


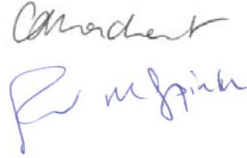
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**Project** : CCI Phase 1 (SST)

**Title** : CCI-SST System Requirements Document

**Abstract** :

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**EUROPEAN SPACE AGENCY  
CONTRACT REPORT**

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## AMENDMENT RECORD

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

### AMENDMENT RECORD SHEET

ISSUE	DATE	REASON FOR CHANGE
0.1	17 Nov 2011	Document structure, TOC
0.3	05 Dec 2011	Document structure updated w.r.t. document template definition proposed by ESA (C. Donlon)
0.6	13 Feb 2012	Document completed for internal team review
0.8	22 Feb 2012	Updates and comments integrated after internal team review
0.9.2	28 Feb 2012	Submitted version for review by ESA
0.9.3	19 March 2012	As a pre-RIDs request of ESA (C Donlon), identified the system requirements arising from points discussed in Section 2 immediately within that section, to aid traceability to Section 3 (although note that all such traceability is also provided for within Section 4).
1.0	23 April 2012	RID telecon discussion of 29 March and RID responses integrated
1.1	30 April 2012	Second RID telecon of 27.04.2012, conclusions integrated
1.2	07 May 2012	PM6, additional comments by C. Donlon, requirements added

### RECORD OF CHANGES IN THIS ISSUE

Issue	Page/Sec.	Reason	Change
1.0	8 / 2.1	RID CD-1	Cloud clearing and sea ice detection added as challenges
1.0	9 / 2.2	RID CD-2	Active role of development team regarding user feedback
1.0	9 / 2.2 + all occurrences in doc	RID CD-3	Science team replaced by SST CCI development team, "supervises production" changed to "directs and prioritizes production" to distinguish its role from the operations team.
1.0	9 / 2.2	RID CD-4	Distinction between internal QA before release and external validation by users with feedback introduced
1.0	13 / 2.3	RID CD-5	Restriction to a subset of DARD inputs removed, numbering of DARD inputs adjusted to current version
1.0	14 / 2.4	RID CD-6	Statement on de-centralised approach re-worded
1.0	14 / 2.4	RID CD-7	Justification added to common services
1.0	14 / 2.4	RID CD-8	Clarified that sharing of services will be defined during design
1.0	15 / 2.5	RID CD-9	Figure updated

Issue	Page/Sec.	Reason	Change
1.0	15 / 2.5	RID CD-10	"continuous improvement added to "problem solving" See RID CD-13
1.0	15 / 2.5	RID CD-11	See change for RID CD-3
1.0	16 / 2.5	RID CD-12	Reference to section 2.6 sensor constellations added
1.0	15 / 2.5	RID CD-13	Caption extended to explain large cycle with user feedback OPS-4 description extended to explicitly name user feedback
1.0	15 / 2.5	RID CD-14	OPS-1 description extended to explain "problem solving"
1.0	16 / 2.5	RID CD-15	Number of cycles in phase 2 removed
1.0	16 / 2.5	RID CD-17	"may" uncover new problems instead of "will"
1.0	16 / 2.5	RID CD-18	"continuously updated" changed to "continuously extended"
1.0	17 / 2.5	RID CD-19	OPS-3 renamed
1.0	17 / 2.6	RID CD-20	Reference to SoW Annex G added
1.0	18 / 2.6.1.1	RID CD-21	Reference to GCOS satellite supplement added
1.0	18 / 2.6.1.1	RID CD-22	Ship-mounted radiometers added for bridging AATSR to SLSTR.
1.0	20 / 2.6.1	RID CD-23	Cloud cover named as advantage of MW sensors in comparison to IR sensors.
1.0	22 / 2.6.1	RID CD-25	Reference to GCOS satellite supplement added
1.0	22 / 2.6.1	RID CD-26	Reasoning for geostationary made more explicit
1.0	23 / 2.6.2	RID CD-28	CMS and OSTIA named as examples for a Metop data provider and L4 analysis system only.
1.0	24 / 2.6.4	RID CD-29	Support for gathering feedback, open access to data, documentation, algorithms
1.0	26 / 2.6.5	RID CD-30	Science team renamed to development team
1.0	30 / 2.7	RID CD-31	Hint added that implementation can expected to be different in CCI phase 2
1.0	36 / 3.1.3	RID CD-35	Note added to SST-SR-6170 that development team maintains URD and collects feedback from users.
1.0	36 / 3.2.1	RID CD-36	Note dropped from SST-SR-1130
1.0	37 / 3.2.1	RID CD-37	Long term preservation of released CDRs added to SST-SR-1240
1.0	38 / 3.2.1	RID CD-38	Note added to SST-SR-1250 that development team maintains ATBD
1.0	38 / 3.2.1	RID CD-39	Note added to SST-SR-1290 that development team maintains PSD
1.0	39 / 3.2.1	RID CD-41	SST-SR-1370 wording modified to make clear that only the types of chains of the prototype are to be supported, but with the actual processors and versions of SST CCI Phase 2
1.0	41 / 3.2.3	RID CD-42	Note added to SST-SR-2180 to explain 72 hours constraint

Issue	Page/Sec.	Reason	Change
1.0	42 / 3.2.3	RID CD-43	Processing speed average specified more explicitly
1.0	42 / 3.2	RID CD-44	Requirement added that system framework development shall follow a tailored ECSS-E-40.
1.0	43 / 3.3.1	RID CD-46	SST-SR-3110 updated to ingest all Phase 1 data, not only a subset
1.0	44 / 3.3.1	RID CD-47	SST-SR-3160 implementation node (RTTOV) dropped
1.0	45 / 3.3.2	RID CD-50	Forward reference added to requirements defining user access to MMS and its outputs
1.0	48 / 3.4.1	RID CD-51	OGC CSW required for a catalogue interface in SST-SR-6250
1.0	49 / 3.4.1	RID CD-52	SST-SR-6280 modified to require read access to the processor repository to any user without restriction.
1.0	49 / 3.4.2	RID CD-54	SST-SR-6330 extended by hint on update frequency of web site
1.0	49 / 3.4.2	RID CD-55	"science team" changed to "development team", see change for RID CD-3
1.0	49 / 3.4.2	RID CD-56	Sentence about involvement of climate users in the process of evaluation and feedback added
1.0	49 / 3.4.2	RID CD-57	SST-SR-5215 modified to make clear that collection and re-assessment of requirements supports the decision making process.
1.0	50 / 3.4.4	RID CD-58	Availability figure in SST-SR-6370 specified "per year" now
1.0	51 / 3.5.1	RID CD-59	Clouds added to SST-SR-5180
1.0	52 / 3.5.1	RID CD-60	SST-SR-5215 modified to remove reference to OSTIA/Met Office.
1.0	52 / 3.5.2	RID CD-62	SST-SR-5250 modified to define participants of decision process for new versions
1.0	52 / 3.5.2	RID CD-63	SST-SR-5260 modified to follow a model of an open initial release of a dataset for validation and later final release
1.0	2.6.1.1	New information	Comments regarding plans for Metop series updated.
1.0	2.6.1.1	New information	Concept of exploiting IASI to monitor/control the calibration stability of Metop added to scenario.
1.1	18 / 2.5	RID CD-2	Figure 2-5 updated to include feedback <i>and evidence</i>
1.1	11 / 2.2	RID CD-3	Development team directs <i>sequence of operations</i> within their agreed scope
1.1	11 / 2.2	RID CD-4	Users <i>independently</i> validate
1.1	11 / 2.2	RID CD-11	Mandate / terms of reference of development team added
1.1	18 / 2.5	RID CD-13	Thin blue lines removed from figure 2-5
1.1	19 / 2.5	RID CD-19	Decisions shall be driven by evidence, sentence added to OPS-6
1.1	25 / 2.6.1	RID CD-26	Team is no longer mentioned
1.1	32 / 2.7.3	RID CD-31	Caption of phase 1 figure extended: provided here for guidance

Issue	Page/Sec.	Reason	Change
1.1	41 / 3.1.3	RID CD-33	Forward reference to performance and sizing requirements of time series production added to output product requirements
1.1	43 / 3.2.1	RID CD-37	Long-term stewardship instead of only long-term preservation of released CDRs
1.1	43 / 3.2.1	RID CD-38	Specified that incremental ATBD version is provided with system freeze for new CDR version
1.1	43 / 3.2.1	RID CD-39	Specified that incremental PSD version is provided with system freeze for new CDR version
1.1	44 / 3.2.1	RID CD-40	Requirements SST-SR-1295 on processor documentation and SST-SR-1365 on system level documentation added to section 3.2.5, references added to SST-SR-1290 and SST-SR-1360.
1.1	56 / 3.4.4	RID CD-58	Explanation for "per year" added to 99% availability requirement
1.1	60 / 3.5.4	RID CD-64	Stability measures for CDR production with respect to development cycle explained more verbose
1.2	49 / 3.2.5	PM6 C. Donlon	Requirement for PUG added
1.2	61 / 3.5.5	PM6 C. Donlon	Requirement for Operator's Manual added
1.2	44 / 3.2.1	PM6 C. Donlon	SST-SR-1240 split into two with one "shall" each, SST-SR-1241 added
1.2	48 / 3.2.4	PM6 C. Donlon	SST-SR-1500 split into two with one "shall" each, SST-SR-1501 added
1.2	40ff / 3	PM6 C. Donlon	All requirements searched for two sentences with "shall", and verified that second "shall" is a more detailed explanation of the first one and not a new requirement (see previous changes for requirements that have been split after check)

## **EXECUTIVE SUMMARY**

This Sea Surface Temperature (SST) System Requirements Document defines a set of requirements for an operational SST system for the European Space Agency (ESA) Climate Change Initiative (CCI). SST is one of 13 Essential Climate Variables (ECV) currently studied by CCI. The SST system will be used to generate and continuously update the SST part of the CCI climate data record (CDR).

The system requirements are derived from input requirements - mainly the Statement of Work and the SST User Requirements document. Because these do not provide wholly sufficient guidelines, the approach of this document is to identify a scenario for the SST 'Phase 2' system defining the sensor constellations used. The development team is assumed to be involved in continuous use of the SST system for CDR development.

As a result, the document defines a set of system requirements for production and reprocessing, for continuous extension of the climate data record, and for the products generated by the system. Requirements cover how the interaction is supported with climate users and the SST community as consumers of the outputs and as source for feedback. Finally, also internal project users require an interface to the system that is defined by a set of requirements.

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## 1. INTRODUCTION

### 1.1 Purpose and scope

This Sea Surface Temperature (SST) System Requirements Document defines a set of requirements for an operational SST system for the European Space Agency (ESA) Climate Change Initiative (CCI). SST is one of 13 Essential Climate Variables (ECV) currently studied by CCI. The SST system will be used to generate and continuously update the SST part of the CCI climate data record (CDR).

There are input documents to the task of deriving requirements from outside and inside the SST CCI project. The Statement of Work (SoW) requires a system requirements document to be a complete, structured collection of individual requirements of the operational ECV production system from a user's point of view. Its annex G lists additional SST-specific requirements. The other inputs are deliverables of the SST project itself. They require a system:

- to generate the products specified in the SST Product Specification Document (PSD) using data specified in the Data Access Requirement Document (DARD);
- to apply the algorithms specified in the SST Algorithm Theoretical Basis Documents (ATBD) for this purpose;
- to make the product accessible to users as specified in the SST User Requirements Document (URD).

However, these inputs provide little information on how the SST CCI system is going to be used, and what performance is expected from it. At the second CCI collocation meeting (12.-14.10.2011 in the European Space Research Institute ESRIN), there was a consensus among the science teams for an agile, responsive process of continuous scientific improvement, and supporting this is also a requirement on the system.

There is no high level requirements document for the entire CCI project (all ECVs); such a document could provide guidance and additional requirements, but is not available at the time of writing. In particular, an outcome of the process of generating high level requirements would be to define what parts of the overall CCI system can be common between ECVs and what should be kept distinct. This in turn influences the requirements of individual ECV SRDs. In the absence of this, some possibilities for commonalities are discussed in section 2.4.

The approach used for this document is to develop a scenario for SST with variants for minimal, satisfactory and optimal configurations. Together with the description of the processing workflow of the SST prototype, this serves as an additional starting point for the derivation of requirements. As far as possible, the requirements are traced to inputs, scenarios and the processing workflow.

The defined SST CCI system requirements will be used as an input to the SST system specification. They may also serve as a basis for a comparison amongst ECVs to find common functions and options.

### 1.2 References

The following documents are applicable to this document:

ID	Title	Issue	Date
[AD 1]	ESA Climate Change Initiative Phase I - Scientific User Consultation and Detailed Specification Statement of Work (SoW), including Annex G: Sea Surface Temperature ECV	1.4	09.11.2009
[AD 2]	Sea Surface Temperature ECV Proposal		16.07.2010
[AD 3]	Sea Surface Temperature CCI User Requirements Document, SST_CCI-URD-UKMO-001 (URD)	2	30.11.2010
[AD 4]	Sea Surface Temperature Data Access Requirements Document, SST_CCI-DARD-UOL-001 (DARD)	1.0	27.01.2012



ID	Title	Issue	Date
[AD 5]	Sea Surface Temperature Product Specification Document, SST_CCI-PSD-UKMO-002 (PSD)	2	11.11.2011
[AD 6]	MMD Content Specification, SST_CCI-REP-UOL-001	C	22.07.2011

The following documents are referenced in this document:

ID	Title	Issue	Date
[RD 1]	ESA CCI Project Guidelines, EOP-DTEX-EOPS-TN-10-0002	1.0	05.11.2010
[RD 2]	Reference Documents List, SST_CCI-REP-UOE-001	1	27.09.2011
[RD 3]	Acronyms List, SST_CCI-REP-UOE-002	1	27.09.2011
[RD 4]	Web site of the Group for High Resolution Sea Surface Temperature at <a href="http://ghrsst-pp.metoffice.com">ghrsst-pp.metoffice.com</a> , see also <a href="http://www.ghrsst.org">www.ghrsst.org</a>		06.01.2011
[RD 5]	Edinburgh Compute and Data Facility web site. 1 August 2007. U of Edinburgh. 7 Jan. 2011 at <a href="http://www.ecdf.ed.ac.uk">www.ecdf.ed.ac.uk</a>		07.01.2011
[RD 6]	European Committee for Space Standardisation - Software, ECSS-E40	C	06.03.2009
[RD 7]	Systematic observation requirements for satellite-based data products for climate, GCOS Satellite Supplement,	Update 2011	Dec 2011

Additional reference documents are listed in [RD 2].

### 1.3 Acronyms

The following SST-specific acronyms are used in this report.

Acronym	Definition
ARC	ATSR Reprocessing for Climate
(A)ATSR	(Advanced) Along-Track Scanning Radiometer
AVHRR	Advanced Very High Resolution Radiometer
BADC	British Atmospheric Data Centre
BEAM	Earth observation toolbox and development platform
CCI	Climate Change Initiative
CF	Climate Forecast
CMIP5	Coupled Model Intercomparison Project Phase 5
DARD	Data Access Requirements Document
DPM	Detailed Processing Model
ECDF	Edinburgh Compute and Data Facility
ECMWF	European Centre for Medium-Range Weather Forecasts
ECSS	European Cooperation for Space Standardisation
ECV	Essential Climate Variable
ESA	European Space Agency
GBCS	Generalised Bayesian Cloud Screening

Acronym	Definition
GDS	GHRSSST Data Processing Specification
GHRSSST	Group for High-Resolution SST
GMPE	GHRSSST Multi Product Ensemble
IR	Infrared
MetOp	Meteorological Operational (EUMETSAT)
MD	Match-up Dataset (single-sensor)
MMD	Multi-sensor Match-up Dataset
MMS	Multi-sensor Match-up System
NOAA	National Oceanic and Atmospheric Administration
NEODC	NERC Earth Observation Data Centre
NERC	Natural Environment Research Council
NWP	Numerical weather prediction
OSI-SAF	Ocean & Sea Ice Satellite Application Facility (EUMETSAT)
OSTIA	Operational Sea Surface Temperature and Sea Ice Analysis
PMW	Passive Microwave
SDI	Saharan Dust Index
SEVIRI	Spinning Enhanced Visible and Infrared Imager
SGE	Sun Grid Engine
SST	Sea Surface Temperature
UoE	University of Edinburgh

Additional acronyms are listed in [RD 3].

## 1.4 Document structure

After this formal introduction,

- sections 2.1 to 2.4 provide an overview of what the SST CCI project will produce, lists the input requirements from the URD and other documents relevant for the system, identifies assumptions about an SST system, and sets the context.
- sections 2.5 - 2.6 describe an operations concept for an SST routine system and identifies SST CCI scenarios for CCI phase 2 with variants for minimal, satisfactory and optimal configurations. Requirements in the end will depend on the variants selected.
- sections 2.7 - 2.9 describe the processing workflows of retrieval, merging and validation as far as known for the prototype, assuming the main parts of this with respective improvements will still be the baseline for CCI phase 2. They further describe the prototype of the multi-sensor matchup system foreseen for continuous algorithm improvement and a set of tools for SST data analysis.
- section 3 lists detailed requirements for the SST CCI system, its outputs, production and reprocessing, the multi-sensor matchup system, user services, and operator interfaces and tools. The sections distinguish main ECSS (European Cooperation for Space Standardization) categories of functional and non-functional requirements.
- section 4 traces input requirements to system requirements.

## 2. SEA SURFACE TEMPERATURE CONCEPTS AND ASSUMPTIONS

### 2.1 Sea Surface Temperature data products

The SST CCI project aims to develop a method, a system and data products for a long-term global SST record.

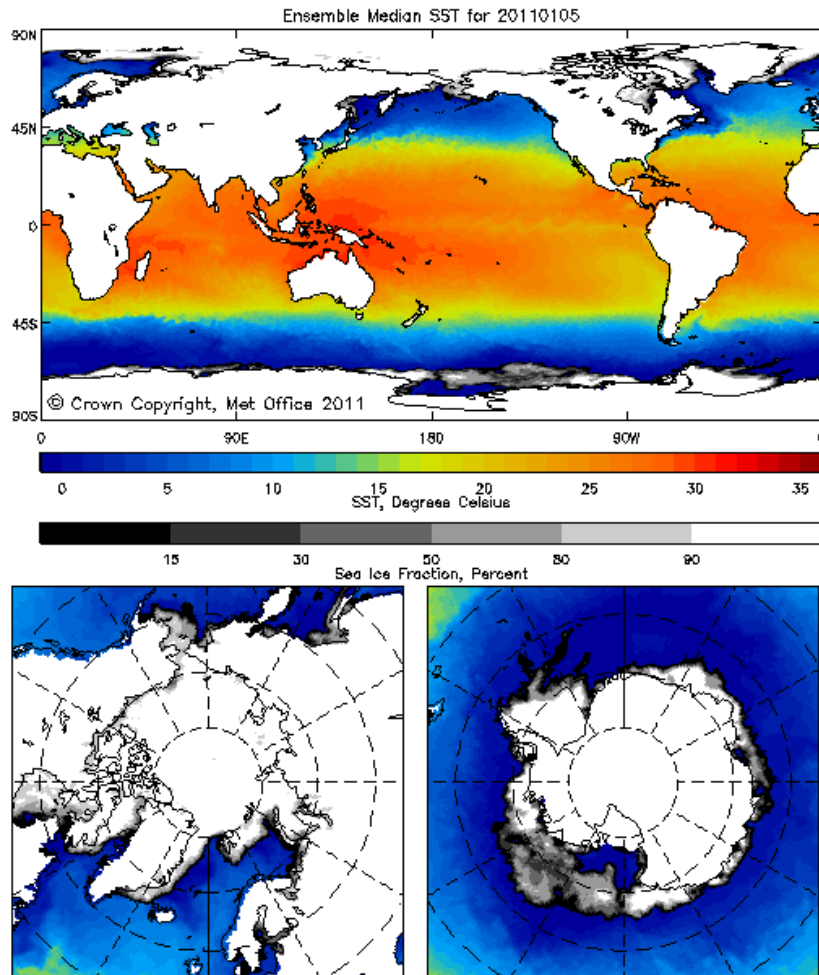
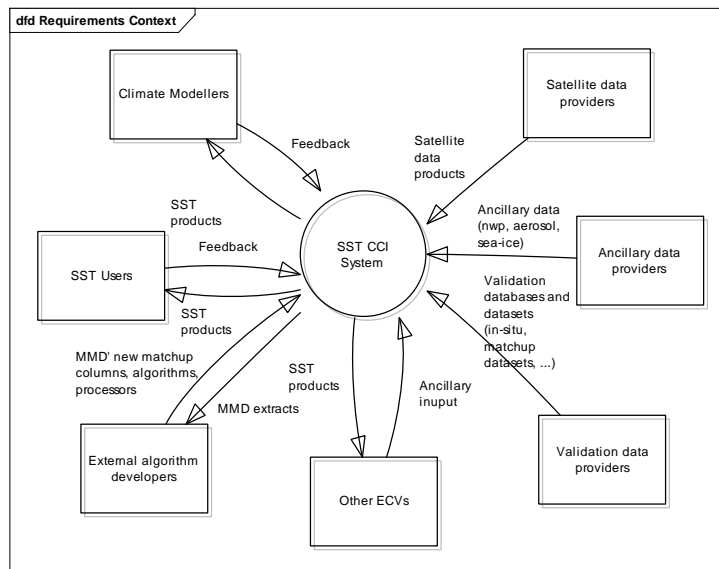


Figure 2-1: GMPE ensemble median SST analysis [RD 4]. The sea ice data shown are derived from OSTIA

The SST CCI Phase 1 prototype CDR will be based on combined ATSR and AVHRR data, covering the period from 1991 to present. As will be described in subsequent subsections, additional sensors will be integrated in the future. Data from geostationary satellites and from passive microwave sensors are merged with the data from IR sensors into a multi-sensor SST product for a Phase 1 demonstration of the full observing system capability. Algorithmic improvements that can be expected during the lifetime of the system comprise among others cloud clearing, sea ice detection, optimal estimation, bias correction with respect to ARC SST, robustness with respect to aerosol, and SST adjustments with respect to reference depth (e.g. skin layer) and reference time of day.

### 2.2 Sea Surface Temperature system context

The SST CCI system has interfaces to its data providers and its users. Figure 2-2 shows the SST CCI system in its context.



**Figure 2-2: Context of the SST CCI system with data providers and users**

- Climate researchers and users from the SST community receive products (and information about them). The SST CCI development team (see below) actively requests feedback from climate users and the SST community. The system shall support the development team in gathering this evidence.
- The interface to satellite data providers usually is the level 1 product.
- Ancillary and validation datasets are provided from different external sources and projects.
- Other ECVs may provide comparison data to SST, e.g. sea level, sea ice, ocean colour, aerosol products. Other ECVs may be receivers of SST products for consistency checks.
- An SST CCI development team shall be established. It consists of experts in Sea Surface Temperature that deliver scientific leadership within the project. It supports, directs sequence of and prioritizes operations within their agreed scope, and helps develop Sea Surface Temperature to meet climate users' needs. The development team has a mandate defined by terms of reference to support continuous improvements in the development cycle (described in section 2.5 below). It is considered part of the SST CCI system with functions assigned to it and therefore does not show up in this diagram.
- Validation is a two step activity.
  - First, validation is part of the process. It is performed as a QA step by the development team before a new CDR is provided to users. It is also performed to identify anomalies.
  - Second, users independently validate the CDR and provide feedback.
- Validation and development may also be undertaken by external algorithm developers, and this is foreseen to take place as an interaction using multi-sensor matchup data (MMD).

## 2.3 Applicable requirements from project documents

This section identifies the input requirements relevant for the SST CCI system. These input requirements for this document stem from:

- the CCI Statement of Work (SoW) [AD 1]
- the SST project documents URD [AD 3], PSD [AD 4], DARD [AD 5]
- CCI Project Guidelines [RD 1]
- Prototype development done for the Round Robin dataset generation

The generic part of the SoW sets the scope of these requirements by defining a set of document requirements rather than by providing specific technical details.

The *System Requirements Document* is a complete, structured collection of individual requirements of the operational ECV production system from a user's point of view.

It shall include

- a description of the scope and the context of the system
- descriptive operational scenarios for the system
- Specification of key parameters that define the required system size, complexity and growth
- a specification of the number, type and qualification of users/operators and the nature of their use of the system
- a complete list of functional, operational, reliability, maintainability, verification, quality and documentation requirements
- detailed requirements for the processing functions, input-output data sets, resource requirements including disk and memory storage volumes,
- archiving requirements (baseline data and interim products and outputs and their safeguarding to allow for reprocessing)
- processing speed and performance requirements
- requirements for modularisation to allow for algorithm improvement or algorithm change while minimising reprocessing temporal constraints, any fundamental interdependencies with other systems, e.g. hosting platform or infrastructure.

**Figure 2-3: SRD document requirements from the Statement of Work [SoW, section D5.1]**

Figure 2-3 reproduces the relevant paragraph of the SoW. The bullets of the list are referred to as:

- **SoW-1** (for "a description of the scope ...")
- ...
- **SoW-9** (for "requirements for modularisation ...")

in the traceability matrix in section 4. As with other inputs defined below in this document, the requirements in Section 3 that derive at least in part from these are listed, for convenience, here:

SoW-1	Scope and context of the system	§1.1 Purpose and scope §2.2 Sea Surface Temperature system context
SoW-2	Descriptive operational scenarios	§2.7 Prototype Sea Surface Temperature production workflow §2.5 Operations concept
SoW-3	Key parameters	§2.7.2 Estimation of system key parameters
SoW-4	Users and operators	SST-SR-1390 Operator SST-SR-1400 Automation SST-SR-1430 Error handling SST-SR-6360 Forum maintainer SST-SR-6340 Science issues SST-SR-5110 Community process
SoW-5	Functional, operational, ... requirements	§3 Detailed system requirements

SoW-6	Processing functions, input, output	§2.7 Prototype Sea Surface Temperature production workflow §3.2 Requirements on SST time series production and reprocessing §3.1 Requirements on the generated output products
SoW-7	Archiving requirements	§2.7.2 Estimation of system key parameters SST-SR-1450 Input storage size SST-SR-1460 Output storage size SST-SR-1470 Online storage SST-SR-1500 Backup archive SST-SR-1501 Bulk archive retrieval SST-SR-1510 Archive reliability
SoW-8	Processing speed and performance	§2.7.2 Estimation of system key parameters SST-SR-1490 Three days per year SST-SR-5300 Performance scalability
SoW-9	Modularisation, improvement, interdependencies	§2.4 Assumptions on common CCI system requirements OPS-2 EO development team assumption-2 Autonomous ECV systems SST-SR-1350 Processor framework SST-SR-1360 Executable integration SST-SR-1520 Autonomous system SST-SR-5115 User requirements re-evaluation SST-SR-5170 New input type SST-SR-5190 New ancillary type SST-SR-5200 New processing chain SST-SR-5210 Transfer to operations SST-SR-5215 L4 analysis system update

The SoW Annex G lists additional SST-specific technical requirements that fall into categories of “methods to be used”, “products to be generated”, and meta-requirements on “how to perform the project”.

- The responses to requirements on “products to be generated” are encapsulated in the PSD. The SST system requirement to generate the products specified in the PSD therefore carries all these requirements into the SST system.
- Responses to requirements on “methods to be used” will be encapsulated in the ATBD v2 (and in v0 and v1 in preliminary form) and the DPM. This is covered by SST system requirements on processors to implement these methods and to be integrated into the SST CCI system.
- Requirements on “how to perform the project” usually will not have immediate implications for the system.

Table 2-1 orders SoW requirements by these three categories (marked as "Products", "Methods", "Project" in table columns). In the "System" column the table indicates which technical requirements should be directly reflected by system requirements. They mainly concern

- the scope of the system defined by sensors, temporal coverage, aggregation periods
- processor functions and algorithms to include
- output definition, in particular format and metadata
- validation, how to support it by the system
- post-processing, extraction and analysis tools

They are considered as input requirements for this SRD.

**Table 2-1: Input requirements from SST CCI SoW, Annex G**

Input Req. ID	Title	Products	Methods	Project	System
SST-TR-1	NetCDF CF	x			x
SST-TR-2	Sensors for level 2 products	x			x
SST-TR-3	SSTskin	x			
SST-TR-4	SSTsub-skin	x			
SST-TR-5	Merged SSTdepth	x			
SST-TR-6	Daily to annual level 3	x			x
SST-TR-7	Temporal coverage 1991-2010	x			x
SST-TR-8	Uncertainties	x	x		
SST-TR-9	Flags not to be used as masks		x		
SST-TR-10	GHRSSST 2.0 GDS	x			x
SST-TR-11	URD to identify current use			x	
SST-TR-12	PSD to identify metadata	x		x	x
SST-TR-13	URD and PSD review			x	
SST-TR-14	Geo-referencing / co-location		x		x
SST-TR-15	Cloud detection		x		x
SST-TR-16	Sun glint		x		x
SST-TR-17	Aerosol		x		x
SST-TR-18	Sea-ice		x		x
SST-TR-19	Quality indicators		x		x
SST-TR-20	IR SST retrieval		x		x
SST-TR-21	Diurnal cycle		x		x
SST-TR-22	In-situ reference data set	x			x
SST-TR-23	Multi-sensor synergy		x		
SST-TR-24	(A)ATSR as reference	x	x		
SST-TR-25	Parallel development			x	
SST-TR-26	Independent validation			x	
SST-TR-27	OI and OE for blending		x		
SST-TR-28	Data OI and OE		x		
SST-TR-29	Observation operators		x		x
SST-TR-30	Use GSICS, HR-DDS, GMPE		x		x
SST-TR-31	Inter-comparison and visualization tools		x		x
SST-TR-32	Best approaches			x	
SST-TR-33	TOA datasets for inter-comparison	x			
SST-TR-34	Trade-off analysis			x	
SST-TR-35	Independent analysis			x	
SST-TR-36	Test products and improvements			x	x
SST-TR-37	Product consistency			x	x
SST-TR-38	Impact of CCI SST products			x	
SST-TR-39	Consistency with other ECVs			x	x
SST-TR-40	Spatial and temporal aspects of validation		x		x
SST-TR-41	High-latitude validation		x		
SST-TR-42	Independent data		x		
SST-TR-43	Multi-way statistical methods		x		
SST-TR-44	Independent in-situ data		x		
SST-TR-45	Maps and time-series inter-comparison		x		x
SST-TR-46	Long-term stability reporting			x	
SST-TR-47	Trend analysis reporting			x	
SST-TR-48	Consistency with established time series		x		
SST-TR-49	Prototype sensors and period	x			x

The URD defines 130 requirements. A questionnaire answered by the science community is one of the sources of these requirements. Again, a large set of the requirements is on the products to be generated. They are summarised by an SST system requirement to generate the products

specified in the PSD. The requirements that should be directly considered to give rise to system requirements concern the following areas:

**Products:**

- data levels L2, L3, L4, single and multi-sensor products (UR-QUF-33, UR-QUF-35)
- temporal coverage of at least 30 years (UR-REF-3, UR-QUF-43)
- independent validation (UR-DIS-125)
- timely availability ranging from year to half a day, (UR-QUF-44, UR-DIS-121, UR-DIS-122)

**Operations:**

- standards for data storage (UR-REF-15)
- highly reliable, routinely operated system (UR-REF-8, UR-QUF-83)
- version control, concurrent data versions (UR-REF-21, UR-DIS-126)

**User Access:**

- users with least developed computing infrastructure, easy access (UR-REF-10, UR-REF-12, UR-DIS-117, UR-LLP-24, UR-QUF-87, UR-QUF-88)
- NetCDF CF, GHRSSST GDS 2.0, metadata (UR-QUF-89, UR-REF-16, UR-REF-17)
- temporal data selection, access to documentation (UR-DIS-124, UR-REF-20)
- access by FTP, Web page, map, OPeNDAP, on media (UR-QUF-90 to -94)
- email notification, up-to-date information on web page (UR-QUF-95, UR-QUF-96, UR-LLP-27, UR-REF-11, UR-REF-18, UR-LLP-29)
- reliability of delivery of 99% (UR-QUF-45)
- feedback on data issues, support (UR-REF-9, UR-REF-23, UR-LLP-25, UR-DIS-119)

**Tools:**

- method for uncertainty aggregation, different resolutions (UR-DIS-128, UR-DIS-123)
- tools for extraction, aggregation, reading, visualisation, uncertainty evaluation, inter-comparison, trend analysis, preferably open-source (UR-QUF-97 to -100 and -102 to -107)
- tools for generation of matchup datasets (UR-QUF-101)
- software libraries for MATLAB, IDL, Fortran (UR-QUF-108 to -110)

These user requirements will be translated into functional requirements and in some cases performance requirements for the CCI system.

The PSD defines content and format of demonstration SST products and long-term SST products for the prototype. The long-term products are

- (A)ATSR L3U 0.05° 1991-2010 (referred to as PSD-1 in this document)
- AVHRR L2P 4km 1991-2010 (PSD-2)
- Analysis L4 0.05° 1991-2010 (PSD-3)

It further defines the

- representation in NetCDF with variables and attributes (PSD-4)
- file name convention following GHRSSST GDS 2.0 (PSD-5)

They translate into requirements to generate these products.

The CCI Data Standards Working Group is also generating requirements that apply to all ECVs. While not yet fully formalised, they include detailed requirements on metadata, both usage (CF-compliance) and discovery (Unidata metadata discovery standard), and on versioning and full traceability (probably via a UUID). These requirements can be expected to become a part of a future PSD for each ECV. The corresponding system requirements are to follow CCI project data standards and to support versioning and traceability.



The DARD specifies the set of input products used for SST in Phase 1. They comprise the main sensor data inputs (A)ATSR and AVHRR level 1, further ancillary data for processing, and various validation datasets. In the DARD the datasets are numbered from 1.01 to 5.06.

- DARD-1.01 to 1.10 for ATSR and AVHRR satellite data and pre-computed matchup databases
- DARD-2.01 to 2.09 for ECMWF ERA-Interim, sea ice, and other ancillary data
- DARD-3.01 to 3.07 for in situ data from ships and buoys
- DARD-4.01 to 4.24 for various inter-comparison datasets from MOHC, NOAA, NASA, ECMWF, and others
- DARD-5.01 to 5.06 for products of other CCI ECVs for ocean colour, sea level, sea ice thickness, sea ice concentration, aerosol optical depth

This translates into requirements for the system to maintain these data, to protect restricted data against unauthorised access, and to provide them as input to the production. The DARD further specifies the volume of input data. This translates into sizing requirements.

## 2.4 Assumptions on common CCI system requirements

One important question for the design of the SST CCI system is the sharing of infrastructure, resources or functions with other ECVs, or their independence. There are currently no requirements on this in the input documents and it is expected they will be an output of the high level requirements discussion recommended in the CCI collocation. One option, discussed at the 2011 CCI collocation, is an approach depicted in Figure 2-4 which may apply to all ECVs jointly or to each member of a cluster of closely related ECVs.

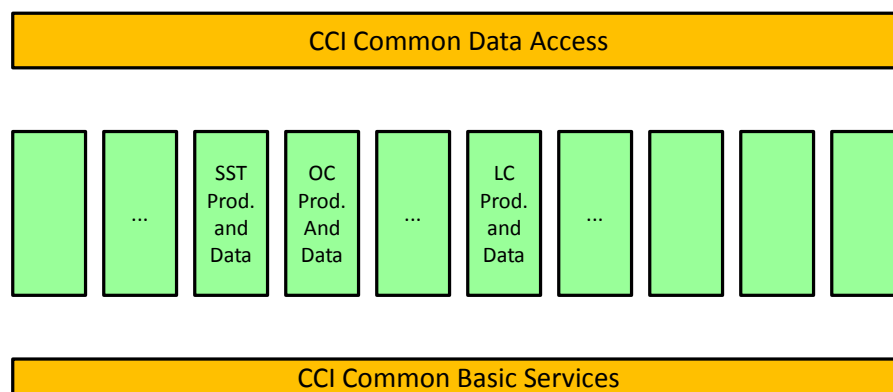


Figure 2-4: Common data access and de-centralised production environments for ECVs

- The common data access layer shared among all or several ECVs provides harmonised access to CCI data for climate researchers. This shall lower the barrier for climate users to use several of the ECVs.
- The individual production and data environments per ECV are close to the scientific groups to support agile, continuous development and nimble reaction to issues with short cycles. The production environments are optimised for re-processing and validation. Strict versioning ensures production of stable product releases. Optionally, sharing of an environment for both production and development allows for access to long time series for the scientific improvement cycle.
- Selected common services may be offered for sharing among ECVs. Among them are: a backup archive for the data; cloud services that can be used by ECVs; and outsourced hosting for bulk download. Sharing such services optimises resources without restricting independence of ECVs regarding their respective production and improvement cycle.

This is an initial framework upon which more concrete solutions can be developed. The allocation of functions and the degree to which basic services can be shared will be defined across ECVs during design.

The approach corresponds to a few abstract requirements, followed in each case by references to the specify requirements that refer to them:

- **assumption-1:** Climate users shall get harmonised access to different ECV outputs with common data formats via a single point of access;
- **assumption-2:** The different ECV production systems (taking L1 and auxiliary data and transforming these into products, managing the data and resources) shall be autonomous and independent of each other, and based in the relevant communities;
- **assumption-3:** The ECV production systems shall be optimised for repeated re-processing and validation as part of an improvement cycle. This must not compromise their use in routine short-delay processing, and is necessary for ensuring CDR quality.

The requirements that make reference to these assumptions are listed below.

assumption-1	Harmonised access	SST-SR-6220 Bulk access
assumption-2	Autonomous ECV systems	SST-SR-1520 Autonomous system
assumption-3	Optimised for repeated re-processing	SST-SR-5250 Version decisions SST-SR-5255 Overlapping versions SST-SR-5275 Internal version storage SST-SR-1220 Input versions SST-SR-1230 Reprocessing input versions SST-SR-1240 Output versions SST-SR-1241 Long-term stewardship SST-SR-2120 Auxiliary update SST-SR-1470 Online storage

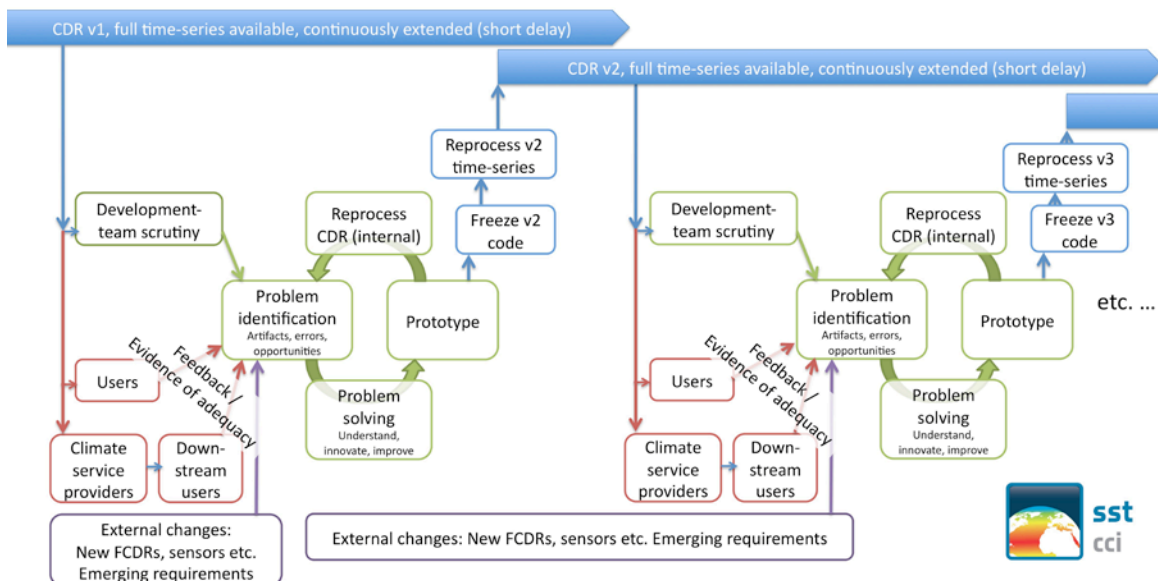
As stated, none of these requirements are formal inputs so far. They are nevertheless helpful as assumptions.

## 2.5 Operations concept

What should a routine system for climate data records look like? The following elements of an operations concept are named OPS-1 ... OPS-9 for reference later in the document.

**OPS-1.** The Climate Change Initiative (CCI) should contribute a long-term scientific legacy of climate-quality satellite retrievals with uncertainty estimates. CCI climate data records (CDRs) should be as precious to Earth System Science in 100 years' time as the fundamental meteorological and oceanographic observations made in the 19th century are to us now. Practically, this implies a transition from the present Phase 1 activities (user consultation, algorithm selection, system definition and prototyping, off-line production) to routine CDR production and problem-solving with continuous improvement. "Problem solving" in this improvement cycle includes analysis of any mismatch of the present CDR to requirements. Routine production will support provision of climate services, the scientific/societal/policy demand for which will likely be long-term.

**OPS-2.** ESA have wisely required scientists and system engineers to work together in the prototyping and system specification in Phase 1. This close co-operation must continue through Phase 2 and thereafter: transition is not merely a software implementation task, and should include embedded development teams to solve problems in the CDRs.



**Figure 2-5: Improvement cycles with user feedback (large cycle including red boxes) and by development team (green short cycle), and stable climate data records (blue) in the SST CCI system**

**OPS-3.** The maturity and functionality of prototype software from Phase 1 will vary between ECVs. For SST and several other variables with functional prototypes, Phase 2 should focus on commissioning existing prototypes in routine reliable infrastructure (with extension to additional sensors assumed in the scenario defined below in section 2.6) and using this for initial operations (including the improvement cycles in Phase 2 – see Figure 2-5). This may involve code revision/refactoring, although rewriting/re-engineering of code from DPMs (Detailed Processing Model documents) shall *not* be necessary (and would likely be scientifically counter-productive).

**OPS-4.** During Phase 2 (in parallel with routine production), we should demonstrate the process of going through cycles of feedback and improvement of the CDR. A concept for this is presented in Figure 2-5. The process is initiated by structured solicitation of climate user and SST user community feedback. It would also allow for the system to support an advisory/management structure via (for example) a steering group, which ESA may elect to have in addition to contractual control of Phase 2. Including this aspect in Phase 2 will prove the approach for the later phases of ‘continuous development and operations’ that should continue the work of the CCI long term.

**OPS-5.** Therefore, ‘routine CDR generation’ must be viewed broadly, as in the figure, to include

- routine, reliable provision of climate-quality observations via robust implementation of excellent scientific methods; and
- the agile scientific work-flow that delivers upgraded CDRs in response to new requirements and problems.

**OPS-6.** Continuous development is essential in parallel to routine generation because

- we continually learn how to reduce uncertainties and improve stability of CDRs
- experiences of users may uncover new problems in these huge, complex data sets
- inputs (level0 and/or level1) will periodically be reprocessed and improved by agencies
- new sensors will require seamless integration into the CDR, while preserving stability and other quality aspects
- new user requirements will emerge, demanding new, value-added or better quality CDRs.

**Decisions for improvements shall be driven by use of evidence that the improvements will improve the CDR, e.g. with respect to what is defined in the URD.**

**OPS-7.** Routine generation must include *continuous availability of a full, consistently reprocessed, continuously extended CDR*. As shown in Figure 2-5, this is the purpose of having overlapping periods between CDR versions. The new version running in parallel would be designated "pre-operational" in a meteorological agency. Pre-operational provision gives users time to move across to the next version CDR.

**OPS-8.** The improvement cycle (loop from problem identification to reprocessing) requires agile implementation of scientific innovations (e.g., new algorithms) within a robust and traceable system environment. The full effect on the CDR is apparent only on reprocessing the full archive. *The system must therefore be capable of maintaining routine delivery of 'new' data while simultaneously undertaking rapid (preferably multiple) reprocessings as part of this improvement cycle.*

**OPS-9.** Distinctions between near-real time operations and routine, short-delay CDR generation are real and should be recognised. One distinction is the need for the CDR improvement cycle as part of the operations, discussed above. Another is that stability and consistency take on a greater importance for a CDR. Lastly, short-time delay mode can, and should, be exploited to maximize the climate-quality aspects of the CDRs, beyond what is possible with near-real time provision. For example: processing for consistency across a constellation and stability in time can take advantage of the short time lag in delayed-mode delivery; more consistent auxiliary data (e.g., re-analyses) may be available.

An evolutionary approach for system development may start from the prototype from CCI Phase 1. While this version is operational the next version of the system is developed and put into operation incrementally. A commissioning phase shall precede the operational phase in which both the prototype and the operational system are operated concurrently.

The system requirements that make reference to the OPS concepts are listed below:

OPS-1	Routine long-term CDR production and climate services	SST-SR-2110 Input ingestion SST-SR-2120 Auxiliary update SST-SR-2125 Validation data update SST-SR-2130 Data-driven processing SST-SR-2150 CDR extension
OPS-2	Involvement of development team	SST-SR-5220 Development team
OPS-3	Cycles of development starting from prototype	SST-SR-5120 Development environment
OPS-4	Model of improvement	SST-SR-5150 Full timeline access SST-SR-5210 Transfer to operations SST-SR-5215 L4 analysis system update SST-SR-5270 Short development cycle SST-SR-5275 Internal version storage SST-SR-5310 Measures for stability
OPS-5	Reliable CDR generation and agile process	SST-SR-5310 Measures for stability SST-SR-5230 Agile requirements selection
OPS-6	Reprocessing needs	SST-SR-2120 Auxiliary update
OPS-7	Availability of consistent CDR	SST-SR-1240 Output versions SST-SR-1241 Long-term stewardship SST-SR-5250 Version decisions SST-SR-5255 Overlapping versions
OPS-8	Robust and traceable environment with access to full archive	SST-SR-5120 Development environment SST-SR-5150 Full timeline access
OPS-9	CDR generation with focus on quality	SST-SR-2140 Wait for ancillary SST-SR-2180 Short-delay processing

## 2.6 Sea Surface Temperature sensor constellations and scenarios

This section identifies SST scenarios for CCI phase 2 with sensor constellations, scope of products, reprocessing capability, and the interaction with users. Variants for minimal, satisfactory and optimal configurations are described.

The System Requirements for SST CCI follow from a number of considerations.

- First, there are User Requirements, where “User” here refers to those looking to use outputs of the SST CCI system. The prime sources of information about User Requirements are (1) the SST CCI User Requirements Document (URD), (2) the SST CCI Technical Note synthesizing URD survey results into quantitative targets for aspects of products, and (3) the GCOS ECV satellite supplement and its update. The user requirements in the URD distinguish three levels: 'Threshold' is the limit at which the observation becomes ineffectual and is of no use. 'Breakthrough' is the level at which a significant improvement would be achieved. 'Objective' is the maximum performance limit beyond which no significant improvement would be achieved for the current application.
- Second, there are ESA requirements for the CCI programme as a whole, expressed as five Cardinal Requirements and as Annex G in the Statement of Work that initiated the present Phase 1 activity within CCI.
- Third, there are development team requirements. A development team will need to work within the SST CCI system to adapt to changes in the satellite constellation over time and deliver the cycle of improvement of the full Climate Data Record (CDR) as understanding and techniques improve. We must also consider the requirements of these “internal users”.
- Fourth, there are judgements, with justifications, by the SST CCI development team of scope for the SST CCI system that is scientifically credible within a conceivable cost, while taking account of all the considerations above. As will be clear below, “a system that does everything possible for SST” in CCI Phase 2 would be extremely costly, in terms of both the infrastructure and volume of research and development that would be required.

### 2.6.1 The potential satellite constellation for SST

It is useful in this section to review what a full constellation of observations for an SST system could encompass, and within that to prioritise and comment on the various components. We then define the components included in the scenario used as the basis for this SRD.

The present SST CCI Phase 1 is funded until mid 2013. The system specified in this document is to be implemented and used for routine production in the period 2013 to 2016 (2013 to 2016 represents CCI Phase 2 in this document, knowing that it may actually start 2014). It is necessary to look beyond 2016, but the constellation up to that time is the focus here.

#### 2.6.1.1 Scientifically credible baseline

Climate users require global SST coverage [UR-REF-2; UR-QUF-42] and products that cover at least 30 years [UR-REF-3; UR-QUF-43]. The only sensor series that addresses these requirements is that of the Advanced Very High Resolution Radiometer (AVHRR), via archives of level 1b Global Area Coverage (GAC) data.

Climate users also require bias to be less than 0.1 K, demonstrated on spatial scales of 100 km [UR-QUF-49] (GCOS satellite supplement, [RD 7]). The 0.1 K bias target has been demonstrated for Advanced Along Track Scanning Radiometer (AATSR) SST-20cm globally at scales of order 1000 km, for SSTs from the ATSR Reprocessing for Climate (ARC) project [RD.184] using radiative transfer based algorithms that are independent of in situ observations. It is likely to have been met for all the ATSRs in the ARC time series, at least back to 1993, except at the end-of-life of ATSR-1 (second quarter of 1996).

On the other hand, for typical AVHRR SST this bias requirement is known to be violated, despite empirical tuning to drifting buoys. The limitations of the non-linear SST retrieval formalism [RD.221, RD.248] lead to biases of up to 0.5 K in the tropics. Within Phase 1 of the CCI pro-

gramme, the SST CCI team has therefore chosen to base its long-term climate data record on ATSR and AVHRR together, with the intention that AVHRR be brought into line with ATSR to address this bias requirement.

Part of the reason ATSRs can obtain lower biases, particularly in the tropics, is the greater information content delivered by having dual view observations. The future dual view sensor will be the Sea and Land Surface Temperature Radiometer (SLSTR). The present launch schedule for SLSTR and end-of-life schedule for AATSR promise an adequate 6 months overlap to give continuity between these dual view sensors. SLSTR will take the role of the ATSRs in the SST CCI system thereafter.

Nonetheless, there is risk that AATSR and SLSTR overlap may not be achieved. The Metop AVHRRs become particularly important in this event. Metop platforms have a stable orbit (most AVHRRs are on platforms whose local times drift) with an equator crossing time within an hour of AATSR and SLSTR. Eumetsat's operating assumption for Metop-A AVHRR (currently operational) is to continue in service until commissioning of Metop-C (2016), which would bridge any AATSR to SLSTR gap. Metop-B should be operational late in 2012, giving some redundancy. The AVHRRs are not by design as stable as AATSR, but in the case of Metop they fly with the Infrared Atmospheric Sounding Interferometer. AATSR/IASI comparisons over 2 years have shown extremely high mutual stability (personal communication, R Saunders, Met Office), and therefore there is an additional scientific opportunity to monitor and control Metop-A AVHRR stability against IASI and (assuming commissioning success) a Metop-B AVHRR and IASI. This gives a credible opportunity to bridge any AATSR and SLSTR gap with satellite SST with estimated stability, maintaining an independent satellite SST record.

Should one or two Metop AVHRRs not be available, any gap will need to be bridged by relying on other satellite sensors. MODIS Terra is also in an appropriate orbit, but is already, at time of writing, over a decade in operation, and therefore the probability of continuity is essentially unknown. In the absence of any of these options, efforts will need to be directed to sensors whose local overpass time is more different from AATSR/SLSTR than Metop or Terra.

Ship mounted radiometers shall be exploited for traceability of the temperature scale for the end of AATSR and the beginning of SLSTR to SI standards. Informative comparisons of AATSR and SLSTR via ship mounted radiometers assumes continuity of ship radiometer campaigns with comparable sampling regimes for both sensors (such as the ISAR campaign operated between Southampton and Spain). Continuity of these observations during any AATSR / SLSTR gap will assist in assuring the bridging of the gap discussed above, using other sensors.

Unlike most AVHRRs, Metop AVHRR is downlinked globally at full spatial resolution. This means that it can, in principle, also bridge AATSR to SLSTR with regards to global 1 km resolution. Cloud detection undertaken at 1 km rather than GAC resolution is also likely to be more effective.

Thus, if it is necessary to carry the independent calibration of AATSR forward to SLSTR indirectly because they do not overlap, the first resort for a bridging sensor will be Metop-A AVHRR, supported with IASI.

There are three options for introducing Metop into the SST CCI system, with different costs.

The lowest cost option, used within CCI Phase 1, is via an interface to the system of the Centre de Meteorologie Spatiale (CMS) (the SST team there is also part of the EUMETSAT Ocean and Sea Ice Satellite Application Facility, OSI-SAF). After full resolution cloud detection, CMS create 0.05 deg resolution clear-sky brightness temperature products with a large range of useful additional information. An interface to CMS brings these intermediate files into the SST CCI system. The breakthrough requirement for spatial resolution of L3 SST is 0.1 deg [UR-QUF-36; UR-QUE-32], and two thirds of climate users would be satisfied at objective level by 0.05 degree, so interfacing to spatially averaged data at 0.05 deg resolution is reasonable. This approach would allow SST CCI to (re)process 0.05 deg data for the SST retrieval step. However, it would mean there is no SST CCI ability to reprocess for cloud and ice detection improvements. Archive reprocessing for Metop is in the plans of CMS, and under this option the future SST CCI system would depend on this for cloud and ice detection improvement. So, with this option, Metop would not bridge between AATSR and SLSTR at full spatial resolution, and the in-house reprocessing capability would be limited to SST retrieval methods.

The middle cost option is to interface with the CMS system at full spatial resolution, to access data at 1 km level 1b, with CMS cloud detection and other auxiliary information that would be determined. This would incur additional costs for both the CMS system and the SST CCI system and the data flows between the systems. Although CMS cloud detection could be used for short-delay mode, the data collected in the SST CCI system would permit in principle reprocessing for cloud and ice detection at full resolution, as well as SST retrieval.

The high cost option is to obtain level 1 full resolution Metop brightness temperatures at the SST CCI system and do all processing (short delay mode and reprocessing). This would increase the consistency between the short-delay Metop SSTs and any reprocessed Metop SSTs, at the cost of not taking advantage of an existing operational system in Europe for short-delay mode production.

The Metop series will be the final AVHRRs flown, and should continue until 2021. The Visible/Infrared Imager Radiometer Suite (VIIRS) has been launched in October 2011 on the NPP mission (planned end of life August 2016), and is the functional replacement for AVHRRs in the Joint Polar Satellite System (JPSS) (JPSS-1 launch planned in July 2017; note there is no continuity therefore with the NPP VIIRS). Relevant VIIRS channels are similar in concept to those of the earlier Moderate-resolution Imaging Spectroradiometer (MODIS). Nonetheless, MODIS and VIIRS are likely to have quite distinct instrumental characteristics that would need to be carefully related to the ATSR and AVHRR series. Moreover, there is a cardinal requirement on the CCI programme [CR-3] to optimize the impact of European sensors in CDR production. This is addressed by the intention to use ATSR/SLSTR as reference sensors in the baseline constellation to which other observations are tied, but may also be taken to imply that MODIS and VIIRS (at least prior to JPSS-1) should be given a lower priority.

Users have requirements for stability of observation [UR-QUF-50] with two thirds of climate users surveyed satisfied at “breakthrough” level by drift of less than 0.05 K per decade for L3 SSTs. On the available evidence (limited to tropical areas by lack of stable long-term in situ observations elsewhere) this objective stability is met for 1993 to 2010 by ARC SSTs, while preserving independence. Assuming adequate AATSR-SLSTR or AATSR-Metop-SLSTR overlap, the SST CCI system must support continuation of this level of stability (after cross-calibration using overlaps), using the ATSR-series as an anchor for AVHRRs. The system needs also to support improvement of stability post-Pinatubo (1991 to 1993). Prior to ATSR, only the AVHRR series are available to meet the temporal coverage requirement, and the system will need to support exploitation of overlaps through the AVHRR record to optimise stability.

To achieve exploitation of overlaps, cross-referencing of sensors and the stability objectives, the system must support a full implementation of the Multi-sensor Matchup System (a concept established in SST CCI Phase 1) for all these sensors.

Stability is arguably the quality that should most distinguish a ‘Climate Data Record’ from a mere ‘Data Record’. It is also a quality that is easily destroyed by using input data streams with markedly different sampling or instrumental characteristics. All the sensors discussed to this point are on polar orbiting platforms and operate in the infra-red with broadly similar channels. They provide a relatively coherent set of input data streams for development of a consistent CDR for SST. Together they should support a baseline SST CDR addressing the central user requirements for coverage, resolution, bias and stability. Table 1 summarises some characteristics and priority within the SST CCI system.

**Table 2-2: Baseline constellation of sensors - characteristic and relative priority**

Sensor series	Temporal coverage	Input data description	Approximate input data volume by 2016	Priority / comments
AVHRR (exc. Metop)	1981 - 2016	GAC (sub-sampled to 4 km at nadir)	25 TB	Essential for baseline [UR-REF-3]

Sensor series	Temporal coverage	Input data description	Approximate input data volume by 2016	Priority / comments
ATSR	1991 - 2014	L1b 1 km	26 TB	Essential for baseline [UR-QUF-50; UR-QUF-49; CR-3]
AVHRR Metop-A and B	A: 2006 - 2016 B: 2012 - 2016+	0.05 deg clear-sky BTs + auxiliary data	1 TB (compressed, corresponds to 15 TB uncompressed NetCDF-3)	Essential for baseline (unless full resolution is used) [UR-QUF-50]
		Full resolution L1b + aux.	15 TB (compressed, corresponds to 50 TB uncompressed)	Highly desirable for baseline (essential if 0.05 deg option is not used, and scientifically preferable) [UR-QUF-50]
IASI Metop A/B	A: 2006 - 2016 B: 2012 - 2016+	Spectra at ~12 km spatial resolution	1 TB (clear-sky samples only to be extracted for stability monitoring of Metop AVHRR)	Highly desirable for baseline, for monitoring and controlling stability. [UR-QUF-50]
SLSTR	2013 - 2016+	L1b 1 km	180 TB	Essential for baseline [UR-QUF-49; CR-3]
VIIRS	2012 - 2016, 2017 onwards	L1b 1 km	40 TB	Highly desirable for baseline. Will become essential, from JPSS-1 in 2017.
MODIS	1999 - 2014(?)	L1b 1 km	200 TB	Desirable for baseline. Priority for Terra mission over Aqua mission if only one were feasible.

The central SST CCI product is and will remain a daily product (day and night separate), including optional adjustments to a fixed local time of observation to eliminate aliasing of variable sampling of the diurnal cycle into the long term record. The essential components in Table 1 will support this, with desirable and highly desirable elements providing increased spatial coverage and decreasing sampling uncertainty.

A significant proportion of climate users require sub-daily temporal resolution of SST, i.e., to have a daily diurnal cycle estimate for each place (e.g. with 3 hourly resolution) [UR-QUF-40] or to obtain SST estimates at fixed synoptic times (in universal time, i.e., a snapshot of different phases of the diurnal cycle with longitude, either daily [UR-QUF-37] or 6-hourly [UR-QUF-41]). Such estimates are supported with the baseline constellation for those periods where a sufficient number of polar orbiting sensors are flying with a range of local equator crossing times. The research has not yet been done to establish how best to do this and for what sample of the full record this is feasible with a given uncertainty. Adding the desirable and highly desirable elements in Table 1 would increase temporal resolution as well as coverage, likely improving the ability to address sub-daily SST.



### Addition of passive microwave sensors

Passive microwave (PMW) sensors have lower intrinsic accuracy than many of the baseline IR constellation, and coarser spatial resolution. However, they give a considerable increase in spatio-temporal coverage in open-ocean areas (roughly, more than 50 km from coasts, islands and sea ice) because their SST observations are prevented or degraded only by actively precipitating clouds and radio frequency interference. MWs therefore give data where persistent cloud prevents any IR observations. This means each PMW sensor obtains SST for a significantly greater proportion of the ocean in a day than does an IR sensor.

PMW sensors therefore could play a useful role in the SST CCI system by (i) reducing sampling uncertainty, and (ii) increasing the observational resolution of the diurnal cycle, thereby improving sub-daily SST information.

However, caution is required, in that:

(i) We don't know the degree to which superior PMW sampling (but with inferior single pixel retrieval uncertainty) will reduce total uncertainty, since propagation of realistic context-sensitive uncertainty from the L1 to L2 retrieval process to L3 and L4 products has never been systematically investigated.

(ii) Having very different instrumental and sampling characteristics, naive inclusion of PMW is most likely to *degrade* the stability of the CDR. This is because they are available comparatively late in the satellite era, there are relatively more significant differences between sensors, and the overlap between missions is not likely to be ideal. In principle, research can be conducted to analyse and learn to remove relative biases compared to the IR constellation. But when dealing with stability targets at the level of 0.005 K/yr, practical success in this is not to be lightly assumed. It will be necessary to maintain the SST CCI Phase 1 approach of having both polar-IR only and polar-IR+PMW versions of L4 products.

(iii) With respect to CR-3 (maximising the impact of European sensors), this is done by research to cross-reference PMW observations to the ATSR/SLSTR series (to obtain both relative bias adjustments and consistent uncertainty estimates). In the current phase, this will be attempted at L2. It is likely that a better approach would be to work from L1 in combination with L2, so this is assumed hereafter.

On the positive side, PMW data streams are relatively modest in data volume, so any benefits they bring may be cost-effective. It will also be an opportunity to increase practical expertise with PMW SST in Europe.

Table 2-3 summarises some characteristics and priority within the SST CCI system.

**Table 2-3: Passive and active microwave extension to constellation of sensors - characteristics and relative priority**

Sensor	Temporal coverage	Input data description	Priority / comments
TMI	1997 - 2013	5 channels (10.7 to 85 GHz), ~25 km resolution	Highly desirable
AMSR-E	2002 - 2011		Highly desirable
AMSR-2	2012 - 2016		Highly desirable
SSMR			Optional: experimental
WindSat			Highly desirable once performance is validated to be as expected

### Addition of geostationary sensors

To address the requirements of some climate users for sub-daily information on SST, a possible extension to the baseline constellation is to include SST-capable sensors on geostationary sensors.

Since global coverage is a requirement, this would require use of geostationary data for the full range of longitudes. This introduces a large diversity of sensors and data formats. While the dual view capability of ATSR/SLSTR makes cross-calibration of geostationary sensors at level 1 feasible using a multi-sensor match-up system (MMS), it is nonetheless a major research effort to do this for a comprehensive suite of geostationary sensors. To achieve climate-quality stability across time and longitudes would demand detailed sensor-by-sensor work. Bayesian approaches to cloud detection are sufficiently general to apply in a consistent manner across all the sensors, but would require development of forward-model adjustments. The design of optimal estimators for geostationary sensors has been demonstrated on SEVIRI, but there are complexities related to trading between SST sensitivity and retrieval noise levels. A very large increase in input data volume would be entailed.

Assuming success, the main benefits would be systematic resolution of diurnal cycle (which is a GCOS requirement [RD 7]) for cloud free areas, increased coverage and reduced sampling uncertainty.

On balance, inclusion of geostationary sensors would be scientifically "Desirable" (not accounting for considerations of cost effectiveness).

However, there is an additional mode of use for geostationaries, as components of the Multi-sensor Match-up System (without being part of the main product stream). This is because diurnally resolved products are specified in the SRD scenario (below). Having SEVIRI in the MMS will provide an independent means of assessing these very effectively. A full constellation of geostationary SST-capable sensors would be "desirable", whereas implementing at least one well-understood geostationary is "essential" for developing and testing techniques to infer information about the diurnal cycle from the remainder of the SST constellation. The use of SEVIRI for this purpose is consistent with CR-3.

### Conclusion on satellite constellation

For the purposes of this SRD, the assumption is that all the "Essential" and "Highly Desirable" data streams will be required in the system. That is, in summary:

- ATSR series
- AVHRR GAC series
- AVHRR Metop A and B series at full global resolution
- SLSTR
- VIIRS
- AMSRE-E
- TMI
- AMSR-2
- WindSat SST

In addition, it will be assumed that matched data from other sensors can be accommodated in the Multi-sensor Match-up System, and that in particular this will include:

- SEVIRI
- IASI

In the formal requirements section (Section 3) the sensor constellation and temporal coverage is referred to as **scenario-1**. Requirements making reference to this scenario are listed below.

scenario-1	Sensor constellations and temporal coverage	SST-SR-6110 L2P outputs SST-SR-1135 PMW inputs SST-SR-1140 Sentinel inputs SST-SR-1150 VIIRS inputs SST-SR-1160 Sentinel data reduction SST-SR-1165 VIIRS data reduction SST-SR-1190 Input data interface SST-SR-2110 Input ingestion SST-SR-2120 Auxiliary update SST-SR-2125 Validation data update SST-SR-2130 Data-driven processing SST-SR-1450 Input storage size SST-SR-1460 Output storage size SST-SR-5160 Other sensor's inputs SST-SR-5170 New input type SST-SR-5190 New ancillary type SST-SR-5200 New processing chain SST-SR-5280 Storage extension SST-SR-5290 Storage extension SST-SR-5300 Performance scalability
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## 2.6.2 Reprocessing capability

The SST CCI system will need to be able to undertake reprocessing of historical data in parallel to routine short-delay processing. The absolute threshold functional requirement is that all input L1b can be reprocessed to L2/3/4 in **six months** of continuous processing---simultaneously to routine processing, use of the multi-sensor match-up system (see below) and computational services to users. This permits an updated cycle on the CDR of order 1 to 2 years.

However, this threshold configuration would be scientifically sub-optimal, in that it does not permit the development team to undertake internal reprocessing (as envisaged above in section 2.5).

To maximise the scientific quality of the CDR (i.e., to maximise the investment in having a development team working on the SST CDR improvement cycle), the internal reprocessing capacity needs to support relatively short internal reprocessing cycles and verification that changes made have had the required positive effects on accuracy, stability, etc, without introducing obvious new artefacts.

The breakthrough requirement scientifically for reprocessing capacity is:

- The system is able to reprocess all data streams from L1 to L2/3/4 in two months, including updating data in the MMS. Individual components of the total data stream can then likely be reprocessed on time scales of weeks, which allows a reasonably interactive and efficient improvement cycle, with possibility of fixing “unintended consequences”.
- The system is able to store outputs of at least the last three internal reprocessing runs for all input streams, for inter-comparison purposes.
- The system is able simultaneously to continue routine processing, use of the multi-sensor match-up system (see below) and computational services to users.

The target requirement scientifically for reprocessing capacity is:

- The system is able to reprocess all data streams from L1 to L2/3/4 in one month, including updating data in the MMS. Individual components of the total data stream can then likely be reprocessed on time scales of days, which facilitates a fully interactive and efficient improvement cycle, with rapid progress on “unintended consequences”.
- The system is able to store outputs of at least the last three internal reprocessing runs for all input streams, for inter-comparison purposes.

- The system is able simultaneously to continue routine processing, use of the multi-sensor match-up system (see below) and computational services to users.

The assumption in this SRD is that the target scientific requirement be met, since maximising the scientific quality of satellite CDRs for climate is the principal reason to have the CCI programme.

A final point on the reprocessing scenario relates specifically to L4 production. In Phase 1, L4 production is located at the Met Office, and is not integrated with the L2/L3 systems prototyped on the University of Edinburgh cluster (with an interface to CMS). This choice was made because of resource limitations within Phase 1. The scenario assumed here is that the Phase 2 system will have a version of an L4 analysis system installed and maintained within a single CCI system. As with the discussion of the Metop data stream above (which can be done via an interface to a system providing this data like CMS or within a CCI system), an alternative solution would be to retain the Phase 1 approach of interfacing to an L4 system like the Met Office OSTIA. This latter approach may be more affordable, although it would also represent an external dependency and some loss of flexibility (since the external L4 system's operational constraints would need to be taken into account).

In the formal requirements section (Section 3) the reprocessing capability is referred to as **scenario-2**. Requirements making reference to this scenario are listed below.

scenario-2	Reprocessing capability	SST-SR-1220 Input versions SST-SR-1230 Reprocessing input versions SST-SR-1470 Online storage SST-SR-1480 Parallel processing SST-SR-1490 Three days per year SST-SR-5250 Version decisions SST-SR-5255 Overlapping versions SST-SR-5270 Short development cycle SST-SR-5275 Internal version storage
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### 2.6.3 Scope of products

The range of SST CCI products to be generated and distributed affects the system requirements in various ways, most obvious in the data volumes associated with these.

The output product assumptions made are as follows:

- L2P SST-skin (or sub-skin) with time-adjusted SST-20cm for all sensors in constellation
- L3U 0.05 deg SST-skin, time-adjusted SST-20cm and clear-sky brightness temperatures for ATSR and SLSTR
- Daily (day and night separate) 0.05 deg L3C SST-skin (or sub-skin) with time-adjusted SST-20cm for all sensors in constellation
- Daily L4 satellite-only analyses at 0.05 deg of
  - SST-skin, SST-20cm and SST-foundation
 for the following sensor sets:
  - full-archive IR analysis (AVHRR GAC, AVHRR Metop, ATSRs, SLSTR, VIIRS)
  - best-coverage analysis (all sensors)
- It should be assumed that enhanced error covariance information is required at all data levels, and (prior to definition of the nature of this information) assume this doubles the output data volume)
- Diurnally resolved (3 hourly) L4 analyses of time-adjusted SST-skin and SST-20cm (assume this is possible since 2002 without geostationary sensors)

In the formal requirements section (Section 3) the scope of products is referred to as **scenario-3**. Most of the above are fully consistent with the requirements carried forward in the PSD. L3U with brightness temperatures and diurnally resolved L4 are not implemented in Phase 1 and will re-

quire an extension of the PSD for Phase 2. Requirements making reference to scenario-3 are listed below.

scenario-3	Scope of products	SST-SR-6110 L2P outputs SST-SR-6120 L3C outputs SST-SR-6130 L3U outputs SST-SR-6140 L4 outputs SST-SR-6150 L4 diurnal outputs SST-SR-5180 Other ECVs as ancillary SST-SR-5190 New ancillary type SST-SR-5200 New processing chain SST-SR-5230 Agile requirements selection SST-SR-5290 Storage extension SST-SR-5300 Performance scalability
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### 2.6.4 Interaction with users

The system needs to accommodate the demands for storage, serving and on-the-fly computation that are seen as necessary to support interactions with users. It further shall support the gathering of feedback from users.

The assumptions about these interactions are:

- All formally released versions of CDRs are accessible to users by http, ftp and OPeNDAP in perpetuity from a long-term facility (meaning, serving in perpetuity need not be supported within the SST CCI system)
- The currently released CDR (full timeseries reprocessed and short-time additions) is accessible to users by http, ftp and OPeNDAP in an SST-specific infrastructure that also supports web services [UR-QUF-90; UR-QUF-91; UR-QUF-93], served from the SST CCI system
- Web services will comprise
  - Time-series, regional averaging and spatio-temporal gridding tools with download, applicable to L2P [UR-QUF-97]
  - Time-series, regional averaging and spatio-temporal regriding tools with download, applicable to L3C and L4 [UR-QUF-97]
  - Extraction of data subsets (including whole-time-series-limited-area requests, and via an interactive map) [UR-QUF-98; UR-QUF-92; UR-DIS-124]
  - Visualisation of data, including of quality and uncertainty information [UR-QUF-99]
  - Climatology and annual average generation [UR-DIS-130]
- These web services must
  - Provide outputs for download in a reasonable time (<1 hour for the maximum request)
  - Provide users with information on progress of the request
  - Be flexible as regards the selection of data sets to include (e.g., a user defined mix of sensors or analyses)
  - Be flexible with regard to the climatology assumed when doing manipulations via SST anomalies (user-defined climatology possible)
- Besides open access to data there is also open access to documentation and read access to the processor and algorithm repository for all users.
- There is a help system for CCI that can be contacted by users. There is a responsibility for the SST CCI development team to answer questions [UR-DIS-119]
- There is a customer relationship management system with issue tracking to trace communication and to route questions to operations or development team

- There are subscription mechanisms (RSS, ATOM, email) in place to inform interested users about new versions, important data issues etc. [UR-QUF-95; UR-QUF-96; UR-LLP-27]
- Users can access MMD extracts from the MMS with a flexible set of criteria for subsetting. There are tools to visualise MMD content and documentation how to access MMD NetCDF files by other tools.
- Users can contribute MMD columns (primarily their SST retrievals) to the MMS (with prior agreement of development team) in order to facilitate future algorithm inter-comparisons, by a means that is user-friendly but also robust against poor quality ingestions. [UR-REF-23]
- Users are enquired and can contribute feedback and raise data issues in a tracked manner, with issues raised visible to other users [UR-REF-9]

In the formal requirements section (Section 3) the interaction with users is referred to as **scenario-4**. Requirements making reference to scenario-4 are listed below.

scenario-4	Interaction with users	SST-SR-6180 Output provision SST-SR-6190 FTP access SST-SR-6200 Web access SST-SR-6210 OPeNDAP access SST-SR-6220 Bulk access SST-SR-4110 Subsetting and regridding SST-SR-6230 Online subsetting and regridding SST-SR-4120 Visualisation and data analysis SST-SR-4130 Data access software SST-SR-6240 Web site SST-SR-6250 Catalogue SST-SR-6260 News feed SST-SR-6270 Forum or help desk SST-SR-6330 Web site SST-SR-6340 Science issues SST-SR-6360 Forum maintainer SST-SR-5230 Agile requirements selection
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### 2.6.5 Further considerations

In the CDR improvement cycle, the development team and authorised scientists will need to work with an efficient Multi-sensor Matchup System (MMS). The assumed capabilities for this MMS are: The MMS will be able to generate a complete MMDB from a new locations list (in situ and dummy), with appropriate quality control and error handling, in a fully automated manner, within 1 month

- The MMS will achieve the routine update of the MMDB with additional in situ observations and locations
- The MMS will support facilities for extraction of small images (for retrieval work) and large images (for classification work)
- MMS tools for subset extract and delivery, plus ingestion tools that ensure validity of ingested data (for development team use, and as an external web service with development team authorisation)

To support the CDR improvement cycle, the system will accommodate an algorithm development environment for use of the development team. In this context, core algorithms used by the development team will be under version control in a place where the development team can experiment with code, test the effect on MMD statistics, and then do internal reprocessing (prior to fixing the code version for formal reprocessing) and assessment of results (using assessment tools).

In the formal requirements section (Section 3) the multi-sensor matchup system and the development environment are referred to as **scenario-5**. Requirements making reference to scenario-5 are listed below.

scenario-5	Multi-sensor matchup system and development environment	SST-SR-3110 Ingest observations of various types SST-SR-3120 Compute multi-sensor matchups SST-SR-3125 Incremental matchup computation SST-SR-3130 Update flag fields SST-SR-3140 Extract satellite sub-scenes SST-SR-3150 Interpolate NWP SST-SR-3160 Process SST SST-SR-3170 Extract multi-sensor matchup datasets SST-SR-3180 Ingest external MMD inputs SST-SR-3190 Support for concurrent versions SST-SR-3220 20 million matchups SST-SR-3225 MMDB re-build SST-SR-1330 Processor configuration control SST-SR-1340 Concurrent processor versions SST-SR-1350 Processor framework SST-SR-1380 Bulk reprocessing SST-SR-6280 Processor repository SST-SR-6290 External algorithm development SST-SR-6300 Matchup datasets SST-SR-6310 Matchup inputs SST-SR-5110 Community process SST-SR-5220 Development team SST-SR-5230 Agile requirements selection SST-SR-5240 Development and evaluation SST-SR-5270 Short development cycle
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## 2.7 Prototype Sea Surface Temperature production workflow

This section describes the processing workflows of retrieval, merging and validation as far as known for the Phase 1 prototype. It will be assumed that parts of this, allowing for respective improvements and extensions, will give guidance about CCI phase 2. But note that all systems named in this section apply to the CCI Phase 1 prototype and can be expected to be replaced by different implementations in CCI Phase 2.

### 2.7.1 Main inputs and outputs

The main input data for the production of CCI SST in the phase 1 prototype are listed in Table 2-4. The data comprise remote sensing observations from ATSR 1, ATSR 2, AATSR, both NOAA and MetOp AVHRRs, SEVIRI and PMW, and numerical weather prediction data produced by ECMWF.

The main outputs of SST CCI are listed in Table 2-5. The data comprise SST retrieval results at several levels. The data file format is NetCDF 4 using a geographic projection and metadata satisfying CF conventions and GHRSSST GDS 2.0 with extensions for CMIP5 compliancy. The data include retrieval uncertainties and confidence limits.

**Table 2-4: Main inputs of the SST CCI processing chain**

Product	Coverage	Volume	Comment
ATSR 1, ATSR 2, AATSR L1b	1991-2012	23 TB	
NOAA AVHRR GAC L1	1991-2012	12 TB	
MetOp AVHRR	2007-2012	3 TB	demonstrator SST processing only
SEVIRI L3C	2003-2012	23 TB	demonstrator SST processing only
PMW SST L2	1999-2012	315 GB	demonstrator SST processing only
ECMWF ERA-Interim NWP	1991-2012	2 TB	

**Table 2-5: Main outputs of the SST CCI project**

Product	Coverage	Volume	Comment
L2P SST	orbit	120 TB	satellite acquisition grid (estimation based on single product size from PSD, without compression, but yet without error covariance information)
L3C SST, single sensor daily (ATSRs and AVHRRs)	global	12 TB	geographic projection, 0.05° resolution (estimation see above)
L4 SST, multi-sensor daily	global	125 GB (20 yrs)	geographic projection, 0.05° grid

### 2.7.2 Estimation of system key parameters

The SST CCI prototype will create a long-term SST record for August 1991 to 2012. The overall data volume and the overall time needed for processing is estimated in Table 2-6.

**Table 2-6: Estimate of overall data volume and processing time**

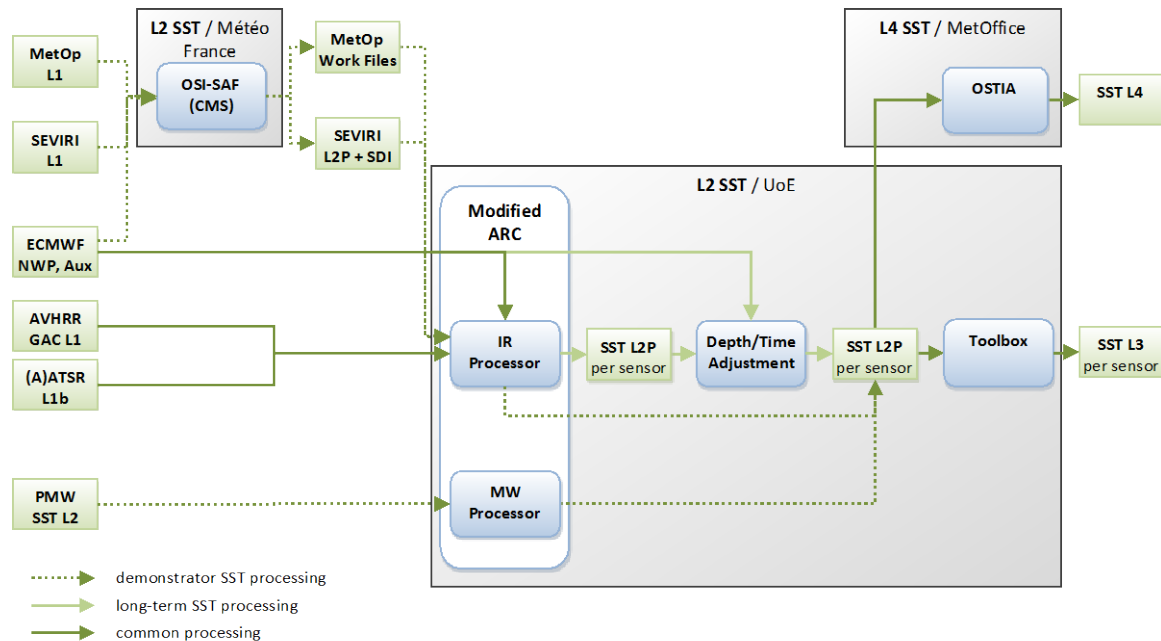
Data	Coverage	Volume	Time	Comment
Single-sensor	Varies	10 TB	7 days	Average per-sensor data volume from Table 2-4; time quoted is that needed by current ARC cluster for reprocessing a complete single-ATSR dataset
Overall level 2	1991-2012	63 TB	46 days	Data volume estimated from Table 2-4; time estimate based on performance of current ARC on current hardware of 14 computing and storage nodes.
Overall level 4	1991-2012	125 GB	66 days	Processing times from first OSTIA re-analysis

### 2.7.3 Processing chain

The distributed Phase 1 SST CCI processing system will comprise three subsystems that will be run at different sites: modified ARC (ECDF), OSI-SAF (Météo-France), and OSTIA (Met Office). The interfaces between these subsystems will be data interfaces for exchanging products online or offline.



The SST CCI processing chain is depicted in Figure 2-6. The figure illustrates two variants: the demonstration SST and the long-term SST processing chains. Both variants share a set of common components. The demonstration chain will be used to generate limited-period demonstration products, not the long-term CDR.



**Figure 2-6: SST CCI Phase 1 processing chain, provided here for guidance (implementation in CCI Phase 2 can be assumed to be different)**

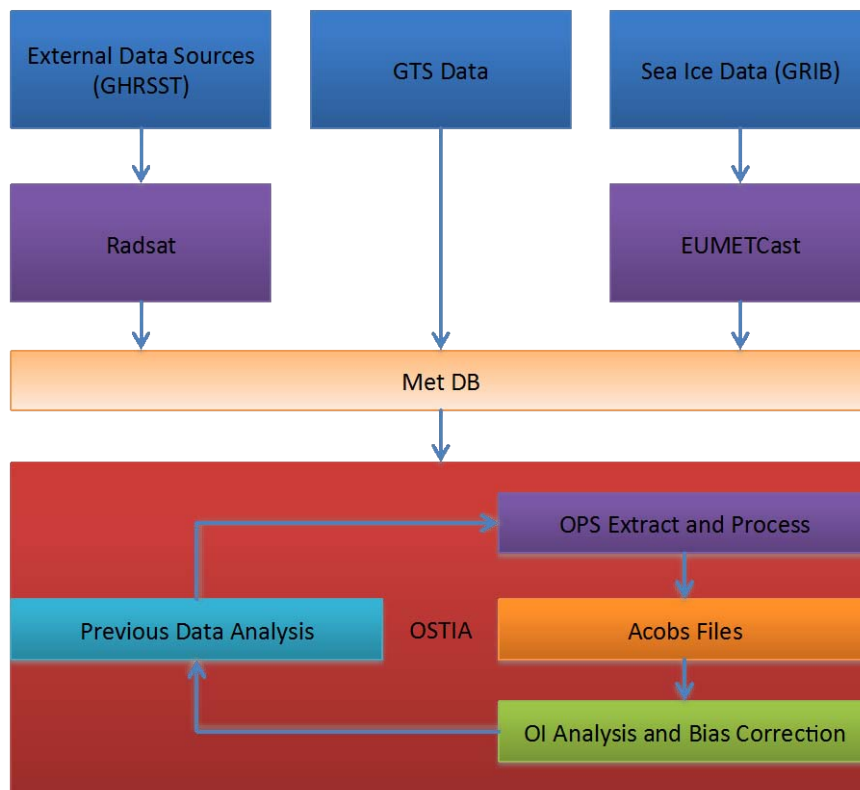
The main difference between the demonstration and the so called long-term SST processing (both in SST CCI phase 1) is the input data used. In addition to the ATSR, AATSR and NOAA/AVHRR data used by both chains, the demonstrator processes data acquired by MetOp AVHRR and SEVIRI, and PMW remote sensing systems. A further difference is that the long-term processing will comprise a step for adjusting the reference depth of the surface layer and the reference time, which will be omitted for the demonstration.

Common components for both chains will be the IR processor, which will be part of the modified ARC processor run at the Edinburgh Compute and Data Facility (ECDF), the SST CCI toolbox based on BEAM, and OSTIA, which is operated at the Met Office and will carry out a daily L4 analysis. The toolbox will aggregate single-sensor L3 SST and comprises additional tools for extracting multi-sensor match-ups and supporting algorithm inter-comparison and validation (see Figure 2-6).

In addition to the common components of the processing, the demonstration will employ a PMW processor for producing L2 SST from PMW systems, and make use of the OSI-SAF, which produces L2 SST and SDI from Metop AVHRR and SEVIRI L1 for ingestion into the IR processor. OSI-SAF is operated by Météo-France.

The modified ARC processor will use the Edinburgh Compute and Data Facility (ECDF). The ECDF is a high-performance cluster of servers including around 1500 processors and currently up to 250 TB of data capacity. The cluster is connected to a large amount of high performance fibre channel disk storage via a number of dedicated machines. These machines then share the data across the cluster using a parallel file system. The ECDF offers a processing grid via the Sun Grid Engine (SGE). Modified ARC processing is integrated in the ECDF SGE environment using SGE batch mode.

OSTIA is a real-time system for producing a daily L4 analysis using various input data sources. An overview of the system and the flow of information are illustrated in Figure 2-7 below.



**Figure 2-7: Overview of the real-time OSTIA system**

All input and output data currently used by the OSTIA system make use of the NetCDF 4 format with CF and GHRSSST GDS 2.0 compliant metadata. Satellite SST data in GHRSSST L2P and L3U format are obtained from a number of external data sources via automatic FTP on a continuous basis. MetOp data are obtained every 3 minutes.

The data are automatically processed on the Radsat computing environment, which is an operational, fully redundant system. The processing system, and its inputs and outputs are automatically monitored, with warnings issued when problems arise and a pre-defined set of procedures for operators to follow when warnings are received. The satellite SST data are sent from the Radsat machines to the Meteorological Database (Met DB) that provides storage and archiving of the data. In situ SST data are obtained continuously over the WMO Global Telecommunications System (GTS) and stored in the MetDB. Sea-ice concentration from the OSI-SAF is obtained over the EUMETCast system and is stored in the Met DB.

Once per day the OSTIA system is run in the operational suite on the Met Office High Performance Computing (HPC) system. The Observation Processing System (OPS) extracts the various data types from the MetDB and processes them, including a quality control step. This produces a number of observation files in an internal Met Office file format. A background file is also created based on the analysis of the previous day with relaxation to climatology. The observations and background files are then passed to the analysis system, which performs a bias correction on the satellite SST data, and an objective analysis. The main output of this analysis is a GHRSSST GDS 2.0 compliant NetCDF file containing an estimate of foundation SST, an error estimate, and sea-ice concentration data, all on a 0.05° latitude-longitude grid. The output files are sent from the HPC to an operational FTP server, which disseminates data to various users over both the Internet and the GTS.

The real-time OSTIA system is implemented on the High Performance Computing (HPC) facility at the Met Office. The HPC consists of approximately 250 IBM Power 6 nodes, each with 32 CPUs. It is currently upgraded to IBM Power 7. The nodes as well as the storage of 600 TB are spread evenly between two computing halls in physically separate locations. Operational production is run on the nominal supercomputer, with fallback to the backup architecture regularly tested. Stor-

age uses IBM's General Parallel File System GPFS. A hierarchical storage management system MASS-R based on IBM HPSS provides an archiving service.

All jobs on the Met Office HPC are managed using the Load Leveler batch subsystem. The same computing facility is available for research and development experiments, pre-operational testing, production of reanalyses, and routine operational jobs. Each type of experiment is allocated its own priority level, with the operational system having dedicated nodes at specific times of the day. The various steps in the main OSTIA system are controlled using the Suite Control System (SCS), a tool developed within the Met Office. The system provides a graphical user interface in order to control and make changes to the various tasks. It also controls the submission of jobs to the HPC using a number of Unix scripts. The SCS is used to submit jobs for both research and development experiments. There are automated monitoring systems in place to supervise the execution of various automated steps. Dedicated operators (available 24/7) monitor the operational OSTIA system and ensure that the system runs correctly. A set of operator instructions are available, with support being provided by the operational team, and further support by scientists and technical experts on a reasonable endeavours basis out of work hours. This set-up ensures the production and delivery of data to the ftp server.

A version of the operational OSTIA system has been set-up for production of reanalyses. This is not run in the same routine manner as the operational system, but on a one-off basis. All the components of the reanalysis system are based on the equivalent component of the real-time system, but with some modifications appropriate for reanalysis mode.

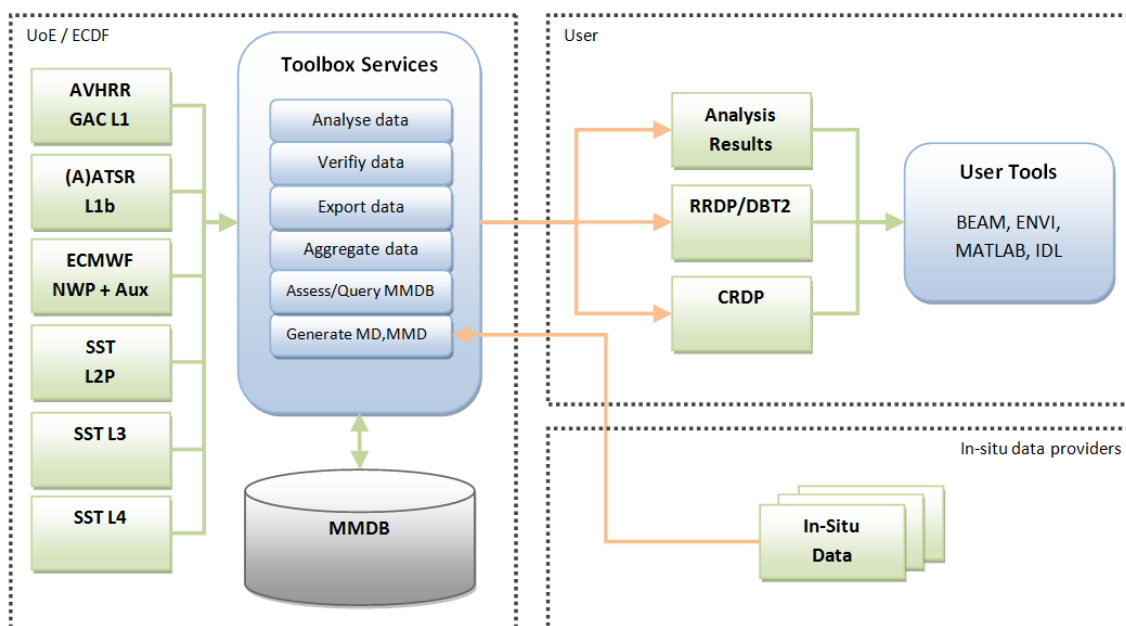
## 2.8 Prototype multi-sensor matchup system

This section describes the prototype of the multi-sensor matchup system.

The SST system shall support continuous algorithm improvement. Considering the algorithm improvement cycle of repeated processing and validation with modified algorithms or parameterisations from the validation end, the way of validation can determine which subset of data has to be processed. This subset may be spatio-temporal extracts that match in-situ data in space and time, or it may be time lines with restricted spatial extent, or it may be selected global datasets, whatever is necessary to assess the results. The multi-sensor matchup system of the prototype supports the case of extracts for matchups with in-situ data.

The key point of this approach is to reduce the processing time for one cycle considerably to a few days or even hours compared to months for complete L2 generation. For this it is essential that the algorithms or processors can process such extracts instead of the complete dataset. This can speed up the cycle because extraction can be done on level 1 and can be pre-computed outside of the cycle, and comparison of different algorithms can be automated. This is the idea of the SST CCI multi-sensor matchup system.

The SST CCI multi-sensor matchup system (MMS) determines matchups of in-situ measurements and several satellite observations, extracts sub-scenes of the satellite image for repeated processing with different algorithms, and controls sub-scene processing. The content is specified in [AD 6]. It further provides tools for analysis and inter-comparison. The prototype system has determined 6 million multi-sensor matchups and has generated and processed 20 million sub-scenes with a single ARC processor version. Figure 2-8 shows its use for the round-robin dataset generation.



**Figure 2-8: SST CCI toolbox for multi-sensor matchups, algorithm development, and product validation**

Input data used by the SST CCI multi-sensor match-up system (MMS) in addition to satellite data are listed in Table 2-7. The data comprise in-situ measurements from several sources along with corresponding sub-scenes extracted from remote sensing observations (listed in Table 2-4) and supplementary data for sea ice and aerosol. In particular, input for the MMS are forward model fields and SST produced by the MMS itself with help of the ARC processor, which can be fed back into the MMS for the purpose of algorithm inter-comparison as part of the improvement cycle.

**Table 2-7: Additional inputs of the MMS**

Product	Coverage	Volume	Comment
Matchup datasets of satellite and in-situ observations from ARGO floats, drifting buoys and ships	1991-2012	110 GB	Pre-computed single-sensor matchups have been used for the prototype because some datasets are available to the project only as such pre-computed matchup datasets.
Aerosol	1991-2012	1 GB	
Sea ice concentration	1991-2012	61 GB	
History of in-situ data	1991-2012	9 GB	
Forward model fields and SST processing results produced by and fed back into the MMS for algorithm inter-comparison		24 GB	CDO and ARC outputs

The prototype of the MMS ingests the data, supports extraction of sub-scenes, processing, re-ingestion of the results, and extraction for inter-comparison or external processing as shown in Figure 2-9.

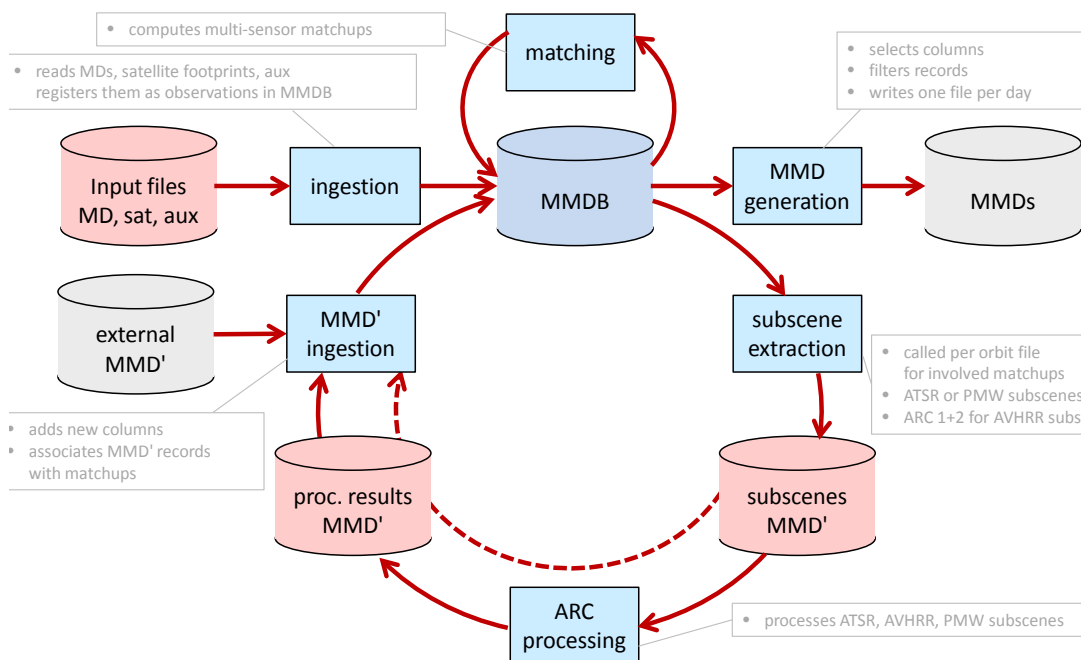


Figure 2-9: Repeated processing and comparison in the SST CCI MMS Prototype

The prototype implementation was a combination of a database system (PostgreSQL and Post-GIS), an archive directory structure and file system, the ECDF Eddie cluster running the Sun Grid Engine, the BEAM toolbox, and a collection of software tools. The MMD exchange data format has been defined and used for all interfaces not determined by external constraints.

Focus of the prototype MMS was the generation of the round-robin dataset which is a single MMD. For an operational MMS sub-scene extraction would have to be moved to before the cycle. The steps in such an MMS would be:

- Matchups are computed from in-situ and from satellite data from different sensors.
- Extracts with e.g. sub-scenes of some size are made from the input L1 data. Also auxiliary data is prepared for processing, e.g. interpolated to the input grid. The extracts are selected such that they match in-situ or reference data. The extracts are stored as extract dataset for repeated use.
- The extracts are processed by an L2 processor. Several different L2 processors may process the dataset; among them may be external processors. The results are L2 of the extracts.
- The L2 of the extracts are analysed and compared with in-situ or reference data, and can be compared with each other.
- The validation result can be used to improve parameterisation, processor implementations, or the selection of algorithms. The improved processor can be compared with its predecessor by comparing the L2 of the extracts.

## 2.9 SST data analysis tools

This section identifies tools besides the MMS to support the development of SST CCI products and which also can be developed to support user services. Some of them will be part of the prototyping in Phase 1 (further details in text below). All of them should be further developed in Phase 2.

Tool Name	Purpose	Main contexts of use
RegionalAverage	Aggregating SST products and propagating uncertainties in space and time, to produce time-series for ocean-basin to global scales	SST time-series generation
Regridder	Aggregating SST products and propagating uncertainties in space and time, to produce lower resolution data and/or time-series	Support to climate assessment report inter-comparisons, background task to SST data visualisation, creation of smaller aggregated SST products
Bias metrics	Calculate mean discrepancies (with various options) from MMs	Algorithm selection, product validation
Bias in uncertainty metrics	Calculate parameters (with various options) from MMs for uncertainty	Algorithm selection, product validation
Precision metrics	Calculate scatter of discrepancies (with various options) from MMs	Algorithm selection, product validation
Stability metrics	Calculate stability of discrepancies (with various options) from MMs	Algorithm selection, product validation
Other validation tools for CAR	Calculate metrics from SST CCI products and comparison data sets	Climate assessment report
MMD Viewer	Presentation of MMD content on maps and in tables, data selection	Algorithm development, algorithm selection, product validation, public MMD users
GridMMS	To verify SST CCI products need to make 0.05 deg ATSR series observations in MMS to compare with product cells	Product verification

Some of the tools are already defined:

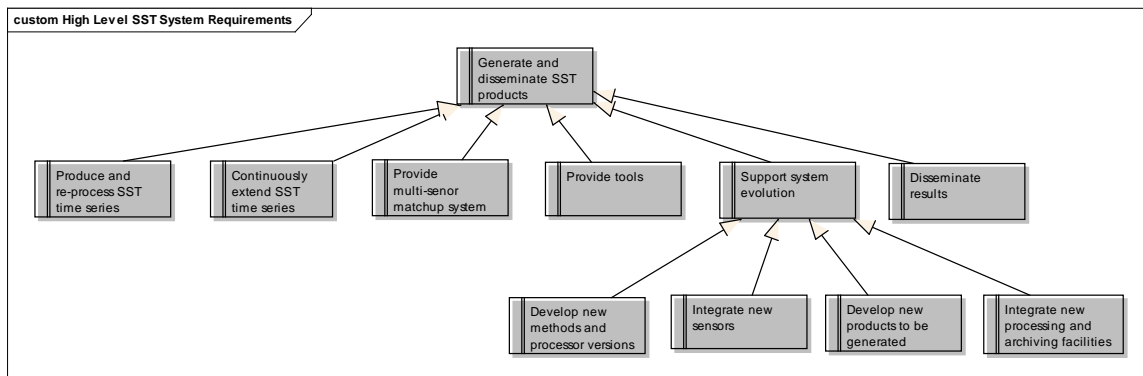
- The regional averaging tool reads in the ARC 0.1° daily and SST CCI L3C and L3U and L4 products at daily 0.05° latitude by longitude resolution and creates regional averages of the SST anomaly relative to a reference climatology, along with estimates of the uncertainty in those averages. The tool also plots those data. Details are defined in a tool specification.
- The regridding tool reads in the SST CCI L3C, L3U and L4 products at daily 0.05° latitude by longitude resolution and outputs on other spatio-temporal resolutions, which are a multiple of this. The tool outputs the SSTs and their uncertainties. Optionally, it extracts sub-regions. Details are defined in a tool specification.
- The various metrics tools calculate metrics of bias, metrics of bias in uncertainty estimation, metrics of SST precision. During phase 1 of the SST CCI project they are used for algorithm selection in the Round Robin comparison as defined in the product validation plan. They operate on an MMD. They generate statistics data files and graphics. Details are defined in tool specifications.

- MMDView is used to open MMD NetCDF files and let users analyse the contained MMD records. Users can visually inspect file contents and export selected MMD records. The tool can also be used to reproject MMD records from satellite coordinates to lat/lon projection. MMDView is a stand-alone desktop application. Details are to be defined in a tool specification.

The processing workflow the foreseen improvement cycle and the identification of tools are important inputs to the detailed system requirements.

### 3. DETAILED SYSTEM REQUIREMENTS

With the source requirements from section 2.3, the SST scenario for CCI phase 2 from section 2.6 and the processing workflow from section 2.7 as basis, this section derives a set of requirements for the SST CCI system from these inputs.



**Figure 3-1: Hierarchy of high level SST CCI system requirements**

Figure 3-1 introduces a number of high level requirements for the SST CCI system. Production and reprocessing the SST time series requires all functions to produce and validate SST products for a large but finite set of inputs. The requirement for continuously extending the time series implies additional functions to extend the CDR by newly acquired data. Providing tools and disseminating results to serve users are the functions of data access, which include the exchange in the SST community and with climate users. Supporting system evolution and providing a multi-sensor matchup system finally comprises requirements to support the improvement cycle and incremental growth of the system.

Requirements are defined by

- **ID**, identifier, e.g. SST-SR-1230, with ranges 1xxx to 6xxx for the six parts of the hierarchy
  - **Type**, one of
    - functional (**fun**)
    - performance and sizing (**per, siz**)
    - interface (**int**)
    - operational (**ope**)
    - reliability, availability, maintainability, security (**ram**)
- with meanings defined in ECSS-E40 [RD 6]
- **Title**, a two-word name for the requirement
  - **Description**, "The SST CCI system shall ..."
  - **Ref.**, reference to the source requirement, one of
    - SoW-x, UR-x, PSD-x, DARD-x
    - assumption-x
    - OPS-x operations concept (referring to section 2.5)
    - scenario-x referring to the choice of section 2.6
    - system key parameters (referring to section 2.7.2)
    - processing workflow (referring to section 2.7 and 2.8)
    - best practice (referring to experience with similar systems)
  - **Vrf.**, verification method, one of
    - review (**R**)
    - test (**T**)
    - inspection (**I**)
    - monitoring in the operational phase (**M**)



### 3.1 Requirements on the generated output products

This section lists requirements for the SST products. They are mainly derived from the scenarios and URD and PSD.

#### 3.1.1 Functional requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-6110	fun	L2P outputs	The SST CCI system shall provide: L2P SST-skin and SST-20cm, for the sensors of ATSR series, AVHRR GAC series, AVHRR Metop series at full global resolution, SLSTR, VIIRS; L2P SST-subskin and SST-20cm, for the sensors of AMSRE-E, TMI, AMSR-2, WindSat SST.	SST-TR-2 scenario-3 scenario-1 PSD-2 UR-QUF-33	R
SST-SR-6120	fun	L3C outputs	The SST CCI system shall provide daily (day and night separate) 0.05 deg L3C SST-skin (or sub-skin) and time-adjusted SST-20cm for all sensors in constellation	scenario-3 UR-QUF-33	R
SST-SR-6130	fun	L3U outputs	The SST CCI system shall provide L3U 0.05 deg SST-skin, time-adjusted SST-20cm and clear-sky brightness temperatures for ATSRs and SLSTR	scenario-3 PSD-1 UR-QUF-33	R
SST-SR-6140	fun	L4 outputs	The SST CCI system shall provide daily L4 satellite-only analyses at 0.05 deg of SST-skin, SST-20cm and SST-foundation for both the full-archive IR analysis (AVHRR GAC, AVHRR Metop, ATSRs, SLSTR, VIIRS) and for the best-coverage analysis (all sensors including PMWs), with enhanced error covariance information.	scenario-3 PSD-3 UR-QUF-35	R
SST-SR-6150	fun	L4 diurnal outputs	The SST CCI system shall provide diurnally resolved (3 hourly) L4 analyses of time-adjusted SST-skin and SST-20cm	SST-TR-21 scenario-3 UR-QUF-35	R
SST-SR-6160	fun	Output format and naming	The SST CCI system shall format and name its output products according to the PSD (which may evolve over time).	SST-TR-1 SST-TR-10 SST-TR-12 PSD-4 PSD-5 UR-QUF-89 UR-REF-16 UR-REF-17	R

#### 3.1.2 Operational requirements

None in this category.

Operational requirements for the generation of the output products are defined in the respective sections below.

### 3.1.3 Performance and sizing requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-6170	per	Product features	The SST CCI system shall document the degree of compliance of its outputs with features required by the URD. The URD is maintained by the development team. The system shall support the collection of new requirements and feedback by users.	SST-TR-6 UR-REF-3, UR-QUF-43	R

More performance and sizing requirements are defined below in section 3.2.3 on performance and sizing for the production of the SST time series. SST-SR-1460 and SST-SR-1490 in particular define output sizing and generation performance.

### 3.1.4 Reliability, availability, maintainability, and security requirements

None in this category.

Relevant requirements can be found in section 3.4.4 on user service requirements below.

## 3.2 Requirements on SST time series production and reprocessing

This section lists requirements on the production of the SST CDR. This comprises the production of a time series from existing data and the continuous extension of this time series by newly acquired data. Note that operational requirements of this section and requirements listed in section 3.5 *Internal user and operator requirements* may have overlapping scope.

### 3.2.1 Functional requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1110	fun	(A)ATSR inputs	The SST CCI system shall include (A)ATSR L1b products since 1991.	SST-TR-7 SST-TR-49 DARD-1.01 UR-REF-3 UR-QUF-43	I
SST-SR-1120	fun	AVHRR GAC inputs	The SST CCI system shall include AVHRR GAC L1b products since 1981.	SST-TR-77 SST-TR-49 DARD-1.03 UR-REF-3 UR-QUF-43	I
SST-SR-1130	fun	AVHRR METOP inputs	The SST CCI system shall include full resolution L1B AVHRR METOP products since 2006.	SST-TR-49 DARD-1.04 UR-REF-3 UR-QUF-43	I
SST-SR-1135	fun	PMW inputs	The SST CCI system shall include PMW L2 and optionally L1 products since 1999.	Scenario-1	I

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1140	fun	Sentinel inputs	The SST CCI system shall include SLSTR L1b products starting from the beginning of the operational phase of the Sentinel 3 mission.	scenario-1	I
SST-SR-1150	fun	VIIRS inputs	The SST CCI system shall include VIIRS L1b products starting from the beginning of the operational phase of the mission.	scenario-1	I
SST-SR-1160	fun	Sentinel data reduction	The SST CCI system shall optionally subset SLSTR L1B inputs to the resolution and channels used for SST CCI and store these subsets to save space.	scenario-1	T
SST-SR-1165	fun	VIIRS data reduction	The SST CCI system shall optionally subset VIIRS L1B inputs to the resolution and channels used for SST CCI and store these subsets to save space.	scenario-1	T
SST-SR-1170	fun	Auxiliary inputs	The SST CCI system shall include auxiliary data required for processing as specified in the DARD.  Note that the DARD can be expected to be updated for Phase 2. The system has to adapt to such updates. Example: For short-delay mode processing operational or forecast NWP data will be required in addition to ERA-interim.	SST-TR-17 SST-TR-18 DARD-12 to -15	I
SST-SR-1180	fun	Validation datasets	The SST CCI system shall include validation datasets as specified in the DARD  Note that the DARD can be expected to be updated for Phase 2. The system has to adapt to such updates.	SST-TR-22 DARD-3.xx DARD-4.xx	I
SST-SR-1190	int	Input data interface	The SST CCI system shall have an interface to ingest its input data. Depending on how the data are accessed or provided, this may include the use of interfaces of data providers.	scenario-1	T
SST-SR-1200	fun	Output preservation	The SST CCI system shall preserve its output products specified in the PSD. For the prototype (long-term time series) these are the L3U ((A)ATSR), L2P (AVHRR), and analysis (L4) output products.	PSD-1 PSD-2 PSD-3	I
SST-SR-1210	fun	Structured storage	The SST CCI system shall store its inputs and outputs in a structured way, e.g. by archiving rules using type, version, year, month, day.	Best practice	I
SST-SR-1220	fun	Input versions	The SST CCI system shall ingest new versions of its input data to replace the previous version. It shall provide some overlap in time to continue the online extension of the former version of the output until the new version is completely reprocessed.	scenario-2 assumption-3	T
SST-SR-1230	fun	Reprocessing input versions	The SST CCI system shall reprocess a new version of its outputs after ingesting new versions of its input data.	scenario-2 assumption-3	T

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1240	fun	Output versions	The SST CCI system shall be able to store several versions of its output product. At least one version shall be consistent and complete at any given time.	assumption-3 UR-DIS-126 OPS-7	R
SST-SR-1241	fun	Long-term stewardship	The SST CCI system shall ensure that all validated and released CDRs are preserved with long-term stewardship.	assumption-3 UR-DIS-126 OPS-7	R
SST-SR-1250	fun	SST retrieval	The SST CCI system shall perform SST retrieval by (a) processor(s) that implement(s) the algorithms specified in the SST ATBD. The ATBD is maintained by the development team. Incremental versions are provided when the system is frozen for a new CDR version.	SST-TR-14 SST-TR-15 SST-TR-16 SST-TR-17 SST-TR-18 SST-TR-20 Processing workflow PSD-2	T
SST-SR-1260	fun	Error characterisation	The SST CCI system shall perform error and uncertainty estimation by (a) processor(s) that implement(s) the algorithms specified in the SST ATBD.	SST-TR-19 Processing workflow PSD-2	T
SST-SR-1270	fun	Projection and compositing	The SST CCI system shall perform level 3 projection and compositing by a processor that implements the algorithm specified in the SST ATBD.	Processing workflow PSD-1	T
SST-SR-1280	fun	Sensor merging	The SST CCI system shall perform sensor merging to generate L4 analysis products by a processor that implements the algorithm specified in the SST ATBD.	SST-TR-29 Processing workflow PSD-3	T
SST-SR-1290	fun	Output products	The SST CCI system with its processing chain shall generate the SST output products specified in the PSD [AD 5], including their specified temporal and spatial resolution, accuracy and other features. The PSD is maintained by the development team. Incremental versions are provided when the system is frozen for a new CDR version. Note: See requirement SST-SR-1365 on system level documentation in section 3.2.5 below	PSD-1 PSD-2 PSD-3 UR-QUF-33 UR-QUF-35	T

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1300	fun	Quality check	The SST CCI system shall quality-check its outputs for formal errors and invalid content. It shall generate quality reports for single products and as a summary.	SST-TR-40 Processing workflow	T
SST-SR-1310	fun	Matchup analysis	The SST CCI system shall systematically perform matchup extraction for its output products against in-situ and reference validation datasets and generate validation reports and reference statistics.	SST-TR-45 Processing workflow	T
SST-SR-1320	fun	Trend analysis	The SST CCI system shall systematically perform time series generation from its output products and generate trend reports and temporal statistics.	SST-TR-45 Processing workflow UR-QUF-105	T
SST-SR-1330	fun	Processor configuration control	The SST CCI system shall support versioning of processors. This includes the parameterisation. The versions shall be under configuration control.  Note: The algorithms required by the ATBD will change over time. The system has to be able to adapt to such changes.	scenario-5 UR-REF-21	I
SST-SR-1340	int	Concurrent processor versions	The SST CCI system shall support the concurrent use of processor versions for different requests. The versions shall co-exist in the system.	scenario-5	R, T
SST-SR-1350	int	Processor framework	The SST CCI system shall provide a processor framework to allow for different implementations (i.e. implementation language, calling conventions, data access) of processors to be integrated into the system.	SoW-9 scenario-5	R
SST-SR-1360	int	Executable integration	The SST CCI system and its processor framework shall at least support the integration of executables as processors (much of the prototype is fortran and python). Dependent on algorithm implementation and selection (which may change over time (Java for level 3 in the prototype) other interfaces shall be supported.  Note: see requirement SST-SR-1295 on processor documentation in section 3.2.5 below	SoW-9 Best practice	R, T
SST-SR-1370	fun	Processing chain	The SST CCI system shall orchestrate the processors to process inputs in their respective processing chain. The types of chains shown in section 2.7.3 Processing chain shall be orchestrated, but with the respective SST Phase 2 processors and workflows, The orchestration may change.	Processing workflow	R, T

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1380	fun	Bulk re-processing	The SST CCI system shall orchestrate the production workflow for bulk reprocessing. It shall do so in chunks of selectable size, e.g. in months of input data.	scenario-2 Processing workflow	R
SST-SR-2110	fun	Input ingestion	The SST CCI system shall ingest new input data to extend the time series for its input products.	scenario-1 OPS-1	T
SST-SR-2120	fun	Auxiliary update	The SST CCI system shall ingest new auxiliary data required for processing. Note: The auxiliary data required by the DARD may change for different algorithms or versions over time. The system has to be able to adapt to such changes, e.g. by versioning auxiliary data.. Example: For short-delay mode processing operational or forecast NWP data will be required in addition to ERA-interim.	scenario-1 OPS-1 assumption-3 OPS-6	T
SST-SR-2125	Fun	Validation data update	The SST CCI system shall ingest new validation data to keep track with new input data that extends the time series. Note: The validation data required by the DARD may change over time. The system has to be able to adapt to such changes, e.g. by versioning validation data.	scenario-1 OPS-1	T
SST-SR-2130	fun	Data-driven processing	The SST CCI system shall continuously and automatically process new available input data in a data-driven way with the current operational processing chain version(s).	scenario-1 OPS-1 UR-REF-8 UR-QUF-83	T
SST-SR-2140	fun	Wait for ancillary	The SST CCI system shall process newly ingested data only after all required high quality inputs (e.g. ancillary data, if used for processing) are available.	OPS-9	T
SST-SR-2150	fun	CDR extension	The SST CCI system shall extend the CDR by the newly processed outputs.	OPS-1	T

### 3.2.2 Operational requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1390	ope	Operator	The SST CCI system shall have an operator that initiates, monitors and controls production	SoW-4 Best practice	R
SST-SR-1400	ope	Automation	The SST CCI system shall process its inputs in an automated way. Operators initiate re-processing by requests (per chunk).	SoW-4 Processing workflow UR-REF-8 UR-QUF-83	R, T

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1410	ope	System status	The SST CCI system shall exhibit the status of the system, in particular the status of requests and the jobs executed for them.	Processing workflow	I
SST-SR-1420	ope	Operating tool	The SST CCI system shall provide an operating tool to monitor and control the system and requests. The operating tool shall be browser-based.	Processing workflow	R
SST-SR-1430	ope	Error handling	The SST CCI system shall handle processing errors. They shall be detected, dependent operations shall not be started, but other processing activities shall continue. Operators shall be able to retry failed steps. The system shall resume processing of the chain in case of success. Operators shall be able to accept partial failure. Dependent steps shall not be executed and the respective input shall be skipped.	SoW-4 Best practice	T
SST-SR-1440	ope	Cancel and resume	The SST CCI system shall allow operators to interrupt, resume, cancel requests and their jobs.	Best practice	T
SST-SR-2160	ope	Online processing status	The SST CCI system shall provide the status of continuous ingestion and online processing of new data. The status shall distinguish the different input data streams and the progress of ingestion, processing, and validation.	Best practice	I
SST-SR-2170	ope	Online processing error handling	The SST CCI system shall provide the same kind of operations with error handling and retry for the online processing chain and for reprocessing. This also includes that an error for one input does not interrupt the chain for subsequent data.	Best practice	T

### 3.2.3 Performance and sizing requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1450	siz	Input storage size	The SST CCI system shall provide storage space for its input products. The size increases over time and depends on the optional reduction of Sentinel inputs. For ATSR and AVHRR up to 2010 the size is 40 TB plus 3 TB per additional year.	SoW-7 scenario-1 System key parameters	I
SST-SR-1460	siz	Output storage size	The SST CCI system shall provide storage space for its output products. The size increases over time and with versions. For (A)ATSR and AVHRR up to 2012 the size for one version is estimated to 132 TB, and 6 TB per additional year, depending on the inclusion of additional sensors.	SoW-7 scenario-1 System key parameters	I

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1470	per	Online storage	The SST CCI system shall store its input data optimised for reprocessing, i.e. in such a way that storage is not a bottleneck for reprocessing. Note: Usually, this requires online storage of the data, and either a fast network or distributed storage. Online storage of large parts of data (e.g. 25% of the total input volume), with systematic, adequately fast staging of data selections, may be an alternative.	SoW-7 assumption-3 scenario-2 UR-REF-1470	R
SST-SR-2180	per	Short-delay processing	The SST CCI system shall process newly ingested data under normal conditions within 72 hours after all required high quality inputs (e.g. ancillary data) are available. Note: 72 hours after availability of all high quality inputs aims at short-delay processing but without the requirement for e.g. operator availability over the weekends.	Best practice UR-QUF-44 UR-DIS-121 UR-DIS-122 OPS-9	R
SST-SR-1480	per	Parallel processing	The SST CCI system shall provide a massive parallel processing infrastructure (i.e. cluster) for bulk reprocessing.	scenario-2	R, T
SST-SR-1490	per	Three days per year	The SST CCI system shall re-process input data for all sensors in a rate (averaged across all years of input data) of 48 hours per year. Note: this requirement must be met on average for the years since 1981, but has to be improved in the future to keep the overall reprocessing time constant with the increasing amount of data from SLSTR, VIIRS and other sensors.	SoW-8 scenario-2	T, M

### 3.2.4 Reliability, availability, maintainability, and security requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1500	ram	Backup archive	The SST CCI system shall make sure that a second copy of its input data is stored in an independent backup archive.	SoW-7 Best practice UR-REF-15	R
SST-SR-1501	ram	Bulk archive retrieval	The SST CCI system's backup archive shall be optimised to allow bulk retrieval of data in chunks of data years.	SoW-7 Best practice UR-REF-15	R
SST-SR-1510	ram	Archive reliability	The SST CCI system shall provide means against data loss of its input products. It shall ensure that the storage together with the backup archive is built in a way that the reliability of storage against loss of input data per year is at least 99.9%.	SoW-7 Best practice UR-REF-15	R



ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1520	ram	Autonomous system	The SST CCI system shall be available for SST operations and processor development independent from other ECVs.	SoW-9 assumption-2	R

### 3.2.5 Other requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1525	des	ECSS compliance	The development of the SST CCI system framework shall comply with a tailored profile of ECSS-E-40.  Note: The processor development is not part of the system framework. It is excluded from this requirement and shall follow an agile, incremental approach instead.	Best practice	R
SST-SR-1365	des	System level documentation	The SST CCI system shall be documented in a system implementation description describing components and their configurations. (see also SST-SR-1367 Operator's Manual in section 3.5.5)	Best practice	R
SST-SR-1366	int	Product User Guide	The SST CCI system shall provide a Product User Guide derived from the PSD.	Best practice	R
SST-SR-1295	des	Processor documentation	The SST CCI processors shall either be documented in the source code repository, or by separate processor documentation.	Best practice	R

### 3.3 Requirements on a SST multi-sensor matchup system

Figure 3-2 shows an overview of the requirements for a multi-sensor matchup system. As already shown in Figure 3-1 they are integrated into the overall hierarchy for the SST CCI system with the high level requirement to generate and disseminate SST products.

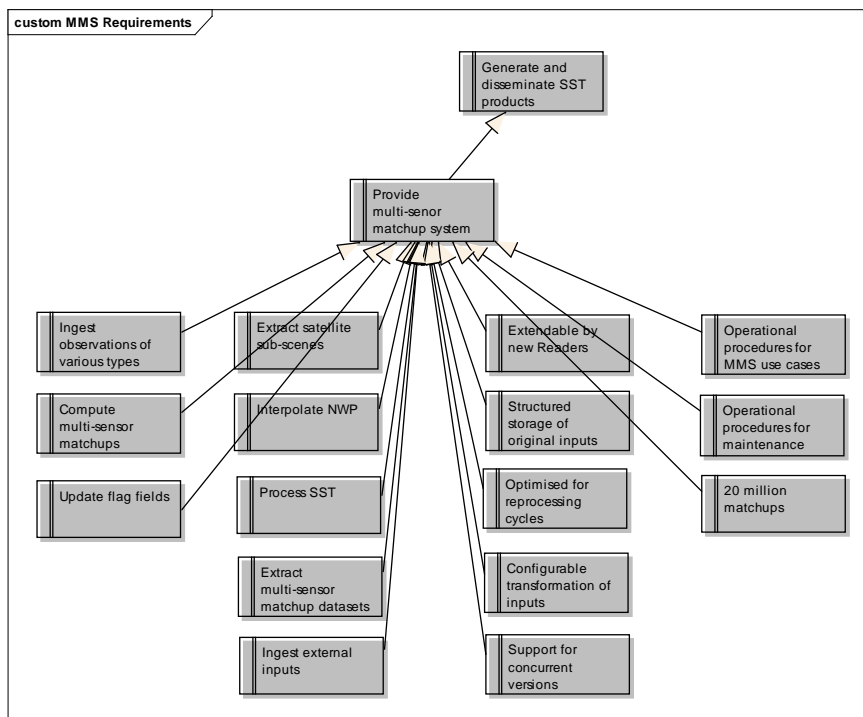


Figure 3-2: Hierarchy of requirements for a multi-sensor matchup system

The requirements on the left define the elementary functions. Requirements on the right cover structure, operations and sizing. The role of the MMS in SST and the prototype has been explained in section 2.

#### 3.3.1 Functional requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-3110	fun	Ingest observations of various types	The MMS of SST CCI shall ingest <ul style="list-style-type: none"> <li>in-situ data (including the in situ time series for +/-18 h of the central match-up time)</li> <li>satellite data from all scenario-1 sensors, e.g. (A)ATSR, AVHRR, AMSR-E, TMI</li> <li>ancillary data of at least NWP ERA-interim, aerosol and sea-ice</li> </ul>	SST-TR-22 scenario-5 workflow-2.8	T
SST-SR-3120	fun	Compute multi-sensor matchups	The MMS of the SST CCI system shall determine multi-sensor matchups <ul style="list-style-type: none"> <li>from in-situ and satellite data</li> <li>from lists of specified locations (“dummies”) matching in time and space with configurable margins, avoiding duplicates that may result from the input data, and shall co-register</li> <li>other matching observations</li> </ul>	scenario-5 workflow-2.8 UR-QUF-101	T

ID	Type	Title	Description	Ref.	Vrf.
			to these matchups. Note: A major difference to the prototype MMS is that the MMS shall start from in-situ and satellite data, not from pre-computed single sensor matchups.		
SST-SR-3125	fun	Incremental matchup computation	The MMS of the SST CCI system shall be able to extend the MMDB incrementally with new matchups on the availability of new in-situ data. It shall also be able to extend the MMDB on the availability of new satellite data.	scenario-5 workflow-2.8	T
SST-SR-3130	fun	Update flag fields	The MMS of the SST CCI shall support the update of MMS variables, in particular those for flags like the reference flag or the validity flag.	scenario-5 workflow-2.8	T
SST-SR-3140	fun	Extract satellite sub-scenes	The MMS of the SST CCI system shall extract sub-scenes of satellite data centred at the respective matchup reference location. The sub-scenes size shall be configurable (e.g. 10km * 10km)	scenario-5 workflow-2.8	T
SST-SR-3150	fun	Interpolate NWP	The MMS of the SST CCI system shall interpolate NWP values and other auxiliary fields for the extracted satellite data sub-scenes and for the matchup reference points. The interpolation results shall be ingested into the MMS as new column. Note: MMS should use the climate data operators (CDO) for this purpose.	scenario-5 workflow-2.8	T
SST-SR-3160	fun	Process SST	The MMS of the SST CCI system shall integrate the SST retrieval processor of SST CCI to process the extracted satellite data sub-scenes. The result of processing shall be ingested into the MMS as new columns.	scenario-5 workflow-2.8	T
SST-SR-3170	fun	Extract multi-sensor matchup datasets	The MMS of the SST CCI shall extract datasets in the MMD format as specified in the MMD definition document [AD 6]. The columns to be included in the MMD shall be selectable. The matchups to be included shall be selectable on the basis of time, geo-location, matched sensors, matchup dataset and optionally other criteria.	scenario-5 workflow-2.8	T
SST-SR-3180	fun	Ingest external MMD inputs	The MMS of the SST CCI system shall ingest external inputs in the MMD format (defined in the MMD definition document) related to any existing matchup. The MMS shall add this data as new columns with unique column identifiers and formalised description.	scenario-5 workflow-2.8	T
SST-SR-3190	fun	Support concurrent versions	The MMS of the SST CCI shall support several versions of a certain type of data in the system at the same time.  Note: This is intended to be used for processing outputs to allow comparison of several processor versions.	scenario-5 workflow-2.8	R

### 3.3.2 Operational requirements

This section lists operational requirements for the MMS system. Requirements regarding access to MMS and its outputs by users (SST-SR-6300, SST-SR-6310) are listed in section 3.4 .

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-3200	ope	Operations procedures for MMS use cases	The MMS of the SST CCI system shall define operational procedures for ingestion, the processing cycle, MMD generation, and external input ingestion.	scenario-5 workflow-2.8	I
SST-SR-3210	ope	Operational procedures for maintenance	The MMS of the SST CCI system shall define operational procedures for data management and backup.	workflow-2.8	I

### 3.3.3 Performance and sizing requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-3220	siz	20 million matchups	The MMS of the SST CCI system shall be able to handle (by 2016) <ul style="list-style-type: none"> <li>• 20 million matchups</li> <li>• 250 million observations, 50% thereof being subscenes</li> <li>• 200 sensor types</li> <li>• 5000 variables, 10% thereof being sub-scenes</li> <li>• 2 million data files</li> <li>• 300 TB inputs</li> </ul> The sizes shall be extendable beyond 2016. Note: The numbers duplicate the prototype MMS size.	scenario-5 workflow-2.8	I
SST-SR-3225	per	MMDB re-build	The MMS of the SST CCI system shall build or re-build the multi-sensor matchups MMDB in no more than 24 hours per year of input data starting from in-situ observations, satellite data, and ancillary data	scenario-5	T

### 3.3.4 Reliability, availability, maintainability, and security requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-3230	mnt	Extendable by new readers	The MMS of the SST CCI system shall be extendable by new readers to read new satellite or ancillary data in different formats. Note: This applies to new sensors. It is assumed that one sensor is homogeneously provided in one format.	scenario-5 scenario-5 workflow-2.8	R

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-3240	mnt	Configurable transformation of inputs	The MMS of the SST CCI system shall provide a configurable mapping of input variables and values to MMD target variables and values. The mapping shall support to change variable names and types. And it shall support value computations, e.g. to transform values from the input formats and units into MMD output values.	scenario-5 workflow-2.8	R

### 3.3.5 Other requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-3250	des	Structured storage of original inputs	The MMS of the SST CCI system shall store the original inputs and intermediate data like processed and re-ingested outputs in a structured way by type, revision, year, month, day. It shall keep these inputs and refer to the information in it instead of copying it.  Note: The multi-sensor matchups shall be represented by references to input files and records in them. The purpose of this is to be able to extract information from these source files in different ways, e.g. by using different sub-scene sizes or different calibration in the future. See also SST-SR-3330.	scenario-5 workflow-2.8	R
SST-SR-3260	des	Optimised for reprocessing cycles	The MMS of the SST CCI system shall be optimised for repeated reprocessing. This means that e.g. repeated copying of input data for processing shall be avoided.  Note: While the multi-sensor matchups in principle shall be represented by references to input files and records in them this shall not exclude pre-extracting sub-scenes. Sub-scenes of satellite data and necessary auxiliary input for processing shall be pre-extracted into MMD files that serve as input to processors. The purpose of this is to quickly re-process with new versions of processors without reading all satellite data and interpolating NWP repeatedly. See also SST-SR-3320.	scenario-5 workflow-2.8	R

### 3.4 User service requirements

This section lists requirements regarding the interaction with climate users and the SST community. They are mainly derived from the URD with its questionnaire.

#### 3.4.1 Functional requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-6180	fun	Output provision	The SST CCI system shall make available quality-checked L2, L3, and L4 output products as specified in the PSD (content, NetCDF format, CF metadata, file naming convention)	SST-TR-1 scenario-3 PSD-1 PSD-2 PSD-3 PSD-4 PSD-5 UR-QUF-33 UR-QUF-35 UR-QUF-89 scenario-4	T
SST-SR-6190	int	FTP access	The SST CCI system shall provide FTP pull access to its output products for users.	UR-QUF-90 UR-REF-12 UR-DIS-117 UR-LLP-24 scenario-4	T
SST-SR-6200	int	Web access	The SST CCI system shall provide access to its output products via a web page.	UR-QUF-91 scenario-4	T
SST-SR-6210	int	OPeNDAP access	The SST CCI system shall provide OPeNDAP access to its output products.	UR-QUF-93 scenario-4	T
SST-SR-6220	fun	Bulk access	The SST CCI system shall support bulk provision of its outputs to climate users.	assumption-1 UR-QUF-94 scenario-4	T
SST-SR-4110	fun	Subsetting and regrid-ding	The SST CCI system shall provide a tool for aggregation, sub-setting and regrid-ding for its output data. The tool shall propagate uncertainties appropriately.	SST-TR-6 UR-QUF-97 UR-QUF-98 UR-QUF-99 UR-QUF-103 UR-QUF-102 UR-QUF-105 UR-DIS-128 scenario-4 §2.9 SST data analysis tools	T

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-6230	fun	Online sub-setting and regridding	The SST CCI system shall provide an online interface to regional averaging, spatio-temporal gridding/re-gridding, and subset extraction tools for its outputs before download, to serve people with low bandwidth internet access.	UR-QUF-87 UR-QUF-88 UR-QUF-97 UR-QUF-98 UR-DIS-123 UR-REF-10 scenario-4	T
SST-SR-4120	fun	Visualisation and data analysis	The SST CCI system shall provide a visualisation uncertainty evaluation, and data analysis tool for its output data. Note: The prototype set of tools is listed in section 2.9.	SST-TR-30 SST-TR-31 UR-QUF-99 UR-QUF-103 scenario-4 §2.9 SST data analysis tools	T
SST-SR-4130	fun	Data access software	The SST CCI system shall provide libraries or examples how to read SST outputs in Matlab, IDL and Fortran.	UR-QUF-108 UR-QUF-109 UR-QUF-110 scenario-4	T
SST-SR-6240	fun	Web site	The SST CCI system shall provide a web site with information about SST CCI (news, access to product documentation, links to product access and services provided, how to raise issues and provide feedback).	UR-REF-20 UR-LLP-27 UR-REF-11 UR-REF-18 UR-LLP-29 UR-QUF-96 scenario-4	I
SST-SR-6250	fun	Catalogue	The SST CCI system shall provide a web-based catalogue for its output products. The catalogue shall provide spatial and temporal search capabilities, a map for data selection, and serve metadata. It shall implement the OGC CSW specification to support a standard interface.	scenario-4 UR-DIS-124 UR-QUF-92	T
SST-SR-6260	fun	News feed	The SST CCI system shall provide a news feed by a broadcasting mechanism (RSS, ATOM or email) where users can subscribe and get information about new product versions, important issues with products and other relevant information for users of the data.	UR-QUF-95 scenario-4	T
SST-SR-6270	fun	Forum or help desk	The SST CCI system shall provide a managed forum and email-based tracked help to allow users to submit questions on the SST products, raise issues, provide feedback. Questions, issues and feedback shall be forwarded to the responsible persons and shall be made persistent in an issue tracker.	UR-REF-9 UR-REF-23 scenario-4	T

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-6280	fun	Processor repository	The SST CCI system shall provide a processor repository that is available to the development team and users for access to processor code. The read access to the repository shall be completely open to all climate and SST users. Only committing to the repository shall be restricted to authorised users. The development team and the operations team maintain the repository and grant access. The repository shall support submission of improvements for review and integration. It shall be possible to restrict write access to the repository to registered users.	scenario-5	I
SST-SR-6290	int	External algorithm development	The SST CCI system shall support a process of external validation and of external development of algorithms and their evaluation by the exchange of matchup datasets and related processing results of various algorithms. The following two requirements provide details.	UR-DIS-125 scenario-5	R
SST-SR-6300	int	Matchup datasets	The SST CCI system shall provide single-sensor and multi-sensor matchup datasets (MMD format) of in-situ, extracted L1B data, and internally processed SST data for algorithm development and for validation.	UR-DIS-125 scenario-5	T
SST-SR-6310	int	Matchup inputs	The SST CCI system shall provide an interface to ingest matchup datasets of in-situ, extracted L1B data, and externally processed SST data for algorithm assessment and validation.	scenario-5 UR-QUF-100	T

### 3.4.2 Operational requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-6330	ope	Web site	The SST CCI system shall maintain and keep up-to-date its web site with information about SST CCI (news, access to product documentation, links to product access and services provided, how to raise issues and provide feedback).  The update frequency shall be adequate for the rate of changes in CDR versions, planning, and e.g. anomalies detected. The Web pages shall be updated within one week after the change.	UR-REF-20 UR-LLP-27 UR-REF-11 UR-REF-18 UR-LLP-29 UR-QUF-96 scenario-4	M
SST-SR-6340	ope	Science issues	The SST CCI system shall accommodate a development team that among other tasks addresses issues raised regarding products or algorithms and shall respond to them on a best effort basis.	SoW-4 UR-DIS-119 scenario-4	M



ID	Type	Title	Description	Ref.	Vrf.
SST-SR-5110	ope	Community process	The SST CCI system's development team shall initiate and maintain a process to evaluate the SST output products and use the MMS and outputs from "internal reprocessing" for algorithm improvement. The development team shall include climate users in the process of evaluation and consider their feedback in this process. Purpose of this process is to meet the requirements of the URD (accuracy, resolution, etc.).	SoW-4 SST-TR-36 scenario-5 UR-DIS-125	M
SST-SR-5115	ope	User requirements re-evaluation	The SST CCI development team shall collect and re-evaluate user requirements periodically in support of the decision making process about deployment of development resources.	SoW-9	M

### 3.4.3 Performance and sizing requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-6360	per fun	Forum maintainer	The SST CCI system shall have an operator to maintain the forum/help in order to react on queries by opening an issue, normally within 2 working days.  Note: any periods during which this normal response can not be met shall be indicated on the forum/help.	SoW-4 scenario-4 UR-LLP-25	M

### 3.4.4 Reliability, availability, maintainability, and security requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-6370	ram	User services availability	The SST CCI system user services web interface and product access shall be available at least 99% per year.  Note: "per year" allows a failure overnight or a weekend and maintenance of longer than 8 hours; in case of "per month" this would be prohibited.	UR-QUF-45	M

### 3.4.5 Other requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-4140	des	Open source tools	The SST CCI system shall provide open-source tools and/or recommend existing open-source tools	SST-TR-30 UR-QUF-107	R

### 3.5 Internal user and operator requirements

This section lists requirements from the internal user's point of view as far as they are not covered by the previous sections, mainly operational requirements from section 3.2 Requirements on SST time series production and reprocessing. They are mainly derived from the operations concept.

#### 3.5.1 Functional requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-5120	fun	Development environment	The SST CCI system shall provide a development environment to test and validate processor versions and new processing chains. The development environment may share components or hardware with the operational environment to process the complete timeline.	scenario-5 OPS-3 OPS-8	R
SST-SR-5130	fun	Development versions	The SST CCI system shall support versioning of processors also in development, but shall allow replacement of development versions without the need to increase the version number in a controlled environment (like the SNAPSHOT versions in git).  Note: In case the output products are used for a scientific comparison the processors shall be versioned in the development environment.	Best practice scenario-5	R
SST-SR-5140	fun	Matchup dataset processing	The SST CCI system shall support a development cycle based on MMS with the matchup datasets with L1B extracts that are also available to external users.	scenario-5	T
SST-SR-5150	fun	Full timeline access	The SST CCI system shall support the test of processors with input product sets ranging from single products to sets for days, months, or years. It shall provide access to the full timeline of inputs for development and evaluation of the (unreleased, "internal version") products from such large-scale tests.	OPS-4 OPS-8	T
SST-SR-5160	fun	Other sensor's inputs	The SST CCI system shall include other L1 products from additional sensors for evaluation. The number of types to be supported may increase over time.	SoW-8 SST-TR-20 SST-TR-49 scenario-1	R
SST-SR-5170	fun	New input type	The SST CCI system shall support the addition of a new input product type by configuration.	SoW-9 SST-TR-49 scenario-1	R
SST-SR-5180	int	Other ECVs as ancillary	The SST CCI system shall be able to store and make available to processors the output of other ECVs as ancillary data to evaluate their use in the SST processing chain.  The variables are in particular sea ice, sea level, ocean colour, clouds and aerosol.	SST-TR-39 DARD-5.xx scenario-3	R

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-5190	fun	New ancillary type	The SST CCI system shall support the addition of a new ancillary input product type by configuration.	SoW-9 DARD-2.xx scenario-1 scenario-3	R
SST-SR-5200	fun	New processing chain	The SST CCI system shall support the addition of a new processing chain by configuration and workflow implementation.	SoW-9 scenario-1 scenario-3	R
SST-SR-5210	fun	Transfer to operations	The SST CCI system shall support the transfer to operations of a new processor version after validation and - if necessary - optimisation by versioning and configuration.	SoW-9 OPS-4	T
SST-SR-5215	fun	L4 analysis system update	If the SST CCI L4 analysis system is derived from an operational L4 analysis system the SST CCI system shall support the routine update of the L4 analysis system when improvements are available for the operational L4 analysis system. Note: This shall ensure that SST CCI does not diverge from the operational L4 analysis system.	SoW-9 OPS-4	M

### 3.5.2 Operational requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-5220	ope	Development team	The SST CCI system shall include a development team that drives the development process interacting with the SST user community and using the system to improve and evaluate methods and algorithms.	SST-TR-36 OPS-2	R
SST-SR-5230	ope	Agile requirements selection	The SST CCI system's development team shall repeatedly select issues or requirements for analysis and development in an agile process. The issues or requirements shall be selected with the goal to improve usage of the products, to defeat weaknesses identified, to come closer to the URD requirements (e.g. frequency, accuracy), to develop new products, and respond to external changes (e.g., changes in input data streams such as a sensor losing a channel).	scenario-4 scenario-3 OPS-5	M
SST-SR-5240	ope	Development and evaluation	The SST CCI system's development team shall perform improvements, select, test and validate processors and parameterisations, and evaluate them.	SST-TR-36 scenario-5	M

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-5250	ope	Version decisions	After validation, consideration of user feedback, and in accordance with management the SST CCI development team shall decide about new versions of the operational SST processing chain and output product on demand. The revisit period of this decision shall be adequate for climate users and for the SST community.	scenario-2 assumption-3 OPS-7	M
SST-SR-5255	ope	Overlapping versions	The SST CCI system shall maintain and update two operational versions of the outputs during transition after a decision to provide a new version for a suitable period (6 months).	scenario-2 assumption-3 OPS-7	M
SST-SR-5260	ope	Version release process	The SST CCI system's development team shall mark the initial release of new versions of the SST product to validators and interested users as "to be validated". After validation the products will be finally released and made accessible marked as "validated".  Products not yet finally released shall be easily recognisable as such.	Best practice	M
SST-SR-5265	ope	Version management	The SST CCI system shall support the management of its operational data as well as of its internal versions data. Deletion of internal versions shall follow an operational procedure to avoid inadvertent deletion of data.	Best practice	M

### 3.5.3 Performance and sizing requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-5270	per	Short development cycle	The SST CCI system shall support the test of new processor versions or parameterisations in a short cycle optimised for frequent update and validation.	OPS-4 scenario-5 scenario-2	R
SST-SR-5275	siz	Internal version storage	The SST CCI system shall store internal-version products temporarily up to a volume equivalent to 2 times the full set of CCI outputs.  Note: This allows the question – is A or B the better improvement?	scenario-2 assumption-3 OPS-4	I
SST-SR-5280	siz	Storage extension	The SST CCI system shall be extendible for larger storage by the addition of new hardware and by configuration.	scenario-1	R
SST-SR-5290	siz	Storage extension	The SST CCI system shall be extendible for more processing power by the addition of new hardware and by configuration.	scenario-1 scenario-3	R

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-5300	per	Performance scalability	The SST CCI system shall be designed in a way that it is scalable to increase performance almost linearly by additional hardware. Note: This calls either for fast networks or data-local processing.	scenario-1 scenario-3	R

### 3.5.4 Reliability, availability, maintainability, and security requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-5310	ram	Measures for stability	The SST CCI system shall take measures not to compromise the stability of the operational chain for systematic reprocessing and online extension of the CDR while running tests for the improvement cycle. This may e.g. be achieved by different accounts and access rights for system operators and the development team.	SST-TR-37 OPS-4 OPS-5 UR-REF-8 UR-QUF-83	R

### 3.5.5 Other requirements

ID	Type	Title	Description	Ref.	Vrf.
SST-SR-1367	ope	Operator's Manual	The SST CCI system shall provide an Operator's Manual for its functions and operational procedures	Best practice	R

## 4. REQUIREMENTS TRACEABILITY

This section traces input requirements identified in section 2.3 (Applicable requirements from project documents) to sections of this document (§) or to particular SST system requirements (SST-SR-xxxx) that implement them.

Input Req. ID	Title	Reference
SoW-1	Scope and context of the system	§1.1 Purpose and scope §2.2 Sea Surface Temperature system context
SoW-2	Descriptive operational scenarios	§2.7 Prototype Sea Surface Temperature production workflow §2.5 Operations concept
SoW-3	Key parameters	§2.7.2 Estimation of system key parameters
SoW-4	Users and operators	SST-SR-1390 Operator SST-SR-1400 Automation SST-SR-1430 Error handling SST-SR-6360 Forum maintainer SST-SR-6340 Science issues SST-SR-5110 Community process
SoW-5	Functional, operational, ... requirements	§3 Detailed system requirements
SoW-6	Processing functions, input, output	§2.7 Prototype Sea Surface Temperature production workflow §3.2 Requirements on SST time series production and reprocessing §3.1 Requirements on the generated output products
SoW-7	Archiving requirements	§2.7.2 Estimation of system key parameters SST-SR-1450 Input storage size SST-SR-1460 Output storage size SST-SR-1470 Online storage SST-SR-1500 Backup archive SST-SR-1501 Bulk archive retrieval SST-SR-1510 Archive reliability
SoW-8	Processing speed and performance	§2.7.2 Estimation of system key parameters SST-SR-1490 Three days per year SST-SR-5300 Performance scalability

Input Req. ID	Title	Reference
SoW-9	Modularisation, improvement, interdependencies	§2.4 Assumptions on common CCI system requirements OPS-2 EO development team assumption-2 Autonomous ECV systems SST-SR-1350 Processor framework SST-SR-1360 Executable integration SST-SR-1520 Autonomous system SST-SR-5115 User requirements re-evaluation SST-SR-5170 New input type SST-SR-5190 New ancillary type SST-SR-5200 New processing chain SST-SR-5210 Transfer to operations SST-SR-5215 L4 analysis system update
SST-TR-1	NetCDF CF	SST-SR-6180 Output provision SST-SR-6160 Output format and naming
SST-TR-2	Sensors for level 2 products	SST-SR-6110 L2P outputs
SST-TR-6	Daily to annual level 3	SST-SR-6170 Product features SST-SR-4110 Sub-setting and regriding
SST-TR-7	Temporal coverage 1991-2010	SST-SR-1110 (A)ATSR inputs SST-SR-1120 AVHRR GAC inputs
SST-TR-10	GHRSSST 2.0 GDS	SST-SR-6160 Output format and naming
SST-TR-12	PSD to identify metadata	SST-SR-6160 Output format and naming
SST-TR-14	Geo-referencing / co-location	SST-SR-1250 SST retrieval
SST-TR-15	Cloud detection	SST-SR-1250 SST retrieval
SST-TR-16	Sun glint	SST-SR-1250 SST retrieval
SST-TR-17	Aerosol	SST-SR-1170 Auxiliary inputs SST-SR-1250 SST retrieval
SST-TR-18	Sea-ice	SST-SR-1170 Auxiliary inputs SST-SR-1250 SST retrieval
SST-TR-19	Quality indicators	SST-SR-1260 Error characterisation
SST-TR-20	IR SST retrieval	SST-SR-1250 SST retrieval SST-SR-5160 Other sensor's inputs
SST-TR-21	Diurnal cycle	SST-SR-6150 L4 diurnal outputs
SST-TR-22	In-situ reference data set	SST-SR-1180 Validation datasets SST-SR-3110 Ingest observations of various types
SST-TR-29	Observation operators	SST-SR-1280 Sensor merging
SST-TR-30	Use GSICS, HR-DDS, GMPE	SST-SR-4120 Visualisation and data analysis SST-SR-4140 Open source tools
SST-TR-31	Inter-comparison, diagnostic and visualization tools	SST-SR-4120 Visualisation and data analysis §2.9 SST data analysis tools

Input Req. ID	Title	Reference
SST-TR-36	Test products and improvements	SST-SR-5220 Development team SST-SR-5110 Community process SST-SR-5240 Development and evaluation
SST-TR-37	Product consistency	SST-SR-5310 Measures for stability
SST-TR-39	Consistency with other ECVs	SST-SR-5180 Other ECVs as ancillary
SST-TR-40	Spatial and temporal aspects of validation	SST-SR-1300 Quality check
SST-TR-45	Maps and time-series inter-comparison	SST-SR-1310 Matchup analysis SST-SR-1320 Trend analysis
SST-TR-49	Prototype sensors and period	SST-SR-1110 (A)ATSR inputs SST-SR-1120 AVHRR GAC inputs SST-SR-1130 AVHRR METOP inputs SST-SR-5160 Other sensor's inputs SST-SR-5170 New input type
UR-QUF-33 UR-QUF-35	data levels L2, L3, L4 single and multi-sensor products	SST-SR-6110 L2P outputs SST-SR-6120 L3C outputs SST-SR-6130 L3U outputs SST-SR-6140 L4 outputs SST-SR-6150 L4 diurnal outputs SST-SR-1290 Output products SST-SR-6180 Output provision
UR-REF-3 UR-QUF-43	temporal coverage of at least 30 years	SST-SR-1110 (A)ATSR inputs SST-SR-1120 AVHRR GAC inputs SST-SR-1130 AVHRR METOP inputs SST-SR-6170 Product features
UR-DIS-125	independent validation	SST-SR-6290 External algorithm development SST-SR-6300 Matchup datasets SST-SR-5110 Community process
UR-QUF-44 UR-DIS-121 UR-DIS-122	timely availability ranging from year to half a day	SST-SR-2180 Short-delay processing
UR-REF-15	standards for data storage	SST-SR-1470 Online storage SST-SR-1500 Backup archive SST-SR-1501 Bulk archive retrieval SST-SR-1510 Archive reliability
UR-REF-8 UR-QUF-83	operational system	SST-SR-1400 Automation SST-SR-2130 Data-driven processing SST-SR-5310 Measures for stability
UR-REF-21	version control	SST-SR-1330 Processor configuration control
UR-DIS-126	concurrent data versions	SST-SR-1240 Output versions SST-SR-1241 Long-term stewardship
UR-REF-10	users with least developed computing infrastructure	SST-SR-6230 Online subsetting and regridding



Input Req. ID	Title	Reference
UR-REF-12 UR-DIS-117 UR-LLP-24	easy access to data	SST-SR-6180 Output provision
UR-QUF-87	download file size	SST-SR-6230 Online subsetting and regridding
UR-QUF-88	download dataset size	SST-SR-6230 Online subsetting and regridding
UR-QUF-89	NetCDF CF, GHRSSST GDS 2.0	SST-SR-6160 Output format and naming SST-SR-6180 Output provision
UR-REF-16	standards for metadata	SST-SR-6160 Output format and naming
UR-REF-17	lineage information metadata	SST-SR-6160 Output format and naming
UR-DIS-124	temporal data selection	SST-SR-6250 Catalogue
UR-REF-20	access to documentation	SST-SR-6240 Web site SST-SR-6330 Web site
UR-QUF-90	Data access by FTP	SST-SR-6180 Output provision
UR-QUF-91	Data from a web page	SST-SR-6200 Web access
UR-QUF-92	Data access via map	SST-SR-6250 Catalogue
UR-QUF-93	Data access by OPeNDAP	SST-SR-6210 OPeNDAP access
UR-QUF-94	Offline delivery on DVD	SST-SR-6220 Bulk access
UR-QUF-95	Email alerts	SST-SR-6260 News feed
UR-QUF-96	Alerts on web page	SST-SR-6240 Web site SST-SR-6330 Web site
UR-LLP-27 UR-REF-11	Information on development	SST-SR-6240 Web site SST-SR-6330 Web site
UR-REF-18	Information on maturity	SST-SR-6240 Web site SST-SR-6330 Web site
UR-LLP-29	Information access via web page	SST-SR-6240 Web site SST-SR-6330 Web site
UR-QUF-45	reliability of delivery of 99%	SST-SR-6370 User services availability
UR-REF-9 UR-REF-23	Feedback on data issues	SST-SR-6270 Forum or help desk
UR-LLP-25	Support reactivity	SST-SR-6360 Forum maintainer
UR-DIS-119	Expert support	SST-SR-6340 Science issues
UR-DIS-128	method for uncertainty aggregation	SST-SR-4110 Subsetting and regridding
UR-DIS-123	Different resolutions	SST-SR-6230 Online subsetting and regridding
UR-QUF-97 UR-QUF-98	Tool for extraction, reading and subsetting	SST-SR-4110 Subsetting and regridding SST-SR-6230 Online subsetting and regridding
UR-QUF-99 UR-QUF-103 UR-QUF-104	Tool for visualisation, data statistics, and uncertainty evaluation	SST-SR-4110 Subsetting and regridding SST-SR-4120 Visualisation and data analysis
UR-QUF-100	Tool for data intercomparison	SST-SR-6310 Matchup inputs

Input Req. ID	Title	Reference
UR-QUF-102 UR-QUF-106	Tool for spatial and temporal averaging, data compositing	SST-SR-4110 Subsetting and regridding
UR-QUF-105	Tool for trend analysis	SST-SR-1320 Trend analysis
UR-QUF-107	Open source tools	SST-SR-4140 Open source tools
UR-QUF-101	Matchup dataset generation	SST-SR-3120 Compute multi-sensor match-ups
UR-QUF-108	Software library for Matlab	SST-SR-4130 Data access software
UR-QUF-109	Software library for IDL	SST-SR-4130 Data access software
UR-QUF-110	Software library for Fortran	SST-SR-4130 Data access software
PSD-1	(A)ATSR L3U 0.05° 1991-2010	SST-SR-6130 L3U outputs SST-SR-1200 Output preservation SST-SR-1270 Projection and compositing SST-SR-1290 Output products SST-SR-6180 Output provision
PSD-2	AVHRR L2P 4km 1991-2010	SST-SR-6110 L2P outputs SST-SR-1200 Output preservation SST-SR-1250 SST retrieval SST-SR-1260 Error characterisation SST-SR-1290 Output products SST-SR-6180 Output provision
PSD-3	Analysis L4 0.05° 1991-2010	SST-SR-6140 L4 outputs SST-SR-1200 Output preservation SST-SR-1280 Sensor merging SST-SR-1290 Output products SST-SR-6180 Output provision
PSD-4	SST NetCDF structure	SST-SR-6160 Output format and naming SST-SR-6180 Output provision
PSD-5	GHRSSST GDS 2.0 filename convention	SST-SR-6160 Output format and naming SST-SR-6180 Output provision
DARD-1.01	(A)ATSR level 1	SST-SR-1110 (A)ATSR inputs
DARD-1.03	AVHRR GAC level 1	SST-SR-1120 AVHRR GAC inputs
DARD-1.04	AVHRR MetOp	SST-SR-1130 AVHRR METOP inputs
DARD-2.01	ECMWF ERA-Interim	SST-SR-1170 Auxiliary inputs SST-SR-5190 New ancillary type
DARD-2.06 to 2.07	Sea ice	SST-SR-1170 Auxiliary inputs SST-SR-5190 New ancillary type
DARD-3.xx	In situ data from ships and buoys	SST-SR-1180 Validation datasets
DARD-4.xx	Inter-comparison datasets	SST-SR-1180 Validation datasets
DARD-5.xx	Outputs of other CCI ECVs	SST-SR-5180 Other ECVs as ancillary
assumption-1	Harmonised access	SST-SR-6220 Bulk access

Input Req. ID	Title	Reference
assumption-2	Autonomous ECV systems	SST-SR-1520 Autonomous system
assumption-3	Optimised for repeated re-processing	SST-SR-5250 Version decisions SST-SR-5255 Overlapping versions SST-SR-5275 Internal version storage SST-SR-1220 Input versions SST-SR-1230 Reprocessing input versions SST-SR-1240 Output versions SST-SR-1241 Long-term stewardship SST-SR-2120 Auxiliary update SST-SR-1470 Online storage
OPS-1	Routine long-term CDR production and climate services	SST-SR-2110 Input ingestion SST-SR-2120 Auxiliary update SST-SR-2125 Validation data update SST-SR-2130 Data-driven processing SST-SR-2150 CDR extension
OPS-2	Involvement of development team	SST-SR-5220 Development team
OPS-3	Continuous development starting from prototype	SST-SR-5120 Development environment
OPS-4	Model of improvement	SST-SR-5150 Full timeline access SST-SR-5210 Transfer to operations SST-SR-5215 L4 analysis system update SST-SR-5270 Short development cycle SST-SR-5275 Internal version storage SST-SR-5310 Measures for stability
OPS-5	Reliable CDR generation and agile process	SST-SR-5310 Measures for stability SST-SR-5230 Agile requirements selection
OPS-6	Reprocessing needs	SST-SR-2120 Auxiliary update
OPS-7	Availability of consistent CDR	SST-SR-1240 Output versions SST-SR-1241 Long-term stewardship SST-SR-5250 Version decisions SST-SR-5255 Overlapping versions
OPS-8	Robust and traceable environment with access to full archive	SST-SR-5120 Development environment SST-SR-5150 Full timeline access
OPS-9	CDR generation with focus on quality	SST-SR-2140 Wait for ancillary SST-SR-2180 Short-delay processing

Input Req. ID	Title	Reference
scenario-1	Sensor constellations and temporal coverage	SST-SR-6110 L2P outputs SST-SR-1135 PMW inputs SST-SR-1140 Sentinel inputs SST-SR-1150 VIIRS inputs SST-SR-1160 Sentinel data reduction SST-SR-1165 VIIRS data reduction SST-SR-1190 Input data interface SST-SR-2110 Input ingestion SST-SR-2120 Auxiliary update SST-SR-2125 Validation data update SST-SR-2130 Data-driven processing SST-SR-1450 Input storage size SST-SR-1460 Output storage size SST-SR-5160 Other sensor's inputs SST-SR-5170 New input type SST-SR-5190 New ancillary type SST-SR-5200 New processing chain SST-SR-5280 Storage extension SST-SR-5290 Storage extension SST-SR-5300 Performance scalability
scenario-2	Reprocessing capability	SST-SR-1220 Input versions SST-SR-1230 Reprocessing input versions SST-SR-1470 Online storage SST-SR-1480 Parallel processing SST-SR-1490 Three days per year SST-SR-5250 Version decisions SST-SR-5255 Overlapping versions SST-SR-5270 Short development cycle SST-SR-5275 Internal version storage
scenario-3	Scope of products	SST-SR-6110 L2P outputs SST-SR-6120 L3C outputs SST-SR-6130 L3U outputs SST-SR-6140 L4 outputs SST-SR-6150 L4 diurnal outputs SST-SR-5180 Other ECVs as ancillary SST-SR-5190 New ancillary type SST-SR-5200 New processing chain SST-SR-5230 Agile requirements selection SST-SR-5290 Storage extension SST-SR-5300 Performance scalability

Input Req. ID	Title	Reference
scenario-4	Interaction with users	SST-SR-6180 Output provision SST-SR-6190 FTP access SST-SR-6200 Web access SST-SR-6210 OPeNDAP access SST-SR-6220 Bulk access SST-SR-4110 Subsetting and regridding SST-SR-6230 Online subsetting and regridding SST-SR-4120 Visualisation and data analysis SST-SR-4130 Data access software SST-SR-6240 Web site SST-SR-6250 Catalogue SST-SR-6260 News feed SST-SR-6270 Forum or help desk SST-SR-6330 Web site SST-SR-6340 Science issues SST-SR-6360 Forum maintainer SST-SR-5230 Agile requirements selection
scenario-5	Multi-sensor matchup system and development environment	SST-SR-3110 Ingest observations of various types SST-SR-3120 Compute multi-sensor matchups SST-SR-3125 Incremental matchup computation SST-SR-3130 Update flag fields SST-SR-3140 Extract satellite sub-scenes SST-SR-3150 Interpolate NWP SST-SR-3160 Process SST SST-SR-3170 Extract multi-sensor matchup datasets SST-SR-3180 Ingest external MMD inputs SST-SR-3190 Support for concurrent versions SST-SR-3220 20 million matchups SST-SR-3225 MMD re-build SST-SR-1330 Processor configuration control SST-SR-1340 Concurrent processor versions SST-SR-1350 Processor framework SST-SR-1380 Bulk reprocessing SST-SR-6280 Processor repository SST-SR-6290 External algorithm development SST-SR-6300 Matchup datasets SST-SR-6310 Matchup inputs SST-SR-5110 Community process SST-SR-5220 Development team SST-SR-5230 Agile requirements selection SST-SR-5240 Development and evaluation SST-SR-5270 Short development cycle