Copernicus Climate Change Service

# System Quality Assurance Document (SQAD)

## Global L4 Sea and Sea Ice Surface Temperature Climate Data Record, Version 1.0

## WP3-SQAD-SST/IST-v1.0

Issued by: Danish Meteorological Institute / Ioanna Karagali

Date: 20/06/2024

Ref: C3S2_312b_WP3-SQAD_SST/IST-202406_SQAD_v1.0

Official reference number service contract: 2022/C3S2_312b_MOi/SC1

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## History of document modifications

| Version | Date | Description of modification | Chapters / Sections |
|---|---|---|---|
| 1.0 | 20/06/2024 | First version submitted for independent review | All |
| | 26/07/2024 | Document amended to account for proof-reading edits suggested by independent review, and document finalised for publication as a Version 1.0. | All |

## List of datasets covered by this document

| Deliverable ID | Product title | Product type (CDR, ICDR) | Version number | Delivery date |
|---|---|---|---|---|
| WP2-FDDP-SST-v1.0 | SST/IST CDR L4 | CDR | 1.0 | |

# Related documents

| Reference ID | Document |
|---|---|
| D1 | Karagali, I. et al. (2024). Global L4 Sea and Sea Ice Surface Temperature Climate Data Records, Version 1.0: Algorithm Theoretical Basis Document. Copernicus Climate Change Service. Document ref. C3S2-312b_WP2-FDDP-SST/IST_2024_ATBD_v1.X. |
| D2 | Karagali, I. et al. (2024). Global L4 Sea and Sea Ice Surface Temperature Climate Data Records, Version 1.0: Product User Guide and Specification. Copernicus Climate Change Service. Document ref. C3S2-312b_WP2-FDDP-SST/IST_2024_PUGS_v1.X. |
| D3 | Karagali, I. et al. (2024). Global L4 Sea and Sea Ice Surface Temperature Climate Data Records, Version 1.0: Product Quality Assessment Report. Copernicus Climate Change Service. Document ref. C3S2-312b_WP2-FDDP-SST/IST_2024_PQAR_v1.X. |
| D4 | Karagali, I. et al. (2024). Global Sea and Ice Surface Temperature ECV: Target Requirements and Gap Analysis Document. Copernicus Climate Change Service. Document ref. C3S2-312b_WP3-TRGAD-SST/IST_2024_TRGAD_v1.X. |
| D5 | Embury, O. et al. (2021). System Quality Assurance Document, Sea Surface Temperature, Version 1.1. Document ref. C3S_D2.SST.3-v3.0_SQAD_of_v2.1SST_products_v1.1. https://datastore.copernicus-climate.eu/documents/satellite-sea-surface-temperature/v2.1/D2.SST.3-v3.0_SQAD_of_v2.1SST_products_v1.1_APPROVED_Ver1.pdf |

# Acronyms

| Acronym | Definition |
|---|---|
| AASTI | Arctic and Antarctic Ice Surface Temperatures from AVHRR |
| AMSR | Advanced Microwave Scanning Radiometer |
| C3S | Copernicus Climate Change Service |
| CCI | Climate Change Initiative |
| CDR | Climate Data Record |
| CEDA | Centre for Environmental Data Analysis |
| DMI | Danish Meteorological Institute |
| ESA | European Space Agency |
| EUMETSAT | European Meteorological Satellites |
| ICDR | Interim Climate Data Record |
| IR | Infrared |
| IST | Sea Ice Surface Temperature |
| L4 | Level 4 |
| L3U | Level 3 Uncollated |
| L3C | Level 3 Collated |
| L2P | Level 2P |
| MIZ | Marginal Ice Zone |
| MetNo | Norwegian Meteorological Institute |
| NP | North Pole |
| OI | Optimal Interpolation |

| | |
|---|---|
| OSISAF | Ocean and Sea Ice Satellite Application Facility |
| PMW | Passive Microwave |
| R&D | Research and development |
| SIC | Sea-ice concentration |
| SST | Sea Surface Temperature |
| UWC-W | United Weather Centres West |

## General definitions

**CDR** – Climate Data Record, defines a time series of measurements of sufficient length, consistency, and continuity to determine climate variability and change. Further satellite-based CDRs can be segmented into Fundamental CDRs (FCDRs), which are calibrated and quality-controlled sensor data that have been improved over time, and Thematic CDRs (TCDRs), which are geophysical variables derived from the FCDRs, such as sea surface temperature and cloud fraction.

**ICDR** – Interim Climate Data Record, defines a dataset that has been forward processed, using the baselined Climate Data Record algorithm and processing environment but whose consistency and continuity have not been verified. Eventually, it will be necessary to perform a new reprocessing of the CDR and ICDR parts together to guarantee consistency, and the new reprocessed data record will replace the old CDR.

**SIC** – Sea-ice concentration as fraction (percentage) of the sea surface area of the grid cell containing sea-ice.

**SST** – Sea Surface Temperature

**$SST_{20cm}$** – Sea Surface Temperature adjusted for the standard depth of 0.2 m and time representative of the daily mean, representative of the water temperature free, or almost free of any diurnal warming.

**IST** – Sea Ice Surface Temperature, representative of the surface skin.

**Open ocean** – Corresponds to ice-free ocean or containing very little ice (<15 %), thus the surface temperature is classified as sea surface temperature (SST).

**Sea Ice** – Corresponds to ocean surface covered by sea ice (>70%) thus the surface temperature is classified as sea-ice surface temperature (IST).

**MIZ** – Marginal Ice Zone, a part of the seasonal ice zone that varies in width (100 to 200 kilometers) that extends from the ice edge into the ice pack, where waves and swells affect the ice; often characterized by highly variable ice conditions; in general, it is wider in the Antarctic than the Arctic.

**L2P** – Geophysical variables derived from Level 1 source data on the Level 1 grid (typically the satellite swath projection). Ancillary data and metadata added following GHRSST Data Specification.

**L3U** – L2 data granules remapped to a regular latitude/longitude grid without combining observations from multiple source files. L3U files will typically be “sparse”, corresponding to a single satellite orbit.

**L3C** – SST observations from a single instrument combined into a space-time grid. In this project, a typical L3C file may contain all the observations from a single instrument in a 24-hour period.
L3S – SST observations from many instruments combined into a space-time grid. In this project, a typical L3S file may contain all the observations from all available instruments in a 24-hour period.

**L4** – SST observations from multiple instruments using an analysis system (e.g. optimal interpolation) to produce a gridded, gap-free product.

## Table of Contents

## Scope of the document

This document is the System Quality Assurance Document (SQAD) for the C3S Sea Surface and Sea Ice Surface Temperature (SST/IST) service. It builds upon the SQAD of the previous dataset on L4 SST CDR [D5]. This document describes all elements and systems that contribute to the processing chain of the input data towards the final L4 combined SST and IST daily files, including all interfaces to the C3S, and to the Research and Development (R&D) component, the hardware used in the processing chain, the procedures to implement new data cycles and to reprocess the products, and those applied in case of system failures or anticipated maintenance work, as well as information on user support.

## Executive summary

This document describes the systems used to produce the Sea Surface Temperature and Sea Ice Surface Temperature (SST/IST) CDR and ICDR products. This product is the first global CDR to include surface temperature over the open ocean (SST), the marginal ice zone (MIZ) and sea-ice (IST). The L4 SST/IST CDR is produced using input from the ESA CCI SST CDR v3.0 (1982-2021) adjusted to a daily mean temperature at 20cm depth (allowing comparison with the historical in situ record) for the SST component, and the AASTI v2.1 and C3S IST CDR v1.0 for the IST component, which represents the skin surface temperature of the sea ice. The L4 SST/IST ICDR is produced using the C3S SST ICDR v3.0 (2022-onward) and the C3S IST CDR v1.0. The two datasets are intended to be used together.

Both ICDR and CDR datasets are generated using the same software and algorithm originally developed within the MyOcean project and currently applied to the operational Multi-Year products for the SST and IST delivered to the Copernicus Marine Service. The main frame of the processing algorithm relies on the bias adjustment among the various single sensor products, the generation of an aggregated observational field from the single sensor input data, and use of an Optimal Interpolation algorithm to fill in the gaps from missing data.

# 1. System overview

## 1.1 System elements and interfaces

The Sea Surface and Sea Ice Surface Temperature (SST/IST) C3S production system ingests Level 2P PMW and L3U IR satellite SSTs and L3C IR satellite ISTs, and processes the data to Level 4 (global gridded, gap-free, SST/IST data) products which are delivered to the Climate Data Store (CDS). Auxiliary data on the Sea Ice Concentration are obtained from the EUMETSAT OSISAF and the ESA ICE CCI+ to produce high resolution and high quality sea ice concentration fields, which are also ingested in the production system to classify the type of surface, i.e. open water (SST), marginal ice zone (combination of SST and IST) and sea ice (IST).

The processing is based on the DMIOI production system and runs at the United Weather Centres West (UWC-W) facility which provides the computation resources and access to the required data streams as shown in Figure 1. Details of the data acquisition are given in section 1.5.

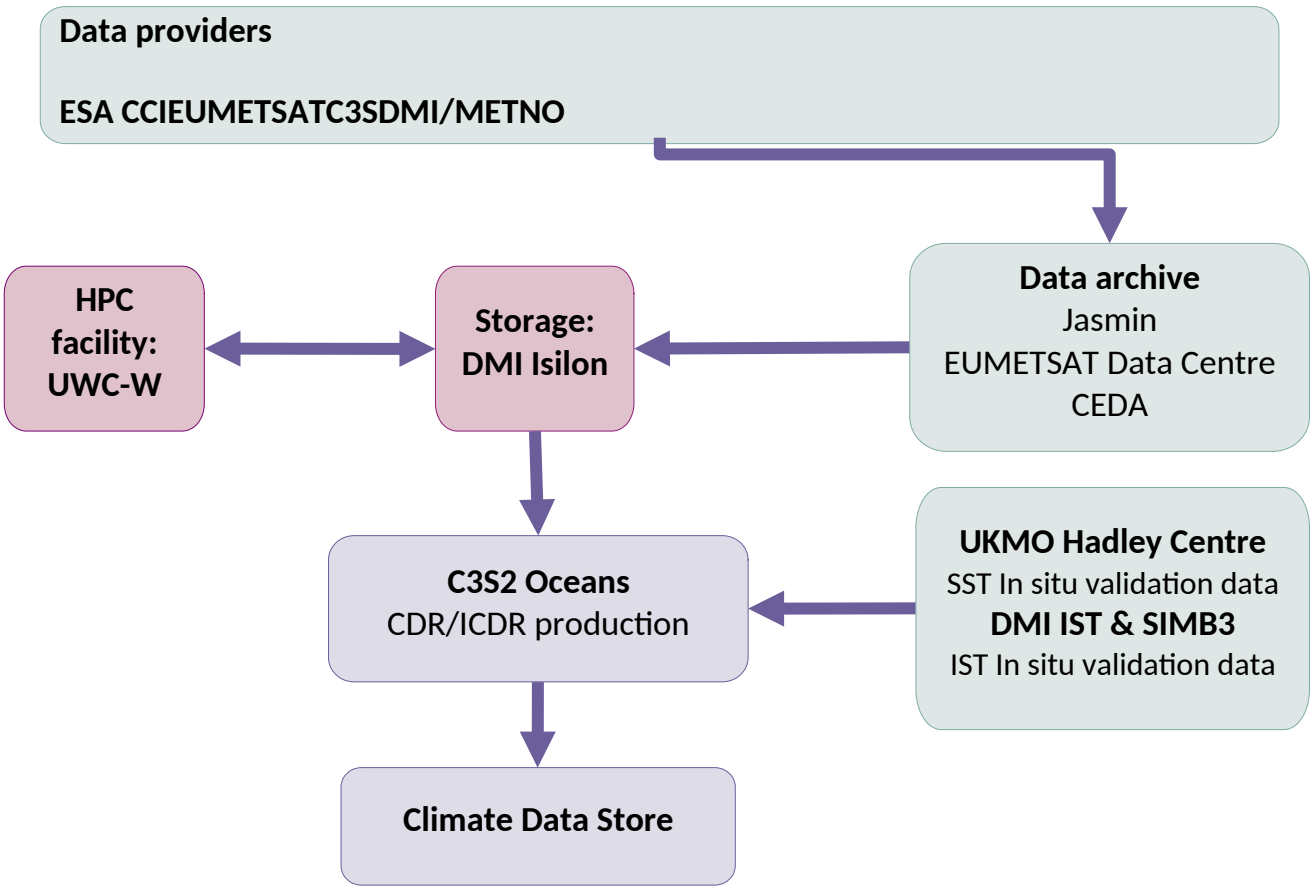


**Figure 1.** Interfaces between the C3S2 Ocean – SST/IST L4 CDR and data and service providers.

## 1.2 Interface with ESA CCI

The ESA CCI SST project produces the L2P/L3U CDR products used as input for the production of the L4 SST/IST CDR and has been responsible for activities including the research and development of new algorithms (cloud detection, SST retrieval, harmonization) and sensors, production of L2P/L3U CDR products, validation and verification activities and detailed assessment of CDR products before release.

Updates to the input CDR are released every few years after each phase of CCI research and development. The v3.0 of the ESA CCI SST is used as input to the C3S SST/IST CDR. After each CDR product release the software and systems are then used by the C3S team to produce an ongoing ICDR complimenting the CDR. The C3S SST team is then responsible for maintaining ICDR production, incremental updates to systems (e.g. due to change in availability of input data streams), ongoing monitoring and validation of ICDR products. The v3.0 C3S SST ICDR is used as input to the C3S L4 SST/IST ICDR.

The ESA ICE CCI+ produces the L2/L3/L4 Sea Ice Concentration CDR from a series of different instruments and at various spatial resolutions. For more information on the project, visit the project page https://climate.esa.int/en/projects/sea-ice/. The AMSR-based CDR on Sea Ice Concentration is used as input to derive the Global Multi-Source Sea Ice Concentration composite produced at DMI (DMI-MSC). The Global DMI-MSC composite is used as input for the surface type classification in the global L4 SST/IST CDR and no updates are foreseen.

## 1.3 Interface with EUMETSAT OSISAF

The EUMETSAT OSISAF project produces global sea ice concentration CDRs from passive microwave observations, among other products. The sea ice concentration CDRs are used as input to derive the Global Multi-Source Sea Ice Concentration composite produced at DMI (DMI-MSC). The Global DMI-MSC composite is used as input for the surface type classification in the global L4 SST/IST CDR and no updates are foreseen.

## 1.4 SST/IST Production System

The SST/IST production system documented here describes the steps followed to generate the L4 SST/IST product. The system is used for both the CDR and ICDR products. Figure 2 shows a schematic overview of the DMI Optimal Interpolation (DMIOI) system, where all input data on surface temperatures over sea, sea ice and the marginal ice zone along with the input SIC fields and the land mask are combined into the final OI L4 product.

The final L4 analysis product is a merged and interpolated daily field with a 0.05° resolution in latitude and longitude, and covers both open ocean, sea ice and the Marginal Ice Zone (MIZ). The optimal interpolation method used to construct the merged and gap free SST/IST analysis is taken from the high latitude SST DMI processing scheme described in Høyer and She (2007); Høyer et al.

(2014). The processes used are described in detail in the C3S Algorithm Theoretical Basis Document [D1] and key steps are also listed below.

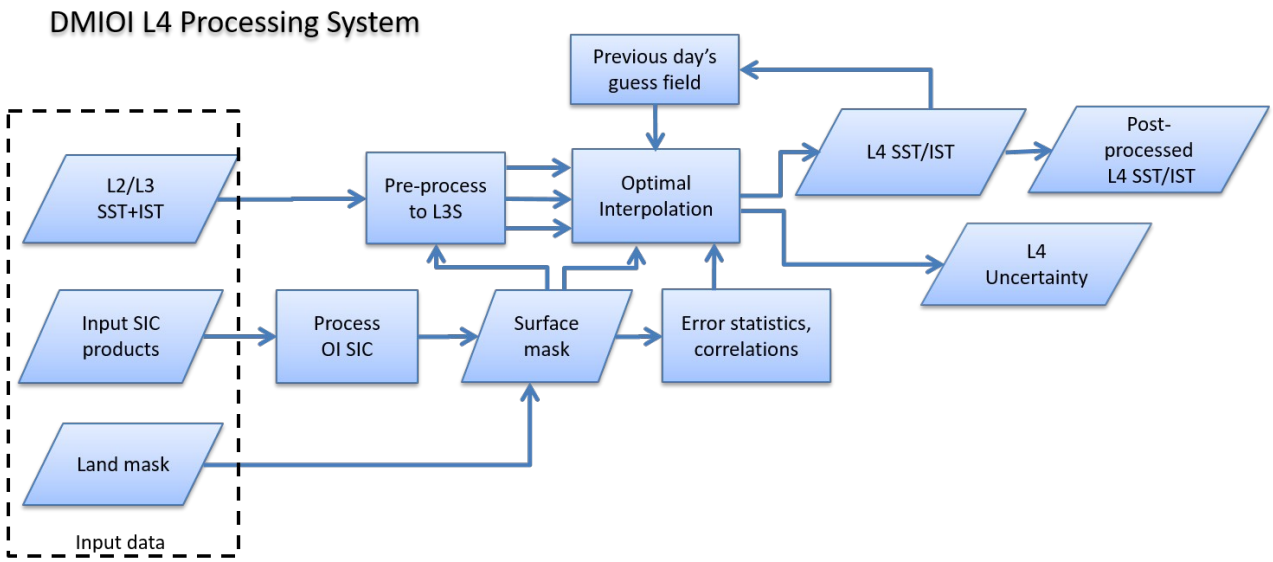


**Figure 2.** Schematic diagram of the DMIOI processing chain at DMI. Level 2 and Level 3 (L2/L3) SST and IST data, Sea Ice Concentration data and land/sea data undergo a series of processes and finally an Optimal Interpolation methodology is applied to produce the Level 4 SST/IST data and its ancillary uncertainty dataset. Rectangles indicate processes, while slanted boxes indicate data products.

**Pre-processing of input SST/IST data -** All satellite data valid for a particular day, within 24 hours from the analysis date are considered. The input L3U SST data undergo various QC and processing steps to generate separate level 3 products. The L3S fields are calculated as a noise weighted average of all available observations. Only satellite data classified as cloud free by the PPS cloud mask are included. For SST from Infrared sensors, quality levels 4 and 5 are used except for SLSTR, where a quality flag of 5 is required. For SST from Passive Microwave, quality levels 3, 4 and 5 are used. For IST from Infrared sensors, quality levels 4 and 5 are used. Satellite observations using an ice algorithm in regions where the sea ice concentration is 0 are discarded.

**Input SIC product DMI-MSC and Land Mask** - The input sea ice concentration DMI-MSC product is converted to the same grid as the final L4 product and, along with the land mask is used as a surface mask to characterise the surface type. For non-land points, depending on the sea ice concentration value ocean surface types are defined as open ocean (<15% sea ice concentration), marginal ice zone (15-70%) and sea-ice (>70%) surface.

**Optimal Interpolation** - The Optimal Interpolation (OI) method works with anomalies from a first guess field (Høyer and She, 2007). In the current approach, a persistence-based method is applied, which uses the previous day's analysis field as the first guess field (Nielsen-Englyst et al., 2023). The SST and IST observations from the previous 24 hours are therefore interpreted as anomalies with respect to the first guess field, i.e. the previous day's analysis. For each grid point, the OI method finds the solution that has the lowest errors, with respect to given statistical inputs (such as a first guess error variance, error covariance functions and uncertainties on the individual observations).

Due to the different physical conditions for ocean and sea ice surface temperature variability, separate statistics have been derived for the open ocean and the sea ice covered regions. The SST and IST first guess variance and error covariance are derived from the observations. The first guess field and the error covariance used in the MIZ is a weighted linear combination of the open waters and the ice values, where the ice concentration was used as the weighting factor. In this context, the MIZ is defined as areas where the ice concentration is between 15% and 70%. The search radius for the OI method is set to 100 km and the maximum number of satellite observations included in the optimal estimation is 8.

## 1.5 Data Acquisition

### 1.5.1 ESA CCI SST CDR v3.0 data

Data were directly downloaded from the public folder of the jasmin server, https://gws-access.jasmin.ac.uk/public/esacci-sst/CDR3.0_release/.

### 1.5.2 C3S ICDR SST data

Data were directly downloaded from the public folder of the jasmin server, https://gws-access.jasmin.ac.uk/public/cds_c3s_sst/data/ICDR_v3/.

### 1.5.3 AASTI v2.1 IST CDR data

Data are available in-house at DMI.

### 1.5.4 C3S IST ICDR v1.0 data

Data were directly downloaded from the C3S Climate Data Store, at https://cds.climate.copernicus.eu/#!/home

### 1.5.5 OSI SAF Sea Ice Concentration CDR

Data were directly downloaded from the OSISAF FTP hosted by MetNo, at ftp.osisaf.met.no.

### 1.5.6 ESA Ice CCI+ Sea Ice Concentration CDR

Data were directly downloaded from the CEDA archive, using the ftp service at http://anon-ftp.ceda.ac.uk/

### 1.5.7 Validation data for SST

Data were downloaded from the Met Office Hadley Centre Integrated Ocean Dataset (HadIOD) v1.2.0.0 (Atkinson et al. 2014).

### 1.5.8 Validation data for IST

Data were downloaded from ECMWF using the MARS archive for the ECMWF-distributed drifting ice buoys. SIMB3 buoy data were downloaded from https://www.cryosphereinnovation.com/data. CRREL mass balance buoy data (Perovich et al., 2016; Richter-Menge et al., 2006), were obtained through http://imb-crrel-dartmouth.org/archived-data/. NP drifting ice stations data, (RU/FSR/HME/AARI and NSIDC, 1993), are accessed through https://rda.ucar.edu/datasets/ds474.0/dataaccess/#. IceBridge flights data (version 2;Studinger, 2020), are accessed through https://nsidc.org/data/iakst1b/versions/2#anchor-data-access-tools.

## 1.6 Hardware, supercomputers and cloud computing

The United Weather Centres (UWC) is a meteorological collaboration between several countries. Denmark is part of UWC-West together with the national weather services of Ireland, Iceland and the Netherlands. In 2024, DMI along with the national weather services of the Netherlands, Ireland and Iceland transitioned to the new United Weather Centres-West (UWC-W) high performance computing (HPC) facility in Iceland (Figure 3). Powered entirely by renewable Icelandic hydropower and geothermal energy sources and taking advantage of the local temperate climate that will keep the supercomputer components cool, the running costs and CO2 footprint are kept to a minimum, saving tonnes of $CO_2$ in line with the four nations' commitments towards net-zero. The machine runs both the weather services' daily forecasts as well as carry out computationally intensive climate research. The procurement of the joint supercomputer is the first visible step in the European meteorological cooperation UWC-West, which by the end of this decade will count the services of ten countries in the UWC. The other six countries are Sweden, Norway, Finland, Estonia, Latvia and Lithuania, which are working on a similar project in UWC-East.

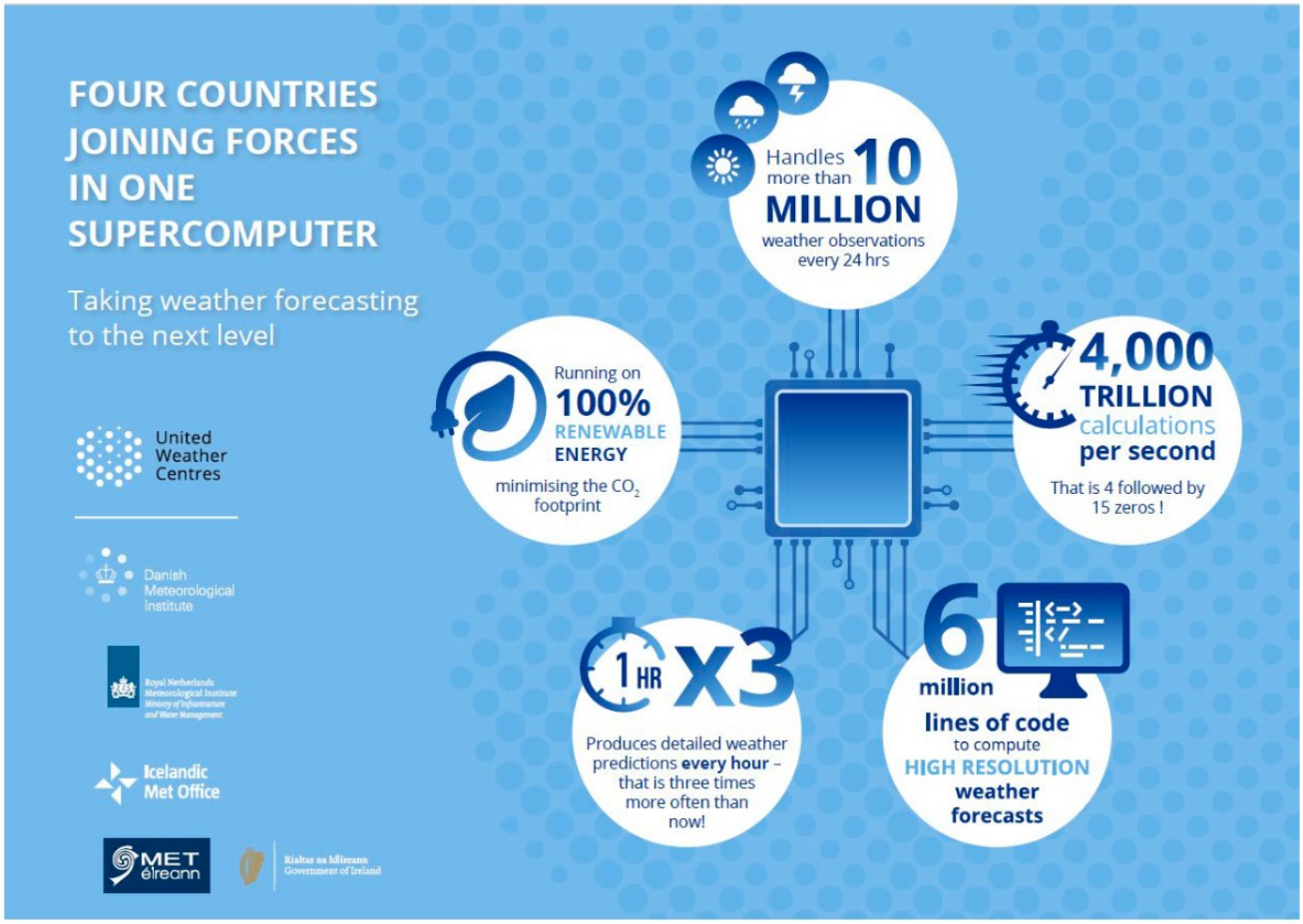


**Figure 3.** Overview of the new HPC system at UWC-W.

The high-performance super-computing facilities consist of two identical systems: One for the operational model and one for research and development. The research and development system acts as backup for the operational system in the unlikely event of a crash of the operational system. In addition, DMI operates a large number of servers used for data processing and visualisation and a massive data storage system.

# 2. Upgrade cycle implementation procedure

ICDR production operates to generate and deliver SST/IST products with a 3-month latency. During normal operation this results in new data being delivered to the CDS in batches with a temporal coverage of 3 months. If there have been interruptions to the production chain (see section 4) then data will be generated as computational resource and input data allow.

## 2.1 Incremental evolutions (C3S updates)

Incremental updates to the production system may be required in order to adapt to changing availability of input data sources. For the period of the current contract and given the scheduled delivery dates of the CDR and ICDR, no C3S updates to the input data are foreseen. The possible addition of a new data stream (not foreseen) may require software updates to support new data formats. In this case the software will be tested offline by generating and validating historical products in parallel to the main productions stream.

Once the software change has been verified in offline testing and validation the update will be applied to the primary production stream. This will allow daily ICDR production to continue without interruption.

## 2.2 CDR/ICDR reprocessing (new CDR/ICDR version)

In the current contract (ECMWF Contract number: C3S2_312b_Moi) no CDR/ICDR reprocessing is foreseen. After a new input data CDR release by the ESA CCI project (not foreseen in the current contract phase) it may be necessary to upgrade the ICDR production chain to match the new input data CDR version.

This typically includes a (re)processing of the ICDR to cover the gap between the end of the CDR and present. Generally, the CDR will extend according to the availability of the input data CDR; ICDR production will start from the end of the CDR and continue according to the availability of input data ICDR. The ICDR production will be halted with the old input data stream and (re)processing with the new version will take over. The new ICDR will be verified, and it will be available with a latency defined based on the availability of input data latency to be integrated into the CDS.

# 3. Procedures for reprocessing CDR's

In the current phase, no reprocessing of the long-term CDR will occur. Full reprocessing of the CDR can be foreseen in a next contract phase, when necessary requirements, e.g. new versions of the input data CDR and new input sources, will make reprocessing relevant. As an example, the ESA CCI LST phase_2 project will include ice surface temperature in the reprocessed versions of a series of instruments (MODIS, AVHRR and SLSTR) and these can be an addition to the SST/IST L4 CDR/ICDR in a next version. Furthermore, a v4.0 of the ESA CCI SST input data (or a new version of the input data CDR under any contract name), released in the future will be a relevant reason for reprocessing the CDR. Finally, improvements to the CDR beyond the version of input data can be foreseen in the next contract phase and these developments will render the reprocessing necessary.

Once reprocessing has been rendered necessary, the procedure in brief will include:

- Review of the requirements and modifications required for the improvements.
- Scientific tests on the CDR with the new requirements/developments for a period of time sufficient for meaningful conclusions.
- Impact assessment of the new developments by comparisons to in situ data and the official CDR version.
- If results are satisfactory, production of the new CDR.

# 4. System maintenance and system failures

Anticipated outages due to planned maintenance work or system upgrades will be reported to the CDS when possible. Both planned and unplanned issues or outages will be reported in the Quarterly Report.

Any possible system maintenance and system failures are relevant for the ICDR production and updates. The production system is configured to operate on an on-demand basis with a latency of 3 months and the production of the ICDRs can be planned around any maintenance and/or failure issues. Systems can only be monitored during standard DK working hours/days. Incidents, especially at weekends and holidays, could result in temporary delays and interruptions to the data delivery.

## 4.1 System Outages

Planned outages on UWC-W are kept to minimum and are not expected to impact the CDR (one off delivery). Regarding the ICDR, production of the 3-month intervals is only expected to occur twice with a final date on mid-January 2025 to finalize the 2024 ICDR.

## 4.2 Input data failure

All input data required for the production of the CDR and the DMI-MSC Sea Ice Concentration product are available.

Input data required for the production of the ICDR are available with a latency of 20 to 28 days and are not expected to impact the production which is scheduled at 3 month intervals.

In case of total sensor/satellite loss the sensor will be removed from the ICDR production chain.

# 5. User support

Front-end user support is provided by ECMWF via the Copernicus User Support desk:

http://copernicus-support.ecmwf.int

Further user support can be provided by the C3S Sea and Sea Ice Surface Temperature team who can be reached with the email address:

myocean_po@dmi.dk

This email is monitored during working hours 9am – 4pm CET during DK working days (Monday-Friday).

# 6. References

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