ESA SST CCI Climatology v2.2
wind_speed	Wind speed (sourced from the ERA Interim or ERA-5 reanalysis).
depth_adjustment	May be added to sea_surface_temperature, if SST at 20cm at observation time is required.
adjustment_alt	May be added to sea_surface_temperature, if alternative SST retrieval is required (e.g. use of two-channel daytime retrieval at night).
Quality information and flags	
quality_level	Indicates the general quality of that pixel – higher values being better. Quantitative analyses should use the higher quality levels (4 or 5). Quality levels 2 and 3 may be useful for qualitative analyses, but the pixels have an increased chance of being cloud contaminated. See Table 10 for details.
l2p_flags	Indicates the type of pixel and what kind of SST retrieval was applied. Pixel type information includes: land, ice, lake, or river. Pixels in the Level 2 products may have these flags set but will not contain any SST data (other than the Caspian Sea). The dual-view bit (6) will be set for retrievals from one of the dual-view sensors (ATSR or SLSTR). The three-channel bit (7) indicates that the more accurate three-channel retrieval has been used. Although the three-channel retrieval can only be used at night, the use of the two-channel retrieval is not a guarantee that the pixel corresponds to a daytime observation (the retrieval may have switched to two-channel due to an instrument failure); therefore, there is a separate daytime flag (8) which indicates if the solar zenith angle was < 90° when the pixel was observed. When written in binary format, each digit of each number provides information about the retrieval in each location. The least significant digit is called bit 0 and there are 16 bits in total, although only 8 are currently in use. The meanings are detailed in Table 11.
sea_surface_temperature_retrieval_type	Type of retrieval used for the primary SST (sea_surface_temperature) <ol style="list-style-type: none"> 1. single view, two channel. 2. single view, three channel. 3. dual view, two channel. 4. dual view, three channel. 5. single view, 11 and 3.7 two channel. 6. single view, one channel.
alt_sst_retrieval_type	Type of retrieval used for the secondary SST (adjustment_alt)

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Uncertainty information	
sea_surface_temperature_total_uncertainty	The total uncertainty in the SSTs in the sea_surface_temperature variable.
sea_surface_temperature_depth_total_uncertainty	The total uncertainty in the SSTs in the sea_surface_temperature_depth variable (not available in all products).
uncertainty_systematic	Component of uncertainty that is correlated over large spatial scales.
uncertainty_correlated	Component of uncertainty that is correlated over synoptic (~100 km) spatial scales.
uncertainty_random	Component of uncertainty that is uncorrelated between SSTs.
uncertainty_correlated_time_and_depth_adjustment	Component of uncertainty associated with adjusting SSTs to a standard depth and time; correlated over synoptic (~100 km) spatial scales.
uncertainty_systematic_alt	As uncertainty_systematic, but for alternate SST.
uncertainty_correlated_alt	As uncertainty_correlated, but for alternate SST.
uncertainty_random_alt	As uncertainty_random, but for alternate SST.
Other	
sst_sensitivity	Estimated sensitivity of the retrieval to actual changes in sea surface temperature.
sses_bias	For ESA SST CCI data only it is safe to ignore this data array (it is filled with zeros). In other GHRST data files this is used to give an indication of bias in the SSTs.
sses_standard_deviation	Not used in ESA SST CCI data, use sea_surface_temperature_total_uncertainty instead.

Table 10: Quality Level definitions used for SST CCI products. Levels 4 and 5 are recommended for quantitative applications. Levels 2 and 3 may be useful for qualitative analyses.

Level	Name	Notes
0	no data	No data – e.g. land pixel
1	bad data	Bad data – e.g. cloudy, SST < 271.15 K, or sea-ice detected
2	worst usable data	Likely to be cloudy, poor quality retrieval, or high view angle
3	low quality	May be cloudy
4	good quality	ATSR: aerosol detected. AVHRR: solar contamination detected (and corrected).
5	best quality	

Table 11: I2p_flags definitions used to indicate the type of pixel and what kind of SST retrieval was applied. Bits 0-5 are defined by GDS, bits 6-8 are SST CCI extensions.

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 satellite views available	One (nadir) view	Two (dual) views
7	Number of satellite radiance channels available	Two	Three
8	Day/night	Night time	Day time (solar zenith angle < 90°)

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6.4.4 'L3U' data format

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

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

time: UNLIMITED (1)

lat: Number of latitude points (3600)

lon: Number of longitude points (7200)

The resolution used for the products is 0.05° hence the full size of the arrays is 7200×3600 . The time dimension is specified as **unlimited**, allowing standard netCDF tools to easily concatenate and manipulate multiple files, but each L3 file contains a single time slice (corresponding to a day).

The dimensions of the data arrays in the L3U files are defined in Table 12 and the coordinate variables found in the files are listed in Table 13, all other variables are the same as the L2P files listed in Table 9.

Table 12: L3U netCDF dimensions.

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

Table 13: List of coordinate variables found in L3U files. Other variables are the same as L2P files shown in Table 9.

Variable name	Description
lat [lat]	Central latitude of each grid cell.
lat_bnds [bnds × lat]	The latitudes of the edges of each grid cell.
lon [lon]	Central longitude of each grid cell.
lon_bnds [bnds × lon]	The longitudes of the edges of each grid cell.
time [time]	A base time from which the time of each SST value is referenced. Here it refers to the start time of the granule. In order to determine the exact time of a specific pixel or grid cell variables, sst_dtime and sst_depth_dtime are provided (see below). These provide the difference in seconds between the pixel observation time and the reference time for the file.
time_bnds [bnds × time]	The start and end times of the data collection for the data in the file.
sst_dtime [time × lat × lon]	The time difference in seconds between the pixel observation time and the reference time for the file (see 'time' above).
sst_depth_dtime [time × lat × lon]	The time difference in seconds between the pixel observation time adjusted to a standard local time and the reference time for the file (not available in all products).

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6.4.5 'L3C' data format

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

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

time: UNLIMITED (1)

lat: Number of latitude points (3600)

lon: Number of longitude points (7200)

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

The dimensions of the data arrays are the same as the L3U files listed in Table 12, as are the variables with coordinate variables listed in Table 13 and non-coordinate variables in the L2P Table 9. In the L3C files are defined in Table 13 and the variables found in the files are listed in Table 14.

Note

In L3C files the base time specified in the "time" variable is the centre time of the collation window (midday for daily files) as opposed to the start time of an uncollated L3U or L2P.

6.4.6 'L4' data format

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

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

time: UNLIMITED (1)

lat: Number of latitude points (3600)

lon: Number of longitude points (7200)

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

The dimensions of the data in an L4 file are described in Table 14 and the variables contained in the files are listed in Table 15.

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Table 14: L4 netCDF dimensions.

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

Table 15: List of variables found in L4 netCDF files. All variables have dimensions [time × lat × lon] unless specified (applies to lat, lon, time, and three “bnds” variables).

Variable name	Description
Coordinates	
lat [lat]	Central latitude of each grid cell.
lat_bnds [lat × bnds]	The latitudes of the edges of each grid cell.
lon [lon]	Central longitude of each grid cell.
lon_bnds [lon × bnds]	The longitudes of the edges of each grid cell.
time [time]	The time (middle of the day) that the data represent.
time_bnds [time × bnds]	The start and end time of the day that the data represent.
Geophysical variables	
analysed_sst	SST at each location. Note it is 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	Sea ice concentrations. These were produced by analysing input data sourced from the EUMETSAT Ocean and Sea Ice Satellite Application Facility (OSI SAF).
Quality information and flags	
mask	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: <ul style="list-style-type: none"> 0. Water 1. Land 2. Lake 3. Sea ice 4. River
Uncertainty information	
analysed_sst_uncertainty	Uncertainty in the SSTs (one error standard deviation).

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7. WORKED EXAMPLES

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 <https://step.esa.int/main/download/>. In this section some example uses of SNAP are provided. Each example makes use of the SNAP-Desktop application, a tool for displaying and analysing satellite data with an easy-to-use graphical user interface. Uses of the SNAP extend far beyond the examples shown here; users are encouraged to experiment with the software themselves.

7.1.1 Examining the contents of the ESA SST CCI products

SNAP can be used to open any of the ESA SST CCI product files using ‘Open Product’ in the file menu and a listing of the file contents is then displayed on the left of the screen. Please use the option “NetCDF following CF conventions” when asked to select a NetCDF format. Clicking on the items brings up additional windows that show the metadata associated with the file or variables, or an image view of the data. Figure 9 shows a screenshot of SNAP being used to display metadata from an AVHRR L2P file. 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 7.2.1 for more information about how to apply these manually).

The screenshot shows the SNAP Desktop application interface. The 'Product Explorer' on the left displays a tree view of metadata for a file named '20100909143121-ESACCI-L2P_GHRSSST-SSTskin-AVHRR18'. The 'Global_Attributes' window in the center shows a table of file-level metadata. The 'sea_surface_temperature' window on the right shows a table of variable-level metadata.

Name	Value	Type
Conventions	CF-1.5, Unidata Observation Dataset v1.0	ascii
references	http://climate.esa.int/en/projects/sea-surf	ascii
institution	ESACCI	ascii
history	Created using GBCS library v3.5.3	ascii
license	Creative Commons Licence by attribution (ascii
naming_authority	org_ghrsst	ascii
uuid	ad8a6ee2-a55b-11ec-a4de-1c34da4be42e	ascii
tracking_id	ad8a6ee2-a55b-11ec-a4de-1c34da4be42e	ascii
gds_version_id	2.0	ascii
netcdf_version_id	4.7.1 of Sep 26 2019 15:57:34	ascii
date_created	20220316T190251Z	ascii
file_quality_level	3	int32
spatial_resolution	4.0 km at nadir	ascii
start_time	20100909T143121Z	ascii
time_coverage_start	20100909T143121Z	ascii
stop_time	20100909T162035Z	ascii
time_coverage_end	20100909T162035Z	ascii
time_coverage_duratio	P0DT01H49M14S	ascii
time_coverage_resoluti	P0DT1H40M00S	ascii
source	AVHRR18_G-ESACCI-L1C-v1.7, ERA_INTERI	ascii
platform	NOAA-18	ascii
sensor	AVHRR_GAC	ascii
Metadata_Conventions	Unidata Dataset Discovery v1.0	ascii
metadata_link	http://climate.esa.int	ascii
keywords	Oceans > Ocean Temperature > Sea Surfac	ascii
keywords_vocabulary	NASA Global change Master Directory (GCI	ascii
standard_name_vocabu	NetCDF Climate and Forecast (CF) Metadati	ascii
geospatial_lat_units	degrees_north	ascii
geospatial_lat_resoluti	0.01	float32
geospatial_lon_units	degrees_east	ascii
geospatial_lon_resoluti	0.01	float32

Name	Value	Type
long_name	sea surface skin temperature	ascii
standard_name	sea_surface_skin_temperature	ascii
units	kelvin	ascii
_FillValue	-32768	int16
add_offset	273.15	float32
scale_factor	0.01	float32
valid_min	-200	int16
valid_max	5000	int16
comment	Temperature of the skin of the ocean;	ascii
references	http://climate.esa.int/en/projects/sea-s	ascii
depth	10 micrometres	ascii
coordinates	lon lat	ascii
ancillary_variables	sea_surface_temperature_total_uncert	ascii
source	AVHRR18_G-ESACCI-L1C-v1	ascii
actual_range.1	271.15	float32
actual_range.2	306.11	float32
_ChunkSizes.1	1	uint32
_ChunkSizes.2	1280	uint32
_ChunkSizes.3	409	uint32

Figure 9: Using SNAP to display metadata about the file and one of the variables stored in the file.

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SNAP can also be used to quickly display and explore the SST data as shown in Figure 10 which illustrates both the land sea mask (extracted from the l2p flag metadata) and the sea_surface_temperature variable. The l2p_flags variable within the NetCDF file has attributes that describe how to interpret the flags. These attributes are shown at the right of the figure – the first tab “l2p_flags” shows how SNAP has interpreted the metadata and is opened from the Product Explorer by following Flag Codings -> l2p_flags; we can also access the full set of metadata for the variable as shown in the second tab “l2p_flags (2)” via Metadata -> Variable Attributes -> l2p_flags. When interpreting the metadata manually the flag_mask and flag_meaning attributes need to be used together. For example, if the l2p_flags variable is masked using the value 2, locations that are land are revealed.

We can extract the land mask as a separate “band” using the Band Maths function: either using the menu Raster -> Band Maths... or right-clicking on the l2p_flags variable and selecting Band Maths... will bring up the dialog shown in Figure 11. The data in the l2p_flags variable has had a bitwise AND operation applied with the number 2, which corresponds to land ('l2p_flags & 2'). Note that SNAP has the facility to use the flag codings directly without extracting them to separate bands. We do this to overlay a mask on the SST data as shown in Figure 10 (central tab) using the Mask Manager tab (far right). Clicking the f(x) button will create a new mask based on a logical band maths expression as shown in Figure 12

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

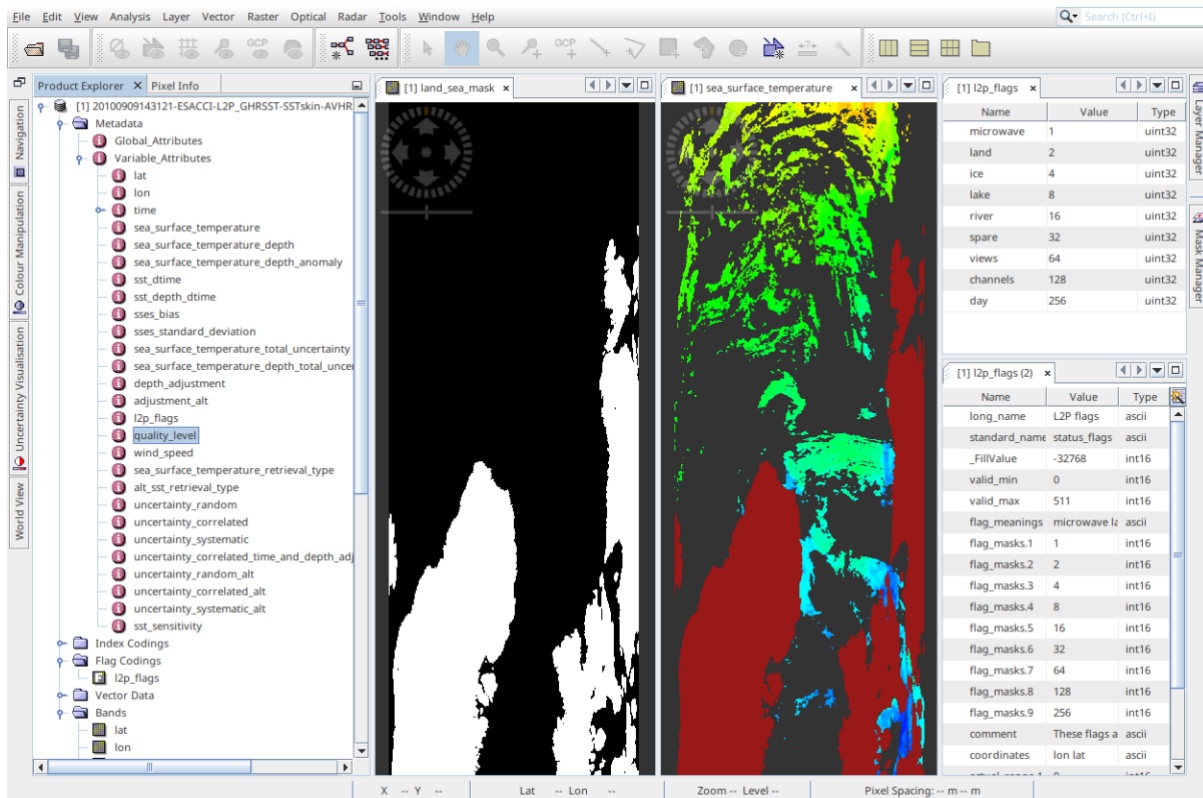


Figure 10: Displaying the SST data and land sea mask in SNAP.

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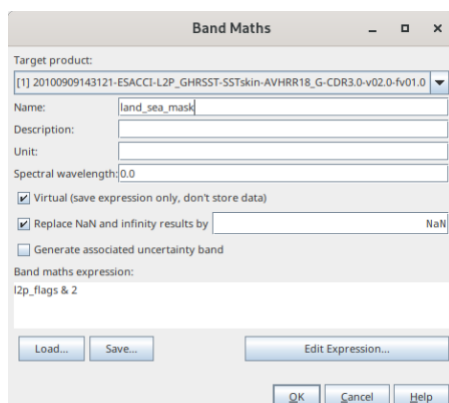


Figure 11: Using the Band Maths dialog to extract a land sea mask from the l2p_flags variable.

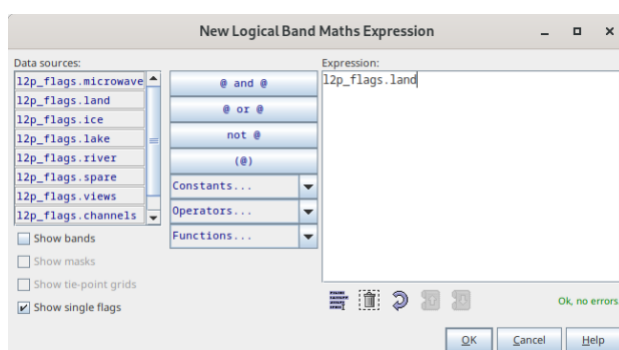


Figure 12: Using the Mask Manager to overlay the land sea mask over the SST data.

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

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

To obtain the difference between the adjusted SSTs and the non-adjusted SSTs, 'Band Maths' was selected from the Raster menu. Then, 'Edit expression' was selected from the window that pops up, which provides an expression editor for defining the mathematics that are required (in this case 'sea_surface_temperature_depth - sea_surface_temperature'). The resulting data are shown in Figure 13. A land mask overlay was also added 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 -0.07°C and 0.42°C and the median was 0.1250°C).

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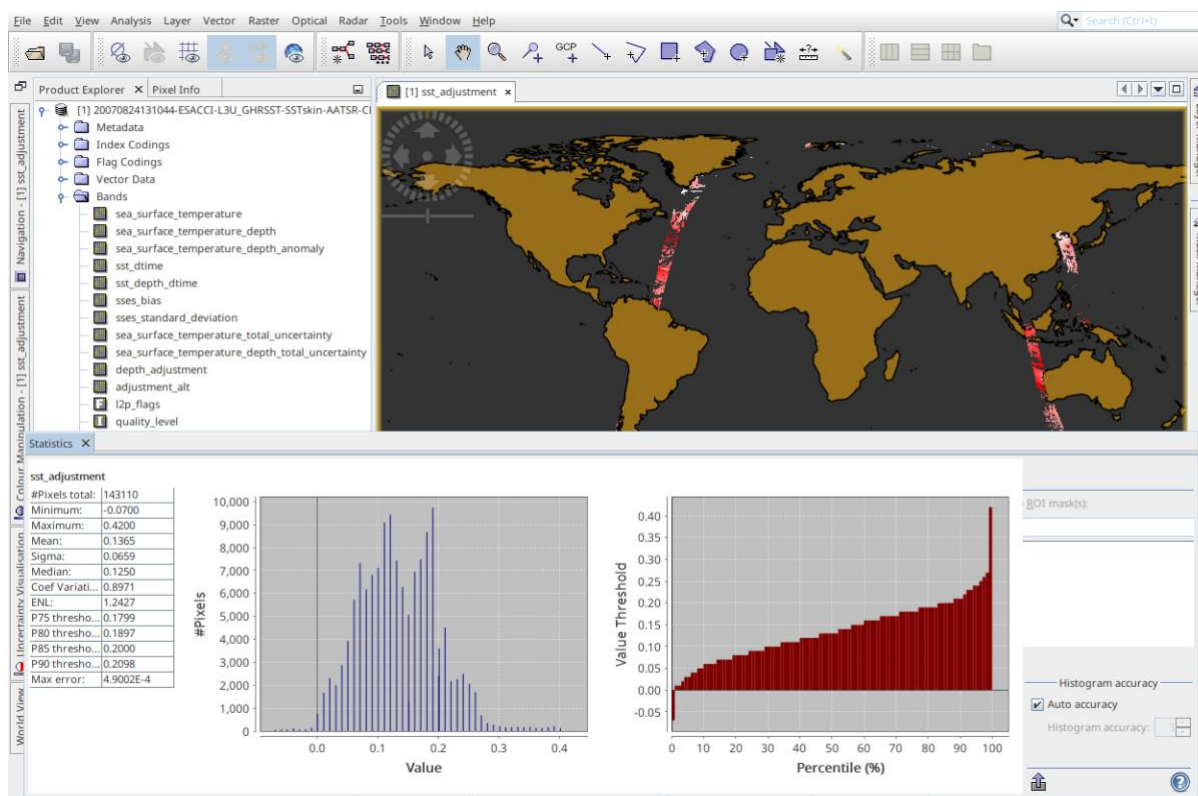


Figure 13: Using SNAP to show the differences between the adjusted and unadjusted SST data in a L3U file. A histogram of the differences is also being displayed.

7.1.3 Detailed example of working with L4 data with SNAP

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

The original data are shown in Figure 14, in which SNAP is being used to display the SST field. The first step of the processing was to apply a Sobel West filter, which approximates the local zonal gradients in the SST field. This is done very simply by selecting 'Filtered Band ...' from the Raster menu. The mask variable is also used, to determine where there are valid ocean SSTs. To do this, right clicking on the filtered data band in the list to left of the screen brings up the 'properties' menu. The button marked '...' to the right of the valid pixel expression box brings up an expression editor which allows the user to define valid data. This process is shown in Figure 15. The same process was then used to apply a Sobel North filter. The range of gradients displayed are much larger meridionally than zonally. The two bands are then combined with the Band Maths option from the Raster Menu as shown in Figure 16.

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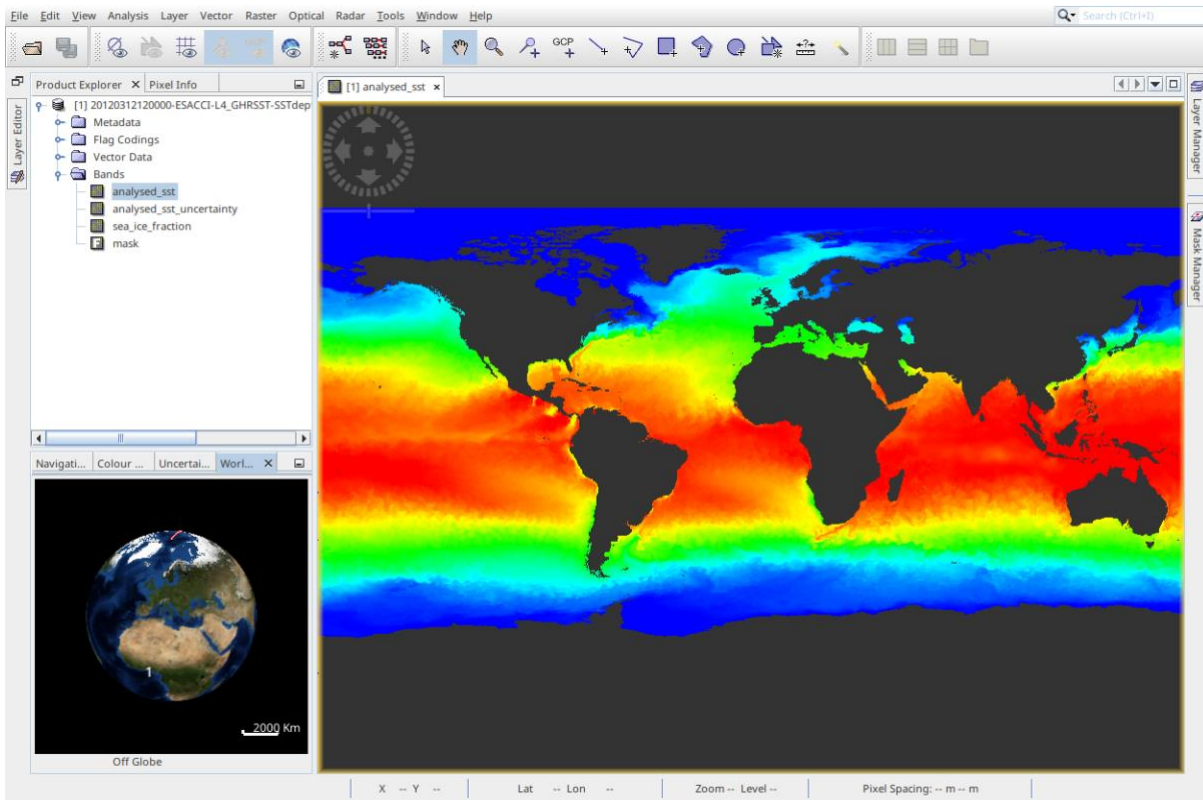


Figure 14: Starting point of the example of filtering with SNAP.

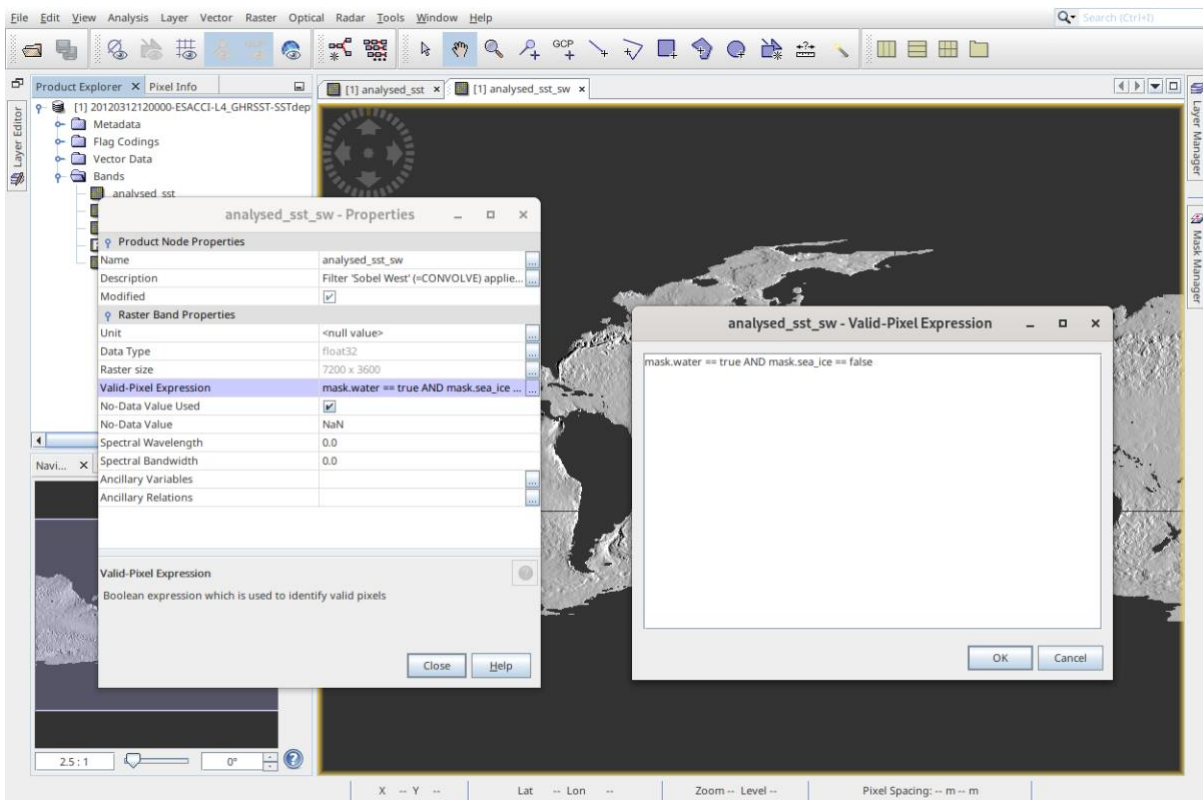


Figure 15: Using the mask to remove data affected by ice etc.

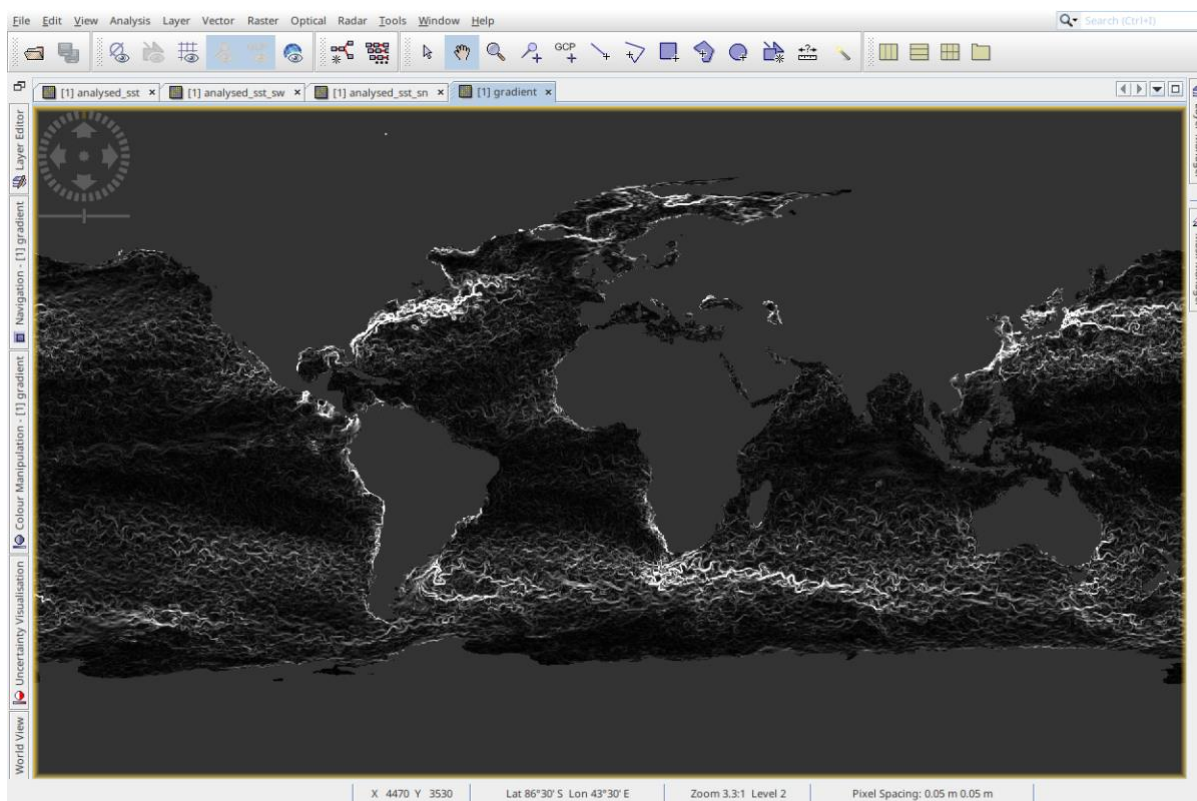
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Figure 16: The final SST gradient calculated by combining the Sobel North and West filters.

7.2 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 – <https://unidata.github.io/netcdf4-python/> – for reading and writing netCDF files.
- Matplotlib – <https://matplotlib.org/> – for scientific plotting [RD.323].
- Cartopy – <https://scitools.org.uk/> – for plotting geospatial data.
- Iris – <https://scitools.org.uk/> – tools for analysing and plotting geophysical data [RD.324].

However, there are dependences on other modules (for example use of the numpy module, <http://www.numpy.org>) that will need to be installed. Python version 3 is used for these examples.

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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.

7.2.1 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 Level 4 Analysis. 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 17.

```
import netCDF4
import cartopy.crs as ccrs
import matplotlib.pyplot as plt

# Open the ESA SST CCI file
nc = netCDF4.Dataset('20061126120000-ESACCI-L4_GHRSSST-SSTdepth-OSTIA-GLOB_CDR3.0-
v02.0-fv01.0.nc')

# Open the SST and ice variables
sst = nc.variables['analysed_sst']
ice = nc.variables['sea_ice_fraction']

# Extract the name and units from the variable attributes
sst_label = f'{sst.long_name} [{sst.units}]'
ice_label = f'{ice.long_name} [{ice.units}]'

# The data variables have dimensions: time, lat, lon
# Where the time dimension is length one. So we extract
# the first slice to get a 2d array for plotting
sst = sst[0]
ice = ice[0]

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

# Latitude values start at south (-90) and increase to north (90)
# so we must specify the origin to be "lower"
ax = fig.add_subplot(2, 2, 1)
ax.imshow(sst, origin='lower')
ax.set_title('Analysed SST')
ax.set_xlabel('Column')
ax.set_ylabel('Row')

# Now plot using cartopy so we can reproject the data and add
# coastlines etc.

# Cartopy projection parameters for the Level 4 data
proj = ccrs.PlateCarree() # Equirectangular grid
extent = (-180, 180, -90, 90) # Global: 180W to 180E, 90S to 90N
```

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```
ax = fig.add_subplot(2, 2, 2, projection=ccrs.PlateCarree())
imsst = ax.imshow(sst, transform=proj, extent=extent, origin='lower',
interpolation='nearest')
ax.coastlines()
ax.set_title('Analysed SST')

# Plot the sea ice data in a polar projection
ax = fig.add_subplot(2, 2, 3, projection=ccrs.Orthographic(0, 90))
imice = ax.imshow(ice, transform=proj, extent=extent, origin='lower',
interpolation='nearest')
ax.coastlines()
ax.set_title('Sea ice area fraction')
ax.set_extent([-180, 180, 50, 90], ccrs.PlateCarree())

ax = fig.add_subplot(2, 2, 4, projection=ccrs.Orthographic(0, -90))
ax.imshow(ice, transform=proj, extent=extent, origin='lower',
interpolation='nearest')
ax.coastlines()
ax.set_title('Sea ice area fraction')
ax.set_extent([-180, 180, -90, -50], ccrs.PlateCarree())

# Add some color bars
fig.colorbar(imsst, ax=fig.axes[0], location='bottom', label=sst_label, pad=0.1)
fig.colorbar(imsst, ax=fig.axes[1], location='bottom', label=sst_label, pad=0.1)
fig.colorbar(imice, ax=fig.axes[2], location='right', label=ice_label, pad=0.1)
fig.colorbar(imice, ax=fig.axes[3], location='right', label=ice_label, pad=0.1)

fig.tight_layout()
fig.savefig('l4_sst.png')
plt.show()
```

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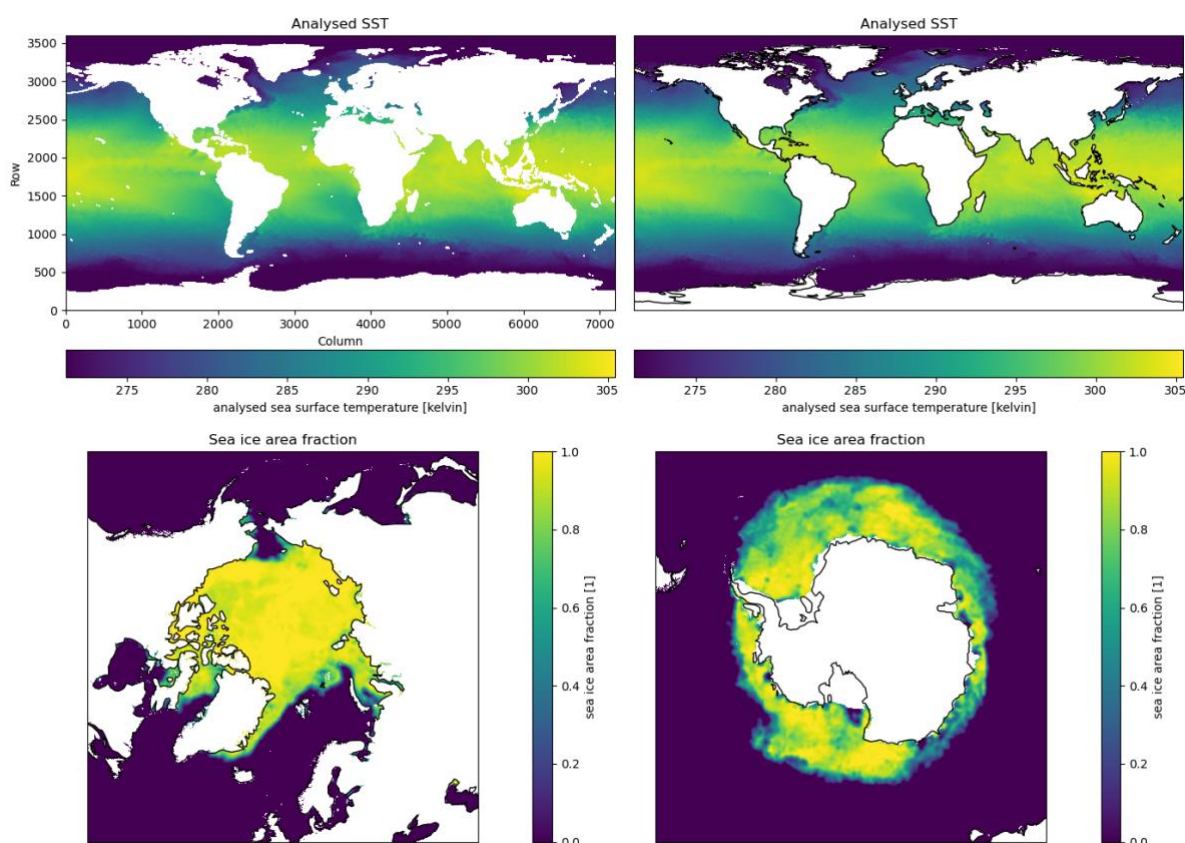


Figure 17: Result of applying the Python code to read and visualise the data.

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: $\text{converted_data} = \text{original_data} \times \text{scale_factor} + \text{add_offset}$.
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 Level 4 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

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arrays rather than longitude and latitude and in the geospatial plots we had to manually specify the geographic extent.

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

7.2.2 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 Level 4 SST data shown in Section 7.2.1 above. The result of running this code is shown in Figure 18.

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

file = '20061126120000-ESACCI-L4_GHRSSST-SSTdepth-OSTIA-GLOB_CDR3.0-v02.0-
fv01.0.nc'

# Load the SST CCI file into iris data structures known as 'cubes'. A Level 4
# SST file will result in two cubes: SST, and sea ice fraction
# Other variables such as the mask and uncertainty field will be loaded as
# 'ancilliary' variables inside the cubes.
cubes = iris.load(file)
print(cubes)
# 0: sea_ice_area_fraction / (1)          (time: 1; latitude: 3600; longitude: 7200)
# 1: sea_water_temperature / (kelvin)    (time: 1; latitude: 3600; longitude: 7200)

# We can extract the SST cube using its standard name (from the CF conventions)
# A slice operation [0] is used to remove the time dimension
sst = cubes.extract_cube('sea_water_temperature')[0]
ice = cubes.extract_cube('sea_ice_area_fraction')[0]

# Plot the SST data
fig = plt.figure()
qplt.contourf(sst)
fig.gca().coastlines()
fig.savefig('iris_sst.png')

# Plot the sea-ice data
fig = plt.figure()
qplt.contourf(ice)
fig.gca().coastlines()
fig.savefig('iris_ice.png')

# We can use the mask variable (standard name = status_flag) to mask
# any areas affected by sea ice etc. The mask variable is read as an
# ancilliary variable of the main data variables
# A value of 1 corresponds to open sea water
mask = sst.ancillary_variable('status_flag').data != 1
fig = plt.figure()
qplt.contourf(iris.util.mask_cube(sst, mask))
fig.gca().coastlines()
fig.savefig('iris_masked.png')
```

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```
plt.show()
```

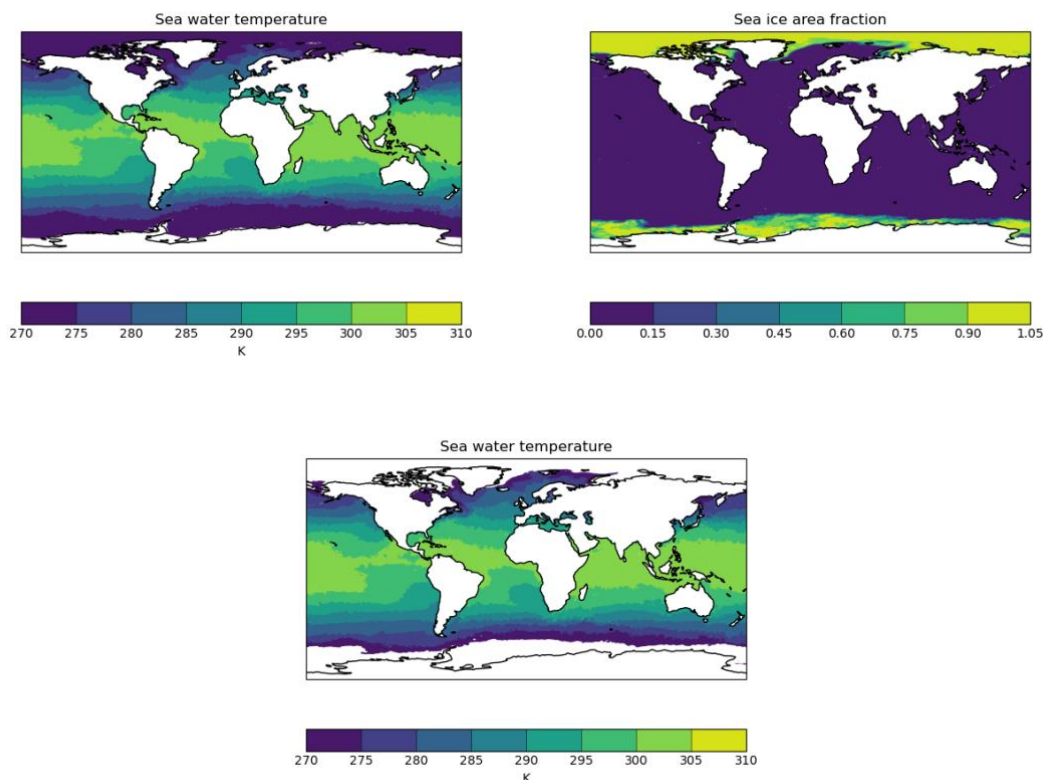


Figure 18: Result of using the iris module to read and plot the analysed SST data. Top-left: plot of all SST data; Top-right: plot of all sea-ice data; Bottom: plot of SST for open-sea only areas (exclude sea-ice and lakes etc.)

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 lower panel in Figure 18 shows the result of masking out any areas corresponding to high sea ice concentrations or lakes.

Similarly, when using L2P, L3U and L3C data, it is desirable to check the flags and quality level information. Use of the `l2p_flags` variable was demonstrated in Section 7.1.1. This provides information about the type of SST retrieval and whether a location is over the land, ice, lake or rivers. Also available, in the `quality_level` variable, is a rating of the quality of each SST. A plot of this variable from an example Phase 1 Release 1 L3U file is shown in Figure 19, with the code used given below. Note that there are more quality levels in version 2 products.

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

```
# Variable is selected using the long_name attribute because there is no
# standard_name attribute for this.
```

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```

cube = iris.load_cube(
    '20061126000044-ESACCI-L3U_GHRSSST-SSTskin-AATSR-LT-v02.0-fv01.0.nc',
    'quality level of SST pixel')
qplt.pcolormesh(cube[0, :, :])
plt.gca().coastlines()
plt.show()

```

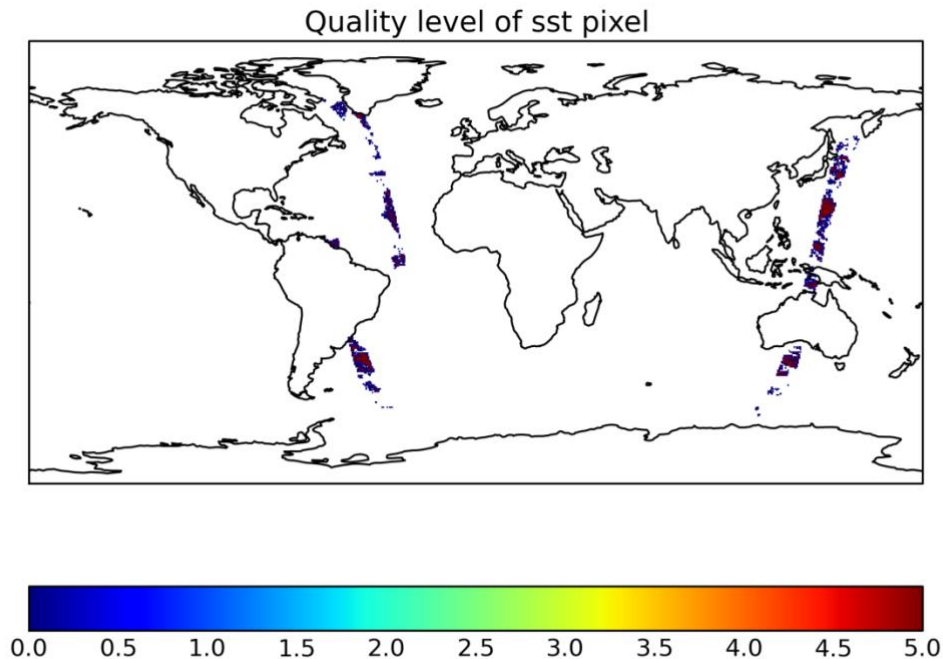


Figure 19: Quick plot of the quality_level variable from a L3U file.

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

```
print SSTCube
```

The result of this is:

```

sea_water_temperature / kelvin      (latitude: 3600; longitude: 7200)
  Dimension coordinates:
    latitude                          x                -
    longitude                          -                x
  Scalar coordinates:
    time: 2006-11-26 12:00:00
  Attributes:
    Conventions: CF-1.5, Unidata Observation dataset v1.0
    Metadata_Conventions: Unidata Observation Dataset v1.0
    acknowledgment: Funded by ESA
    cdm_data_type: grid
    comment: SST analysis produced for ESA SST CCI project using the OSTIA
system in...
    creator_email: science.leader@esa-sst-cci.org
    creator_name: ESA SST CCI
    creator_processing_institution: These data were produced at the Met
Office as part of the ESA SST CCI ...
    creator_url: http://www.esa-sst-cci.org

```

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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: GHRSSST 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

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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.

7.3 Example of working with the uncertainty information

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

More detailed information about uncertainty information for the SST CCI products can be found in material presented at a user workshop on uncertainties (<https://climate.esa.int/en/projects/sea-surface-temperature/SST-key-documents/#sst-cci-user-workshop-on-uncertainties-18--20-november-2014>). As well as material from presentations on the uncertainties, practical exercises on using the uncertainties can also be found there.

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

1. Random uncertainty components should be aggregated by:
 - a. Square the random uncertainty numbers that correspond to the SSTs to be averaged.
 - b. Sum the values obtained in a.
 - c. Calculate the square root of the result of b.
 - d. Divide result of c by the number of SST values being averaged.

Mathematically this is represented by: $\frac{1}{n} \sqrt{\sum_{i=1}^n \sigma_i^2}$ 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:

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- i. Square the synoptically correlated uncertainty numbers that correspond to the SSTs to be averaged.
 - ii. Sum the values obtained in a(i).
 - iii. Divide a(ii) by the number of SSTs.
 - b. Calculate the effective number of synoptic areas in the grid box:
 - i. Find the mean spatial separation of the SSTs that are being averaged (in km) and divide the result by the spatial correlation length scale of the uncertainties (100 km).
 - ii. Find the mean temporal separation of the SSTs that are being averaged (in days) and divide the result by the temporal correlation length scale (1 day).
 - iii. Calculate the reciprocal of the exponent of the average of b(i) and b(ii).
 - iv. Calculate the result of b(iii) multiplied by the number of SSTs being averaged minus one, and then add one to the result.
 - v. The effective number of synoptic areas is the number of SSTs being averaged divided by the result of b(iv).
 - c. Divide the result of a by the result of b and calculate the square root
- Mathematically, this is:

$$\sqrt{\frac{1}{\eta} \frac{\sum_{i=1}^n \sigma_i^2}{n}}$$

Where

$$\eta = \frac{n}{1 + \exp\left(-\frac{1}{2}\left(\frac{d_{xy}}{100} + d_t\right)\right)}(n - 1)$$

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

3. Large scale correlated uncertainties should be aggregated by:
 - a. Sum the large scale correlated uncertainty values that correspond to the SSTs to be averaged.
 - b. Divide the result of a by the number of SSTs being averaged.

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

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8. DICTIONARY OF ACRONYMS, ABBREVIATIONS AND JARGON

Item	Definition
(A)ATSR	(Advanced) Along Track Scanning Radiometer
AVHRR	Advanced Very High Resolution Radiometer
AMSR	Advanced Microwave Scanning Radiometer
C3S	Copernicus Climate Change Service
CCI	Climate Change Initiative
CDR	Climate Data Record
CEDA	Centre for Environmental Data Analysis
CF	Climate Forecast
DMI	Danmarks Meteorologiske Institut (Danish Meteorological Institute)
ECV	Essential Climate Variable
Envisat	Environment Satellite; an ESA satellite
EOCIS	UK Earth Observation Climate Information Service
EOS	Earth Observing System
EPS	EUMETSAT Polar System
ERS	European Remote-Sensing Satellite
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
EXP	Experimental product release
GAC	Global Area Coverage
GCOM	Global Change Observation Mission
GCOS	Global Climate Observing System
GDS	GHRSSST Data Processing Specification
GHRSSST	Group for High-Resolution SST
HadCRUT4	The Met Office Hadley Centre and University of East Anglia dataset of gridded historical surface temperature anomalies version 4.
HadSST2 and HadSST3	The Met Office Hadley Centre dataset of gridded in situ temperature anomalies, versions 2 and 3.
HadISST1	The Met Office Hadley Centre sea ice and sea surface temperature dataset version 1.
ICDR	Interim Climate Data Record
IR	Infrared
in situ observations	Observations made by an instrument at the position of the thing being measured.
L2P	Level 2 Pre-processed data; see Section 3.1.3.
L3U	Level 3 Uncollated data; see Section 3.1.3.
L3C	Level 3 Collated data; see Section 3.1.3.
L4	Level 4 data; see Section 3.1.3.
MCAS	Marine Climate Advisory Service
MD	Matchup Dataset

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Item	Definition
MMD	Multi-sensor Matchup Dataset
MetOp	Meteorological Operational (EUMETSAT satellite)
MSG	Meteosat Second Generation
NetCDF	Network Common Data Format
NOAA	National Oceanic and Atmospheric Administration
OSI SAF	Ocean and Sea Ice Satellite Application Facility
OSTIA	Operational Sea Surface Temperature and Sea Ice Analysis
PMWR	Passive Microwave Radiometers
POES	Polar Operational Environmental Satellites
Retrieval	A term used for the process of calculating SST from the measurements made by a satellite instrument.
SEVIRI	Spinning Enhanced Visible and Infrared Imager
SLSTR	Sea and Land Surface Temperature Radiometer
SNAP	Sentinel Application Platform software
SST	Sea Surface Temperature
UNFCCC	United Nations Framework Convention on Climate Change
UTC	Coordinated Universal Time

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