

Sea surface temperature intercomparison in the framework of the Copernicus Climate Change Service (C3S)

Article

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1	Sea Surface Temperature intercomparison in the framework of the Copernicus
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24	
25	Abstract
26	A joint effort between the Copernicus Climate Change Service (C3S) and the Group
27	for High Resolution Sea Surface Temperature (GHRSST) has been dedicated to an
28	intercomparison study of eight global gap-free Sea Surface Temperature (SST)
29	products to assess their accurate representation of the SST relevant to climate
30	analysis. In general, all SST products show consistent spatial patterns and temporal
31	variability during the overlapping time period (2003-2018). The main differences
32	between each product are located in western boundary current and Antarctic

33	Circumpolar Current regions. Linear trends display consistent SST spatial patterns
34	among all products and exhibit a strong warming trend from 2012 to 2018 with the
35	Pacific Ocean basin as the main contributor. SST discrepancy between all SST
36	products is very small compared to the significant warming trend. Spatial power
37	spectral density shows that the interpolation into 1° spatial resolution has negligible
38	impacts on our results. The global mean SST time series reveals larger differences
39	among all SST products during the early period of the satellite era (1982-2002) when
40	there were fewer observations, indicating that the observation frequency is the main
41	constraint of the SST climatology. The maturity matrix scores, which present the
42	maturity of each product in terms of documentation, storage, and dissemination but
43	not the scientific quality, demonstrate that ESA-CCI and OSTIA SST are well
44	documented for users' convenience. Improvements could be made for MGDSST and
45	BoM SST. Finally, we have recommended that these SST products can be used for
46	fundamental climate applications and climate studies (e.g. El Nino).

1. Introduction

49	Sea surface temperature (SST) as one of the Essential Ocean Variables (EOVs), and
50	the Essential Climate Variables (ECVs), plays a crucial role in heat, freshwater, and
51	momentum flux exchange at the ocean-atmosphere interface. The variation of SST at
52	different temporal and spatial scales modulates the atmospheric lower boundary
53	layer (e.g. Renault et al., 2019) eventually driving small and large-scale changes at
54	interannual to decadal time scales in the atmosphere (Perlin et al., 2014, McPhaden,
55	2012). Additionally, the SST changes can influence the biogeochemical marine
56	environment, contributing to modulating the primary production and related carbon
57	absorption in the ocean (Behrenfeld et al, 2006). Besides its importance for assessing
58	and monitoring the state of the global climate system, SST is widely used as
59	boundary conditions in weather and climate operational forecast systems (Robinson
60	2012) and as initial conditions in ocean operational forecast systems (Le Traon et al.,
61	2019). Therefore, assessing the quality of SST data is critical from several
62	perspectives, from operational to climate studies, marine environment and related
63	services.

65	SST observations are mainly obtained from low-Earth orbit infrared and microwave
66	satellite imagery and geostationary infrared imagery, and from various in situ
67	platforms including moored and drifting buoys, Argo floats, ships of opportunity,
68	autonomous sailing drones, and radiometers (O'Carroll et al., 2019). All these
69	instruments provide observations characterized by different representativeness,
70	resolution, and accuracy. Different retrieval methods and reanalysis techniques are
71	thus applied to obtain temporally and spatially consistent long-term SST products
72	with global coverage (Minnett et al, 2019).
73	
74	The Group for High-Resolution Sea Surface Temperature (GHRSST, www.ghrsst.org;
75	Donlon et al, 2009) is an international initiative aimed at coordinating the provision
76	of SST products developed and distributed by different agencies and research
77	institutes. Among GHRSST products, level 4 data (L4) provide gap-free SST maps at
78	regional and global scales, obtained with different algorithms that combine and
79	interpolate satellite based SST data, acquired by a variety of different sensors,

80	sometimes also including in situ observations. Different interpolation techniques and
81	related configurations (e.g. observation/background error correlation scales),
82	interpolation grid size, input data bias-correction, and the sampling adopted by
83	GHRSST data providers induce a significant diversity among L4 SST products (Dash
84	et al., 2012). Understanding the consistency and discrepancy of the different SST L4
85	products will not only help data providers to improve their algorithms, but also
86	represents an important step to inform users about the characteristics of the
87	different products, helping them to select the one that may better suit their
88	applications.
89	
90	Several previous global SST analysis intercomparison studies have already been
91	performed, among which, most noticeably, the Global Climate Observing System
92	(GCOS) SST-Sea Ice intercomparison project
93	(https://www.nodc.noaa.gov/SatelliteData/ghrsst/intercomp.html), and the GMPE
94	(Group for High-Resolution SST, GHRSST, Multi-Product Ensemble) system,

96	(2012) and Dash et al. (2012), which were focused on a relatively short time series
97	over the satellite period (for the year 2010), has recently been extended to
98	intercompare longer-term analyses over the overlapping period of 1991 to 2010
99	(Fiedler et al., 2019a). A much shorter period (one year) is considered in the
100	intercomparison of satellite-based analyses performed by Okuro et al. (2014), while a
101	comparison study on the historical SST datasets based on in situ data alone is
102	described in Yasunaka and Hanawa (2011). With the recent reprocessing of several
103	global high resolution daily L4 products from the start of the operational satellite
104	SST era (1981) to recent years, it is now timely to perform an intercomparison of
105	additional SST analyses over a significantly longer period.
106	
107	In the framework of the European Copernicus Climate Change Service (C3S), an
108	Independent Assessment of Essential Climate Variables (ECVs) present in the C3S
109	Climate Data Store (CDS) is foreseen. The C3S CDS distributes and provides access
110	to quality-assured climate dataset and tools in the clouds for users. The independent
111	assessment aims to evaluate the quality, usability and consistency of available ECVs

112	for different applications, ranging from scientific studies (e.g. on climate change), to
113	commercial and private sector uses. SST is one of the ECVs considered in the
114	assessment framework of C3S and the intercomparison of SST products available in
115	the CDS will help the users to understand the quality of different SST products and
116	choose the right one for their specific applications.
117	
118	The study presented hereafter represents the joint effort between the GHRSST SST
119	Analysis Intercomparison Task Team (https://www.ghrsst.org/about-ghrsst/task-
120	teams/) and the C3S SST assessment activities. The objective of this study is to
121	evaluate the basic characteristics and the maturity of eight state of the art global
122	SST analysis products; to describe how SST climatology and variability is represented
123	in each SST product, and to understand the consistency and discrepancy between all
124	these long-term eight SST analyses available in or outside of CDS (some of the SST
125	products are provided in GHRSST L4 format), and eventually to provide guidance on
126	which product might be better suited for users' applications.

The paper is organized as follows: Section 2 introduces the characteristics of SST analysis products included in this study, the basic diagnostics are presented in section 3, and the data maturity of all SST products is described in section 4, and finally, the summary of the evaluation and the recommendations to users are discussed in sections 5 and 6.

132

133 **2. Datasets**

134 Currently, two global SST analysis datasets are distributed through the CDS, namely 135 European Space Agency (ESA) Climate Change Initiative (ESA CCI) version 2.1 and European Centre for Medium-Range Weather Forecasts Atmospheric Reanalysis 136 137 version 5 (ERA5). They are compared here with a selection of six state of the art SST 138 analyses distributed outside the CDS, obtained from different input data and analysis 139 system configurations. These are: 140 Hadley Centre Sea Ice and Sea Surface Temperature (HadISST1) (Rayner et • 141 al., 2003);

142	· UK MetOffice Operational Sea Surface Temperature and Sea Ice Analysis
143	(OSTIA) system (Good et al., 2020)
144	• NOAA Daily OISST v2.1 daily reanalysis also referred to as Reynolds SST
145	(Reynolds et al., 2007; Banzon et al., 2016; Huang et al., 2020);
146	• Multi-scale Ultra-high Resolution 0.25 deg. (MUR25) SST analysis v.4.2
147	(Chin et al., 2017);
148	· Merged satellite and in situ data Global Daily Sea Surface Temperature
149	(MGDSST) (Sakurai et al., 2005; Kurihara et al., 2006);
150	• Australian Bureau of Meteorology Global Monthly SST Analysis (BoM
151	Monthly SST) (Smith et al., 1999).
152	
153	These eight datasets combine satellites and in many cases in situ temperature
154	measurements to generate gap-free (optimally interpolated) SST fields at the globa
155	scale. All these datasets are specifically designed to provide accurate high spatial
156	and temporal resolution SST estimates that can be used in operational applications
157	such as assimilation and/or boundary conditions in numerical weather prediction

158	models (e.g., MGDSST and OSTIA SST), and/or analysed for climate applications (e.g.
159	HadISST1, NOAA Daily OISST analysis, MUR25, BoM Monthly SST). Some of the
160	selected datasets, namely ESA CCI v2.1, OSTIA, NOAA Daily OISST v2.1, MUR25 and
161	BoM Monthly are provided in GHRSST L4 format (GHRSST Science Team, 2012).
162	
163	Below, we detail the characteristics of all the SST products included in this
164	intercomparison study.
165	
166	2.1 ESA-CCI SST
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Temperature Radiometer (SLSTR) series of sensors (Merchant et al., 2019, 2014).
These data are provided at different processing levels: single-sensor data on the
native swath grid (Level-2); uncollated single-sensor (Level-3U) and collated multisensor (Level-3C) gridded data; and blended multi-sensor and optimally interpolated
(Level-4) data.

178 The ESA CCI Level-4 product considered here consists of gap-free (optimally 179 interpolated) maps of daily average SST at 20 cm depth at 0.05° x 0.05° latitude-180 longitude grid (approximately 5x5 km at the equator). The Level-4 data have been 181 produced by running the OSTIA system (Donlon et al., 2012) using CCI Level-3U 182 SSTs as inputs, no in situ data are included. Estimates of standard uncertainty 183 (considered as the standard deviation of the estimated error distribution) are provided for every SST at all product levels. The evaluated global median uncertainty 184 185 is 0.18 K (Merchant et al., 2019). The multiannual stability of the whole time series, 186 evaluated relative to drifting buoy measurements, is within 0.003K/year (Merchant et 187 al., 2019). Given the high temporal and spatial resolution and the performance

188	statistics, this dataset gives an accurate representation of SST spatio-temporal
189	variability of relevance to climate applications. Target applications of the ESA CCI
190	SST dataset include climate and ocean model assessment; accurate definitions of
191	climatic indices; quantification of climate variability and its impacts on weather
192	extremes (including marine heatwaves), marine ecosystems, and related services.
193	
194	2.2 ERA5
195	The ERA5 SST dataset is produced by ECMWF to be used for ERA5 atmospheric
196	reanalysis (Hirahara et al., 2016). It consists of hourly global gap-free SST data at
197	0.25°x0.25° latitude-longitude grid covering the period from 1979 to the present.
198	ERA5 SST data are based on the HadISST2 (Kennedy et al., 2016) product from 1979
199	to August 2007, and the daily operational OSTIA (Donlon et al., 2012) product from
200	September 2007 to present. The HadISST1 version 2 was developed by the UK Met
201	Office Hadley Centre, and its "pentad" dataset consists of spatially complete, 5-daily
202	mean fields on a 0.25° spatial resolution grid. OSTIA is a high resolution (0.05°x0.05°)

203	operational daily product developed by the UK MetOffice and distributed through
204	the Copernicus Marine Environment Monitoring Service (CMEMS). These two SST
205	datasets are aggregated into one continuous data record and interpolated onto the
206	ERA5 model grid (Dee et al., 2011) to be used as boundary conditions for ERA5
207	atmospheric reanalysis. There are two types of Sea Surface Temperature in ERA5
208	including Sea Surface Skin Temperature and Sea Surface Temperature. In this study
209	we have used monthly ERA5 Sea Surface Temperature. ERA5 SST is calculated as
210	the SST from an ocean model with increment as the difference between OSTIA SST
211	and the ocean analysis. Since the input of SST comes from both OSTIA and
212	HadISST2, the ERA5 SST is a mixture of SST in the absence of diurnal variation,
213	"foundation SST" (OSTIA), and SST at indeterminate depth, "SSTdepth" (HadISST2),
214	following the SST definitions in Minnett and Kaiser-Weiss (2012). Here we give the
215	SST type as SSTdepth for ERA5 SST.

216 2.3 HadISST1

217	Hadley Centre Sea Ice and Sea Surface Temperature dataset (HadISST1) is available
218	at_https://www.metoffice.gov.uk/hadobs/hadisst/data/download.html. This dataset
219	includes a combination of monthly globally-complete fields of SST and sea ice
220	concentration on a 1°x1° latitude-longitude grid from 1870 to present. HadISST1
221	data have been produced using SST measurements from the Met Office Marine Data
222	Bank (MDB), mainly ship tracks, and a blend of in situ and adjusted satellite-derived
223	SSTs for 1982-onwards. A bias adjustment of the satellite SST data is performed by
224	subtracting the in situ fields from the AVHRR fields. Specifically, the difference fields
225	are smoothed using a moving window average with a radius of 2224 km (20 degrees
226	of latitude). The smoothed bias fields are then subtracted from the monthly AVHRR
227	SST (see Appendix C in Rayner et al. 2003 for further details).

In order to enhance data coverage, monthly median SSTs for 1871-onward from the
Comprehensive Ocean-Atmosphere Data Set (COADS) (now ICOADS) were also used
where MDB data were not available. Information on sea ice concentrations is also

232	included in the HadISST product. This information is derived from several sources
233	that include digitized sea ice charts and satellite data. Temperatures are
234	reconstructed using a two-stage reduced-space optimal interpolation procedure
235	(Kaplan et al., 1997), followed by superposition of quality-improved gridded
236	observations onto the reconstructions to restore local detail (Rayner et al., 2003).
237	
238	2.4 NOAA (Daily OISST)
239	The NOAA Daily OISST v2.1 dataset (Reynolds et al., 2007; Banzon et al., 2016;
240	Huang et al., 2020), also known as the "Reynolds" Daily Optimum Interpolation SST
241	analysis, consists of global daily spatially-complete SST data on a 0.25°x0.25°
242	latitude-longitude grid from 1981 to present (https://www.nodc.noaa.gov/oisst). This
243	dataset is routinely produced by NOAA/NESDIS/NCEI and publicly provided at

245 interpolation/v2.1/.

GHRSST GDS2 L4 format (GHRSST Science Team, 2012) files are also available from
1981 to 2015 from https://podaac.jpl.nasa.gov/dataset/AVHRR_OI-NCEI-L4-GLOBv2.0 and 2016 to present from https://podaac.jpl.nasa.gov/dataset/AVHRR_OI-NCEIL4-GLOB-v2.1.

251	The NOAA optimal interpolation analysis uses both in situ and satellite-derived SST
252	data. Satellite SSTs are estimated from NOAA/AVHRR and MetOp/AVHRR
253	observations. This dataset also utilizes the in situ ICOADS dataset to correct the
254	residual satellite SST biases. OISST has been updated from v2.0 to v2.1 from January
255	2016 onward. The updates include the following five aspects: (a) MetOp-B replaces
256	NOAA-19 while MetOp-A remains unchanged, (b) freezing-point temperature
257	replaces ice-SST regression in SST proxy in ice-covered oceans, (c) the estimated
258	ship SST bias is reduced from 0.14°C to 0.01°C, (d) ship and buoy observations from
259	ICOADS-D R3.0.2 are used instead of NCEP GTS receipts, and (e) Argo observations
260	above 5 m depth are included. The Argo observations were first used as

independent data to validate the improvements in the updates from (a) to (d), and
the Argo observations were finally included in OISST in (e).

263

264 **2.5 MUR25**

265 The Multi-scale Ultra-high Resolution 0.25 degree. (MUR25) SST analysis (v.4.2) is a global daily spatially-complete SST dataset on a 0.25° x 0.25° grid covering the 266 period from mid-2002 to present. The analyzed SST is representative of the 267 268 foundation temperature (namely, the temperature free, or nearly free, of any diurnal 269 cycle (Minnett and Kaiser-Weiss, 2012). This dataset is a reprocessed version of the 270 MUR dataset v.4.1 (Chin et al., 2017), which provides global daily spatially-complete 271 SST analyses at 0.01° spatial resolution. MUR25 is provided by NASA's Jet Propulsion 272 Laboratory (JPL) Physical Oceanography Distributed Active Archive Center (PO.DAAC) and is available at https://podaac.jpl.nasa.gov/dataset/MUR25-JPL-L4-GLOB-v04.2. 273 274 The MUR L4 analysis is built by using only nighttime SST observations derived from 275 different types of satellite sensors, which include microwave and infrared

276	measurements from, e.g., Advanced Microwave Scanning Radiometer (AMSR) for
277	Earth Observing System (AMSR-E) and NOAA/AVHRR observations. In addition,
278	MUR25 ingests in situ SST measurements from the NOAA iQuam data set (Xu and
279	Ignatov, 2014) to improve the estimate of the foundation temperature, and ice
280	concentration data from the EUMETSAT Ocean and Sea Ice Satellite Application
281	Facility (OSI SAF), which are used for an improved SST parameterization in the polar
282	regions. Satellite and in situ data are combined using MRVA, a meshless multi-scale
283	interpolation method which uses wavelets as basis functions in order to build the
284	daily MUR SST analysis (Chin et al., 2017).

286 **2.6 MGDSST**

The Merged satellite and in situ data Global Daily SST (MGDSST) analysis dataset provides global daily spatially-complete SST fields on a 0.25°x0.25° latitudelongitude grid covering the period from 1982 to present. This dataset is derived from infrared satellite sensors (NOAA/AVHRR and MetOp/AVHRR), microwave

291	satellite sensors (Coriolis/WINDSAT, GCOM-W1/AMSR-2), and in situ temperature
292	measurements (from buoys and ships). This dataset is provided by The Japanese
293	Meteorological Agency (JMA) and is available at
294	https://ds.data.jma.go.jp/gmd/goos/data/rrtdb/jma-pro/mgd_sst_glb_D.html.
295	SSTs from the microwave sensor AQUA/AMSR-E are used in the analysis from May
296	2002 through 5th October, 2011. In the reanalysis data, SSTs under sea ice are
297	determined according to the statistical relation between sea-ice concentration and
298	SST. The lowest SST is -1.8 degree Celsius where the sea-ice concentration is 100%.
299	Additional information is provided by Kurihara et al. (2006) and Sakurai et al. (2005)
300	

2.7 BoM Monthly

The Monthly Optimal Interpolation (OI) SST Analysis is the global monthly spatially complete SST dataset on a 1°x1° grid produced by the Australian Bureau of Meteorology (BoM), covering the period of 1994 to present (Smith et al., 1999), formed by averaging the BoM Weekly OI SST analyses over each month. In this

306	study, we use the GHRSST version 1 L4 format files of this dataset covering the
307	period 2002 to present (Beggs and Pugh, 2009). The SST observations are obtained
308	from in situ SST observations from drifting and moored buoys, ships, Argo floats,
309	Conductivity Temperature Depth (CTD) and Expendable Bathythermographs (XBTs),
310	and satellite-derived SST from infrared AVHRR sensors aboard NOAA Polar-Orbiting
311	Environmental Satellites (POES) and ESA/EUMETSAT MetOp satellites. Weekly OI
312	analyses of the in situ data are used to correct for biases in the satellite data (Smith
313	et al., 1999), similar to the method used in the NOAA Weekly 1°x1° OISST v2
314	(Reynolds et al., 2002). The resulting outputs of the Weekly and Monthly OI
315	analyses of in situ and satellite data are therefore SST values of indeterminate depth,
316	SSTdepth.
317	At high latitudes, the BoM weekly analysis system uses the daily sea-ice
318	concentration analysis from NOAA/NCEP
319	(https://polar.ncep.noaa.gov/seaice/Analyses.shtml) to constrain the SST, by setting
320	SST at a given grid point to –1.8°C if the concentration of NCEP ice data in that grid

321	cell is greater than 50 per cent. Until 12 March 2008, the 0.5° resolution sea-ice
322	analysis was used and after that date, the 1/12° resolution sea-ice analysis
323	(Grumbine, 1996).
324	Maps of these weekly and monthly SST analyses are available at
325	http://www.bom.gov.au/marine/sst.shtml, and they are used operationally by BoM to
326	generate El Niño indices, monitor the Indian Ocean Dipole and produce SST
327	anomaly maps for climate applications
328	(http://www.bom.gov.au/climate/enso/#tabs=Sea-surface). The BoM Weekly and
329	Monthly OI SST analysis GHRSST L4 format files are available on request
330	(http://www.bom.gov.au/climate/data-services/data-requests.shtml). It should be
331	noted that higher resolution (0.25°x0.25°) global daily OI SST analyses have been
332	produced operationally at the Bureau of Meteorology since 2008 (Zhong and Beggs,
333	2008; http://www.bom.gov.au/marine/sst.shtml) but these only cover the period 2008
334	to present so were not included in this study.

2.8 UK Met Office OSTIA SST

337	The UK Met Office OSTIA (Good et al., 2020) system is a daily global SST product
338	with a resolution of 1/20° (approximately 5-6km). Monthly and seasonal frequency
339	datasets are also available. The version of OSTIA SST we use in this study is the
340	CMEMS reprocessed SST analysis based on the OSTIA configuration reported in
341	Good et al. (2020), covering the period 1 October 1981 to 31 December 2018. This
342	OSTIA reanalysis is formed by the combination of satellite SST data provided by the
343	GHRSST project with additional AATSR, SLSTR and AVHRR data from ESA CCI SST
344	v2.1, C3S projects, and in situ observations from the HadIOD by using NEMOVAR, a
345	variational assimilation (Fiedler et al., 2019b), instead of the optimal interpolation
346	algorithm (Martin et al., 2007, Donlon et al., 2012). Note that ESA CCI SST v2 and
347	V2.1 only differ in the file specification, but no scientific differences. Bias correction
348	is performed for all the input satellite data (except the satellite data in the reference
349	dataset) by carrying out match-ups between satellite and reference measurements.
350	The depth of the SST analysis represents the sub-skin temperature immediately

351	before sunrise also referred to as foundational SST that is free of diurnal variability
352	(Donlon et al., 2012). The OSTIA reanalysis is publicly available from
353	https://resources.marine.copernicus.eu/?option=com_csw&task=results?option=com_
354	csw&view=details&product_id=SST_GLO_SST_L4_REP_OBSERVATIONS_010_011.
355	In order to verify the accuracy of reprocessed SST analysis, near-surface Argo data
356	that are not included in SST analysis are used as independent data for quality
357	assessment as shown in CMEMS quality information documentation of OSTIA SST
358	(https://resources.marine.copernicus.eu/documents/QUID/CMEMS-SST-QUID-010-
359	011.pdf). Note that the drifting buoy SSTs used for validation are ingested into the
360	analyses, however the validation process uses OSTIA background fields without data
361	assimilating buoy SSTs to compare with drifting buoys from analysis day plus 1 day
362	to avoid the validation data independence issue.
363	OSTIA SST has been used as boundary conditions for operational forecast models at
364	the UK Met Office and European Centre for Medium-range Weather Forecasting
365	(ECMWF) and is also part of the CMEMS project. The validation, assessment activities

366 update regularly through the CMEMS project, the data, and relevant documentations

367 are available at

368 https://resources.marine.copernicus.eu/?option=com_csw&view=details&product_id=

369 SST_GLO_SST_L4_REP_OBSERVATIONS_010_011.

370

371 3 Basic diagnostics

372

373	In order to compare the selected datasets (see Section 2) especially against global
374	SST climatology, all the SST products need to be mapped on a common temporal
375	and spatial resolution (regular 1°x1° latitude-longitude grid.). Apart from HadISST1,
376	the majority of the SST products have higher resolution than 1°x1° and the
377	advantage of high resolution is to resolve small scale ocean processes. The
378	interpolation from higher resolution to low resolution may exclude the impacts of
379	important small-scale signals in the SST products. Before we present the basic
380	diagnostics such as mean climatology and variability, we have performed spatial

381	spectral analysis (Section 3.1.1 - methods and Section 3.2.1 - results) to quantify the
382	impact of interpolation to the common 1°x1° resolution we have performed in our
383	basic diagnostics.
384	
385	The grid of HadISST1 has been chosen as the reference grid (at $1^{\circ}x1^{\circ}$ nominal
386	resolution). The HadISST1 land-sea mask has then been applied to all products. In
387	addition, a sea-ice mask was built from HadISST1 and used as a common sea-ice
388	mask for all datasets.
389	
390	To homogenize the datasets' temporal and spatial resolution we have used CDO
391	(Climate Data Operator) command line operators (see the user guide at
392	https://code.mpimet.mpg.de/projects/cdo/embedded/cdo.pdf). In particular, we have
393	chosen a bilinear interpolation for gridding all datasets on the HadISST1 spatial grid.
394	
395	For all the selected SST products, the overlapping period is 2003-2018 (Figure 1) and
396	the intercomparison of all SST products are performed for the period 2003-2018,

397	when observations are abundant compared to the beginning of the satellite era.
398	Recent period increased quantities of observations ingested in the SST analysis may
399	reduce the spread of ensemble SST products produced with different algorithms. In
400	order to understand deeper the discrepancy and consistency between all the SST
401	analyses produced with different algorithms, similar intercomparison diagnostics of
402	SST products (ESA-CCI, ERA5, OSTIA, NOAA OISST, MGDSST and HadISST1) that
403	have the common period from 1982-2018 (Figure 1) are also carried out for the
404	earlier period of the satellite era (1982-2002) when the observations are scarce
405	compared to the later period of the satellite era.
406	
407	In this section, we first introduce the methodologies we applied to produce the
408	basic diagnostics, and the spatial spectral analysis method used to investigate the
409	impact of spatial resolution is also presented. Then we present the results generated
410	by these diagnostics in terms of intercomparison for the period 2003-2018, and the
411	intercomparison of SST products that cover the period 1982-2002 is presented at
412	the end of this section.

3.1 Statistical Methods

415	A set of basic diagnostics have been defined to evaluate the similarity and
416	disagreements between selected SST datasets, as detailed in the following
417	subsections. Some of these metrics, such as the mean climatology, quantify the
418	long-term mean spatial distribution (climatology) of the SST for each single dataset
419	and can be used to qualitatively evaluate the capability of SST in representing the
420	climatological spatial patterns and the temporal variability of globally averaged
421	SSTs . Other metrics, such as difference, root-mean-square difference (RMSD), and
422	correlation, measure the distance between a single product and a "reference". The
423	latter can be either a previously validated dataset (if available) or any other dataset
424	that is arbitrarily chosen as reference. In this report, we have taken the median of all
425	datasets (hereafter the Ensemble median) as a reference and used it to measure the
426	difference among different SST products. Finally, we choose a specific case study of
427	the El Niño Southern Oscillation (ENSO) Nino3.4 Index to evaluate the capability of

representing ENSO events in all SST products. Nino3.4 is the average SST anomaly in
the region bounded by 5°N to 5°S, from 170°W to 120°W.

430

3.1.1 Spatial Spectral Analysis

431 The spectral analysis method we adopted in this study is the Multitaper Power 432 Spectral Density Estimate (MTM) (Thomson, 1982), which is a very useful tool for the 433 analysis of relatively short and noisy series that may contain both broadband and 434 line components. Different from several other techniques, MTM multiplies the data 435 by a small set of orthogonal tapers rather than a single taper to minimize the 436 spectral leakage due to the finite length of the series. 437 MTM power spectral estimates were performed using the pmtm matlab function (https://www.mathworks.com/help/signal/ref/pmtm.html). For more details please 438 439 refer to Ghil et al. (2002) Section 3.4. 440 We have chosen four datasets, ESA-CCI and OSTIA with the original spatial 441

442 resolution of 0.05° and MGDSST and NOAA Daily OISST (Reynolds 0.25 x 0.25° SST)

443	with the original resolution of 0.25° all covering the same period 1982-2018 with
444	daily frequency. Meanwhile, we chose the Pacific equator pixel line, spanning from
445	Indonesian to South America as the study region (0°N, 120°E-80°W). For each
446	dataset the spatial power spectral density has been estimated on a daily basis over
447	the common period (1982-2018) and then time averaged. The detailed results and
448	discussion are given in Section 3.2.1.
449	3.1.2 Trend analysis
450	
451	SST trends have been estimated by using the X-11 seasonal adjustment procedure
452	(see e.g. Pezzulli et al., 2005). Given X_t is the input time series (namely, an SST time
453	series), the X-11 procedure generates the following decomposition:
454	$X_t = T_t + S_t + I_t$
455	
456	where T_t is the trend component, S_t the seasonal component and I_t the irregular

457 component, which accounts for the residual irregular variations such as sub-annual

458	fluctuations. The decomposition is obtained through iterative application of different
459	running means, which have the effect of a low-pass filter for T_{t} estimation and a
460	seasonal filter for S _t estimation.
461	In addition, the Mann-Kendall test is used to assess whether a monotonic upward or
462	downward trend in T_{t} exists (against the null hypothesis of no trend), Sen's method
463	is applied to estimate the slope of $T_{t\scriptscriptstyle t}$ i.e. the trend (as the median of the slopes of
464	all pairs of sample points), and a bootstrap procedure is used to estimate the 95%
465	confidence interval of the trend (Mann, 1945; Sen, 1968; Kendall, 1975; Efron and
466	Tibshirani, 1993).
467	
468	3.2 Results

3.2.1 Spatial Spectrum Analysis

471 In order to verify the suitableness of our choice of interpolation, we have performed472 spatial power spectral analysis (section 3.1.1) based on the chosen SST products

473	(Figure 2). With rapid growth of computing power and storage capacity, along with
474	advancement of scientific knowledge and users' needs, spatial resolution of SST gap-
475	free analyses has increased dramatically to resolve smaller scale features in the
476	ocean. The spatial resolution of SST products used in this study spans from 1° to
477	0.05°, meaning that the highest resolution is 20 times the lowest resolution. In the
478	high resolution SST products, the meso-scales might be resolved, by contrast in the
479	low resolution SST products only large scale features are represented.
480	
481	All of the SST products we chose for the spectral analysis cover the same period
482	from 1982 to 2018 with daily frequency. OSTIA and ESA-CCI SST have the original
483	spatial resolution of 0.05° and MGDSST and NOAA Daily OISST have the spatial
484	resolution of 0.25°. If the power spectra gradient becomes flat at a certain
485	wavelength it means that the analysis carried out at a wavelength shorter than this
486	certain wavelength contains only noise. The power spectrum density of these four
487	datasets shows that even though all of these SST products have higher grid
488	resolution than the chosen common grid, 1°, the power density of all SST products

489	starts to decline at spatial wavelengths greater than their grid-resolution. The
490	prominent differences between NOAA OISST and MGDSST are most likely due to
491	different background correlation length scales being used in the optimal
492	interpolation and different methodology used to correct satellite-based observations.
493	For high resolution datasets, the 0.05° products, the power density significantly
494	declined after \sim 100 km (wavenumber 10 ⁻²), which is close to 1° spatial resolution
495	near the equator and the gradient becomes flat at wavelengths \sim 70 km. It means
496	that the signals within a wavelength of 100 km are noise, with no physical meaning
497	in 0.05° SST products, and that also applies to 0.25° resolution SST products. Similar
498	results were shown in Fiedler et al. (2019a) that in the Gulf Stream regions for the
499	2017 northern winter the spectral density of SST starts to depart from the
500	$II^{11/3}$ cascade of SST field (equivalent to kinetic energy power spectrum cascade of
501	$I I^{-5/3}$ based on Le Traon et al., 1990; 2008) at wavelengths around 90km. This
502	confirms that the interpolation to 1° does not undermine the interpretation of
503	results presented in our study.

505	Additionally, the diagnostics performed in the following sections mainly focus on the
506	general features (mean climatology and long-term temporal variability) of the
507	representation of all the SST products. We believe the interpolation of all SST
508	products to 1° brings minor issues to the interpretation of the results. Certainly, the
509	intercomparison between all the SST products in terms of specific details, for
510	example, the representation of the Gulf Stream and meso-scale features are not in
511	the scope of this study. Related activities are underway and will be presented by the
512	GHRSST SST Analysis Intercomparison Task Team in the near future.

514 **3.2.2 Mean and Variability (2003-2018)**

In terms of the basic diagnostics, we have first calculated the mean climatology of the global SST distribution of the eight selected SST datasets during 16 years from 2003 to 2018 plus the median of all the eight SST products, i.e., the climatology of the ensemble median (Figure 3). In all eight cases, the average correctly reveals the dominant latitudinal spatial SST pattern: higher at the tropics, milder at middle latitudes and lower in the polar regions. Regions impacted by occasional or
521	persistent presence of sea ice are flagged, i.e., only complete years have been
522	considered for the average estimate in each grid point.
523	
524	A first qualitative inspection of the eight mean SST fields suggests that all products
525	reproduce a very similar spatial distribution of SST with minor differences not
526	appreciable from Figure 3. Considering a confidence level of 95%, the eight global
527	mean SST estimates for the period 2003 to 2018 range in an interval between
528	20.02°C and 20.17°C. The ensemble median obviously falls close to the middle of
529	this range (i.e., 20.12 °C).
530	In order to have a further investigation of the consistency and discrepancy between
531	all SST products, we calculated the difference between each SST product and the
532	ensemble median displayed in Figure 4. Considering a 95% confidence interval, the
533	global mean difference between each single product and the ensemble median
534	ranges between -0.05 and 0.1 °C with relevant spatial variability (Figure 4). In fact,
535	differences are more pronounced in the Southern ocean where distances between

536	single product values and the ensemble median reach values higher than 1°C. This is
537	particularly evident in the case of HadISST1 data. In general, higher difference areas
538	correspond to the western boundary current systems such as the Gulf Stream
539	Current, the Kuroshio Current in the Northern Hemisphere, Brazil currents in the
540	Southern Atlantic Ocean, and the Antarctic Circumpolar Current (ACC), where eddies
541	are extremely active. In some datasets, especially ESA-CCI SST, MGDSST and OSTIA,
542	the greatest differences from the ensemble median are also located within eastern
543	boundary currents which represent the main upwelling systems, e.g., Peru-Chilli,
544	Benguela, North West-African coast and along the southern Saudi Arabia coast.
545	These discrepancies could be due to mismatch in the position of the main streams,
546	especially the eddy representation in different SST products. Along the coast, the
547	disagreement may come from the interpolation methodology implemented in
548	different SST datasets by data providers. Especially regions where upwelling is active
549	add difficulties to retrieving satellite observations for representing SST patterns and
550	variability. For the case of ESA CCI SSTs, it has been shown that cool biases off the
551	North West-African coast and in the Arabian Sea arise from influences of mineral

552	dust aerosol on IR retrievals of SST, and a large-scale adjustment (not used here) for
553	the dust-related biases has been devised (Merchant and Embury, 2020).
554	The RMSD is defined as the square root of the average squared difference between
555	the SST value of each dataset and the ensemble median, which is an absolute
556	measure of the distance between each single product value and the ensemble
557	median. Considering the 95% confidence interval, the global average RMSD ranges
558	from 0.02 to 0.18 °C. Extreme RMSD values (Figure 5) are concentrated in the
559	Southern ocean and correspond to the ACC, as also evidenced by the mean
560	difference (Figure 4), particularly evident in HadISST1 data. These higher RMSD
561	values are also observed in correspondence to large differences between each SST
562	product and the ensemble median that are mainly located in the western boundary
563	currents, namely, the Gulf Stream in the North Atlantic Ocean and the Kuroshio
564	Current in the North Pacific Ocean, and the ACC regions.
565	The spatial distribution of the Pearson correlation coefficient (Figure 6) highlights the
566	different behavior of HadISST1 with respect to the other seven products. In

567	particular, in the southern ocean region, the correlation falls down to values as low
568	as 0.5 or even less. Similar but less extended discrepancies are also observed for
569	BoM, NOAA Daily OISSTs, ESA-CCI, MUR25, ERA5, OSTIA and MGDSST. In particular,
570	ESA-CCI seems well representative of the ensemble median. MUR25, ERA5, MGDSST
571	and OSTIA are well representative of the ensemble median as well but with slightly
572	higher discrepancies than other SST products. However, the low correlation
573	especially along the coastal regions could be due to the interpolation method
574	adopted during the SST production by data providers because it is still a challenge
575	to correctly retrieve satellite observations at the coastal upwelling regions where SST
576	is highly variable.
577	The temporal variability of globally averaged monthly mean SSTs (Figure 7) clearly
578	exhibits the annual oscillation around the mean value of 20.12 $^\circ$ C (Figure 3). This
579	oscillation has an amplitude of about 0.6 $^\circ$ C as a result of the opposite seasonal
580	cycle in the southern and northern hemispheres. SST anomalies from 2003 to 2018
581	(Figure 8) are obtained by subtracting from all SST products the annual cycle of the

582	ensemble median, i.e., the mean of each month over the whole period (2003-2018).
583	Two main periods are observed with distinct mean values: the first period before
584	2012 where the temperature oscillates around a constant mean value of about
585	20.1°C and a second period where a positive (warming) trend is observed. All the
586	eight datasets show temperatures that vary coherently over all time scales but with
587	relative absolute biases in the range from zero to 0.4 °C.
588	
589	3.2.3 Global linear trends (2003-2018)
590	Global SST trend maps have been computed for each product over the common 16
591	years period from 2003 to 2018 (Figure 9). All the datasets exhibit a global mean
592	warming SST trend ranging from 0.012 (HadISST1) to 0.022 (MGDSST) °C/year, with
593	an average value of 0.019 °C/year (ensemble median). Within the 95% confidence
594	interval, these results are close to the global ocean warming trend of 0.011 °C/year
595	from 1980 to 2005 reported in the last IPCC report (Pachauri et al., 2014) and the
596	differences are due to the different calculating period. The prominent warming

597	trends shown in all SST products are located in the subtropical North Atlantic Ocean,
598	South Indian Ocean, eastern tropical Pacific Ocean close to the American continent.
599	Especially at the Gulf Stream area all SST products (apart from HadISST1 which has
600	slightly weaker signals compared to other dataset) exhibit distinguished warming
601	trends for the period of 2003 to 2018.
602	In the North Atlantic Ocean, between 40 and 70 °N, negative trends are observed in
603	the sub polar gyre region extending up to the coastal areas of Ireland. A second
604	common negative trend area is present in the Southern Ocean at longitudes
605	centered around the Drake Passage. In the tropical Atlantic Ocean, a large area of
606	negative trends is observed only in ERA5 and a smaller area in BoM, OSTIA and
607	HadISST1. For all the other products this area is characterized by no significant
608	trends (i.e., areas where, given the $p=0.05$ limit, the null hypothesis cannot be
609	refuted) with few sparse negative trend points.

611	The Mediterranean Sea shows an evident positive trend in all products in contrast
612	with a close to zero trend region in the adjacent northeast Atlantic Ocean. This is in
613	agreement with what was recently published by Pisano et al. (2020) who observe
614	that, after 1990, SST in the Mediterranean Sea continues to increase in contrast with
615	the adjacent areas of the Atlantic Ocean where a pause of the general warming
616	trend occurred. The larger area of positive SST trends is present in the Indian Ocean.
617	Intense (positive) trends cover more uniformly and densely the reddish areas in ESA
618	CCI, MUR, NOAA OISST and MGDSST data, while a more patchy and less intense
619	positive trend coverage is observed in ERA5, BoM, OSTIA and HadISST1 data.
620	Besides a bias that separates the curves by a maximum of 0.2°C, the trend
621	component of the eight spatially averaged global SST time series (Figure 10a),
622	obtained using the X-11 procedure with a 2-year low-pass filter (section 3.1.2),
623	shows a very similar behaviour for all the products. The time evolution of the trend
624	component reveals an apparently neutral period until 2011 included with a single
625	maximum centered on the year 2009. After this period, a continuous warming phase

is observed with an increase of the temperature of nearly 0.3°C, that is, about
0.06°C/year which is consistent with the signal observed in the time series anomalies
(Figures 7 and 8).

In order to understand better the contribution to the significant warming trends for 629 the period of 2012-2018 observed in all SST products, we have calculated the SST 630 631 trend component in different ocean basins, i.e. Pacific Ocean (Figure 10b), Atlantic Ocean (Figure 10c) and Indian Ocean (Figure 10d). Quantitatively, the warming 632 trends for the period 2012-2018 ranges from 0.036°C/year (BoM) to 0.062°C/year 633 634 (MUR25) with 0.049°C/year in the ensemble median. The major contributor to this 635 warming trend comes from the Pacific Ocean where warming trends span from 636 0.045°C/year (BoM) to 0.084°C/year (MUR25) with 0.064°C/year in the ensemble median. The contribution from the Atlantic (0.02°C/year from BoM to 0.52°C/year 637 638 from MUR25) is smaller compared to the Pacific Ocean, and the warming trends in 639 the Indian Ocean from 2012 to 2018 are relatively very small (from 0.002°C/year, MGDSST to 0.030°C/year, BoM), which are evidently exhibited in Figure 10d. 640

3.2.4 Intercomparison during the early period (1982-2002)

643	In this section, we present the intercomparison of all SST products covering the
644	period 1982-2002. First we have shown the global mean SST time series (Figure 11)
645	that covers the time period originally obtained in each SST product allows us to
646	detect the consistency and disagreement between all SST products for a longer
647	period to fully take advantage of SST products which covers the period beyond 2003
648	and 2018. As we have discussed, all the SST products are very similar to the period
649	of 2003-2018 when there are abundant observations. On the contrary, during the
650	period of early satellite era (1982-2002), the disagreement between all the SST
651	products is larger compared to the later period (2003-2018), which may be due to
652	fewer observations ingested in the SST analysis.
653	To quantify the consistency and discrepancy of SST products for the early satellite
654	era (1982-2002) we have calculated the mean climatology (Figure 12) for all SST
655	products which cover the period back to 1982 (Figure 1), including ESA-CCI, OSTIA,

656	ERA5, NOAA OISST, MGDSST and HadISST1 and the differences between each
657	member with the ensemble median (Figure 13). The mean climatology of SST during
658	the period of 1982-2002 spans the range from 19.76°C (NOAA OISST) to 20.05°C
659	(HadISST1) with the ensemble median as 19.79°C. The differences of each member
660	relative to the ensemble median for the period of 1982-2002 range from 0.03°C to
661	0.26°C that is much higher than that during the period of 2003-2018 which range
662	from 0.01°C to 0.1°C. The discrepancy of all SST products (Figure 13) are located in
663	the areas that are similar to the period of 2003-2018 (Figure 4), but with amplified
664	signals. However, in some SST products, the differences relative to the ensemble
665	median change signs. For example, during the period of 2003-2018 the MGDSST
666	mean climatology is higher than the ensemble median in the eastern Indian Ocean.
667	On the contrary, the mean climatology differences between MGDSST and the
668	ensemble median became negative during the period of 1982-2002. ERA5 SST is
669	based on OSTIA SST, however, there are differences between them because ERA5 is
670	forced by SST from an ocean model with increment based on the difference

between ocean analysis and OSTIA, which contains information from the OSTIA SSTbut is not exactly identi.

673	These results are consistent with what is shown in Figure 11 that during the early
674	period of the satellite era (1982-2002, fewer SST observations) all the SST products
675	have larger differences compared to the later period (2003-2018, more SST
676	observations), indicating that observation number is the main factor to constrain the
677	climatology of all the SST products developed with different algorithms. The total
678	number of valid in situ SST observations from drifting buoys, ships, Argo floats and
679	moorings, used for bias-correcting satellite SST ingested into ERA5, HadISST1, OSTIA,
680	Daily OISST and BoM Monthly, indeed increases over time (Xu and Ignatov, 2014;
681	https://www.star.nesdis.noaa.gov/socd/sst/iquam).
682	In 2002, the microwave radiometer AMSR-E, which measures ocean brightness
683	temperatures through clouds, commenced operation on Aqua satellite. This
684	improvement in spatial coverage is another important factor affecting SST data

685	ingested into OSTIA, ERA5, MGDSST and MUR25, and it is notable that all SST
686	products studied converge more after 2003 compared to before 2003.
687	
688	
689	3.2.5 Niño 3.4 Index
690	
691	In order to have a deeper evaluation of the quality of the SST for climate studies, we
692	investigated the capability of representing the climate modes in all SST products for
693	the period of 1982-2018 in order to include more ENSO events, here the Nino3.4
694	index (Trenberth 2020). Niño 3.4 is one of the most used indexes to monitor the
695	occurrence and variability of El Niño and la Niña events, defined as the average
696	equatorial SST anomalies across the Pacific in the region 5°S-5°N, 170W°-120W°.
697	Figures 14 show the time evolution of the Niño 3.4 index during the 1982-2018
698	"common period" for each product time series after applying a 5-month running
699	mean filter.

700	All products give evidence of the very strong El Niño events in the period selected.
701	The procedure used here to independently compute the Niño 3.4 index for all the
702	data sets is the same applied by Trenberth (2020). The time evolution of the Niño
703	3.4 SST anomaly is nearly identical for all the products with minor differences (Figure
704	14). The three strong El Niño events that occurred during this investigation period,
705	namely 1982-1983, 1997-1998, and 2015-2016, are reproduced, with a similar
706	intensity, by all products. Moreover, the larger intensity of the El Niño positive
707	anomalies with respect to the negative La Niña events confirms the asymmetry
708	hypothesis of Monahan and Dai (2004).

4. Data Maturity Matrix

The concept of the data maturity matrix is to evaluate the basic characteristics of a
dataset initiated by the World Meteorological Organization (WMO) to develop
technical guidance and standards for collecting, processing, and managing datasets.
The assessment of the maturity of the individual dataset is essential to guarantee

715	and further improve the documentation, storage, and dissemination of datasets that
716	are applicable for users (Peng et al., 2019).
717	The System Maturity Matrix (SMM) for Climate Data Records (CDRs) is first
718	developed in the Coordinating Earth Observation Data Validation for Reanalysis for
719	Climate Services project (CORE-CLIMAX) (Su et al., 2018). The objective is to
720	develop a tool to evaluate different aspects of the CDRs combining scientific and
721	engineering views. (EUMETSAT, 2014). In the SMM framework assessments are made
722	in six major category areas and a score of 1 to 6 is assigned that reflects the
723	maturity of the CDR with respect to a specific category;
724	
725	1. Software readiness
726	2. Metadata
727	3. User documentation
728	4. Uncertainty characterization
729	5. Public access, feedback, and update

730	6.	Usage
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731	However, the assessment of maturity can only reflect aspects of process maturity. It
732	does not interpret the scientific quality of a dataset. For example, a mature product
733	may not be scientifically reliable thus the maturity matrix only provides the
734	assessment of fitness-of-purpose of a given product for climate service practitioners
735	in terms of the categories mentioned above.
736	Additionally, the SMM scores recognize that at the early evaluation stage in the life
737	cycle of the product the low scores in some of the categories do not demonstrate
738	the possible future maturity of the dataset. Instead, low SMM scores indicate a
739	recently released and evolving product at a less mature stage being made available
740	to users.
741	In the context of the C3S_511 project, the aim of our assessment is to evaluate the
742	maturity of the dataset instead of the whole CDRs. We have adopted the SMM
743	methodology of the CORE-CLIMAX for our use to evaluate individual datasets. We
744	defined our matrix as the Maturity Matrix (MM) since we evaluate the dataset

745	instead of the system of the dataset. Not all the categories from CORE-CLIMAX are
746	included because some of them are not suitable for our usage. A guidance
747	document is developed in the framework of C3S_511 project , and the assessment
748	scores given in this study are based on our guidance document
749	(https://confluence.ecmwf.int/display/CKB/Guidance+document+on+applying+the+M
750	aturity+Matrix+as+part+of+the+Evaluation+and+Quality+Control). The MM, as
751	important as the scientific quality, provides data providers important information in
752	which aspects they need to improve their dataset for potential easy access and
753	usage for users.
754	The MM of ESA-CCI and ERA5 SST (Table 2), showing that ESA-CCI SST is much
755	more mature compared to ERA5 SST in terms of documentation, uncertainty
756	characterization, and usage. As we mentioned above, low MM scores do not suggest
757	the scientific quality of ERA5 SST is lower than ESA-CCI SST. However, in terms of
758	the documentation of the dataset, ESA-CCI SST is much more advanced than ERA5
759	SST.

760	In this study we have extended the evaluation of the MM to the dataset outside of
761	CDS (Table 2). Due to the length limit, detailed defensible traces to score MM for
762	SST products are given in the Appendix. In terms of metadata, MGDSST has a lower
763	score because it is provided in text format not following any standards with limited
764	global attributes. The rest of the SST analysis products follow the NetCDF format
765	and CF compliance with detailed information on Metadata. Compared with other
766	datasets, BoM, MGDSST and MUR25 lack user documentation including the formal
767	description of scientific methodology, validation report and product user guide. A
768	formal user guide is not found for HadISST1 either. Very few SST products (OSTIA
769	and ESA-CCI SST) have automated quality monitoring in terms of the uncertainty
770	characterisation category. Thanks to GHRSST activities, all GHRSST L4 products
771	follow internationally agreed GHRSST specifications, which provide uncertainty
772	calculations. Several SST analysis products (HadISST1, MGDSST, BoM and ERA5)
773	have very limited validation, standards or uncertainty quantification documentation.
774	All SST products are publicly available via the online portal, except that BoM SST is
775	available on request from the data provider via their website. However, the

776	versioning, user feedback, and updates to records in the category of public access to
777	SST products are not fully developed for BoM and MGDSST. All SST products except
778	ERA5 are widely used in multiple research fields, and most of them either support
779	decision support systems or usage and benefits of the SST products are emerging.
780	Overall, most of the SST products are well documented and user friendly. As we
781	mentioned before, this scoring does not judge the scientific quality of the SST
782	product. However, the low scoring of some products might give data providers
783	important information to improve the documentation of their products in order to
784	make the product more user friendly.
785	
786	5. Summary of evaluations
787	SST is an essential climate variable (ECV) to assess the state of the global climate
788	system and monitor its variations on interannual and (multi)decadal timescales.
789	Accurate SST observations at high spatial and temporal resolution over a long-term

period are needed to evaluate the present state of the oceans and the impact ofglobal surface warming.

792	In this report, eight different SST datasets have been analyzed and intercompared
793	for the overlapping period from 2003-2018. The ESA CCI SST v.2.1 and ERA5
794	reanalysis are available through the C3S Climate Data Store while the remaining six
795	datasets (OSTIA, HadISST1, NOAA Daily OISST, MUR, MGDSST, BoM) are provided
796	outside the CDS. All these datasets provide global gap-free (optimally interpolated)
797	SST maps but at different spatial and temporal resolutions. Then, to be comparable,
798	all the datasets have been gridded to a common grid (i.e., $1^{\circ}x1^{\circ}$) and averaged to a
799	common temporal frequency (i.e., monthly) over the overlapping period from 2003
800	to 2018. Finally, the average of the median of all the datasets (namely, the Ensemble
801	median) has been defined in order to analyze differences among these datasets.
802	In general, all the SST datasets show consistent climatological spatial patterns
803	(section 3.2). The global monthly mean and anomaly SST time series of these
804	datasets show very good agreement. When compared to the Ensemble median,

805	higher differences (in terms of mean difference, root-mean-square difference and
806	correlation) are found in correspondence to the main current systems, such as the
807	Gulf Current, the Kuroshio Current and the Antarctic circumpolar current. These
808	discrepancies are due to the different retrieval methods used to derive the spatially-
809	complete SST analyses. Differences can originate from several factors: interpolation
810	technique and related configuration (e.g. observation/background error correlation
811	scales), interpolation grid size, input data bias-correction and, if present, the
812	correction applied to obtain the foundation temperature or the temperature at 0.2
813	m. As an example, OSTIA, MUR25, MGDSST and ERA5 (via OSTIA from 2007
814	onwards) are the only L4 analyses included in the study that ingested microwave SST
815	data. Since these datasets (OSTIA, MUR25, MGDSST and ERA5) would ingest possibly
816	cooler daytime SST observations over cloudy regions, they may therefore exhibit
817	slightly cooler biases after 2002 compared with the other analyses that ingest only
818	infrared SST observations and in situ data. This effect may be offset in some
819	analyses, such as BoM Monthly and NOAA Daily OISST v2.1, where in situ data at 0.2
820	m to several meters depth are used to bias-correct the infrared AVHRR SST data.

821 However, on average, the Taylor diagram confirms the very close similarity between 822 the different datasets.

All the datasets reproduce very similar spatial patterns of global SST trends (section 3.3). In addition, global mean warming trends as estimated from all the datasets are consistent (within the 95% confidence interval) with the global ocean warming trend as reported in the last IPCC report, estimated at 0.011 °C/year from 1980 to 2005. The linear trend in different basins shows that the main contributor from 2012 to 2018 is the Pacific Ocean.

829

The global mean SST time series for the whole period originally covered by all the SST products reveals that the disagreement between all SST products is larger in the early period (1982-2002) of the satellite era during which fewer observations are available compared to the later period (2003-2018) of the satellite era. Specifically, the difference between each ensemble member and the ensemble median ranges from 0.03°C to 0.26°C during the early period (1982-2002) and from 0.01°C to 0.1°C

836	during the later period (2003-2018), respectively. It indicates that the observations
837	ingested into each SST analysis plays a significant role in constraining the SST
838	climatology. Satellite sensor improvements (e.g., the launch of AMSR-E in 2002 that
839	could measure ocean brightness temperatures through clouds) is another important
840	factor affecting SST quality after 2003. Note that the impact of natural variability on
841	SST climatology is embedded in the analysis, that is, it is difficult to differentiate
842	from the constraint of SST observations on the SST climatology. Additionally, the
843	discrepancy between each product due to algorithms, observations ingested etc. is
844	very small compared to the significant warming trends shown in the linear trends
845	and time series.
846	
847	Finally, the tropical Pacific region has been selected, as a test case, to assess the
848	capability of the different SST products, with a longer common temporal period, to
849	capture the main modes of variability of a well-known climate oscillatory mode, e.g.
850	ENSO. This analysis confirmed the close similarity of all the five datasets selected
851	and their capability to reproduce, in the same way, the main components of the

tropical Pacific region space and time variability at time scales compatible with thelength of the selected time series.

854

855	The maturity matrix score of all SST products (Table 2), that aims to demonstrate the
856	maturity of data documentation during the life cycle of one product, shows that
857	most of SST products are user friendly and provide sufficient information. Low scores
858	of some SST products (Table 2) indicate a direction where data providers could
859	improve their products in terms of data documentation, storage and dissemination
860	for users. Thanks to the GHRSST effort, all GHRSST products are well documented
861	for their uncertainty characteristics (GHRSST Science Team, 2012).
862	

863 6. Recommendations to users

All the datasets presented here provide state-of-the-art spatially-complete SST
products at the global scale. These datasets are characterized by different spatial

and temporal resolutions and temporal coverage that can fulfil the requirements ofa large variety of users.

868	Intercomparison results and a test case analysis suggest these datasets provide an
869	accurate representation of the SST spatio-temporal variability. These datasets can
870	then be used for fundamental climate applications compatible with the length of
871	each time series, such as long-term monitoring of SST changes (e.g., trends) and
872	comparison to or initialization of numerical models. Other target applications include
873	the use of these datasets in the definition of climatic indices, assessment and
874	monitoring of weather extreme events (including marine heatwaves) and their
875	impact on marine ecosystem, and related services.
876	
877	In this study we have interpolated all SST products into 1 degree and monthly
878	frequency in order to facilitate intercomparison studies. However, to understand
879	which dataset is suitable for specific case studies where spatial and/or temporal
880	resolution are critical, such as the separation of the Gulf Stream and the diurnal

cycle of the SST products, specific intercomparison studies are required. Indeed, in the framework of the GHRSST intercomparison team, several such intercomparison tasks are ongoing and scientific findings will be available in the near future.

884

885 Finally, users are strongly encouraged to consider also the type of SST offered by 886 each producer and to distinguish between, e.g., skin SST, subskin or SSTdepth, and foundation SST according to the specific application for which the data are intended 887 888 to be used. For example, in conditions of high insolation and low surface ocean 889 mixing skin SST is strongly impacted by diurnal warming, SST at 0.2 m depth 890 somewhat impacted, SSTdepth below 1 m minimally impacted and foundation SST 891 has no diurnal signature (Gentemann et al., 2009; Minnett and Kaiser-Weiss, 2012). In our study, we have used SSTdepth, foundation SST and SST at 0.2 m depth, which 892 893 appears to have had minor impacts on the results.

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899	Andrea Pisano, Vincenzo Artale, Rosalia Santoleri and Vincenzo De Toma.
900	The BoM Monthly OI SST analysis GHRSST L4 format files were provided by the
901	Australian Bureau of Meteorology and are available on request from
902	http://www.bom.gov.au/climate/data-services/data-requests.shtml.
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904	at the Jet Propulsion Laboratory, California Institute of Technology, under a contract
905	with the National Aeronautics and Space Administration (80NM0018D0004). The
906	authors declare no conflict of interest.

907

908 Data Availability Statement

909	The download	website o	f all datasets	used in this stud	y has been	included in th	he
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910 manuscript in section 2.

911

912 Appendix

- 913 This section provides defensible traces for Maturity Matrix Score given to all SST
- 914 products shown in Table 2 based on the guidance document
- 915 (https://confluence.ecmwf.int/display/CKB/Guidance+document+on+applying+the+M
- 916 aturity+Matrix+as+part+of+the+Evaluation+and+Quality+Control) developed within
- 917 the C3S independent assessment project (C3S_511).

- 919 1. ESA-CCI SST
- 920 Metadata
- 921 Standard (Score: 6/6)
- 922 The ESA CCI SST data files follow the GHRSST Data Specification v2.0 (GDS) and are
- 923 provided in NetCDF-4 format CompactFlash (CF)-1.5 compliant. Files specifications

924	are fully detailed in the ESA CCI Product User Guide (PUG). The NetCDF files contain
925	detailed metadata describing the data by means of global attributes, which are
926	applicable to the whole file, and variable attributes, which apply to a specific data
927	field.
928	
929	Collection Level (Score: 6/6)
930	The ESA CCI SST data files follow the GHRSST Data Specification v2.0 (GDS). Global
931	attributes provide all information available on the data and relative references. In
932	addition the Product Specification Document (PSD) with detailed information of
933	Metadata is available.
934	
935	User Documentation
936	Formal description of scientific methodology (Score: 6/6)
937	The formal description of the ESA CCI SST product is detailed in the Algorithm
938	Theoretical Background Document (ATBD), published by the data provider, which
939	describes and justifies the algorithms used for obtaining SST estimates. A synthesis

940	of the formal ATBD is also available in the CDS. In addition, the ESA CCI SST dataset
941	has been published in Nature Scientific Data (Merchant et al., 2019).
942	

- 943 Formal validation report (Score: 6/6)For the formal validation report of the ESA CCI
- 944 SST L4 product users can refer to Merchant et al. (2019), Product User Guide (PUG),
- 945 and Climate Assessment Report (CAR).
- 946
- 947 Formal product user guide (Score: 6/6)
- 948 The formal product user guide ESA CCI SST product is published by the data
- 949 provider (PUG). A synthesis of the formal user product guide is also available in the
- 950 CDS.
- 951
- 952 Uncertainty Characterization
- 953 Standards (Score: 6/6)

954	Uncertainty characterization follows the internationally agreed GHRSST standard
955	specifications, which are detailed in the GHRSST Data Specification v2.0 (GDS)
956	document.
957	
958	<i>Validation</i> (Score: 6/6)
959	A detailed and comprehensive validation of the ESA CCI SST L4 product is provided
960	in the Product User Guide (PUG), Climate Assessment Report (CAR), and in Merchant
961	et al. (2019). The validation of the ESA CCI SST L4 product is based on different
962	procedures, from automated and visual inspection to comparison of SST data with
963	co-located in situ measurements.
964	
965	Uncertainty quantification (Score: 6/6)
966	Uncertainty in the ESA CCI SST L4 data at each location (i.e., the analysed_sst field in
967	the NETCDF file) is quantified and provided (i.e., in the analysis_error field) through
968	an analysis quality methodology. The methodology used to derive the uncertainty is
969	based on the optimal interpolation theory and described in the ATBD and PUG,

970	giving comprehensive information of validation of the quantitative uncertainty
971	estimates and error covariance.
972	
973	Automated Quality monitoring (Score: 6/6)
974	The identification of valid observations for SST estimation and algorithms used in
975	the preparatory preprocessing are described in the ATBD and PUG. Moreover, a
976	confidence level on a scale 0 to 5 is provided for each SST as a quality indicator,
977	following the international GHRSST conventions. Five indicates the highest
978	confidence. Quality levels 4 and 5 should be used for climate applications.
979	Automated check is implemented to valid the data quality (Merchant et al., 2019).
980	
981	Public access, feedback and update
982	Public Access/Archive (Score: 5/6)
983	The ESA CCI SST dataset v2.0 is available on the data provider's website. Detailed
984	information available in the PUG. However, the source code is not publically

985 available.

987 *Version* (Score: 6/6)

988 The version is fully established by the data provider.

989

990 User feedback (Score: 6/6)

991 The ESA CCI SST dataset v2.0 is also provided through the CMEMS and is part of

992 GHRSST. Within CMEMS, a Multi-Year Product Quality Working Group is established

993 with the aim of periodically assessing the status of the CMEMS climate data records,

994 including ESA CCI SST, integrating users' needs and feedback. Feedback from users

995 are also included in the Climate Assessment Report (CAR). In addition, ESA CCI data

996 provider provides an email contact to collect users' feedback.

997

998 Updates to record (Score: 6/6)

999 Currently the ESA CCI SST dataset v2.0 covers the period from late-1981 to 2018.

1000 Updates through to the near-present are expected this year (2020). Extensions are

- 1001 expected to be produced by the Copernicus Climate Change Service (C3S) with only
- 1002 ~5 days delay to real time
- 1003
- 1004 Usage
- 1005 Research (Score: 6/6)
- 1006 The ESA CCI SST dataset v.2.0 is very recent. However, it has already been used in
- 1007 some research publications.
- 1008
- 1009 Decision support system (Score: 6/6)
- 1010 ESA-CCI SST is part of the ESA Climate Change Initiative, and one of the essential
- 1011 climate variables. The objective of ESA-CCI SST is to establish a long term data
- 1012 record to monitor the global climate system required by UNFCCC (http://cci.esa.int/)
- 1013 for decision making.
- 1014
- 1015 2. ERA5 SST
- 1016 Metadata

1017	Standard	(Score:	6/6)
------	----------	---------	------

1018	ERA5 SST data can be downloaded from the CDS in both GRIB and NetCDF formats.
1019	The native data format is GRIB, but they can be converted to NetCDF format
1020	through the CDS. In NetCDF global attributes reference to CF-1.6 conventions is
1021	made. This represents a mature state-of-the-art metadata standard according to
1022	guidance.
1023	
1024	Collection Level (Score 5/6)
1025	The standardized attributes on the collection level of the dataset are sufficient to
1026	understand the data's origins without further documents, including standardized
1027	information on how to obtain raw data and its preprocessing procedures.
1028	Note: The collection level in this case includes the ECMWF confluence wiki.
1029	(https://confluence.ecmwf.int/display/CKB/ERA5%3A+data+documentation)
1030	
1031	User Documentation
1032	Formal description of scientific methodology (Score 6/6)

1033	The scientific description is comprehensive and publicly available in the form of a
1034	scientific report/ATBD and elibrary of ECMWF. The description is kept up to date
1035	with the updated dataset. There is also a peer reviewed methodological journal
1036	paper published.
1037	
1038	Formal validation report (Score: 3/6)
1039	There is no formal validation report for ERA5 SST. The ERA5 documentation available
1040	at confluence wiki can be regarded as a user guide but does not have any clear
1041	version number with a publication date and is a document that is changing. Due to
1042	the nature of ERA5 being in development it makes sense to have an evolving
1043	documentation, but the creation of a formal product validation report in the future
1044	is recommended. An assessment report evaluating HadISST2 and OSTIA SST datasets
1045	(from which ERA5 SST is built) is available (Hirahara 2016).
1046	

1047 *Formal product user guide* (Score 6/6)

1048	There is a regularly updated comprehensive formal Product User Guide (PUG) for the
1049	dataset publicly available.
1050	Note: In this case the confluence wiki is regarded as the Product User Guide (PUG).
1051	
1052	Uncertainty Characterization
1053	Standards (Score 3/6)
1054	Uncertainty information follows standard nomenclature.
1055	Note: In this case the ensemble members are regarded as uncertainty measures.
1056	
1057	Validation (Score: 3/6)
1058	A formal validation report of ERA5 SST is not available. However, an assessment
1059	report evaluating HadISST2 and OSTIA SST datasets (from which ERA5 SST is built) is
1060	available (Hirahara 2016), and users can refer to HadISST2 and OSTIA
1061	documentation.
1062	
1063	Uncertainty quantification (Score 3/6)
1064 A comprehensive uncertainty quantification of systematic and random effects is

1065 available.

1066 Note: In this case the ensemble members are regarded as uncertainty measures.

1067

- 1068 Automated quality monitoring (Score 2/6)
- 1069 There is no automated quality monitoring documented for the dataset.
- 1070 Note: Although there is no automated quality monitoring documented, data
- 1071 assimilation itself could be regarded as a quality check.
- 1072
- 1073 Public access, feedback and updates
- 1074 Access and Archive (Score 5/6)
- 1075 The dataset is publicly available. The different versions of data including
- 1076 documentation and source code is archived by the data provider. Source code is not
- 1077 publically available.

1078

1079 Version Control (Score 6/6)

1080	There is full information on version control of documentation, data and/or metadata
1081	available for the dataset. The documented version control information is fully
1082	traceable from the files.
1083	Note: In this case the version control is referring to the confluence wiki.
1084	
1085	User Feedback (Score 6/6)
1086	There is a public reach-out/feedback form/contact point for collecting feedback for
1087	the dataset. There are regular events, groups, 2-way feedback mechanisms, etc.
1088	organized by the data provider. The established feedback fed back into data
1089	production is documented, including third party international data quality
1090	assessment results.
1091	
1092	Updates to Record (Score 6/6)
1093	There are regular operational updates available for the dataset, depending on the
1094	availability of input data and including improved methodology.
1095	

- 1097 *Research* (Score: 3/6)
- 1098 Although ERA5 reanalysis has been largely used in many research publications, it
- 1099 seems that there are few relevant publications based on ERA5 SST data (as e.g.
- 1100 Wang et al., 2020). This could arise from the prevalent use of ERA5 in atmospheric
- 1101 research.

- 1103 *Decision support system* (Score: 1/6)
- 1104 To the evaluators' knowledge the product is not used yet for the decision support
- 1105 system. .
- 1106
- 1107 3. OSTIA SST

1108 Metadata

- 1109 Standard (Score: 6/6)
- 1110 The OSTIA SST data files are provided in NetCDF-4 format CF-1.5 compliant through
- 1111 CMEMS and the Recommended GHRSST Data Specification (GDS). File specifications

1112	are fully detailed in the OSTIA Product User Manual (PUM) available in CMEMS. The
1113	NetCDF files contain detailed metadata describing the data by means of global
1114	attributes, which are applicable to the whole file, and variable attributes, which apply
1115	to a specific data field.
1116	
1117	Collection Level (Score: 6/6)
1118	Global attributes provide all information available on the data and relative
1119	references. In addition the Product User Manual (PUM,) with detailed information on
1120	Metadata is available.
1121	
1122	User Documentation
1123	Formal description of scientific methodology (Score: 6/6)
1124	The formal description of the OSTIA product is detailed in the peer-reviewed paper
1125	(Good et al., 2020), published by the data provider, which describes and justifies the
1126	algorithms used for obtaining SST estimates. A synthesis of the Product User Manual
1127	(PUM) is also available in the CMEMS.

- 1129 *Formal validation report* (Score: 6/6)
- 1130 For the formal validation report of the OSTIA product users can refer to the Quality
- 1131 Information Document (QUID) available in the CMEMS service.
- 1132
- 1133 Formal product user guide (Score: 6/6)
- 1134 The formal product user guide OSTIA product is published by the data provider
- 1135 (PUM) as a peer-reviewed journal article Good et al. (2020). A synthesis of the formal
- 1136 user product guide (PUM) is also available in the CMEMS.
- 1137
- 1138 Uncertainty Characterization
- 1139 Standards (Score: 6/6)
- 1140 Uncertainty characterization follows the internationally agreed GHRSST standard
- 1141 specifications, which are detailed in the GHRSST Data Specification v2.0 (GDS)
- 1142 document (GHRSST Science Team, 2012).
- 1143

1144	Validation	(Score:	6/6)
------	------------	---------	------

A validation of the OSTIA product is provided in the Quality Information Document through CMEMS. The validation of the OSTIA SST product is based on comparison of SST data with co-located in situ measurements.

1148

1149 Uncertainty quantification (Score: 6/6)

1150 Uncertainty in the OSTIA data at each location (i.e., the analysed_sst field in the

1151 NETCDF file) is quantified and provided (i.e., in the analysis_error field) through an

analysis quality methodology. The methodology used to derive the uncertainty is

1153 produced using a special "observation influence" analysis (Good et al., 2020).

1154

1155 Automated Quality monitoring (Score: 6/6)

1156 Automatic quality is monitored during the production of the SST product. The real-

1157 time OSTIA SST analysis is routinely validated by the UK MetOffice against the

1158 GHRSST Multi-product ensemble (http://ghrsst-pp.metoffice.gov.uk/ostia-

- 1159 website/gmpe-monitoring.html) and Argo SST (http://ghrsst-
- 1160 pp.metoffice.gov.uk/ostia-website/gmpe-argo-stats.html).

- 1162 Public access, feedback and update
- 1163 Public Access/Archive (Score: 5/6)
- 1164 The OSTIA SST is available on the CMEMS website. Detailed information available in
- 1165 the PUM. However, the source code is not publically available.

1166

- 1167 *Version* (Score: 6/6)
- 1168 The version is fully established by the data provider.

1169

1170 User feedback (Score: 6/6)

- 1171 The OSTIA is provided through the CMEMS and is part of GHRSST. Within CMEMS, a
- 1172 Multi-Year Product Quality Working Group is established with the aim of periodically
- 1173 assessing the status of the CMEMS data records, including OSTIA, integrating users'
- 1174 needs and feedback.

1176	Updates to re	<i>ecord</i> (Score: 6/6)
------	---------------	---------------------------

- 1177 Currently the OSTIA SST dataset covers the period from late-1981 to 2018. Updates
- 1178 through to the near-present are expected this year (2020). Extensions are expected
- 1179 to be produced by the CMEMS with only ~5 days delay to real time

- 1181 Usage
- 1182 *Research* (Score: 6/6)
- 1183 The current version of OSTIA SST is very recent. However, it has already been used
- 1184 in some research publications.

1185

- 1186 *Decision support system* (Score: 6/6)
- 1187 OSTIA SST is part of the CMEMS project and the information derived from SST
- 1188 products is used in the CMEMS ocean state report for decision making.

1189

1190 4. BoM

1191 M	etadata
--------	---------

1192	Standard (Score:	6/6))
		`		

- 1193 The BoM SST files are provided in the GHRSST Data Specification version 1.7 NetCDF
- 1194 classic format CF-1 (Beggs and Pugh, 2009) on request from the data providers. The
- 1195 NetCDF files contain detailed metadata describing the data by means of global
- 1196 attributes, which are applicable to the whole file, and variable attributes, which apply
- 1197 to a specific data field.
- 1198
- 1199 *Collection Level* (Score: 5/6)
- 1200 Global attributes provide all information available on the data and relative
- 1201 references. However, the reference shown in the Metadata (Beggs and Pugh, 2009) is
- 1202 not accessible at the moment of writing this report although it is available by
- 1203 request from library@bom.gov.au.

- 1205 User Documentation
- 1206 Formal description of scientific methodology (Score: 4/6)

1207	The formal description of the BoM Monthly OI SST is published in a conference
1208	paper (Smith et al., 1999) and a peer-reviewed paper (Beggs et al., 2011), however
1209	the peer-reviewed paper focuses on the BoM higher resolution daily 1/12 degree
1210	regional analyses available from 2006, which uses a modified version of the Fortran
1211	"SIANAL" code used to produce the original BoM Weekly and Monthly OI SST
1212	analyses.
1213	
1214	
1215	Formal validation report (Score: 2/6)
1216	BoM Monthly OI 1 degree L4 SST is part of the GHRSST suite of L4 products, and
1217	intercomparison of the BoM higher resolution daily SST analyses with other SST
1218	products have been published in peer reviewed journals (Beggs et al., 2011; Dash et
1219	al., 2012; Martin et al., 2012). However, the only previously published comparison of
1220	the lower resolution BoM Weekly 1 degree OI SST analysis with other SST analysis
1221	products is in a BoM Operations Bulletin (Zhong and Beggs, 2008).
1222	
1223	Formal product user guide (Score: 4/6)

1224	The description of the BoM Monthly OI SST analysis methodology is published in
1225	Smith et al. (1999) and Beggs et al. (2011), and a user guide is provided (Beggs and
1226	Pugh, 2009). However, (Beggs and Pugh, 2009) is not accessible at the moment of
1227	writing this report although it is available by request from library@bom.gov.au.
1228	
1229	
1230	Uncertainty Characterization
1231	Standards (Score: 6/6)
1232	Uncertainty characterization follows the internationally agreed GHRSST standard
1233	specifications (analysis_error), which are detailed in the GHRSST Data Specification
1234	v2.0 (GDS) document (GHRSST Science Team, 2012).
1235	
1236	Validation (Score: 5/6)
1237	No validation report is found for BoM SST. However, BoM is part of the GHRSST
1238	community and intercomparison activities of the BoM Daily Global SST analyses have
1239	been performed in the framework of GHRSST (Dash et al., 2011; Martin et al., 2011).

1240	Although routine verification of the BoM Global Daily 0.25 degree OI SST analysis
1241	(GAMSSA) are performed by UK MetOffice (http://ghrsst-pp.metoffice.gov.uk/ostia-
1242	website/gmpe-argo-stats.html) and NOAA/NESDIS/STAR
1243	(https://www.star.nesdis.noaa.gov/socd/sst/squam/analysis/l4), there are no routine
1244	verifications of the BoM Monthly or Weekly OI SST analyses.
1245	
1246	
1247	Uncertainty quantification (Score: 6/6)
1248	Uncertainty in the BoM data at each location (i.e., the analysed_sst field in the
1249	NETCDF file) is quantified and provided (i.e., in the analysis_error field) through an
1250	analysis quality methodology (Beggs et al., 2011).
1251	
1252	Automated Quality monitoring (Score: 1/6)
1253	No Automatic quality is provided.
1254	
1255	Public access, feedback and update
1256	Public Access/Archive (Score: 4/6)

- 1257 BoM Monthly SST product is available on request from the data provider website for
- 1258 both real-time and archived GHRSST L4 files.

- 1260 *Version* (Score: 2/6)
- 1261 No information is found for the version control for BoM SST.

1262

- 1263 User feedback (Score: 3/6)
- 1264 Data providers collect and evaluate feedback from the scientific community through
- 1265 the data provider's website, but no feedback mechanisms set up from data

1266 providers.

1267

- 1268 Updates to record (Score: 5/6)
- 1269 BoM Daily, Weekly and Monthly SST analyses are published in real time for climate
- 1270 monitoring on the BoM website.

- 1272 Usage
- 1273 *Research* (Score: 4/6)

1274	The BoM Weekly and Monthly SST analyses have been used by the BoM for
1275	research, especially climate studies.
1276	
1277	Decision support system (Score: 6/6)
1278	BoM Monthly SST is an operational SST analysis which serves for climate monitoring
1279	that is an essential service of the Australian Government Bureau of Meteorology.
1280	
1281	5. MGDSST
1282	Metadata
1283	Standard (Score: 3/6)
1284	The MGDSST is provided in the txt format and variable attributes are limited.
1285	
1286	Collection Level (Score: 2/6)
1287	There is limited information about standard attributes, but extra information
1288	published in the data provider's website is needed to use and understand the data.
1289	

1290 User Documentation

- 1291 Formal description of scientific methodology (Score: 3/6)
- 1292 Limited information is provided on the data provider's website, but the method is
- 1293 documented in two non peer-reviewed reports
- 1294
- 1295 Formal validation report (Score: 4/6)
- 1296 No JMA validation report is found for MGDSST at the time of writing this report.
- 1297 However, MGDSST was compared with other SST analyses and independent
- observations in Martin et al. (2012) and Fiedler et al. (2019a) for the periods 2010
- and 1992 to 2011. The UK MetOffice routinely compares MGDSST with the GHRSST
- 1300 Multi-product ensemble (http://ghrsst-pp.metoffice.gov.uk/ostia-website/gmpe-
- 1301 monitoring.html) and Argo SST (http://ghrsst-pp.metoffice.gov.uk/ostia-
- 1302 website/gmpe-argo-stats.html).
- 1303
- 1304 *Formal product user guide* (Score: 3/6)
- 1305 Limited product user guide from the data provider.

1307	Uncertainty Characterization
1308	Standards (Score: 1/6)
1309	No information is available at this stage.
1310	
1311	Validation (Score: 6/6)
1312	MGDSST is part of the GHRSST and intercomparison with other SST products has
1313	been performed and published in peer-review journals (Fiedler et al., 2019a; Martin
1314	et al., 2012).
1315	
1316	Uncertainty quantification (Score: 1/6)
1317	No uncertainty quantification is found.
1318	
1319	Automated Quality monitoring (Score: 2/6)
1320	No automatic quality is monitored during the production of the SST product.
1321	
1322	Public access, feedback and update

- 1323 Public Access/Archive (Score: 4/6)
- 1324 The MGDSST is publicly accessible from the data provider's website and brief
- 1325 information of the data is provided in the data provider's website.

- 1327 Version (Score: 2/6)
- 1328 No information is found for the version control.

1329

- 1330 User feedback (Score: 3/6)
- 1331 Data providers collect and evaluate feedback from the scientific community through
- 1332 the data provider's website.

1333

- 1334 Updates to record (Score: 4/6)
- 1335 MGDSST is published in real time for climate monitoring and Numerical Weather
- 1336 Prediction on the data provider's website.

- 1338 <u>Usage</u>
- 1339 *Research* (Score: 6/6)

1340 The data has already been used in some research publications.

1341

- 1342 *Decision support system* (Score: 6/6)
- 1343 MGDSST is an operational SST analysis which serves for climate monitoring and
- 1344 Numerical Weather Prediction that is an essential service of the Japanese
- 1345 Meteorological Agency (JMA).

1346

- 1347 6. MUR25
- 1348 Metadata
- 1349 Standard (Score: 6/6)
- 1350 The MUR25 SST is provided in NetCDF format. The NetCDF files contain detailed
- 1351 metadata describing the data by means of global attributes, which are applicable to
- 1352 the whole file, and variable attributes, which apply to a specific data field.

1353

1354 *Collection Level* (Score: 6/6)

1355 Global attributes provide all information available on the data and relati	ive
---	-----

- 1356 references.
- 1357

1358 User Documentation

- 1359 Formal description of scientific methodology (Score: 6/6)
- 1360 The formal description of the MUR25 product is detailed in the peer-reviewed
- 1361 journal (Chin et al., 2017), published by the data provider.

1362

- 1363 Formal validation report (Score: 4/6)
- 1364 No formal validation report is available, however, the validation is performed in the
- 1365 peer-reviewed paper (Chin et al., 2017). Additional validation of the 1km product
- 1366 occurred with direct comparisons with the Saildrone autonomous vehicle with the
- 1367 published article. The validation focused on an exemplary coastal area, the
- 1368 California/Baja Coast.

- 1370 Formal product user guide (Score: 2/6)
- 1371 No formal product user guide is available for MUR25 SST.

1373	Uncertainty Characterization
1374	Standards (Score: 6/6)
1375	Uncertainty characterization follows the internationally agreed GHRSST standard
1376	specifications, which are detailed in the GHRSST Data Specification v2.0 (GDS)
1377	document.
1378	
1379	Validation (Score: 6/6)
1380	Intercomparison of MUR25 has been performed in the framework of GHRSST.
1381	
1382	Uncertainty quantification (Score: 6/6)
1383	Uncertainty in the MUR25 data at each location (i.e., the analysed_sst field in the
1384	NETCDF file) is quantified and provided (i.e., in the analysis_error field) through an
1385	analysis quality methodology.
1386	
1387	Automated Quality monitoring (Score: 4/6)

1388	No automatic o	quality	monitoring i	is found for	MUR25 SST	product,	but the 1	km
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- 1389 resolution version of the MUR SST analysis is routinely validated with the GHRSST
- 1390 Multi-product ensemble (http://ghrsst-pp.metoffice.gov.uk/ostia-website/gmpe-
- 1391 monitoring.html; https://www.star.nesdis.noaa.gov/socd/sst/squam/analysis/l4). Since
- 1392 Argo SST are ingested into MUR25 they are not useful for verification.
- 1393
- 1394 Public access, feedback and update
- 1395 Public Access/Archive (Score: 5/6)
- 1396 The MUR25 SST is published in the data provider's archive center. However, source
- 1397 code is not publically available.
- 1398
- 1399 *Version* (Score: 6/6)
- 1400 The version is fully established by the data provider.
- 1401
- 1402 User feedback (Score: 6/6)
- 1403 Public contact information is given in the data provider's website for users to give
- 1404 feedback. Users can give all feedback through the Physical Oceanography

- 1405 Distributed Active Archive Center (PO.DAAC) user services and forum. All feedback
- 1406 is publicly available.

- 1408 Updates to record (Score: 5/6)
- 1409 Regular updates are available from the data provider. There is no immediate
- 1410 production of interim data products.
- 1411
- 1412 <u>Usage</u>
- 1413 *Research* (Score: 6/6)
- 1414 The MUR25 is used in research in multiple fields.

1415

- 1416 Decision support system (Score: 3/6)
- 1417 No decision support system is found for MUR25 SST, however use is occurring and
- 1418 benefits are emerging.

1419

1420 7. NOAA Daily OISSTv2.1 SST

- 1422 *Standard* (Score: 6/6)
- 1423 The NOAA Daily OISST data files are provided in NetCDF-4 format CF-1.0 compliant
- 1424 data provider's website. The NetCDF files contain detailed metadata describing the
- 1425 data by means of global attributes, which are applicable to the whole file, and
- 1426 variable attributes, which apply to a specific data field.
- 1427
- 1428 Collection Level (Score: 6/6)
- 1429 Global attributes provide all information available on the data and relative
- 1430 references.
- 1431
- 1432 User Documentation
- 1433 Formal description of scientific methodology (Score: 6/6)
- 1434 The formal description of the NOAA Daily OISST v2.1 is provided in the data
- 1435 provider's website (https://www.ncdc.noaa.gov/oisst), third party data resource
- 1436 website (https://podaac.jpl.nasa.gov/dataset/AVHRR_OI-NCEI-L4-GLOB-v2.1) and is

1437	also detailed in several peer-reviewed papers (Reynolds et al., 2007; Banzon et al.,
1438	2016; Huang et al., 2020), published by the data provider, which describe and justify
1439	the algorithms used for obtaining SST estimates.
1440	
1441	Formal validation report (Score: 6/6)
1442	Formal validation report of NOAA Daily OISST is along with data access.
1443	
1444	<i>Formal product user guide</i> (Score: 6/6)
1445	The formal product user guide is provided in the peer review journal (Banzon et al.,
1446	2016).
1447	
1448	Uncertainty Characterization
1449	Standards (Score: 6/6)
1450	Uncertainty characterization follows the internationally agreed GHRSST standard
1451	specifications, which are detailed in the GHRSST Data Specification v2.0 (GDS)
1452	document.

- 1454 Validation (Score: 6/6)
- 1455 A validation of NOAA Daily OISST is provided through peer-review journals (Dash et
- 1456 al., 2012; Martin et al., 2012; Banzon et al., 2016; Fiedler et al., 2019a; Huang et al.,
- 1457 2020).
- 1458
- 1459 Uncertainty quantification (Score: 6/6)
- 1460 Uncertainty in the NOAA Daily OISST data at each location (i.e., the analysed_sst
- 1461 field in the NETCDF file available from
- 1462 https://podaac.jpl.nasa.gov/dataset/AVHRR_OI-NCEI-L4-GLOB-v2.1) is quantified and
- 1463 provided (i.e., in the analysis_error field) through an analysis quality methodology.

- 1465 Automated Quality monitoring (Score: 4/6)
- 1466 The Daily OISST v2.1 SST analyses are validated in near real-time against the
- 1467 GHRSST Multi-Product Ensemble by NOAA/STAR at

1468	https://www.star.nesd	is.noaa.gov/socd/sst	/squam/analysis/l4.	Since Argo SST are

1469 ingested into Daily OISST v2.1 they are not useful for verification.

1470

1471 Public access, feedback and update

- 1472 Public Access/Archive (Score: 5/6)
- 1473 The data is publicly accessible through the data provider's website and also other
- 1474 data portals with documentation. No source code is available publically.

1475

- 1476 *Version* (Score: 6/6)
- 1477 The version is fully established by the data provider.

1478

- 1479 User feedback (Score: 3/6)
- 1480 Contact information of the data provider is publicly available for user feedback.

- 1482 Updates to record (Score: 6/6)
- 1483 Data providers regularly update the data record.

- 1485 Usage
- 1486 Research (Score: 6/6)
- 1487 The NOAA Daily OISST is widely used in multiple research fields.

- 1489 Decision support system (Score: 3/6)
- 1490 No decision support system is found for NOAA Daily OISST, however use is
- 1491 occurring and benefits are emerging.
- 1492
- 1493 8. HadISST1
- 1494 Metadata
- 1495 Standard (Score: 6/6)
- 1496 The HadISST1data files are provided in NetCDF classic format CF compliant through
- 1497 the data provider's website. The NetCDF files contain detailed metadata describing
- 1498 the data by means of global attributes, which are applicable to the whole file, and
- 1499 variable attributes, which apply to a specific data field.

1501 *Collection Level* (Score: 6/6)

1502 Global attributes provide all information available on the data and relative

- 1503 references.
- 1504
- 1505 User Documentation
- 1506 Formal description of scientific methodology (Score: 6/6)
- 1507 The formal description of the HadISST1 is detailed in the peer-reviewed journal
- 1508 (Rayner et al., 2003), published by the data provider, which describes and justifies
- 1509 the algorithms used for obtaining SST estimates.
- 1510
- 1511 Formal validation report (Score: 6/6)
- 1512 Formal validation report is published in a peer reviewed journal.

1513

1514 Formal product user guide (Score: 3/6)

- 1516 data provider's website.
- 1517
- 1518 Uncertainty Characterization
- 1519 Standards (Score: 1/6)
- 1520 No information is available at this stage.

- 1522 Validation (Score: 6/6)
- 1523 The validation is available through peer reviewed journal paper.

1524

- 1525 Uncertainty quantification (Score: 1/6)
- 1526 No uncertainty quantification is found.

1527

- 1528 Automated Quality monitoring (Score: 1/6)
- 1529 No automatic quality is monitored during the production of the SST product.

1531 Public access, feedback and update

- 1532 Public Access/Archive (Score: 5/6)
- 1533 The data is published through the data provider's website, but no source code is
- 1534 publically available.

1535

- 1536 *Version* (Score: 6/6)
- 1537 The version is fully established by the data provider.

1538

- 1539 User feedback (Score: 3/6)
- 1540 Contact information of the data provider is given for collecting user feedback.

1541

- 1542 Updates to record (Score: 6/6)
- 1543 The data is regularly updated by the data provider.

1544

1545 <u>Usage</u>

1546 *Research* (Score: 6/6)

1547 HadISST1 has been widely used in multiple research fields.

- 1549 Decision support system (Score: 6/6)
- 1550 Up to now no decision support system is found for HadISST1, however, influence on
- 1551 decision making is demonstrated.
- 1552

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Dataset	Institution	Type of	Time Range	Observation input	Type of SST	Horizontal Grid spacing	Vertical resolution	Temporal resolution	Main Reference
ESA CCI SST (v.2.0)	Met Office	SST analysis	1981- 2018	IR	SST at 0.2 m	global 0.05°x0.05°	surface	daily	Merchant et al. (2019)
ERA5	ECMWF	SST analysis	1979- 2018	IR + MW + in situ	SSTdepth	global 0.25°x0.25°	surface	hourly	Hirahara et al. (2016)
HadISST1	Met Office	SST analysis	1870- 2018	IR + in situ	SSTdepth	global 1°x1°	surface	monthly	Rayner et al. (2003)
NOAA Daily OISST v2.1	NOAA	SST analysis	1981- 2018	IR + in situ	SST at 0.2 m	global 0.25°x0.25°	surface	daily	Huang et al., (2020)
MUR25 (v.4.2)	PODACC	SST analysis	2003- 2018	IR + MW + in situ	Foundation SST	global 0.25°x0.25°	surface	daily	Chin et al. (2017)
MGDSST	Japanese Met. Agency (JMA)	SST analysis	1982- 2018	IR + MW + in situ	SSTdepth	global 0.25°x0.25°	surface	daily	Sakurai et al. (2005)
BoM Monthly SST	Australian Bureau of Met. (BoM)	SST analysis	2002- 2018	IR + in situ	SSTdepth	global 1°x1° (weekly/monthly)	surface	weekly/monthly	Smith et al. (1999)
OSTIASST	UK MeOffice	SST analysis	1981- 2018	IR + MW + in situ	Foundation SST	0.05°x0.05°	surface	daily/weekly/monthly	Good et al., 2020

1842	Table 1. Descriptive product comparison summary for the described products from
1843	sections 2. Input observations are derived from satellite infrared (IR) and/or
1844	microwave (MW) sensors and/or in situ measurements.
1845	
1846	
1847	
1848	

Name	ESA CCI SST	ERA5 SST	OSTIA	ВоМ	MGDSST	MUR25	NOAA Daily	HadISST1
C3S_511 MM Category							UISST	
Metadata								
Standards	6	6	6	6	3	6	6	6
Collection level	6	5	6	5	2	6	6	6
User Documentation								
Formal description of scientific methodology	6	6	6	4	3	6	6	6
Formal validation report	6	3	6	2	4	4	6	6
Formal product user guide	6	6	6	4	3	2	6	3
Uncertainty Characterisation								
Standards	6	3	6	6	1	6	6	1
Validation	6	3	6	5	6	6	6	6
Uncertainty quantification	6	3	6	6	1	6	6	1
Automated quality monitoring	6	2	6	1	2	4	4	1
Public Access, feedback, and update								
Public Access/Archive	5	5	5	4	4	5	5	5
Version	6	6	6	2	2	6	6	6
User feedback mechanism	6	6	6	3	3	6	3	6
Updates to record	6	6	6	5	4	5	6	6
Usage								
Research	6	3	6	4	6	6	6	3
Decision support system	6	1	6	6	6	3	3	6

1850 Table 2. Maturity Matrix for all SST products



1854 Figure 1. Temporal range (years) covered by each SST dataset. The common period

1855 for all datasets is highlighted (2003-2018) and the secondary common period is

1856 1982-2018 with less SST products included.

1857





1861 Figure 2. Power Spectral Density at the equator in the Pacific Ocean (0°N, 120°E-

1862 80°W) for ESA-CCI (green), OSTIA (dashed dark blue), NOAA Daily OISST (Reynolds

1863 0.25 Degree. red) and MGDSST (cyan) based on the daily temporal and original

1864 spatial resolution for the period 1982-2018



1867 Figure 3. Global SST climatologies for the period 2003-2018. Global SST average

1868 value and its 95% confidence interval is also shown.



1871 Figure 4 The difference between each SST product and the ensemble median for the

1872 period of 2003-2018

1873



1876 Figure 5 The RMSD between each SST product and the ensemble median for the

1877 period of 2003-2018



1880 Figure 6 The correlation between each SST product and the ensemble median for

1881 the period of 2003-2018	1881	the period of 2003-2018
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- Figure 8. Global SST monthly anomalies time series, obtained by subtracting the climatology of the ensemble median to all the SST ensemble members from 2003 to 2018.



Figure 9. Global linear trend maps (2003-2018) (°C/year) of each ensemble member and ensemble median. Areas with no significant (95% significance level) trends are covered by grey points.







1902 3.1.2), the same calculation but for (b) the Pacific Ocean basin (c) Atlantic Ocean

1903 basin and (d) Indian Ocean Basin for the period of 2003-2018.





1908 the whole covered period originally obtained in each SST product.



1911 Figure 12 Global SST climatologies for the period 1982-2002. Global SST average

1912 and its 95% confidence interval is also shown in brackets above each map.



1916 Figure 13 The difference between each SST product and the ensemble median for

- 1917 the period of 1982-2002



1921 Figure 14 Intercomparison between El Niño 3.4 time series of the five SST products:

1922 HadISST1, ERA5, ESA CCI SST, MGDSST, NOAA OISST.

<u>±</u>

1	Sea Surface Temperature intercomparison in the framework of the Copernicus
2	Climate Change Service (C3S)
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24	
25	Abstract
26	A joint effort between the Copernicus Climate Change Service (C3S) and the Group
26 27	A joint effort between the Copernicus Climate Change Service (C3S) and the Group for High Resolution Sea Surface Temperature (GHRSST) has been dedicated to an
26 27 28	A joint effort between the Copernicus Climate Change Service (C3S) and the Group for High Resolution Sea Surface Temperature (GHRSST) has been dedicated to an intercomparison study of eight global and-gap-free Sea Surface Temperature (SST)
26 27 28 29	A joint effort between the Copernicus Climate Change Service (C3S) and the Group for High Resolution Sea Surface Temperature (GHRSST) has been dedicated to an intercomparison study of eight global and-gap-free Sea Surface Temperature (SST) products to assess their accuraterepresentation of the SST relevant to climate
 26 27 28 29 30 	A joint effort between the Copernicus Climate Change Service (C3S) and the Group for High Resolution Sea Surface Temperature (GHRSST) has been dedicated to an intercomparison study of eight global and-gap-free Sea Surface Temperature (SST) products to assess their accuraterepresentation of the SST relevant to climate analysis. In general, all SST products show consistent climatological s patial patterns
 26 27 28 29 30 31 	A joint effort between the Copernicus Climate Change Service (C3S) and the Group for High Resolution Sea Surface Temperature (GHRSST) has been dedicated to an intercomparison study of eight global and-gap-free Sea Surface Temperature (SST) products to assess their accuraterepresentation of the SST relevant to climate analysis. In general, all SST products show consistent climatological spatial patterns and temporal variability during the overlapping time period (2003-2018). The main

33	and Antarctic Circumpolar Current (ACC) -regions. <u>L-Global-l</u> inear trends display
34	consistent SST spatial patterns among all_ the -products and <u>exhibit</u> evidencing a
35	strong warming trend from 2012 to 2018 with the Pacific Ocean basin as the main
36	contributor. SST discrepancy between all SST products is very small compared to the
37	significant warming trend. Spatial pPower spectral density shows that the
38	interpolation into 1° spatial resolution has negligible impacts on our results. The
39	global mean SST time series reveals larger differences among all SST products
40	during the early period of the satellite era (1982-2002) when there were $\frac{fewerless}{fewerless}$
41	observations compared to the latter period, indicating that the observation
42	frequencys are-is the main constraint of the SST climatology. The maturity matrix
43	scores, which present the maturity of each product in terms of documentation,
44	storage, and dissemination but not <u>the</u> scientific quality, -of a dataset, demonstrate
45	that ESA-CCI and OSTIA SST are well documented for users' convenience.
46	Improvements could be made for MGDSST and BoM SST. Finally, we have
47	recommended to users that these SST products can be used for fundamental climate
48	applications and climate studies (e.g. El Nino).

1. Introduction

51	Sea surface temperature (SST) as one of the Essential Ocean Variables (EOVs), and
52	the Essential Climate Variables (ECVs), plays a crucial role in heat, freshwater, and
53	momentum flux $\frac{1}{2}$ exchange at the ocean-atmosphere interface. The variation of SST
54	at different temporal and spatial scales modulates the atmospheric lower boundary
55	layer (e.g. Renault et al., 2019) eventually driving small and large-scale changes at
56	interannual to decadal time scales in the atmosphere (Perlin et al., 2014, McPhaden,
57	2012). Additionally, the SST changes can influence the biogeochemical marine
58	environment, contributing to modulating the primary production and related carbon
59	absorption in the ocean (Behrenfeld et al, 2006). Besides its importance for assessing
60	and monitoring the state of the global climate system, SST is widely used as
61	boundary conditions in weather and climate operational forecast systems (Robinson
62	2012) and as initial conditions in ocean operational forecast systems (Le Traon et al.,
63	2019). Therefore, assessing the quality of SST data is critical from several

64 perspectives, from operational to climate studies, marine environment and related

65 services preservation.

67	SST observations are mainly obtained from low-Earth orbit infrared and microwave
68	satellite imagery and geostationary infrared imagery, and from various in situ
69	platforms including moored and drifting buoys, Argo floats, ships of opportunity,
70	autonomous sailing drones, and radiometers (O'Carroll et al., 2019). All these
71	instruments provide observations characterized by different representativeness,
72	resolution, and accuracy. Different retrieval methods and reanalysis techniques are
73	thus applied toapplied in to obtain temporally and spatially consistent long-term
74	SST products with global coverage (Minnett et al, 2019).
75	
76	The Group for High-Resolution Sea Surface Temperature (GHRSST, www.ghrsst.org;
77	Donlon et al, 2009) is an international initiative aimed at coordinating the provision
78	of SST products developed and distributed by different agencies and research
79	institutes. Among GHRSST products, level 4 data (L4) provide gap-free SST maps at

80	regional and global scales, obtained with different algorithms that combine and
81	interpolate satellite based SST data, acquired by a variety of different sensors,
82	sometimes also including in situ observations. Different interpolation techniques and
83	related configurations (e.g. observation/background error correlation scales),
84	interpolation grid size, input data bias-correction, and the sampling adopted by
85	GHRSST data providers induce a significant diversity among L4 SST products (Dash
86	et al., 2012). Understanding the consistency and discrepancy of the different SST L4
87	products will not only help data providers to improve their algorithms, but also
88	represents an important step to inform users about the characteristics of the
89	different products, helping them to select the one that may better suit their
90	applications.
91	
92	Several previous global SST analysis intercomparison studies have already been
93	performed, among which, most noticeably, the Global Climate Observing System
94	(GCOS) SST-Sea Ice intercomparison project

95 (https://www.nodc.noaa.gov/SatelliteData/ghrsst/intercomp.html), and the GMPE
96	(Group for High-Resolution SST, GHRSST, Multi-Product Ensemble) system,
97	performed as a contribution to GHRSST activities-under the umbrella of the <u>SST</u>
98	Analysis lintercomparison Ttask Tteam of GHRSST. The initial work by Martin et al.
99	(2012) and Dash et al. (2012), which were focused on a relatively short time series
100	over the satellite period (for the year 2010), has recently been extended to
101	intercompare longer-term analyses analyses over the overlapping period of 1991 to
102	2010 (Fiedler et al., 2019a). A much shorter period (one year) is considered in the
103	intercomparison of satellite-based analyses performed by Okuro et al. (2014), while a
104	comparison study on the historical sea surface temperature <u>SST</u> datasets based on in
105	situ data alone is described in Yasunaka and Hanawa (2011). With the recent
106	reprocessing of several global high resolution daily L4 products from the start of the
107	operational satellite SST era (1981) to recent years, it is now timely to perform an
108	intercomparison of additional SST analyses over a significantly longer period.
109	
110	In the framework of the European Copernicus Climate Change Service (C3S), an

111 Independent Assessment of Essential Climate Variables (ECVs) present in the C3S

112	Climate Data Store (CDS) is foreseen. The C3S CDS distributes and provides access
113	to quality-assured climate dataset and tools in the clouds for usersThe
114	independentis assessment aims to evaluate the quality, usability and consistency of
115	available ECVs for different applications, ranging from scientific studies (e.g. on
116	climate change), to commercial and private sector uses. SST is one of the ECVs
117	considered in the assessment framework of C3S and the intercomparison of SST
118	products available in the CDS will help the users to understand the quality of
119	different SST products and choose the right one for their specific applications.
120	
121	The study presented hereafter represents the joint effort between the GHRSST \underline{SST}
122	<u>Analysis I</u> intercomparison <u>T</u> task <u>T</u> team (https://www.ghrsst.org/about-ghrsst/task-
123	teams/) and the C3S SST assessment activities. The objective of this study is to
124	evaluate the basic characteristics and the maturity of eight states of the art global
125	SST analysis products; to describe how SST climatology and variability is represented
126	in each SST product, and to understand the consistency and discrepancy between all
127	these long-term eight SST analyses available in or outside of CDS (some of the SST

128	products are	provided in	GHRSST L4	format),	and eve	ntually to	provide	guidance	on
-----	--------------	-------------	-----------	----------	---------	------------	---------	----------	----

- 129 which product might be better suited for users' applications.
- 130 The paper is organized as follows: Section 2 introduces the characteristics of SST
- 131 analysis products included in this study, the basic diagnostics are presented in
- 132 section 3, and the data maturity of all SST products is described in section 4, and
- 133 finally, the summary of the evaluation and the recommendations to users are
- 134 discussed in sections 5 and 6.
- 135

136 **2. Datasets**

- Currently, two global SST analysis datasets are distributed through the CDS, namely
 <u>European Space Agency (ESA) Climate Change Initiative (ESA CCI)</u> version 2.1 and
 <u>European Centre for Medium-Range Weather Forecasts Atmospheric Reanalysis</u>
- 140 version 5 (ERA5). They are compared here with a selection of six state of the art SST
- 141 analyses distributed outside the CDS, obtained from different input data and analysis
- 142 system configurations. These are:

143	Hadley Centre Sea Ice and Sea Surface Temperature (HadISST1) (Rayner et
144	al., 2003);
145	· UK MetOffice Operational Sea Surface Temperature and Sea Ice Analysis
146	(OSTIA) system (Good et al., 2020)
147	• NOAA Daily OISST v2.1 daily reanalysis also referred to as Reynolds SST
148	(Reynolds et al., 2007; Banzon et al., 2016; Huang et al., 2020);
149	• Multi-scale Ultra-high Resolution 0.25 deg. (MUR25) SST analysis v.4.2
150	(Chin et al., 2017);
151	• Merged satellite and in situ data Global Daily Sea Surface Temperature
152	(MGDSST) (Sakurai et al., 2005; Kurihara et al., 2006);
153	• Australian Bureau of Meteorology Global Monthly SST Analysis (BoM
154	Monthly SST) (Smith et al., 1999).
155	
156	These eight datasets combine satellite and in many cases in situ temperature
157	measurements to generate gap-free (optimally interpolated) SST fields at the global
158	scale. All these datasets are specifically designed to provide accurate high spatial

159	and temporal resolution SST estimates that can be used in operational applications
160	such as assimilation and/or boundary conditions in numerical weather prediction
161	models (e.g., MGDSST and OSTIA SST), and/or analysed for climate applications (e.g.
162	HadISST1, NOAA Daily OISST analysis, MUR25, BoM Monthly SST).Some of the
163	selected datasets, namely ESA CCI v2.1, OSTIA, NOAA Daily OISST v2.1, MUR25 and
164	BoM Monthly are provided in GHRSST L4 format (GHRSST Science Team, 2012).
165	
166	Below, we detail the characteristics of all the SST products included in this
167	intercomparison study.
168	
169	2.1 ESA-CCI SST
170	The ESA CCI SST dataset (version 2.1) provides global daily SST estimates based on
171	observations acquired from different satellite sensors covering the period from

- 172 September 1981 to December 2018 (at the time of the study). The CCI SSTs are
- 173 designed to provide a stable, low-bias climate data record derived from different

174	infrared sensors, i.e., the <u>Advanced Vvery-Hhigh-Rresolution Rradiometer (</u> AVHRR <u>)</u> ,
175	Aadvanced Aalong Ttrack Secanning Readiometer ((A)ATSR) and Sea and Land
176	Surface Temperature Radiometer (SLSTR) series of sensors (Merchant et al., 2019,
177	2014). These data are provided at different processing levels: single-sensor data on
178	the native swath grid (Level-2); uncollated single-sensor (Level-3U) and collated
179	multi-sensor (Level-3C) gridded data; and blended multi-sensor and optimally
180	interpolated (Level-4) data.
181	The ESA CCI Level-4 product considered here consists of gap-free (optimally
182	interpolated) maps of daily average SST at 20 cm depth at 0.05° x 0.05° latitude-
183	longitude grid <u>(approximately 5x5 km at the equator)</u> . The Level-4 data have been
184	produced by running the Operational Sea Surface Temperature and Sea Ice Analysis
185	(OSTIA) system (Donlon et al., 2012) using CCI Level-3U SSTs as inputs, no in situ
186	data are included. Estimates of standard uncertainty (considered as the standard
187	deviation of the estimated error distribution) are provided for every SST at all
188	product levels. The evaluated global median uncertainty is 0.18 K (Merchant et al.,

189	2019). The multiannual stability of the whole time series, evaluated relative to
190	drifting buoy measurements, is within 0.003K/year (Merchant et al., 2019). Given the
191	high temporal and spatial resolution and the performance statistics, this dataset
192	gives an accurate representation of SST spatio-temporal variability of relevance to
193	climate applications. Target applications of the ESA CCI SST dataset include climate
194	and ocean model assessment; accurate definitions of climatic indices; quantification
195	of climate variability and its impacts on weather extremes (including marine
196	heatwaves), marine ecosystems, and related services.
197	
198	2.2 ERA5
199	The ERA5 Sea Surface Temperature (SST) dataset is produced by ECMWF to be used
200	for ERA5 atmospheric reanalysis (Hirahara et al., 2016). It consists of hourly global
201	gap-free SST data at 0.25°x0.25° latitude-longitude grid covering the period from
202	1979 to the present. ERA5 SST data are based on the HadISST2 (Kennedy et al.,
203	2016) product from 1979 to August 2007, and the daily operational OSTIA (Donlon

204	et al., 2012) product from September 2007 to present. The HadISST1 version 2 was
205	developed by the UK Met Office Hadley Centre, and its "pentad" dataset consists of
206	spatially complete, 5-daily mean fields on a 0.25° spatial resolution grid. OSTIA is a
207	high resolution (0.05°x0.05°) operational daily product developed by the UK
208	MetOffice and distributed through the Copernicus Marine Environment Monitoring
209	Service (CMEMS). These two SST datasets are aggregated into one continuous data
210	record and interpolated onto the ERA5 model grid (Dee et al., 2011) to be used as
211	boundary conditions for ERA5 atmospheric reanalysis. There are two types of Sea
212	Surface Temperature in ERA5 including Sea Surface Skin Temperature and Sea
213	Surface Temperature. In this study we have used monthly ERA5 Sea Surface
214	Temperature. ERA5 SST is calculated as the SST from an ocean model with
215	increment as the difference between OSTIA SST and the ocean analysis. Since the
216	input of SST comes from both OSTIA and HadISST2, the ERA5 SST is a mixture of
217	SST in the absence of diurnal variation, "foundation SST" (OSTIA), and SST at
218	indeterminate depth, "SSTdepth" (HadISST2), following the SST definitions in Minnett
219	and Kaiser-Weiss (2012). Here we give the SST type as SSTdepth for ERA5 SST.

220 2.3 HadISST1

221	Hadley Centre Sea Ice and Sea Surface Temperature dataset (HadISST1) is available
222	at_https://www.metoffice.gov.uk/hadobs/hadisst/data/download.html. This dataset
223	includes a combination of monthly globally-complete fields of SST and sea ice
224	concentration on a 1°x1° latitude-longitude grid from 1870 to present. HadISST1
225	data have been produced using SST measurements from the Met Office Marine Data
226	Bank (MDB), mainly ship tracks, and a blend of in situ and adjusted satellite-derived
227	SSTs for 1982-onwards. A bias adjustment of the satellite SST data is performed by
228	subtracting the in situ fields from the AVHRR fields. Specifically, the difference fields
229	are smoothed using a moving window average with <u>a radius of 2224radius 2224</u> km
230	(20 degrees of latitude). The smoothed bias fields are then subtracted from the
231	monthly AVHRR SST (see Appendix C in Rayner et al. 2003 for further details).

232

In order to enhance data coverage, monthly median SSTs for 1871-onward from the
Comprehensive Ocean-Atmosphere Data Set (COADS) (now ICOADS) were also used

235	where MDB data were not available. Information on sea ice concentrations isare also
236	included in the HadISST product. This information is derived from several sources
237	that include digitized sea ice charts and satellite data. Temperatures are
238	reconstructed using a two-stage reduced-space optimal interpolation procedure
239	(Kaplan et al., 1997), followed by superposition of quality-improved gridded
240	observations onto the reconstructions to restore local detail (Rayner et al., 2003).
241	
242	2.4 NOAA (Daily OISST)
243	The NOAA Daily OISST v2.1 dataset (Reynolds et al., 2007; Banzon et al., 2016;
244	Huang et al., 2020), also known as the "Reynolds" Daily Optimum Interpolation SST
245	
210	analysis, consists of global daily spatially-complete SST data on a 0.25°x0.25°
246	analysis, consists of global daily spatially-complete SST data on a 0.25°x0.25° latitude-longitude grid from 1981 to present (https://www.nodc.noaa.gov/oisst). This
246 247	analysis, consists of global daily spatially-complete SST data on a 0.25°x0.25° latitude-longitude grid from 1981 to present (https://www.nodc.noaa.gov/oisst). This dataset is routinely produced by NOAA/NESDIS/NCEI and publicly provided at
246 247 248	analysis, consists of global daily spatially-complete SST data on a 0.25°x0.25° latitude-longitude grid from 1981 to present (https://www.nodc.noaa.gov/oisst). This dataset is routinely produced by NOAA/NESDIS/NCEI and publicly provided at https://www.ncei.noaa.gov/data/sea-surface-temperature-optimum-

250	GHRSST GDS2 L4 format (GHRSST Science Team, 2012) files are also available from
251	1981 to 2015 from https://podaac.jpl.nasa.gov/dataset/AVHRR_OI-NCEI-L4-GLOB-
252	v2.0 and 2016 to present from https://podaac.jpl.nasa.gov/dataset/AVHRR_OI-NCEI-
253	L4-GLOB-v2.1.
254	

255 The NOAA optimal interpolation analysis uses both in situ and satellite-derived SST data. Satellite SSTs are estimated from NOAA/AVHRR and MetOp/AVHRR 256 observations. This dataset also utilizes the in situ ICOADS dataset to correct the 257 residual satellite SST biases. OISST has been updated from v2.0 to v2.1 from January 258 259 2016 onward. The updates include the following five aspects: (a) MetOp-B replaces 260 NOAA-19 while MetOp-A remains unchanged, (b) freezing-point temperature replaces ice-SST regression in SST proxy in ice-covered oceans, (c) the estimated 261 ship SST bias is reduced from 0.14°C to 0.01°C, (d) ship and buoy observations from 262 ICOADS-D R3.0.2 are used instead of NCEP GTS receipts, and (e) Argo observations 263

above 5 m depth are included. The Argo observations were first used as

independent data to validate the improvements in the updates from (a) to (d), and
the Argo observations were finally included in OISST in (e).
267
268 2.5 MUR25

269	The Multi-scale Ultra-high Resolution 0.25 degree. (MUR25) SST analysis (v.4.2) is a
270	global daily spatially-complete SST dataset on a 0.25° x 0.25° grid covering the
271	period from mid-2002 to present. The analyzed SST is representative of the
272	foundation temperature (namely, the temperature free, or nearly free, of any diurnal
273	cycle (Minnett and Kaiser-Weiss, 2012). This dataset is a reprocessed version of the
274	MUR dataset v.4.1 (Chin et al., 2017), which provides global daily spatially-complete
275	SST analyses at 0.01° spatial resolution. MUR25 is provided by NASA's Jet Propulsion
276	Laboratory (JPL) Physical Oceanography Distributed Active Archive Center (PO.DAAC)
277	and is available at https://podaac.jpl.nasa.gov/dataset/MUR25-JPL-L4-GLOB-v04.2.
278	The MUR L4 analysis is built by using only nighttime SST observations derived from
279	different types of satellite sensors, which include microwave and infrared

280	measurements from, e.g., Advanced Microwave Scanning Radiometer (AMSR) for
281	Earth Observing System (AMSR-E) and NOAA/AVHRR observations. In addition,
282	MUR25 ingests in situ SST measurements from the NOAA iQuam data set (Xu and
283	Ignatov, 2014)project to improve the estimate of the foundation temperature, and
l 284	ice concentration data from the EUMETSAT Ocean and Sea Ice Satellite Application
285	Facility (OSI SAF), which are used for an improved SST parameterization in the pola
286	regions. Satellite and in situ data are combined using MRVA, a meshless multi-scale
287	interpolation method which uses wavelets as basis functions in order to build the
288	daily MUR SST analysis (Chin et al., 2017).

290 **2.6 MGDSST**

The Merged satellite and in situ data Global Daily <u>Sea Surface TemperatureSST</u> (MGDSST) analysis dataset provides global daily spatially-complete SST fields on a 0.25°x0.25° latitude-longitude grid covering the period from 1982 to present. This dataset is derived from infrared satellite sensors (NOAA/AVHRR and MetOp/AVHRR),

295	microwave satellite sensors (Coriolis/WINDSAT, GCOM-W1/AMSR-2), and in situ
296	temperature measurements (from buoys and ships). This dataset is provided by The
297	Japanese Meteorological Agency (JMA) and is available at
298	https://ds.data.jma.go.jp/gmd/goos/data/rrtdb/jma-pro/mgd_sst_glb_D.html.
299	SSTs from the microwave sensor AQUA/AMSR-E are used in the analysis from May
300	2002 through 5th October, 2011. In the reanalysis data, SSTs under sea ice are
301	determined according to the statistical relation between sea-ice concentration and
302	SST. The lowest SST is -1.8 degree Celsius where the sea-ice concentration is 100%.
303	Additional information is provided by Kurihara et al. (2006) and Sakurai et al. (2005).
304	

305 2.7 BoM Monthly

306	The Monthly Optimal Interpolation (OI) SST Analysis is the global monthly spatially
307	complete SST dataset on a $1^{\circ}x1^{\circ}$ grid produced by the Australian Bureau of
308	Meteorology (BoM), covering the period of 1994 to present (Smith et al., 1999)_ $_{\!\scriptscriptstyle L}$
309	formed by averaging the BoM Weekly OI SST analyses over each month. In this

310	study, we use the GHRSST version 1 L4 format files of this dataset covering the
311	period 2002 to present (Beggs and Pugh, 2009) Each Monday a weekly SST analysis
312	on a 1°x1° grid is formed from optimally interpolated SST observations collected
313	over the preceding week (Monday to Sunday) (Smith et al., 1999). The BoM monthly
314	OI SST analysis is formed on the first Monday of each month from an average of the
315	weekly OI SST analyses for the preceding calendar month, where the middle date of
316	each weekly analysis falls within that month (Beggs and Pugh, 2009).—The SST
317	observations used to derive the global weekly and monthly SST analyses are
318	obtained from in situ SST observations from drifting and moored buoys, ships, Argo
319	floats, Conductivity Temperature Depth (CTD) and Expendable Bathythermographs
320	(XBTs), and satellite-derived SST from infrared AVHRR sensors aboard NOAA Polar-
321	Orbiting Environmental Satellites (POES) and ESA/EUMETSAT MetOp satellites.
322	Weekly OI analyses of the in situ data are used to correct for biases in the satellite
323	data (Smith et al., 1999), similar to the method used in the NOAA Weekly $1^{\circ}x1^{\circ}$
324	OISST v2 (Reynolds et al., 2002). The resulting outputs of the Weekly and Monthly

....

OI analyses of in situ and satellite data are therefore SST values of indeterminate

326 depth, SSTdepth.

- 327 At high latitudes, the BoM weekly analysis system uses the daily sea-ice
- 328 concentration analysis from NOAA/NCEP
- 329 (https://polar.ncep.noaa.gov/seaice/Analyses.shtml) to constrain the SST, by setting
- 330 SST at a given grid point to -1.8°C if the concentration of NCEP ice data in that grid
- 331 cell is greater than 50 per cent. Until 12 March 2008, the 0.5° resolution sea-ice
- analysis was used and after that date, the 1/12° resolution sea-ice analysis
- 333 (Grumbine, 1996).
- 334 Maps of these weekly and monthly SST analyses are available at
- 335 http://www.bom.gov.au/marine/sst.shtml, and they are used operationally by BoM to
- 336 generate El Niño indices, monitor the Indian Ocean Dipole and produce SST
- 337 anomaly maps for climate applications
- 338 (http://www.bom.gov.au/climate/enso/#tabs=Sea-surface). The BoM Weekly and
- 339 Monthly OI SST analysis GHRSST L4 format files are available on request

340	(http://www.bom.gov.au/climate/data-services/data-requests.shtml). It should be
341	noted that higher resolution (0.25°x0.25°) global daily OI SST analyses have been
342	produced operationally at the Bureau of Meteorology since 2008 (Zhong and Beggs,
343	2008; http://www.bom.gov.au/marine/sst.shtml) but these only cover the period 2008
344	to present so were not included in this study.

346 2.8 UK Met Office OSTIA SST

347 The UK Met Office Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA) (Good et al., 2020) system is a daily global SST product with a resolution of 348 1/20° (approximately 5-6km). Monthly and seasonal frequency datasets are also 349 350 available. The version of OSTIA SST we use in this study is the Copernicus Marine 351 Environment Monitoring Service (CMEMS) reprocessed SST analysis based on the 352 OSTIA configuration reported in Good et al. (2020), covering the period 1 October 1981 to 31 December 2018. This OSTIA reanalysis is formed by the combination of 353 354 satellite SST data provided by the GHRSST project with additional (A)ATSR, SLSTR

355	and AVHRR data from ESA CCI SST v2. <u>1</u> ,1 (note that ESA CCI SST v2 and V2.1 only
356	differ in the file specification, but no scientific differences) and C3S projects, and in
357	situ observations from the HadIOD by using NEMOVAR, a variational assimilation
358	(Fiedler et al., 2019b), instead of the optimal interpolation algorithm (Martin et al.,
359	2007, Donlon et al., 2012). Note that ESA CCI SST v2 and V2.1 only differ in the file
360	specification, but no scientific differences. Bias correction is performed for all the
361	input satellite data (except the satellite data in the reference dataset) by carrying out
362	match-ups between satellite and reference measurements. The depth of the SST
363	analysis represents the sub-skin temperature immediately before sunrise also
364	referred to as foundational SST that is free of diurnal variability (Donlon et al., 2012).
365	The OSTIA reanalysis is publicly available from
366	https://resources.marine.copernicus.eu/?option=com_csw&task=results?option=com_
367	csw&view=details&product_id=SST_GLO_SST_L4_REP_OBSERVATIONS_010_011.
368	In order to verify the accuracy of reprocessed SST analysis, drifting buoys and near-
369	surface Argo data that are not included in SST analysis are used as independent

370	data for quality assessment <u>as</u> shown in Copernicus Marine Environment Monitoring
371	Service (CMEMS) quality information documentation of OSTIA SST
372	(https://resources.marine.copernicus.eu/documents/QUID/CMEMS-SST-QUID-010-
373	011.pdf). Note that the drifting buoy SSTs used for validation are ingested into the
374	analyses, however the validation process uses OSTIA background fields without data
375	assimilating buoy SSTs -to compareed with to drifting buoys from analysis day plus
376	1 day to , as the time offset between the background fields and these drifting buoys
377	avoid s the validation data independence issue.
378	OSTIA SST has been used as boundary conditions for operational forecast models at
379	the UK Met Office and European Centre for Medium-range Weather Forecasting
380	(ECMWF) and is also part of the CMEMS project. The validation,and-assessment
381	activities update regularly through the CMEMS projectand-the dataand relevant
382	documentations are available at
383	https://resources.marine.copernicus.eu/?option=com_csw&view=details&product_id=

384 SST_GLO_SST_L4_REP_OBSERVATIONS_010_011.

3 Basic diagnostics

388	In order to compare the selected datasets (see Section 2) especially against global
389	SST climatology, all the SST products need to be mapped on a common temporal
390	and spatial resolution (regular 1°x1° latitude-longitude grid.). Apart from HadISST1,
391	the majority of the SST products have higher resolution than $1^{\circ}x1^{\circ}$ and the
392	advantage of high resolution is to resolve small scale ocean processes. The
393	interpolation from higher resolution to low resolution may exclude the impacts of
394	important small-scale signals in the SST products. Before we present the basic
395	diagnostics such as mean climatology and variability, we have performed spatial
396	spectral analysis (Section 3.1.1 - methods and Section 3.2.1 - results) to quantify the
397	impact of interpolation to the common 1°x1° resolution we have performed in our
398	basic diagnostics.

400	The grid of HadISST1 has been chosen as the reference grid (at 1°x1° nominal
401	resolution). The HadISST1 land-sea mask has then been applied to all products. In
402	addition, a sea-ice mask was built from HadISST1 and used as a common sea-ice
403	mask for all datasets.
404	
405	To homogenize the datasets' temporal and spatial resolution we have used CDO
406	(Climate Data Operator) command line operators (see the user guide at
407	https://code.mpimet.mpg.de/projects/cdo/embedded/cdo.pdf). In particular, we have
408	chosen a bilinear interpolation for gridding all datasets on the HadISST1 spatial grid.
409	
410	For all the selected SST products, the overlapping period is 2003-2018 (Figure 1) and
411	the intercomparison of all SST products are performed for the period 2003-2018,
412	when observations are abundant compared to the beginning of the satellite era.
413	Recent period increased quantities of observations ingested The richness of
414	observation numbers used in the SST analysismay reduce the spread of ensemble
415	help all the SST products produced with different algorithms converge . In order to

416	understand deeper the discrepancy and consistency between all the SST analyses
417	produced with different algorithms, similar intercomparison diagnostics of SST
418	products (ESA-CCI, ERA5, OSTIA, NOAA OISST, MGDSST and HadISST1) that have the
419	common period from 1982-2018 (Figure 1) are also carried out for the earlier period
420	of the satellite era (1982-2002) when the observations are scarce compared to the
421	later period of the satellite era.
422	
423	In this section, we first introduce the methodologies we applied to produce the
424	basic diagnostics, and the spatial spectral analysis method used to investigate the
425	impact of spatial resolution is also presented. Then we present the results generated
426	by these diagnostics in terms of intercomparison for the period 2003-2018, and the
427	intercomparison of SST products that cover the period 1982-2002 is presented at

3.1 Statistical Methods

431	A set of basic diagnostics have been defined to evaluate the similarity and
432	disagreements between selected SST datasets, as detailed in the following
433	subsections. Some of these metrics, such as the mean climatology, quantify the
434	long-term mean spatial distribution (climatology) of the sea surface temperature <u>SST</u>
435	for each single dataset and can be used to qualitatively evaluate the capability of
436	SST in representing the climatological spatial patterns and the temporal variability of
437	globally averaged SSTs . Other metrics, such as difference, root-mean-square
438	difference (RMSD), and correlation, measure the distance between a single product
439	and a "reference". The latter can be either a previously validated dataset (if available)
440	or any other dataset that is arbitrarily chosen as reference. In this report, we have
441	taken the median of all datasets (hereafter the Ensemble median) as a reference and
442	used it to measure the difference among different SST products. Finally, we choose a
443	specific case study of the El Niño Southern Oscillation (ENSO) Nino3.4 Index to
444	evaluate the capability of representing ENSO events in all SST products. Nino3.4 is
445	the average sea surface temperature<u>SST</u> anomaly in the region bounded by 5°N to
1 446	5°S, from 170°W to 120°W.

447 3.1.1 Spatial Spectral Analysis

448	The spectral analysis method we adopted in this study is the Multitaper Power
449	Spectral Density Estimate (MTM) (Thomson, 1982), which is a very useful tool for the
450	analysis of relatively short and noisy series that may contain both broadband and
451	line components. Different from several other spectra-techniques, MTM
452	multipliesmultiply the data by a small set of orthogonal tapers rather than a single
453	taper to minimize the spectral leakage due to the finite length of the series.
454	MTM requires, as input, to fix number of tapers (k) and the integer bandwidth
455	parameter (p) that imply a choice of a bandwidth equal to 2pf, in which f is the
456	Rayleigh frequency f=1/(NDT), N is the number of samples and DT is the sampling
457	interval. As in many other practical cases the selection of p and k represents a
458	classical trade off between spectral resolution, defined by the selection of p, and the
459	need of a variance reduction related to the number of tapers k that pre-multiply
460	the series. Note that the choice p=1 and k=1 is simply the single tapered discrete
461	Fourier transform.

462	MIM power spectral estimates were performed using the pmtm matlab function
463	(https://www.mathworks.com/help/signal/ref/pmtm.html), setting the time-
464	halfbandwidth product p equal to 2. This is equivalent to the choice resolution $p=2$
465	and number of tapers, $k=(2*p \ 1)=3$ in the SSA MTM toolkit
466	(https://dept.atmos.ucla.edu/tcd/documentation)We_preferred to use the matlab
467	function rather than the University California Los Angeles (UCLA) toolkit because we
468	needed to recursively compute spectra on a daily basis for time series of several
469	years before_ to applying a time average and this was not feasible with the very user
470	friendly toolkit that requires to process individually each series. For more details
471	please refer to Ghil et al. (2002) Section 3.4.
472	
473	We have chosen four-representative datasets, ESA-CCI and OSTIA with the original
474	spatial resolution of 0.05° and MGDSST and NOAA Daily OISST (Reynolds 0.25 \boldsymbol{x}
475	0.25° SST) with the original resolution of 0.25° all covering the same period 1982-
476	2018 with daily frequency. Meanwhile, we chose the Pacific equator pixelpixels line,
l 477	spanning from Indonesian to South America as the study region (0°N, 120°E-80°W).

.

478	For each dataset the spatial power spectral density has been estimated on a daily
479	basis over the common period (1982-2018) and then time averaged. The detailed
480	results and discussion are given in Section 3.2.1.
481	3.1.2 Trend analysis
482	
483	Sea surface temperatureSST trends have been estimated by using the X-11 seasonal
484	adjustment procedure (see e.g. Pezzulli et al., 2005). Given X_t is the input time series
485	(namely, an SST time series), the X-11 procedure generates the following
486	decomposition:
487	$X_t = T_t + S_t + I_t$
488	
489	where T_t is the trend component, S_t the seasonal component and I_t the irregular
490	component, which accounts for the residual irregular variations such as sub-annual
491	fluctuations. The decomposition is obtained through iterative application of different

493	seasonal filter for S _t estimation.	
494	In addition, the Mann-Kendall test is used to assess whether a monotonic upward or	
495	downward trend in T_{t} exists (against the null hypothesis of no trend), Sen's method	
496	is applied to estimate the slope of $T_{t\prime}$ i.e. the trend (as the median of the slopes of	
497	all pairs of sample points), and a bootstrap procedure is used to estimate the 95%	
498	confidence interval of the trend (Mann, 1945; Sen, 1968; Kendall, 1975; Efron and	
499	Tibshirani, 1993).	
500		
501	3.2 Results	
502		
503	3.2.1 Spatial Spectrum Analysis	
504	4	Formatted: Heading 3
505	With rapid growth of computing power and storage capacity, along with	
506	advancement of scientific knowledge and users' needs, spatial resolution of SST gap-	
507	free analyses has increased dramatically to resolve smaller scale features in the	

running means, which have the effect of a low-pass filter for $T_{t}\xspace$ estimation and a

508	ocean. The spatial resolution of SST products used in this study spans from 1° to
509	0.05°, meaning that the highest resolution is 20 times smaller than the lowest
510	resolution. In the high resolution SST products, the meso scales might be resolved,
511	by contrast in the low resolution SST products only large scale features are
512	represented.
513	
514	In order to verify the suitableness of our choice of interpolation, we have performed
515	spatial power spectral analysis (section 3.1.1) based on the chosen SST products
516	(Figure 2). With rapid growth of computing power and storage capacity, along with
517	advancement of scientific knowledge and users' needs, spatial resolution of SST gap-
518	free analyses has increased dramatically to resolve smaller scale features in the
519	ocean. The spatial resolution of SST products used in this study spans from 1° to
520	0.05°, meaning that the highest resolution is 20 times smaller than the lowest
521	resolution. In the high resolution SST products, the meso-scales might be resolved,
522	by contrast in the low resolution SST products only large scale features are
523	represented.

524	
525	All of the SST products we chose for the spectral analysis cover the same period
526	from 1982 to 2018 with daily frequency. OSTIA and ESA-CCI SST have the original
527	spatial resolution of 0.05° and MGDSST and NOAA Daily OISST have the spatial
528	resolution of 0.25°. If the power spectra gradient becomes flat at a certainat certain
529	wavelength it means that the analysis carried out at a wavelength shorter than this
530	certain wavelength contains only noise. The resultThe power spectrum density of
531	these four datasets shows that even though all of these SST products have higher
532	grid resolution than the chosen common grid, 1°, the power density of all SST
533	products starts to decline at spatial wavelengths greater than their grid-resolution.
534	The prominent differences between NOAA OISST and MGDSST are mostly likely due
535	to different background correlation length scales being used in the optimal
536	interpolation and different methodology used to correct satellite-based
537	observationsArgo SSTs ingestion in NOAA OISST and different methodology to
538	correct satellite based observations. For high resolution datasets, the 0.05° products,
539	the power density-is significantly declined after by $\sim 80 \sim 100$ km (wavenumber 10^{-2}),

540	which is close to 10.7° spatial resolution near the equator and the gradient becomes
541	flat at wavelengths ~70 km. It means that the signals within a wavelength of 100 km
542	are noise, s with no physical meaning in 0.05° SST products, and that also applies to
543	0.25° resolution SST products. —Similar results were shown in Fiedler et al. (2019a)
544	that in the Gulf Stream regions for the 2017 northern winter the spectral density of
545	SST starts to depart from the ${\it I\!I}^{-11/3}$ cascade of SST field (equivalent to kinetic
546	energy power spectrum cascade of $D^{-5/3}$ based on Le Traon et al., 1990; 2008) at
547	wavelengths around 90km. This confirms that the interpolation to 1° does not
548	undermine the interpretation of results presented in our study.
549	
550	Additionally, the diagnostics performed in the following sections mainly focus on the
551	general features (mean climatology and long-term temporal variability) of the
552	representation of all the SST products. <u>W that we</u> believe the interpolation of all SST
553	products to 1° brings minor issues to the interpretation of the results. Certainly, the
l 554	intercomparison between all the SST products in terms of specific details, for
555	example, the representation of the Gulf Stream and meso-scale features are not in

the scope of this study. Related activities are <u>underway</u>undergoing and will be presented by the GHRSST <u>SST Analysis l</u>intercomparison <u>Task T</u>team in the near future.

559

560 **3.2.2 - Mean and Variability (2003-2018)**

561	In terms of the basic diagnostics, we have first calculated the mean climatology of
562	the global SST distribution of the eight selected SST datasets during 16 years from
563	2003 to 2018 plus the median of all the eight SST products, i.e., the climatology of
564	the ensemble median (Figure 3). In all eight cases, the average correctly reveals the
565	dominant latitudinal spatial SST pattern: higher at the tropics, milder at middle
566	latitudes and lower in the polar regions. Regions impacted by occasional or
567	persistent presence of sea ice are flagged, i.e., only complete years have been
568	considered for the average estimate in each grid point.
569	

- 570 A first qualitative inspection of the eight mean SST fields suggests that all products
- 571 reproduce a very similar spatial distribution of SST with minor differences not

572	appreciable from Figure 3. Considering a confidence level of 95%, the eight global
573	mean SST estimates for the period 2003 to 2018 range in an interval between
574	20.02°C and 20.17°C. The ensemble median obviously falls close to the middle of
575	this range (i.e., 20.12 °C).
576	In order to have a further investigation of the consistency and discrepancy between
577	all SST products, we calculated the difference between each SST product and the
578	ensemble median displayed in Figure 4. Considering a 95% confidence interval, the
579	global mean difference between each single product and the ensemble median
580	ranges between -0.05 and 0.1 $^\circ$ C with relevant spatial variability (Figure 4). In fact,
581	differences are more pronounced in the Southern ocean where distances between

single product values and the ensemble median reach values higher than 1°C. This is

583 particularly evident in the case of HadISST1 data. In general, higher difference areas

correspond to the western boundary current systems such as the Gulf Stream

585 Current, the Kuroshio Current in the Northern Hemisphere, Brazil currents in the

586 Southern Atlantic Ocean, and the Antarctic Circumpolar Current Antarctic

587	Circumpolar Current (ACC), where eddies are extremely active. In some datasets,
588	especially ESA-CCI SST <u>, and MGDSST and OSTIA</u> , the <u>greatest</u> differences from the
589	ensemble median are also located withinat eastern boundary currents which where
590	<u>re</u> present the main upwelling systems, e.g., Per o u-Chi <u>l</u> li, Benguela, North West-
591	African coast and along the southern Saudi Arabia coast. These discrepancies could
592	be due to the mismatching in the position of the main streams, especially the eddy
593	representation in different SST products. Along the coast, the disagreement may
594	come from the interpolation methodology implemented in different SST datasets by
595	data providers. Especially regions where upwelling is active add difficulties to
596	retrievinge satellite observations for representing SST patterns and variability. For the
597	case of ESA CCI SSTs, it has been shown that cool biases off the North West-African
598	coast and in the Arabian Sea arise from influences of mineral dust aerosol on IR
599	retrievals of SST, and a large-scale adjustment (not used here) for the dust-related
600	biases has been devised (Merchant and Embury, 2020).

ī

601	The RMSD is defined as the square root of the average squared difference between
602	the SST value of each dataset and the ensemble median, which is an absolute
603	measure of the distance between each single product value and the ensemble
604	median. Considering the 95% confidence interval, the global average RMSD ranges
605	from 0.02 to 0.18 °C. Extreme RMSD values (Figure 5) are concentrated in the
606	Southern ocean <u>andthat</u> correspond s to the Antarctic Circumpolar Current<u>ACC</u>, as
607	also evidenced by the mean difference (Figure 4), particularly evident in HadISST1
608	data. These higher RMSD values are also observed in correspondence $to of the$ large
609	differences between each SST product and the ensemble median that are mainly
610	located in the western boundary currents, namely, the Gulf Stream in the North
611	Atlantic Ocean and the Kuroshio Current in the North Pacific Ocean, and the ACC
612	currents regions.
613	The spatial distribution of the Pearson correlation coefficient (Figure 6) highlights the
614	different behavior of HadISST1 with respect to the other seven products. In
615	particular, in the southern ocean region, the correlation falls down to values as low

616	as 0.5 or even less. Similar but less extended discrepancies are also observed for
617	BoM <u>, and</u> NOAA Daily OISSTs <u>, ESA-CCI, MUR25, ERA5, OSTIA and MGDSST.</u> In
618	particular, -ESA-CCI seems well representative of the ensemble median. MUR25,
619	ERA5, MGDSST and OSTIA are well representative of the ensemble median as well
620	but with slightly higher discrepancies than other SST products. However, the low
621	correlation especially along the coastal regions could be due to the interpolation
622	method adopted during the SST production by data providers because it is still a
623	challenge to correctly retrieve satellite observations at the coastal upwelling regions
624	where SST is highly variable.
625	The temporal variability of globally averaged monthly mean SSTs (Figure 7) clearly
626	exhibits the annual oscillation around the mean value of 20.12 °C (Figure 3). This
627	oscillation has an amplitude of about 0.6 $^\circ C$ as a result of the opposite seasonal
628	cycle in the southern and northern hemispheres. SST anomalies from 2003 to 2018
629	(Figure 8) are obtained by subtracting from all SST products the annual cycle of the
630	ensemble median, i.e., the mean of each month over the whole period (2003-2018).

631	Two main periods are observed with distinguished <u>distinct</u> mean values: the first
632	period before 2012 where the temperature oscillates around a constant mean value
633	of about 20.1°C and a second period where a positive (warming) trend is observed.
634	All the eight datasets show temperatures that vary coherently over all time scales
635	but with relative absolute biases in the range from zero to 0.4 $^\circ$ C.
636	
637	3.2.3 Global linear trends (2003-2018)
638	Global SST trend maps have been computed for each product over the common 16
639	years period from 2003 to 2018 (Figure 9). All the datasets exhibit a global mean
640	warming SST trend ranging from 0.012 (HadISST1) to 0.022 (MGDSST) $^{\circ}$ C/year, with

 $\,$ 641 $\,$ an average value of 0.019 °C/year (ensemble median). Within the 95% confidence

642 interval, these results are close to the global ocean warming trend of 0.011 °C/year

643 from 1980 to 2005 reported in the last IPCC report (Pachauri et al., 2014) and the

644 differences are due to the different calculating period. The prominent warming

645 trends shown in all SST products are located in the subtropical North Atlantic Ocean,
646	South Indian Ocean, eastern tropical Pacific Ocean close to the American continent.
647	Especially at the Gulf Stream area all SST products (apart from HadISST1 which has
648	slightly weaker signals compared to other dataset) exhibit distinguished warming
649	trends for the period of 2003 to 2018.
650	In the North Atlantic Ocean, between 40 and 70 °N, negative trends are observed in
651	the sub polar gyre region extending up to the coastal areas of Ireland. A second
652	common negative trend area is present in the Southern Ocean at longitudes
653	centered around the Drake Passage. In the tropical Atlantic Ocean, a large area of
654	negative trends is observed only in ERA5 and a smaller area in BoM, OSTIA and
655	HadISST1. For all the other products this area is characterized by no significant
656	trends (i.e., areas where, given the p=0.05 limit, the null hypothesis cannot be
657	refu <u>t</u> sed) with few sparse negative trend points.
658	
659	The Mediterranean Sea shows an evident positive trend in all products in contrast

with a close to zerono trend region in the adjacent northeast Atlantic Ocean. This is

660

661	in agreement with what was recently published by Pisano et al. (2020) who observe
662	that, after 1990, SST in the Mediterranean Sea continues to increase in contrast with
663	the adjacent areas of the Atlantic Ocean where a pause of the general warming
664	trend occurred. The larger area of positive SST trends is present in the Indian Ocean.
665	Intense (positive) trends cover more uniformly and densely the reddish areas in ESA
666	CCI, MUR, NOAA OISST and MGDSST data, while a more patchy and less intense
667	positive trend coverage is observed in ERA5, BoM, OSTIA and HadISST1 data.
668	Besides a bias that separates the curves by a maximum of 0.2°C, the trend
669	component of the eight spatially averaged global SST time series (Figure 10a),
670	obtained using the X-11 procedure with a 2-year low-pass filter (section 3.1.2),
671	shows a very similar behaviour for all the products. The time evolution of the trend
672	component reveals an apparently neutral period until 2011 included with a single
673	maximum centered on the year 2009. After this period, a continuous warming phase
674	is observed with an increase of the temperature of nearly 0.3°C, that is, about

675 0.06°C/year which is consistent with the signal observed in the time series anomalies676 (Figures 7 and 8).

677	In order to understand better the contribution to the significant warming trends for
678	the period of 2012-2018 observed in all SST products, we have calculated the SST
679	trend component in different ocean basins, i.e. Pacific Ocean (Figure 10b), Atlantic
680	Ocean (Figure 10c) and Indian Ocean (Figure 10d). Quantitatively, the warming
681	trends for the period of 2012-2018 ranges from 0.036°C/year (BoM) to 0.062°C/year
682	(MUR25) with 0.049°C/year in the ensemble median. The major contributor to this
683	warming trend comes from the Pacific Ocean where warming trends span from
684	0.045°C/year (BoM) to 0.084°C/year (MUR25) with 0.064°C/year in the ensemble
685	median. The contribution from the Atlantic (0.02°C/year from BoM to 0.52°C/year
686	from MUR25) is smaller compared to the Pacific Ocean, and the warming trends in
687	the Indian Ocean from 2012 to 2018 are relatively very small (from 0.002°C/year,
688	MGDSST to 0.030°C/year, BoM), which are evidently exhibited in Figure 10d.

690 3.2.4 Intercomparison during the early period (1982-2002)

691	In this section, we present the intercomparison of all SST products covering the
692	period 1982-2002. First we have shown t ⁺ he global mean SST time series (Figure 11)
693	that covers the time period originally obtained in each SST product allows us to
694	detect the consistency and disagreement between all SST products for a longer
695	period to fully take advantage of SST products which covers the period beyond 2003
696	and 2018. As we have discussed, all the SST products are very similar <u>tofor the</u>
697	period of 2003-2018 when there are abundant observations. On the contrary, during
698	the period of early satellite era (1982-2002), the disagreement between all the SST
699	products is larger compared to the later period (2003-2018), which may be due to
700	fewerless observations ingested in the SST analysis.
701	To quantify the consistency and discrepancy of SST products for the early satellite
702	era (1982-2002) we have <u>calculatedperformed the mean climatology (Figure 12) for</u>
703	all SST products which cover the period back to 1982 (Figure 1), including ESA-CCI,
l 704	OSTIA, ERA5, NOAA OISST, MGDSST and HadISST1 and the differences between

705	each member with the ensemble median (Figure 13). The mean climatology of SST
706	during the period of 1982-2002 spans the range from 19.76°C (NOAA OISST) to
707	20.05°C (HadISST1) with the ensemble median as 19.79°C. The differences of each
708	member relative to the ensemble median for the period of 1982-2002 range from
709	0.03°C to 0.26°C that is much higher than that during the period of 2003-2018
710	which range from 0.01°C to 0.1°C. The discrepancy of all SST products (Figure 13)
711	are located in the areas that are similar to the period of 2003-2018 (Figure 4), but
712	with amplified signals. However, in some SST products, the differences relative to the
713	ensemble median change signs. For example, during the period of 2003-2018 the
714	MGDSST mean climatology is higher than the ensemble median in the eastern
715	Indian Ocean. On the contrary, the mean climatology differences between MGDSST
716	and the ensemble median became negative during the period of 1982-2002. <u>ERA5</u>
717	SST is based on OSTIA SST, however, there are differences between them because
718	ERA5 is forced by SST from an ocean model with increment based on the difference
719	between ocean analysis and OSTIA, which contains information fromof the OSTIA
720	SST but is not exactly identithe same.

721	These results are consistent with what is shown in Figure 11 that during the early
722	period of the satellite era (1982-2002, <u>fewerless_SST</u> observations) all the SST
723	products have larger differences compared to the later period (2003-2018, more
724	SST observations), indicating that observation numbers is the main factor to
725	constrain the climatology of all the SST products developed with different
726	algorithms.— <u>The total number of valid in situ SST observations from drifting buoys</u> ,
727	ships, Argo floats and moorings, used for bias-correcting satellite SST ingested into
728	ERA5, HadISST1, OSTIA, Daily OISST and BoM Monthly, number indeed increases
729	over time (Xu and Ignatov, 2014; https://www.star.nesdis.noaa.gov/socd/sst/iquam).
730	In 2002, the microwave radiometer AMSR-Ethe Advanced Microwave Scanning
731	Radiometer (AMSR) for Earth Observing System (EOS) started to be in operation on
732	Aqua and Terra satellites, which measures ocean brightness temperatures through
733	clouds, commenced operation on Aqua satellite. This improvement in spatial
734	coverage of sensors in the satellite sensors-is another important factor affectingon
735	SST data-quality ingested into OSTIA, ERA5, MGDSST and MUR25, and it is notable

736 that all SST products studied converge more after year-2003 compared to that

737 <u>before year 2003.</u>

738

739

740 3.2.5 Niño 3.4 Index

742	In order to have a deeper evaluation of the quality of the SST for climate studies, we
743	investigated the capability of representing the climate modes in all SST products for
744	the period of 1982-2018 in order to include more ENSO events, here the Nino3.4
745	index (Trenberth 2020). Niño 3.4 is one of the most used indexes to monitor the
746	occurrence and variability of El Niño and la Niña events, defined as the average
747	equatorial SST anomalies across the Pacific in the region 5°S-5°N, 170W°-120W°.
748	Figures 14 show the time evolution of the Niño 3.4 index during the 1982-2018
749	"common period" for each product time series after applying a 5-month
750	<u>running</u> moving meanaverage filter.

751	All products give evidence of the very strong El Niño events in the period selected.
752	The procedure used here to independently compute the Niño 3.4 index for all the
753	data sets is the same applied by Trenberth (2020). The time evolution of the Niño
754	3.4 SST anomaly is nearly identical for all the products with-very minor differences
755	(Figure 14). The three strong El Niño events that occurred during this investigation
756	period, namely 1982-1983, 1997-1998, and 2015-2016, are reproduced, with <u>a</u>
757	similarthe same intensity, by all products. Moreover, the larger intensity of the El
758	Niño positive anomalies with respect to the negative La Niña events confirms the
759	asymmetry hypothesis of Monahan and Dai (2004).

4. Data Maturity Matrix

The concept of the data maturity matrix is to evaluate the basic characteristics of a
dataset initiated by the World Meteorological Organization (WMO) to develop
technical guidance and standards for collecting, processing, and managing datasets.
The assessment of the maturity of the individual dataset is essential to guarantee

766	and further improve the documentation, storage, and dissemination of datasets that
767	are applicable for users (Peng et al., 2019).
768	The System Maturity Matrix (SMM) for Climate Data Records (CDRs) is first
769	developed in the Coordinating Earth Observation Data Validation for Reanalysis for
770	Climate Services project (CORE-CLIMAX) (Su et al., 2018). The objective is to
771	develop a tool to evaluate different aspects of the CDRs combining scientific and
772	engineering views. (EUMETSAT, 2014). In the SMM framework assessments are made
773	in six major category areas and a score of 1 to 6 is assigned that reflects the
774	maturity of the CDR with respect to a specific category;
775	
776	1. Software readiness
777	2. Metadata
778	3. User documentation
779	4. Uncertainty characterization
780	5. Public access, feedback, and update

781 6. Usage

782	However, the assessment of maturity can only reflect speak about aspectsspeak
783	aspects of process maturity. It does not interpret the scientific quality of a dataset.
l 784	For example, a mature product may not be scientifically reliable thus the maturity
785	matrix only provides the assessment of fitness-of-purpose of a given product for
786	climate service practitioners in terms of the categories mentioned above.
787	Additionally, the SMM scores should be recognized <u>recognize</u> that at the early
788	evaluation stage in the life cycle of the product the low scores in some of the
789	categories do not demonstrate the possible future maturity of the dataset. Instead,
790	low SMM scores indicate a recently released and evolving product at a less mature
791	stage being made available to users.
792	In the context of the C3S_511 project, the aim of our assessment is to evaluate the
793	maturity of the dataset instead of the whole CDRs. We have adopted the SMM
794	methodology of the CORE-CLIMAX for our use to evaluate individual datasets. We
795	defined our matrix as the Maturity Matrix (MM) since we evaluate the dataset

796	instead of the system of the dataset. Not all the categories from CORE-CLIMAX are
797	included because some of them are not suitable for our usage. A guidance
798	document is developed in the framework of C3S_511 project , and the assessment
799	scores given in this study are based on our guidance document
800	(https://confluence.ecmwf.int/display/CKB/Guidance+document+on+applying+the+M
801	aturity+Matrix+as+part+of+the+Evaluation+and+Quality+Control). The MM, as
802	important as the scientific quality, provides data providers important information in
803	which aspects they need to improve their dataset for potential easy access and
804	usage for users.
805	The MM of ESA-CCI and ERA5 SST (Table 2), showing that ESA-CCI SST is much
806	more mature compared to ERA5 SST in terms of documentation, uncertainty
807	characterization, and usage. As we mentioned above, low MM scores do not suggest
808	the scientific quality of ERA5 SST is lower than ESA-CCI SST. However, in terms of
809	the documentation of the dataset, ESA-CCI SST is much more advanced than ERA5
810	SST.

811	In this study we have extended the evaluation of the MM to the dataset outside of
812	CDS (Table 2). Due to the length limit, detailed defensible traces to score MM for
813	SST products are given in the Appendix. In terms of metadata, MGDSST has a lower
814	score because it is provided in text format not following any standards with limited
815	global attributes. The rest of the SST analysis products follow the NetCDF format
816	and CF compliance with detailed information on Metadata. Compared with other
817	datasets, BoM, MGDSST and MUR25 lack user documentation including the formal
818	description of scientific methodology, validation report and product user guide. A
819	formal user guide is not found for HadISST1 either. Very few SST products (OSTIA
820	and ESA-CCI SST) have automated quality monitoring in terms of the uncertainty
821	characterisation category. Thanks to GHRSST activities, all GHRSST L4 products
822	follow internationally agreed GHRSST specifications, which provide uncertainty
823	calculations. Several SST analysis products (HadISST1, MGDSST, BoM and ERA5)
824	have very limited validation, standards or uncertainty quantification documentation.
825	All SST products are publicly available via the online portal, except that BoM SST is
826	available on request from the data provider via their website. However, the

827	versioning, user feedback, and updates to records in the category of public access
828	toof SST products are not fully developed for BoM and MGDSST. All SST products
829	except ERA5 are widely used in multiple research fields, and most of them either
830	support decision support systems or usage and benefits of the SST products are
831	emerging.
832	Overall, most of the SST products are well documented and user friendly. As we
833	mentioned before, this scoring does not judge the scientific quality of the SST
834	product. However, the low scoring of some products might give data providers
835	important information to improve the documentation of their products in order to
836	make the product more user friendly.
837	
838	5. Summary of evaluations
839	Sea Surface Temperature (SST) is an essential climate variable (ECV) to assess the
840	state of the global climate system and monitor its variations on interannual and
841	(multi)decadal timescales. Accurate SST observations at high spatial and temporal

842	resolution over a long-term period are needed to evaluate the present state of the
843	oceans and the impact of global surface warming.
844	In this report, eight different SST datasets have been analyzed and intercompared
845	for the overlapping period from 2003-2018. The ESA CCI SST v.2.1 and ERA5
846	reanalysis are available through the C3S Climate Data Store while the remaining six
847	datasets (OSTIA, HadISST1, NOAA Daily OISST, MUR, MGDSST, BoM) are provided
848	outside the CDS. All these datasets provide global gap-free (optimally interpolated)
849	SST maps but at different spatial and temporal resolutions. Then, to be comparable,
850	all the datasets have been gridded to a common grid (i.e., $1^{\circ}x1^{\circ}$) and averaged to a
851	common temporal frequency (i.e., monthly) over the overlapping period from 2003
852	to 2018. Finally, the average of the median of all the datasets (namely, the Ensemble
853	median) has been defined in order to analyze differences among these datasets.
854	In general, all the SST datasets show consistent climatological spatial patterns
855	(section 3.2). The global monthly mean and anomaly SST time series of these
856	datasets show very good agreement. When compared to the Ensemble median,

857	higher differences (in terms of mean difference, root-mean-square difference and
858	correlation) are found in correspondence to the main current systems, such as the
859	Gulf Current, the Kuroshio Current and the Antarctic circumpolar current. These
860	discrepancies can be<u>are</u> due to the different retrieval methods used to derive the
861	spatially-complete SST analyses. Differences can originate from several factors:
862	interpolation technique and related configuration (e.g. observation/background error
863	correlation scales), interpolation grid size, input data bias-correction and, if present,
864	the correction applied to obtain the foundation temperature or the temperature at
865	0.2 m. As an example, OSTIA, MUR25, MGDSST and ERA5 (via OSTIA from 2007
866	onwards) are the only L4 analyses included in the study that ingested microwave SST
867	data. Since these datasets (OSTIA, MUR25, MGDSST and ERA5) would ingest possibly
868	cooler daytime SST observations over cloudy regions, they may therefore exhibit
869	slightly cooler biases after 2002 compared with the other analyses that ingest only
870	infrared SST observations and in situ data. This effect may be offset in some
871	analyses, such as BoM Monthly and NOAA Daily OISST v2.1, where in situ data at 0.2 $$
872	m to several meters depth are used to bias-correct the infrared AVHRR SST data.

873 However, on average, the Taylor diagram confirms the very close similarity between

the different datasets.

875	All the datasets reproduce very similar spatial patterns of global SST trends (section
876	3.3). In addition, global mean warming trends as estimated from all the datasets are
877	consistent (within the 95% confidence interval) with the global ocean warming trend
878	as reported in the last IPCC report, estimated at 0.011 °C/year from 1980 to 2005.
879	The linear trend s in different basins show <u>s</u> that the main contributor from 2012 to
880	2018 is the Pacific Ocean.

881

882	The global mean SST time series for the whole period originally covered by all the
883	SST products reveals that the disagreement between all SST products is larger in the
884	early period (1982-2002) of the satellite era during which fewerless observations are
885	available compared to the later period (2003-2018) of the satellite era. Specifically,
886	the difference between each ensemble member and the ensemble median ranges
887	from 0.03°C to 0.26°C during the early period (1982-2002) and from 0.01°C to 0.1°C

888	during the later period (2003-2018), respectively. It indicates that the observations
889	ingested into \underline{each} the SST analysis plays a significant role in constraining the SST
890	climatology. The Satellite sensor improvements in the satellite (e.g., the
891	launchoperation of AMSR-EOS in 2002 that could measure ocean brightness of
892	temperatures through clouds) is another important factor affectingon the SST quality
893	after 2003. Noted that the impact of natural variability on SST climatology is
894	embedded in the analysis, that is, it is difficult to differentiate from the constraint of
895	SST observations on the SST climatology. Additionally, the discrepancy between each
896	product due to algorithms, observations ingested etc. is very small compared to the
897	significant warming trends shown in the linear trends and time series.
898	
899	Finally, the tropical Pacific region has been selected, as a test case, to assess the
900	capability of the different SST products, with a longer common temporal period, to
901	capture the main modes of variability of a well-known climate oscillatory mode <u>i</u> e.g.
902	the El Niño Southern Oscillation (ENSO). This analysis confirmed the close similarity
 903	of all the five datasets selected and their capability to reproduce, in the same way,

904	the main components of the tropical Pacific region space and time variability at time
905	scales compatible with the length of the selected time series.
906	
907	The maturity matrix score of all SST products (Table 2), that aims to demonstrate the
908	maturity of data documentation during the life cycle of one product, shows that
909	most of SST products are user friendly and provide sufficient information. Low scores
910	of some SST products (Table 2) , which do not indicate low scientific quality of the
911	dataset, but showsindicate a direction where data providers could improve their
912	products in terms of data documentation, storage and dissemination for users.
913	Thanks to the Group for High Resolution SST (GHRSST) effort, all GHRSST products
914	are well documented for their uncertainty characteristics (GHRSST Science Team,
915	2012).

917 6. Recommendations to users

918	All the datasets presented here provide state-of-the-art spatially-complete SST
919	products at the global scale. These datasets are characterized by different spatial
920	and temporal resolutions and temporal coverage that can fulfil the requirements of
921	a large variety of users.
922	Intercomparison results and a test case analysis suggest these datasets provide an
923	accurate representation of the SST spati <mark>gal</mark> -temporal variability. These datasets can
924	then be used for fundamental climate applications compatible with the length of
925	each time series, such as long-term monitoring of SST changes (e.g., trends) and
926	comparison to or initialization of numerical models. Other target applications include
927	the use of these datasets in the definition of climatic indices, assessment and
928	monitoring of weather extreme events (including marine heatwaves) and their
929	impact on marine ecosystem, and related services.

931	In this study we have interpolated all SST products into 1 degree and monthly
932	frequency in order to facilitate intercomparison studies. However, to understand
933	which dataset is suitable for specific case studies where spatial and/or temporal
934	resolution are critical, such as the separation of the Gulf Stream and the diurnal
935	cycle of the SST products, specific intercomparison studies are required. Indeed, in
936	the framework of the GHRSST intercomparison team, several <u>such</u> intercomparison
937	tasks are ongoing and scientific findings will be available in the near future.
938	
939	Finally, users are strongly encouraged to consider also the type of SST offered by

each producer<u>and to</u>r distinguish between, e.g., skin SST, subskin or SSTdepth, and foundation SST according to the specific application for which the data are meant intended to be used. For example, <u>skin SST_in conditions of high insolation and low</u> surface ocean mixing skin SST is-strongly impacted by diurnal warmingcontains diurnal cycle_-but-SST at 0.2 m depth somewhat impacted, SSTdepth_below 1 m minimally impacted and foundation SST <u>has no diurnal signaturedo not have the</u>

946	diurnal cycle involved (Gentemann et al., 2009; Minnett and Kaiser-Weiss, 2012). In
947	our study, we have used SSTdepth, foundation SST and SST at 0.2 <u>m depth,</u> which
948	appears to have had minor impacts on the interpretation of the results.

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- 956 Australian Bureau of Meteorology and are available on request from
- 957 http://www.bom.gov.au/climate/data-services/data-requests.shtml.
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960	with the	National	Aeronautics	and	Space	Administration	(80110018000	104).	ine

961 authors declare no conflict of interest.

962

963	Data	Availability	Statement
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964 The download website of all datasets used in this study has been included in the

965 manuscript in section 2.

966

- 967 Appendix
- P68 This section provides dDefensible traces for Maturity Matrix Score given to all SST
- products shown in Table 2 based on the guidance document
- 970 (https://confluence.ecmwf.int/display/CKB/Guidance+document+on+applying+the+M
- aturity+Matrix+as+part+of+the+Evaluation+and+Quality+Control) developed within
- 972 <u>the C3S independent assessment project (C3S_511).</u>
- 973

974 1. ESA-CCI SST

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975	Metadata 🔹		Formatted: Font: Not Bold, Underline
		\frown	Formatted: Left
976	Standard (Score: 6/6)		Formatted: Font: (Default) Times New Roman, Not Bold, Underline
			Formatted: Font: (Default) Arial, 11 pt, Font color: Black
977	The ESA CCI SST data files follow the GHRSST Data Specification v2.0 (GDS) and are		Formatted: Font: Not Bold
978 979 980 981	provided in NetCDF-4 format <u>CompactFlash (</u> CF <u>)</u> -1.5 compliant. Files specifications are fully detailed in the ESA CCI Product User Guide (PUG). The NetCDF files contain detailed metadata describing the data by means of global attributes, which are applicable to the whole file, and variable attributes, which apply to a specific data		
982 983	field.		
i			
984	Collection Level (Score: 6/6)		Formatted: Left
			Formatted: Font: (Default) Times New Roman
985	The ESA CCI SST data files follow the GHRSST Data Specification v2.0 (GDS). Global		Formatted: Font: Not Bold
986	attributes provide all information available on the data and relative references. In		
987	addition the Product Specification Document (PSD) with detailed information of		Formatted: Font: Not Bold
988	Metadata is available.		
989		/	Formatted: Font: Not Bold, Underline
		1	Formatted: Left
990	User Documentation		Formatted: Font: (Default) Times New Roman, Not Bold
I	65		

I		
991	Formal description of scientific methodology (Score: 6/6)	Formatted: Font: (Default) Arial, 11 pt, Font color: Black
992	The formal description of the ESA CCI SST product is detailed in the Algorithm	
993	Theoretical Background Document (ATBD), published by the data provider, which	Formatted: Font: Not Bold
994	describes and justifies the algorithms used for obtaining sea surface temperatureSST	
995	estimates. A synthesis of the formal ATBD is also available in the CDS. In addition,	
996	the ESA CCI SST dataset has been published in Nature Scientific Data (Merchant et	Formatted: Font: Not Bold
997	al., 2019).	
998	•	Formatted: Font: (Default) Times New Roman
		Formatted: Left
999	Formal validation report (Score: 6/6)	Formatted: Space After: 0 pt
1000	For the formal validation report of the ESA CCI SST L4 product users can refer to	Formatted: Font: (Default) Times New Roman
1001	Merchant et al. (2019), Product User Guide (PUG), and Climate Assessment Report	Formatted: Font: Not Bold
		Formatted: Font: Not Bold
1002	(CAR).	Formatted: Font: Not Bold
		Formatted: Font: (Default) Times New Roman
1003		
1004	Formal product user quide (Score: 6/6)	Formatted: Left
	· · · · · · · · · · · · · · · · · · ·	Formatted: Font: (Default) Arial, 11 pt, Font color: Black

1005	The formal product user guide ESA CCI SST product is published by the data	
1006	provider (PUG). A synthesis of the formal user product guide is also available in the	Formatted: Font: Not Bold
1007	CDS.	
1008	•	Formatted: Font: (Default) Times New Roman
		Formatted: Left
1009	Uncertainty Characterization	Formatted: Font: Not Bold, Underline
		Formatted: Font: (Default) Times New Roman, Not Bold. Underline
1010	Standards (Score: 6/6)	Formatted: Font: (Default) Arial 11 pt Font color: Black
1011	Uncertainty characterization follows the internationally agreed GHRSST standard	
1012	specifications, which are detailed in the GHRSST Data Specification v2.0 (GDS)	Formatted: Font: Not Bold
 1013 1014	document.	
1015	Validation (Score: 6/6)	Formatted: Left
		Formatted: Font: (Default) Times New Roman
1016	A detailed and comprehensive validation of the ESA CCI SST L4 product is provided	
1017	in the Product Product-User Guide (PLIG) Climate Assessment Report (CAR) and in	Formatted: Font: Not Bold
1017		Formatted: Font: Not Bold
1018	Merchant et al. (2019). The validation of the ESA CCI SST L4 product is based on	Formatted: Font: Not Bold
1019	different procedures, from automated and visual inspection to comparison of SST	
1020	data with co-located in situ measurements.	

1021 1022 Formatted: Left Uncertainty quantification (Score: 6/6) Formatted: Font: (Default) Times New Roman 1023 Uncertainty in the ESA CCI SST L4 data at each location (i.e., the analysed_sst field in the NETCDF file) is quantified and provided (i.e., in the analysis_error field) through 1024 1025 an analysis quality methodology. The methodology used to derive the uncertainty is 1026 Formatted: Font: Not Bold based on the optimal interpolation theory and described in the ATBD and PUG, Formatted: Font: Not Bold 1027 giving comprehensive information of validation of the quantitative uncertainty 1028 estimates and error covariance. 1029 Formatted: Left 1030 Automated Quality monitoring (Score: 6/6) Formatted: Font: (Default) Times New Roman 1031 The identification of valid observations for sea surface temperatureSST estimation and algorithms used in the preparatory preprocessing are described in the ATBD Formatted: Font: Not Bold 1032 Formatted: Font: Not Bold 1033 and PUG. Moreover, a confidence level on a scale 0 to 5 is provided for each SST as

1035 the highest confidence. Quality levels 4 and 5 should be used for climate

1034

a guality indicator, following the international GHRSST conventions. Five indicates

1036	applications. Automated check is implemented to valid the data quality (Merchant et		
1037	<u>al., 2019).</u>		
1038			
1039	Public access, feedback and update		Formatted: Font: Not Bold, Underline
1000			Formatted: Font: (Default) Times New Roman, Not
1040	Public Access/Archive (Score: 56/6)		Bold
		\rightarrow	Formatted: Font: (Default) Arial. 11 pt. Font color: Black
1041	The FSA CCLSST dataset v2.0 is available on the data provider's website. Detailed		Formatted: Font: Not Bold
1041	The LSA CCI SST dataset v2.0 is available on the data provider's website. Detailed	/ (
1042	information available in the PUG. However, the source code is not publically		Formatted: Font: Not Bold
1043	available.		
1044			
1045	Version (Score: 6/6)		Formatted: Font: (Default) Times New Roman
10.10		\sim	Formatted: Left
1046	The version is fully established by the data provider.		
1047			
1048	User feedback (Score: 6/6)		Formatted: Left
1010		-	Formatted: Font: (Default) Times New Roman
1049	The ESA CCI SST dataset v2.0 is also provided through the Copernicus Marine		
1050	Environment Monitoring Service (CMEMS) and is part of GHRSST. Within CMEMS, a		
1051	Multi-Year Product Quality Working Group is established with the aim of periodically		
	69		

1052	assessing the status of the CMEMS climate data records, including ESA CCI SST,	
1053	integrating users' needs and feedback. Feedback from users are also included in the	
1054	Climate Assessment Report (CAR). In addition, ESA CCI data provider provides an	Formatted: Font: Not Bold
1055	email contact to collect users' feedback.	
1056		
1057	Updates to record (Score: 6/6)	Formatted: Font: (Default) Times New Roman
		Formatted: Left
1058	Currently the ESA CCI SST dataset v2.0 covers the period from late-1981 to 2018.	
1059	Updates through to the near-present are expected this year (2020). Extensions are	
1060	expected to be produced by the Copernicus Climate Change Service (C3S) with only	
1061	~5 days delay to real time	
1062	·*	Formatted: Font: (Default) Times New Roman
10.00		Formatted: Left
1063	Usage	Formatted: Font: Not Bold, Underline
1064	Research (Score: 6/6)	Formatted: Font: (Default) Times New Roman, Not Bold, Underline
		Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1065	The ESA CCI SST dataset v.2.0 is very recent. However, it has already been used in	

1066 some research publications.

1068	Decision support system (Score: 6/6)		Formatted: Font: (Default) Times New Roman
10/0		Ą	Formatted: Left
1069	ESA-CCI SST is part of the ESA Climate Change Initiative, and one of the essential		
1070	climate variables. The objective of ESA-CCI SST is to establish a long term data		
1071	record to monitor the global climate system required by UNECCC (http://cci.esa.int/)		
10,11			
1072	for decision making.		
1073			
1075			
1074	2. ERA5 SST		Formatted: Font: Not Bold
			Formatted: Indent: Left: 0", First line: 0"
1075	Matadata		Formatted: Font: Not Bold
1075	Metadata		Formatted: Font: (Default) Times New Roman, Not Bold
1076	Standard (Score: 6/6)		Formatted: Font: Not Bold, Underline
1070			Formatted: Font: Italic
1077	ERA5 SST data can be downloaded from the CDS in both GRIB and NetCDF formats.		
1078	The native data format is GRIB, but they can be converted to NetCDF format		
1079	through the CDS. In NetCDF global attributes reference to CF-1.6 conventions is		
1080	made. This represents a mature state-of-the-art metadata standard according to		
1081	guidance.		
1082			
			Formatted: Font: Italic
1002	Collection Level (Score E/G)	1	Formatted: Left
1083			Formatted: Font: (Default) Times New Roman
	71		

1084	The standardized attributes on the collection level of the dataset are sufficient to		
1085	understand the data's origins without further documents, including standardized		
1086	information on how to obtain raw data and its preprocessing procedures.		Formatted: Font: (Default) Times New Roman
1087	Note: The collection level in this case includes the <u>ECMWF</u> confluence wikiconfluence		Formatted: Font: Not Bold
1088	wiki. (https://confluence.ecmwf.int/display/CKB/ERA5%3A+data+documentation)		
1089			
1090	User Documentation		Formatted: Font: Not Bold, Underline
1070		$\langle \rangle$	Formatted: Left
1091	Formal description of scientific methodology (Score—5 6/6)		Formatted: Font: (Default) Times New Roman, Not Bold
			Formatted: Font: Italic
1092	The scientific description is comprehensive and publicly available in the form of a $\begin{tabular}{c} \bullet \end{array}$	(Formatted: Left
1093	scientific report/ATBD <u>and elibrary of ECMWF</u> . The description is kept up to date		
1094	with the updated dataset. There is also a peer reviewed methodological journal		
1095	paper published.		Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1096	Note: In this case the confluence wiki is regarded as the scientific report/ATBD_and		Formatted: Font: Not Bold
1097	also elibrary of ECMWF.		Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1098		ſ	Formattad Foot: Holis
		1	
1099	Formal validation report (Score: 3/6)		Formatted: Len
		L	
I	72		

1100	There is no formal validation report for ERA5 SST. The ERA5 documentation available		
1101	at confluence wiki can be regarded as a user guide but does not have any clear		
1102	version number with a publication date and is a document that is changing. Due to		
1103	the nature of ERA5 being in development it makes sense to have an evolving		
1104	documentation, but the creation of a formal product validation report in the future		
1105	is recommended. An assessment report evaluating HadISST2 and OSTIA SST datasets		
1106	(from which ERA5 SST is built) is available (Hirahara 2016).		Formatted: Font: Not Bold
1107			
1108	Formal product user guide (Score 6/6)		Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman
1109	There is a regularly updated comprehensive formal Product User Guide (PUG) for the	Ì	Formatted: Left
1109	There is a regularly updated comprehensive formal Product User Guide (PUG) for the	Y	Formatted: Left
1109 1110	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available.		Formatted: Left Formatted: Font: (Default) Times New Roman
1109 1110 1111	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available.		Formatted: Left Formatted: Font: (Default) Times New Roman Formatted: Font: Not Bold
1109 1110 1111	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available. Note: In this case the confluence wiki is regarded as the Product User Guide (PUG).		Formatted: Left Formatted: Font: (Default) Times New Roman Formatted: Font: Not Bold
1109 1110 1111 1111	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available. Note: In this case the confluence wiki is regarded as the Product User Guide (PUG).		Formatted: Left Formatted: Font: (Default) Times New Roman Formatted: Font: Not Bold
1109 1110 1111 1112	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available. Note: In this case the confluence wiki is regarded as the Product User Guide (PUG).		Formatted: Left Formatted: Font: (Default) Times New Roman Formatted: Font: Not Bold
1109 1110 1111 1111 1112 1113	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available. Note: In this case the confluence wiki is regarded as the Product User Guide (PUG).		Formatted: Left Formatted: Font: (Default) Times New Roman Formatted: Font: Not Bold Formatted: Font: Not Bold, Underline
1109 1110 1111 1111 1112 1113	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available. Note: In this case the confluence wiki is regarded as the Product User Guide (PUG).		Formatted: Left Formatted: Font: (Default) Times New Roman Formatted: Font: Not Bold Formatted: Font: Not Bold, Underline Formatted: Left Formatted: Left Formatted: Font: (Default) Times New Roman Net
11109 11110 11111 11112 11113 11114	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available. Note: In this case the confluence wiki is regarded as the Product User Guide (PUG). Uncertainty Characterization		Formatted: Left Formatted: Font: (Default) Times New Roman Formatted: Font: Not Bold Formatted: Font: Not Bold, Underline Formatted: Left Formatted: Font: (Default) Times New Roman, Not Bold
11109 11110 11111 11112 11113 11114	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available. Note: In this case the confluence wiki is regarded as the Product User Guide (PUG). <u>Uncertainty Characterization</u> Standards <u>(Score 3/6)</u>		Formatted: Left Formatted: Font: (Default) Times New Roman Formatted: Font: Not Bold Formatted: Font: Not Bold, Underline Formatted: Left Formatted: Font: (Default) Times New Roman, Not Bold Formatted: Left Formatted: Left
11109 11110 11111 11112 11113 11114 11115	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available. Note: In this case the confluence wiki is regarded as the Product User Guide (PUG). Uncertainty Characterization Standards (Score 3/6) Uncertainty information follows standard nomenclature.		Formatted: Left Formatted: Font: (Default) Times New Roman Formatted: Font: Not Bold Formatted: Font: Not Bold, Underline Formatted: Left Formatted: Font: (Default) Times New Roman, Not Bold Formatted: Left Formatted: Left Formatted: Left Formatted: Font: (Default) Times New Roman, Underline
11109 11110 11111 11112 11113 11114 11115	There is a regularly updated comprehensive formal Product User Guide (PUG) for the dataset publicly available. Note: In this case the confluence wiki is regarded as the Product User Guide (PUG). Uncertainty Characterization Standards (Score 3/6) Uncertainty information follows standard nomenclature.		Formatted: Left Formatted: Font: (Default) Times New Roman Formatted: Font: Not Bold Formatted: Font: Not Bold, Underline Formatted: Left Formatted: Font: (Default) Times New Roman, Not Bold Formatted: Left Formatted: Font: (Default) Times New Roman, Underline

1116	Note: In this case the ensemble members are regarded as uncertainty measures.		Formatted: Font: Not Bold
1117			
1118	Validation (Score: 3/6)		Formatted: Font: Italic
1110		$\overline{\langle}$	Formatted: Font: (Default) Times New Roman
1110	A formal validation report of EDAE SST is not available. However, an accessment		Formatted: Left
1119	A formal validation report of EKAS SST is not available. However, all assessment		
1120	report evaluating HadISST2 and OSTIA SST datasets (from which ERA5 SST is built) is		
1121	available (Hirahara 2016), and users can refer to HadISST2 and OSTIA		Formatted: Font: Not Bold
1122	documentation.		
1123			
1125			
1124	Uncortainty quantification (Score 2/6)		Formatted: Font: Italic
1124		$\langle \cdot \rangle$	Formatted: Font: (Default) Times New Roman
			Formatted: Left
1125	A comprehensive uncertainty quantification of systematic and random effects is		
1126	available.		Formatted: Font: (Default) Times New Roman
1127	Note: In this case the ensemble members are regarded as uncertainty measures.		Formatted: Font: Not Bold
1128			
1129	Automated quality monitoring (Score 2/6)		Formatted: Font: Italic
		\bigtriangledown	Formatted: Left
1130	There is no automated quality monitoring documented for the dataset		Formatted: Font: (Default) Times New Roman
1.50			Formatted: Font: (Default) Times New Roman

1131	Note: Although there is no automated quality monitoring documented, data	Formatted: Font: Not Bold
1132	assimilation itself could be regarded as a quality check.	
1122		
1133	•	Formatted: Font: (Default) Times New Roman
1134	Public access feedback and undates	Formatted: Left
1154		Formatted: Font: Not Bold, Underline
1135	Access and Archive (Score 5 6 /6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman,
1136	The dataset is publicly available. The different versions of data including	Undernine
1137	documentation and source code is archived by the data provider. Source code is not	
1138	publically available.	
1139		
1140	Version Control (Score 6/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1141	There is full information on version control of documentation, data and/or metadata	Formatted: Left
1142	available for the dataset. The documented version control information is fully	
1143	traceable from the files.	Formatted: Font: (Default) Times New Roman
_		
1144	Note: In this case the version control is referring to the confluence wiki.	Formatted: Font: Not Bold
 1145		
1175		
11/16	User Feedback (Score 6/6)	Formatted: Font: Italic
1140	OSCI TECADACK (SCOTE 0/0)	Formatted: Font: (Default) Arial, 11 pt, Font color: Black

1147	There is a public reach-out/feedback form/contact point for collecting feedback for	
1148	the dataset. There are regular events, groups, 2-way feedback mechanisms, etc.	
1149	organized by the data provider. The established feedback fed back into data	
1150	production is documented, including third party international data quality	
1151	assessment results.	
1152		
11.50	Undeter to Departd (Cooke (16)	Formatted: Font: Italic
1155		Formatted: Left
		Formatted: Font: (Default) Arial. 11 pt. Font color: Black
1155	availability of input data and including improved methodology.	
1156	۸	Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1157	Usage	Formatted: Font: Not Bold, Underline
		Formatted: Left
1158	Research (Score: 3/6)	Formatted: Font: (Default) Times New Roman, Not Bold, Underline
		Formatted: Font: Italic
1159	Although ERA5 reanalysis has been largely used in many research publications, it	Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1160	seems that there are few relevant publications based on ERA5 SST data (as e.g.	
1161	Wang et al., 2020). This could arise from the prevalent use of ERA5 in atmospheric	Formatted: Font: Not Bold
1162	research.	

1163 Formatted: Font: Italic 1164 Decision support system (Score: 1/6) Formatted: Font: (Default) Times New Roman Formatted: Left 1165 To the evaluators' knowledge the product is not used yet for the decision support 1166 system. this DSS. 1167 Formatted: Font: (Default) Times New Roman Formatted: Left 1168 OSTIA SST 3. Formatted: Font: Not Bold Formatted: Font: Not Bold 1169 Formatted: Font: (Default) Times New Roman, Not Metadata Bold Formatted: Left, Indent: Left: 0", First line: 0" 1170 Standard (Score: 6/6) Formatted: Left Formatted: Font: Not Bold, Underline Formatted: Font: (Default) Arial, 11 pt, Not Bold, Font The OSTIA SST data files are provided in NetCDF-4 format CF-1.5 compliant through 1171 color: Black Formatted: Font: Italic 1172 Copernicus Marine Environment Monitoring Service (CMEMS) and the Formatted: Font: (Default) Arial, 11 pt, Font color: Black Recommended GHRSST Data Specification (GDS)-. File specifications are fully 1173 1174 detailed in the OSTIA Product User Manual (PUM) available in CMEMS. The NetCDF

- 1175 files contain detailed metadata describing the data by means of global attributes,
- 1176 which are applicable to the whole file, and variable attributes, which apply to a
- 1177 specific data field.
- 1178

1179	Collection Level (Score: 6/6)	\sim	Formatted: Font: Italic
		$\langle \rangle$	Formatted: Left
1180	Global attributes provide all information available on the data and relative		Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1181	references. In addition the Product User Manual (PUM,) with detailed information on		
1182	Metadata is available.		
1183			
1184	User Documentation	\sim	Formatted: Font: Not Bold, Underline
1.0.		$\langle \rangle$	Formatted: Left
1185	Formal description of scientific methodology (Score: 6/6)		Formatted: Font: (Default) Times New Roman, Not Bold
			Formatted: Font: Italic
1186	The formal description of the OSTIA product is detailed in the peer-reviewed paper		Formatted: Font: (Default) Times New Roman
1187 1188	(Good et al., 2020), published by the data provider, which describes and justifies the algorithms used for obtaining sea surface temperature <u>SST</u> estimates. A synthesis of		
1189	the Product User Manual (PUM) is also available in the CMEMS.		
1190			
1191	Formal validation report (Score: 6/6)	5	Formatted: Font: Italic
			Formatted: Left
1192	For the formal validation report of the OSTIA product users can refer to the Quality		Formatted: Font: (Default) Times New Roman
1193	Information Document (QUID) available in the CMEMS service.		
1194		\sim	Formatted: Font: (Default) Times New Roman
-			Formatted: Left
	78		
1195	Formal product user quide (Score: 6/6)		Formatted: Font: Italic
------	--	---	---
			Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1196	The formal product user guide OSTIA product is published by the data provider		
1197	(PUM) as a peer-reviewed journal article Good et al. (2020). A synthesis of the forma		
1198	user product guide (PUM) is also available in the CMEMS.		
1199			
1200	Uncertainty Characterization	•	Formatted: Font: Not Bold, Underline
			Formatted: Left
1201	Standards (Score: 6/6)	_	Formatted: Font: (Default) Times New Roman, Not Bold
			Formatted: Font: Italic
1202	Uncertainty characterization follows the internationally agreed GHRSST standard		Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1203	specifications, which are detailed in the GHRSST Data Specification v2.0 (GDS)		Formatted: Font: Not Bold
1204	document (GHRSST Science Team, 2012).		
1205			
1206	Validation (Score: 6/6)	•	Formatted: Font: Italic
1207	A validation of the OSTIA product is provided in <u>the</u> Quality Information Document		Formatted: Left Formatted: Font: (Default) Times New Roman
1208	through CMEMS. The validation of the OSTIA SST product is based on comparison		
1209	of SST data with co-located in situ measurements.		

1211	Uncertainty quantification (Score: 6/6)		Formatted: Font: Italic
		\frown	Formatted: Left
1212	Uncertainty in the OSTIA data at each location (i.e., the analysed_sst field in the		Formatted: Font: (Default) Times New Roman
1213	NETCDF file) is quantified and provided (i.e., in the analysis_error field) through an		
1214	analysis quality methodology. The methodology used to derive the uncertainty is		
1215	produced using a special "observation influence" analysis (Good et al., 2020).	/	Formatted: Font: (Default) Times New Roman
1216			
1217	Automated Quality monitoring (Score: 6/6)	<	Formatted: Font: Italic Formatted: Left
1218	Automatic quality is monitored during the production of the SST product. The real-		Formatted: Font: (Default) Times New Roman
1219	time OSTIA SST analysis is routinely validated by the UK MetOffice against the		
1220	GHRSST Multi-product ensemble (http://ghrsst-pp.metoffice.gov.uk/ostia-		
1221	website/gmpe-monitoring.html) and Argo SST (http://ghrsst-		
1222	pp.metoffice.gov.uk/ostia-website/gmpe-argo-stats.html).	/	Formatted: Font: (Default) Times New Roman
 1223			
1024	Public access feedback and undate		Formatted: Font: Not Bold, Underline
1224		<	Formatted: Left
1225	Public Access/Archive (Score:-6 5/6)		Formatted: Font: (Default) Times New Roman, Not Bold
		$\langle \rangle$	Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman

1226	The OSTIA SST is available on <u>the CMEMS</u> website. Detailed information available in		
1227	the PUM. However, the source code is not publically avaiable.		
1228			
1229	Version (Score: 6/6)		Formatted: Font: Italic
122)		$\langle \rangle$	Formatted: Left
			Formatted: Font: (Default) Times New Roman
1230	The version is fully established by the data provider.		Formatted: Font: (Default) Times New Roman
1231			
1232	User feedback (Score: 6/6)	\checkmark	Formatted: Font: Italic
		\leq	Formatted: Left
1233	The OSTIA is provided through the Copernicus Marine Environment Monitoring	J	Formatted: Font: (Default) Times New Roman
1234	Service (CMEMS) and is part of GHRSST. Within CMEMS, a Multi-Year Product		
1235	Quality Working Group is established with the aim of periodically assessing the		
1236	status of the CMEMS data records, including OSTIA, integrating users' needs and		
1237	feedback.		
1238			
1239	Undates to record (Score: 6/6)		Formatted: Font: Italic
1237		$\langle \cdot \rangle$	Formatted: Left
1			Formatted: Font: (Default) Times New Roman

1240	Currently the OSTIA SST dataset covers the period from late-1981 to 2018. Updates	
1241	through to the near-present are expected this year (2020). Extensions are expected	
1242	to be produced by the CMEMS with only \sim 5 days delay to real time	
1243		
1044		Formatted: Font: Not Bold, Underline
1211		Formatted: Left
1245	Research (Score: 6/6)	Formatted: Font: (Default) Times New Roman, Not Bold
	· · · · · · · · · · · · · · · · · · ·	Formatted: Font: Italic
1246	The <u>current version of OSTIA SST</u> is very recent. However, it has already been used	Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1247	in some research publications.	Formatted: Font: (Default) Times New Roman
1248		
1249	Decision support system (rScore: 6/6)	Formatted: Font: Italic
		Formatted: Left
1250	OSTIA SST is part of the CMEMS project and the information derived from SST	Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1251	products is used in the CMEMS ocean state report for decision makingers.	
1252		
1232		Formatted: Font: Not Bold
.h		Formatted: Font: Not Bold
1253	4. BOM	Formatted: Font: Not Bold, Underline
		Formatted: Left
1254	Metadata	Formatted: Font: (Default) Times New Roman, Not Bold, Underline
1055	Standard (Score: 616)	Formatted: Font: Italic
1233		Formatted: Font: (Default) Times New Roman

1256	The BoM SST files are provided in the GHRSST Data Specification version 1.7 NetCDF		
1257	classic format CF-1 (Beggs and Pugh, 2009) on request from the data providers. The		
1258	NetCDF files contain detailed metadata describing the data by means of global		
1259	attributes, which are applicable to the whole file, and variable attributes, which apply		
1260	to a specific data field.		
1261		F	Formatted: Font: (Default) Times New Roman
	•	F	Formatted: Left
1262	Collection Level (Score: 5/6)	F	Formatted: Font: Italic
		F	Formatted: Font: (Default) Times New Roman
1263	Global attributes provide all information available on the data and relative		
1264	references. However, the reference shown in the Metadata (Beggs and Pugh, 2009) is		
1265	not accessible at the moment of writing this report although it is available by		
1266	request from library@bom.gov.au.	F	Formatted: Font: (Default) Times New Roman
1267			
12.68	User Documentation	F	Formatted: Font: Not Bold, Underline
		F	Formatted: Font: (Default) Times New Roman, Not Sold, Underline
1269	Formal description of scientific methodology (Score: 4/6)		Formatted: Font: Italic
		F	Formatted: Font: (Default) Times New Roman
1270	The formal description of the BoM Monthly OI SST is published in a conference		
1271	paper (Smith et al., 1999) and a peer-reviewed paper (Beggs et al., 2011), however		



1289	Pugh, 2009). However, (Beggs and Pugh, 2009) is not accessible at the moment of		
1290	writing this report although it is available by request from library@bom.gov.au.		
1291	However, the product user guide is not up to date for the current version of the SST		
1292	we have used.		
1293			
1294	Uncertainty Characterization		Formatted: Font: Not Bold, Underline
		F	Formatted: Font: (Default) Times New Roman, Not Bold
1295	Standards (Score: 6/6)		Formatted: Left
		$\overline{\ }$	Formatted: Font: Italic
1296	Uncertainty characterization follows the internationally agreed GHRSST standard		Formatted: Font: (Default) Times New Roman
1297	specifications (analysis_error), which are detailed in the GHRSST Data Specification		
1298	v2.0 (GDS) document (GHRSST Science Team, 2012).		Formatted: Font: Not Bold
			Formatted: Font: (Default) Times New Roman
1299			
1300	<i>Validation</i> (Score: 5 3 /6)		Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman
1301	No validation report is found for BoM SST. However, BoM is part of the GHRSST		
1302	community and intercomparison activities of the BoM Daily Global SST analyses have		
1303	been performed in the framework of GHRSST (Dash et al., 2011; Martin et al., 2011).		
1304	Although routine verification of the BoM Global Daily 0.25 degree OI SST analysis		

1305	(GAMSSA) are performed by UK MetOffice (http://ghrsst-pp.metoffice.gov.uk/ostia-		
1306	website/gmpe-argo-stats.html) and NOAA/NESDIS/STAR		
1307	(https://www.star.nesdis.noaa.gov/socd/sst/squam/analysis/l4), there are no routine		
1308	verifications of the BoM Monthly or Weekly OI SST analyses.		Formatted: Font: (Default) Times New Roman
1309			
1310			Formatted: Font: (Default) Times New Roman
1311	Uncertainty quantification (Score: 6/6)		Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman
1312	Uncertainty in the BoM data at each location (i.e., the analysed_sst field in the		
1313	NETCDF file) is quantified and provided (i.e., in the analysis_error field) through an		
1314	analysis quality methodology (Beggs et al., 2011).		
1315			
1316	Automated Quality monitoring (Score: 1/6)		Formatted: Font: Italic
			Formatted: Left
1817	No Automatic quality is provided		Formatted: Font: (Default) Times New Roman
1017		(1	Formatted: Font: (Default) Times New Roman
1318			
1319	Public access feedback and update		Formatted: Font: Not Bold, Underline
			Formatted: Font: (Default) Times New Roman, Not Bold, Underline
1320	Public Access/Archive (Score: 4/6)		Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman
1		<u> </u>	

1321	BoM Monthly SST product is available on request from the data provider website for		
1322	both real-time and archived GHRSST L4 files.		Formatted: Font: (Default) Times New Roman
1323			
1324	Version (Score: 2/6)		Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman
1325	No information is found for the version control for BoM SST.		
1326	•	•	Formatted: Font: (Default) Times New Roman
			Formatted: Left
1327	User feedback (Score: 3/6)		Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman
1328	Data providers collect and evaluate feedback from the scientific community through		
1329	the data provider's website, but no feedback mechanisms set up from data		
1330	providers		Formatted: Font: (Default) Times New Roman
1331			
1332	Undates to record (Score: 5/6)	•	Formatted: Font: Italic
100-			Formatted: Left
1333	BoM Daily, Weekly and Monthly SST analyses are published in real time for climate		Formatted: Font: (Default) Times New Roman
1334	monitoring on the BoM website.		Formatted: Font: (Default) Times New Roman
1005			
1335			Formatted: Font: Not Bold Underline
1336	Usage		Formatted: Font: (Default) Times New Roman, Not Bold, Underline
100-			Formatted: Font: Italic
1337	Kesearch (Score: 4/b)		Formatted: Font: (Default) Times New Roman

1338	The BoM Weekly and Monthly SST analyses have been used by the BoM for		
1339	research, especially climate studies.		Formatted: Font: (Default) Times New Roman
1340			
1341	Decision support system (Score: 6/6)		Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman
1342	BoM Monthly SST is an operational SST analysis which serves for climate monitoring		Formatted: Left
1343	that is an essential service of the Australian Government Bureau of Meteorology.		
1344			
1345	5. MGDSST		Formatted: Font: Not Bold
			Formatted: Font: Not Bold
1346	Metadata		Formatted: Font: Not Bold, Underline
		$\langle \rangle$	Formatted: Left
1347	Standard (Score: 3/6)		Formatted: Font: (Default) Times New Roman, Not Bold, Underline
			Formatted: Font: Italic
1348	The MGDSST is provided in the txt format and variable attributes are limited.		Formatted: Font: (Default) Times New Roman
1349			
1350	Collection Level (Score: 2/6)	\checkmark	Formatted: Font: Italic
		$\langle \rangle$	Formatted: Left
1351	There is limited information about standard attributes, but extra information		Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1352	published in the data provider's website is needed to use and understand the data.		
1853			Formatted: Font: (Default) Times New Roman
1000	۸	\frown	Formatted: Left
·	88		

1354	User Documentation	Formatted: Font: Not Bold, Underline
		Formatted: Font: (Default) Times New Roman, Not Bold, Underline
1355	<i>Formal description of scientific methodology</i> (Score: <u>3</u> 4/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1356	Limited information is provided on the data provider's website, but the method is	
1357	documented in two non peer-reviewed reports	
1358		
1359	Formal validation report (Score: 4/6)	Formatted: Font: Italic
		Formatted: Left
1360	No JMA validation report is found for MGDSST at the time of writing this report.	Formatted: Font: (Default) Times New Roman
1361	However, MGDSST was compared with other SST analyses and independent	
1362	observations in Martin et al. (2012) and Fiedler et al. (2019a) for the periods 2010	
1363	and 1992 to 2011. The UK MetOffice routinely compares MGDSST with the GHRSST	
1364	Multi-product ensemble (http://ghrsst-pp.metoffice.gov.uk/ostia-website/gmpe-	
1365	monitoring.html) and Argo SST (http://ghrsst-pp.metoffice.gov.uk/ostia-	
1366	website/gmpe-argo-stats.html).	
1367	•	Formatted: Font: (Default) Times New Roman
		Formatted: Left
1368	Formal product user guide (Score: 3/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1869	Limited product user guide from the data provider.	Formatted: Font: (Default) Times New Roman

1370		
1371	Uncertainty Characterization	Formatted: Font: Not Bold, Underline
		Formatted: Font: (Default) Times New Roman, Not Bold
1372	Standards (Score: 1/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1373	No information is available at this stage.	
1374	•	Formatted: Font: (Default) Times New Roman
		Formatted: Left
1375	Validation (Score: 6/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1376	MGDSST is part of the GHRSST and intercomparison with other SST products has	
1377	been performed and published in peer-review journals (Fiedler et al., 2019a; Martin	
1378	et al., 2012).	Formatted: Font: (Default) Times New Roman
1379		
1380	Uncertainty quantification (Score: 1/6)	Formatted: Font: Italic
1000		Formatted: Font: (Default) Times New Roman
1381	No uncertainty quantification is found.	
1382	•	Formatted: Font: (Default) Times New Roman
		Formatted: Left
1383	Automated Quality monitoring (Score: 2/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1384	No automatic quality is monitored during the production of the SST product.	Formatted: Font: (Default) Times New Roman
1385		
1386	Public access, feedback and update	Formatted: Font: Not Bold, Underline
		Formatted: Font: (Default) Times New Roman, Not Bold, Underline

1887	Public Access/Archive (Score: 4/6)	Formatted: Font: Italic
1007		Formatted: Font: (Default) Times New Roman
1388	The MGDSST is publicly accessible from the data provider's website and brief	
1389	information of the data is provided in the data provider's website.	Formatted: Font: (Default) Times New Roman
1390		
1391	Version (Score: 2/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1392	No information is found for the version control.	Formatted: Font: (Default) Times New Roman
1393		
1394	User feedback (Score: 3/6)	Formatted: Font: Italic
1074		Formatted: Font: (Default) Times New Roman
1395	Data providers collect and evaluate feedback from the scientific community through	
1396	the data provider's website.	Formatted: Font: (Default) Times New Roman
1397		
1398	Updates to record (Score: 4/6)	Formatted: Font: Italic
		Formatted: Left
1399	MGDSST is published in real time for climate monitoring and Numerical Weather	Formatted: Font: (Default) Times New Roman
1400	Prediction on the data provider's website.	Formatted: Font: (Default) Times New Roman
1401		Formatted: Font: (Default) Times New Roman
101	<u>۸</u>	Formatted: Font: Not Bold. Underline
1402	Usage	Formatted: Font: (Default) Times New Roman, Not Bold, Underline
1402	Pacaarch (Copro: 6/6)	Formatted: Font: Italic
1403		Formatted: Font: (Default) Times New Roman

1404	The data has already been used in some research publications.	
1405		
1406	Decision support system (Score: 6/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1407	MGDSST is an operational SST analysis which serves for climate monitoring and	Formatted: Left
1408	Numerical Weather Prediction that is an essential service of the Japanese	
1409	Meteorological Agency (JMA).	Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1410		
1411		Formatted Font: Not Pold
1411	b. MUK25	Formatted, Indenty Lefty 0"
		Formatted: Indent: Left: 0
1412	Metadata	Formatted: Font: Not Bold
		Bold
1/13	Standard (Score: 6/6)	Formatted: Font: Not Bold, Underline
1415		Formatted: Left
 1414	The MUR25 SST is provided in NetCDF format. The NetCDF files contain detailed	Formatted: Font: (Default) Times New Roman, Not Bold, Underline
		Formatted: Font: Italic
1415	metadata describing the data by means of global attributes, which are applicable to	Formatted: Font: (Default) Times New Roman
1416	the whole file, and variable attributes, which apply to a specific data field.	
1417	<u>ــــــــــــــــــــــــــــــــــــ</u>	Formatted: Left
		Formatted: Font: (Default) Times New Roman
1418	Collection Level (Score: 6/6)	Formatted: Font: Italic
1		

1419 Global attributes provide all information available on the data and relative

1420 references.

1421	•	Formatted: Font: (Default) Times New Roman
		Formatted: Left
1422	User Documentation	Formatted: Font: Not Bold, Underline
1423	Formal description of scientific methodology (Score: 6/6)	Formatted: Font: (Default) Times New Roman, Not Bold, Underline
1+23		Formatted: Font: Italic
1424	The formal description of the MUR25 product is detailed in the peer-reviewed	Formatted: Font: (Default) Times New Roman
1425	iournal (Chin et al., 2017), published by the data provider.	Formatted: Font: Not Bold
		Formatted: Font: (Default) Times New Roman
1426		
1427	<i>Formal validation report</i> (Score: 4 3 /6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1428	No formal validation report is available, however, the validation is performed in the	
1429	peer-reviewed paper (Chin et al., 2017). Additional validation of the 1km product	Formatted: Font: Not Bold
1430	occurred with direct comparisons with the Saildrone autonomous vehicle with $\frac{\mathrm{the}}{\mathrm{the}}$	
l 1431	published article. The validation focused on an exemplary coastal area, the	
1432	California/Baja Coast.	
1433	•	Formatted: Font: (Default) Arial, 11 pt, Font color: Black
		Formatted: Left
1434	Formal product user guide (Score: 2/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1	No formal product user quide is available for MUR25 SST	

1436		
1437	Uncertainty Characterization	Formatted: Font: Not Bold, Underline
		Formatted: Font: (Default) Times New Roman, Not Bold, Underline
1438	Standards (Score: 6/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1439	Uncertainty characterization follows the internationally agreed GHRSST standard	
1440	specifications, which are detailed in the GHRSST Data Specification v2.0 (GDS)	Formatted: Font: Not Bold
1441	document.	Formatted: Font: (Default) Times New Roman
1442		
1443	Validation (Score: 6/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1444	Intercomparison of MUR25 has been performed in the framework of GHRSST.	Formatted: Font: (Default) Times New Roman
1445		
1446	Uncertainty quantification (Score: 6/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
l 1447	Uncertainty in the MUR25 data at each location (i.e., the analysed_sst field in the	
1448	NETCDF file) is quantified and provided (i.e., in the analysis_error field) through an	
1449	analysis quality methodology.	
1450	•	Formatted: Font: (Default) Times New Roman
		Formatted: Left
1451	Automated Quality monitoring (Score: 4/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman

1452	No automatic quality monitoring is found for MUR25 SST product, but the 1 km		
1453	resolution version of the MUR SST analysis is routinely validated with the GHRSST		
1454	Multi-product ensemble (http://ghrsst-pp.metoffice.gov.uk/ostia-website/gmpe-		
1455	monitoring.html; https://www.star.nesdis.noaa.gov/socd/sst/squam/analysis/l4). Since		
1456	Argo SST are ingested into MUR25 they are not useful for verification.		Formatted: Font: (Default) Times New Roman
1457			
1458	Public access, feedback and update		Formatted: Font: Not Bold, Underline
			Formatted: Font: (Default) Times New Roman, Not Bold, Underline
1459	Public Access/Archive (Score: <u>5</u> 6 /6)	<	Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman
1460 1461	The MUR25 SST is published in the data provider's archive center. <u>However, source</u> code is not publically available.		
1462	۸		Formatted: Font: (Default) Times New Roman
1462	Version (Score: 6/6)		Formatted: Font: Italic
1405		$\left<$	Formatted: Left
1464	The version is fully established by the data provider.		Formatted: Font: (Default) Times New Roman
1465	*		Formatted: Loft
100	•		Formatted: Font: (Default) Times New Roman
1466	User feedback (Score: 6/6)		Formatted: Font: Italic
	A	\leq	Formatted: Font: (Default) Times New Roman
1467	Public contact information is given in the data provider's website for users to give		
1468	feedback. Users can give all feedback through the Physical Oceanography		

1469	Distributed Active Archive Center (PO.DAAC) user services and forum. All feedback	
1470	is publicly available.	
1471		
1472	Undates to record (Score: 5/6)	Formatted: Font: Italic
1,2		Formatted: Left
1473	Regular updates are available from the data provider. There is no immediate	Formatted: Font: (Default) Times New Roman
1474	production of interim data products.	
1475		Formatted: Font: (Default) Times New Roman
		Formatted: Left
1476	Usage	Formatted: Font: Not Bold, Underline
1477	Research (Score: 6/6)	Formatted: Font: (Default) Times New Roman, Not Bold, Underline
		Formatted: Font: Italic
1478	The MUR25 is used in research in multiple fields.	Formatted: Font: (Default) Times New Roman
1479		
1480	Decision support system (Score: 3/6)	Formatted: Font: Italic
		Formatted: Left
1481	No decision support system is found for MUR25 SST, however use is occurring and	Formatted: Font: (Default) Times New Roman
1482	benefits are emerging.	
1483		
1484	7. NOAA Daily OISSTv2.1 SST	Formatted: Font: Not Bold
		Formatted: Font: Not Bold
I		

1485	Metadata	Formatted: Font: Not Bold, Underline
		Formatted: Left
1486	Standard (Score: 6/6)	Formatted: Font: (Default) Times New Roman, Not Bold, Underline
		Formatted: Font: Italic
1487	The NOAA Daily OISST data files are provided in NetCDF-4 format CF-1.0 compliant	Formatted: Font: (Default) Times New Roman
1488	data provider's website. The NetCDF files contain detailed metadata describing the	
1489	data by means of global attributes, which are applicable to the whole file, and	
1490	variable attributes, which apply to a specific data field.	
1491		Formatted: Font: (Default) Arial 11 nt Font color: Black
		Formatted: Left
1492	Collection Level (Score: 6/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1493	Global attributes provide all information available on the data and relative	
1494	references.	
1495	•	Formatted: Font: (Default) Times New Roman
		Formatted: Left
1496	User Documentation	Formatted: Font: Not Bold, Underline
1497	Formal description of scientific methodology (Score: 6/6)	Formatted: Font: (Default) Times New Roman, Not Bold, Underline
1477		Formatted: Font: Italic
1498	The formal description of the NOAA Daily OISST v2.1 is provided in the data	Formatted: Font: (Default) Times New Roman
1499	provider's website (https://www.ncdc.noaa.gov/oisst), third party data resource	
1500	website (https://podaac.ipl.nasa.gov/dataset/AVHRR_OI-NCEI-L4-GLOB-v2.1) and is	

1501	also detailed in several peer-reviewed papers (Reynolds et al., 2007; Banzon et al.,		
1502	2016; Huang et al., 2020), published by the data provider, which describe and justify		
1503	the algorithms used for obtaining sea surface temperatureSST estimates.		
1504			
1505	Formal validation report (Score: 6/6)		Formatted: Font: Italic
1505		\sim	Formatted: Left
			Formatted: Font: (Default) Times New Roman
1506	Formal validation report of NOAA Daily OISST is along with data access.		
1507	•		Formatted: Font: (Default) Arial 11 pt Font color: Black
			Formatted: Left
1508	Formal product user guide (Score: 6/6)		Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman
1509	The formal product user quide is provided in the peer review journal (Banzon et al.,		
1510	2016).		
1511	<u>۸</u>	~	Formatted: Font: (Default) Times New Roman
			Formatted: Left
1512	Uncertainty Characterization		Formatted: Font: Not Bold, Underline
1512	Standards (Saara: 6/6)		Formatted: Font: (Default) Times New Roman, Not Bold, Underline
1515	Standards (Score. 6/6)		Formatted: Font: Italic
			Formatted: Font: (Default) Times New Roman
1514	Uncertainty characterization follows the internationally agreed GHRSST standard		
1515	specifications, which are detailed in the GHRSST Data Specification v2.0 (GDS)		Formatted: Font: Not Bold
1516	document.		

1518	Validation (Score: 6/6)	F	Formatted: Font: Italic
		F	Formatted: Left
1519	A validation of NOAA Daily OISST is provided through peer-review journals (Dash et	F	Formatted: Font: (Default) Times New Roman
1520	al., 2012; Martin et al., 2012; Banzon et al., 2016; Fiedler et al., 2019a; Huang et al.,		
1521	2020).		
1522		F	ormatted: Font: (Default) Times New Roman
		F	ormatted: Left
1523	Uncertainty quantification (Score: 6/6)		ormatted: Font: Italic
		F	ormatted: Font: (Default) Times New Roman
1524	Uncertainty in the NOAA Daily OISST data at each location (i.e., the analysed_sst		
1525	field in the NETCDF file available from		
1526	https://podaac.jpl.nasa.gov/dataset/AVHRR_OI-NCEI-L4-GLOB-v2.1) is quantified and		
1527	provided (i.e., in the analysis_error field) through an analysis quality methodology.		
1528			
1529	Automated Quality monitoring (Score: 4/6)	F	Formatted: Font: Italic
		F	Formatted: Left
1530	The Daily OISST v2.1 SST analyses are validated in near real-time against the	F	Formatted: Font: (Default) Times New Roman
1531	GHRSST Multi-Product Ensemble by NOAA/STAR at		

1532	https://www.star.nesdi	s.noaa.gov/socd,	/sst/squam/ana	alysis/l4.	Since Argo	SST are
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1533 ingested into Daily OISST v2.1 they are not useful for verification.

Data providers regularly update the data record.

1534

1535	Public access, feedback and update	Formatted: Font: Not Bold, Underline
		Formatted: Left
1536	Public Access/Archive (Score: 56/6)	Formatted: Font: (Default) Times New Roman, Not Bold
		Formatted: Font: Italic
1537	The data is publicly accessible through the data provider's website and also other	Formatted: Font: (Default) Times New Roman
1538	data portals with documentation. No souce code is available publically.	
1539	<u>۸</u>	Formatted: Font: (Default) Times New Roman
		Formatted: Left
1540	Version (Score: 6/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1541	The version is fully established by the data provider.	
1542	<u>۸</u>	Formatted: Font: (Default) Times New Roman
		Formatted: Left
1543	User feedback (Score: <u>3</u> 6 /6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1544	Contact information of the data provider is publicly available for user feedback.	
1545		
1546	Updates to record (Score: 6/6)	Formatted: Font: Italic
		Formatted: Font: (Default) Times New Roman
1		Formatted: Left

1549	Usage	Formatted: Font: Not Bold, Underline
		Formatted: Left
1550	Research (Score: 6/6)	Formatted: Font: (Default) Times New Roman, Not Bold
		Formatted: Font: Italic
1551	The NOAA Daily OISST is widely used in multiple research fields.	
1552		
1553	Decision support system (Score: 3/6)	Formatted: Font: Italic
		Formatted: Left
1554	No decision support system is found for NOAA Daily OISST, however use is	Formatted: Font: (Default) Times New Roman
1555	occurring and benefits are emerging.	
1556		
1557	8. HadISST1	Formatted: Font: Not Bold
	AA	Formatted: Font: Not Bold
1558	Metadata	Formatted: Font: Not Bold, Underline
		Formatted: Left
1559	Standard (Score: 6/6)	Formatted: Font: (Default) Arial, 11 pt, Not Bold, Font color: Black
		Formatted: Font: Italic
1560	The <u>HadISST1OSTIA SST data files are provided in NetCDF classic format CF</u>	Formatted: Font: (Default) Times New Roman
1561	compliant through the data provider's website. The NetCDF files contain detailed	
1562	metadata describing the data by means of global attributes, which are applicable to	
1563	the whole file, and variable attributes, which apply to a specific data field.	

1564			
1565	Collection Level (Score: 6/6)	•	Formatted: Font: Italic
			Formatted: Left
1566	Global attributes provide all information available on the data and relative		Formatted: Font: (Default) Arial, 11 pt, Font color: Black
1567	references.		
1568			
1569	User Documentation	•	Formatted: Font: Not Bold, Underline
			Formatted: Left
1570	Formal description of scientific methodology (Score: 6/6)		Formatted: Font: (Default) Times New Roman, Not Bold
1571	The formal description of the HadISST1 is detailed in the peer-reviewed journal		Formatted: Font: Italic
1572	(Rayner et al., 2003), published by the data provider, which describes and justifies		Formatted: Font: Not Bold
1573	the algorithms used for obtaining sea surface temperature <u>SST</u> estimates.		
1 1574			
1575	Formal validation report (Score: 6/6)		Formatted: Font: Italic
1576	Formal validation report is published in a peer reviewed journal.		
1577			
1570	Formal product user quide (Score: 2/6)		Formatted: Font: Italic
10/8			Formatted: Font: (Default) Times New Roman
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1579	No formal product user guide is provided. Product information is provided on the in		
1580	the data provider's website.		
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1582	Uncertainty Characterization		Formatted: Font: Not Bold, Underline
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1583	Standards (Score: 1/6)		Formatted: Left
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1586	Validation (Score: 6/6)	\checkmark	Formatted: Font: Italic
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1587	The validation is available through peer reviewed journal paper.		Formatted: Left
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1589	Uncertainty quantification (Score: 1/6)	\times	Formatted: Font: Italic
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1592	Automated Quality monitoring (Score: 1/6)		Formatted: Font: Italic
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1595	Public access, feedback and update	•	Formatted: Font: Not Bold, Underline
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1596	Public Access/Archive (Score: 5 6 /6)		Formatted: Left
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1597	The data is published through data provider's website, but no source code is		Formatted: Font: (Default) Times New Roman
1598	publically available.		
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1600	Version (Score: 6/6)	•	Formatted: Font: Italic
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1601	The version is fully established by the data provider.		Formatted: Left
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1603	<i>User feedback</i> (Score: 3 6 /6)	•	Formatted: Font: Italic
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1604	Contact information of the data provider is given for collecting user feedback.		Formatted: Font: (Default) Times New Roman
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1607	The data is regularly updated by the data provider.		Formatted: Font: (Default) Times New Roman
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1610	Research (Score: 6/6)	/	Formatted: Font: Italic
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1611	HadISST1 has been widely used in multiple research fields.		
1612			
1613	Decision support system (Score: 6/6)	<	Formatted: Font: Italic
1614	Up to now no decision support system is found for HadISST1, however, influence on		Formatted: Font: (Default) Times New Roman
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Dataset	Institution	Type of product	Time Range	Observation input	Type of SST	Horizontal Grid spacing	Vertical resolution	Temporal resolution	Main Reference
ESA CCI SST (v.2.0)	Met Office	SST analysis	1981- 2018	IR	SST at 0.2 m	global 0.05°x0.05°	surface	daily	Merchant et al. (2019)
ERA5	ECMWF	SST analysis	1979- 2018	IR + MW + in situ		global 0.25°x0.25°	surface	hourly	Hirahara et al. (2016)
HadISST1	Met Office	SST analysis	1870- 2018	IR + in situ		global 1°x1°	surface	monthly	Rayner et al. (2003)
NOAA Daily OISST V2.1	NOAA	SST analysis	1981- 2018	IR + in situ	SST at 0.2 m	global 0.25°x0.25°	surface	daily	Huang et al., (2020)
MUR25 (v.4.2)	PODACC	SST analysis	2003- 2018	IR + MW + in situ	Foundation SST	global 0.25°x0.25°	surface	daily	Chin et al. (2017)
MGDSST	Japanese Met. Agency (JMA)	SST analysis	1982- 2017	IR + MW + in situ		global 0.25°x0.25°	surface	daily	Sakurai et al. (2005)
BoM Monthly SST	Australian Bureau of Met. (BoM)	SST analysis	2002- 2018	IR + in situ	SST at 0.2 m	global 1°x1° (weekly/monthly)	surface	weekly/monthly	Smith et al. (1999)
OSTIASST	UK MeOffice	SST analysis	1981- 2018	IR + MW + in situ	Foundation SST	0.05°x0.05°	surface	daily/weekly/monthly	Good et al., 2020

Dataset	Institution	Type of product	Time Range	Observation input	Type of SST	Horizontal Grid spacing	Vertical resolution	Temporal resolution	Main Reference
ESA CCI SST (v.2.0)	Met Office	SST analysis	1981- 2018	IR	SST at 0.2 m	global 0.05°x0.05°	surface	daily	Merchant et al. (2019)
ERA5	ECMWF	SST analysis	1979- 2018	IR + MW + in situ	SSTdepth	global 0.25°x0.25°	surface	hourly	Hirahara et al. (2016)
HadISST1	Met Office	SST analysis	1870- 2018	IR + in situ	SSTdepth	global 1°x1°	surface	monthly	Rayner et al. (2003)
NOAA Daily OISST v2.1	NOAA	SST analysis	1981- 2018	IR + in situ	SST at 0.2 m	global 0.25°x0.25°	surface	daily	Huang et al., (2020)
MUR25 (v.4.2)	PODACC	SST analysis	2003- 2018	IR + MW + in situ	Foundation SST	global 0.25°x0.25°	surface	daily	Chin et al. (2017)
MGDSST	Japanese Met. Agency (JMA)	SST analysis	1982- 2018	IR + MW + in situ	SSTdepth	global 0.25°x0.25°	surface	daily	Sakurai et al. (2005)
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v2.1									
MUR25 (v.4.2)	PODACC	SST analysis	2003- 2018	IR + MW + in situ	Foundation SST	global 0.25°x0.25°	surface	daily	Chin et al. (2017)
MGDSST	Japanese Met. Agency (JMA)	SST analysis	1982- 2017	IR + MW + in situ	SSTdepth	global 0.25°x0.25°	surface	daily	Sakurai et al. (2005)
BoM Monthly SST	Australian Bureau of Met. (BoM)	SST analysis	2002- 2018	IR + in situ	SSTdepth	global 1°x1° (weekly/monthly)	surface	weekly/monthly	Smith et al. (1999)
OSTIASST	UK MeOffice	SST analysis	1981- 2018	IR + MW + in situ	Foundation SST	0.05°x0.05°	surface	daily/weekly/monthly	Good et al., 2020

Commented [1]: Please change BoM Monthly SST Type of SST to SSTdepth

- 1903 Table 1. Descriptive product comparison summary for the described products from
- 1904 sections 2. Input observations are derived from satellite infrared (IR) and/or
- 1905 microwave (MW) sensors and/or in situ measurements.

1907

Name	ESA CCI SST	ERA5 SST	OSTIA	ВоМ	MGDSST	MUR25	NOAA Daily OISST	HadISST1
C3S_511 MM Category								
Metadata								
Standards	6	6	6	6	3	6	6	6
Collection level	6	5	6	5	2	6	6	6
User Documentation								
Formal description of scientific methodology	6	5	6	4	4	6	6	6
Formal validation report	6	3	6	2	4	3	6	6
Formal product user guide	6	6	6	4	3	2	6	3
Uncertainty Characterisation								
Standards	6	3	6	6	1	6	6	1
Validation	6	3	6	3	6	6	6	6
Uncertainty quantification	6	3	6	6	1	6	6	1
Automated quality monitoring	6	2	6	1	2	4	4	1
Public Access, feedback, and update								
Public Access/Archive	6	6	6	4	4	6	6	6
Version	6	6	6	2	2	6	6	6
User feedback mechanism	6	6	6	3	3	6	6	6
Updates to record	6	6	6	5	4	5	6	6
Usage								
Research	6	3	6	4	6	6	6	6
Decision support system	6	1	6	6	6	3	3	6

Name	ESA CCI SST	ERA5 SST	OSTIA	ВоМ	MGDSST	MUR25	NOAA Daily OISST	HadISST1
C3S_511 MM Category								
Metadata								
Standards	6	6	6	6	3	6	6	6
Collection level	6	5	6	5	2	6	6	6
User Documentation								
Formal description of scientific methodology	6	6	6	4	3	6	6	6
Formal validation report	6	3	6	2	4	4	6	6
Formal product user guide	6	6	6	4	3	2	6	3
Uncertainty Characterisation								
Standards	6	3	6	6	1	6	6	1
Validation	6	3	6	5	6	6	6	6
Uncertainty quantification	6	3	6	6	1	6	6	1
Automated quality monitoring	6	2	6	1	2	4	4	1
Public Access, feedback, and update								
Public Access/Archive	5	5	5	4	4	5	5	5
Version	6	6	6	2	2	6	6	6
User feedback mechanism	6	6	6	3	3	6	3	6
Updates to record	6	6	6	5	4	5	6	6
Usage								
Research	6	3	6	4	6	6	6	3
Decision support system	6	1	6	6	6	3	3	6

1911 Table 2. Maturity Matrix for all SST products





1915 Figure 1. Temporal range (years) covered by each SST dataset. The common period

1916 for all datasets is highlighted (2003-2018) and the secondary common period is

1917 1982-2018 with less SST products included.

1918







80°W) for ESA-CCI (green), OSTIA (dashed dark blue), NOAA Daily OISST (Reynolds

- 0.25 Degree. red) and MGDSST (cyan) based on the daily temporal and original
- spatial resolution for the period 1982-2018



- 1928 Figure 3. Global SST climatologies for the period 2003-2018. Global SST average
- 1929 value and its 95% confidence interval is also shown.



- 1932 Figure 4 The difference between each SST product and the ensemble median for the
- 1933 period of 2003-2018
- 1934
- 1935





1938 Figure 5 The RMSD between each SST product and the ensemble median for the

¹⁹³⁹ period of 2003-2018



- 1942 Figure 6 The correlation between each SST product and the ensemble median for
- 1943 the period of 2003-2018



1949 Figure 7 Global monthly mean SST time series from 2003 to 2018.



- 1952 Figure 8. Global SST monthly anomalies time series, obtained by subtracting the
- 1953 climatology of the ensemble median to all the SST ensemble members from 2003 to

1954 2018.

1955





- 1960 Figure 9. Global linear trend maps (2003-2018) (°C/year) of each ensemble member
- 1961 and ensemble median. Areas with no significant (95% significance level) trends are

¹⁹⁶² covered by grey points.



1964

1965 Figure 10. (a) Global average SST trend component deduced from the global

1966 average monthly mean time series (Figure 3.2.2) using the X-11 procedure (section

1967 3.1.2), the same calculation but for (b) the Pacific Ocean basin (c) Atlantic Ocean

- 1969
- 1970

¹⁹⁶⁸ basin and (d) Indian Ocean Basin for the period of 2003-2018.



1973 Figure 11. Global monthly mean SST time series for all the ensemble members for





1977 Figure 12 Global SST climatologies for the period 1982-2002. Global SST average

1978 and its 95% confidence interval is also shown<u>in brackets above each map</u>. 1979



Figure 13 The difference between each SST product and the ensemble median for





- 1986 Figure 14 Intercomparison between El Niño 3.4 time series of the five SST products:
- 1987 HadISST1, ERA5, ESA CCI SST, MGDSST, NOAA OISST.