# A New Operational Mediterranean Diurnal Optimally Interpolated

# 2 SST Product within the Copernicus Marine Environment

## 3 Monitoring Service

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10 Abstract, Within the Copernicus Marine Environment Monitoring Service (CMEMS), a new operational MEDiterranean Diurnal Optimally Interpolated Sea Surface Temperature (MED DOISST) product has been developed. This product provides 11 12 hourly mean maps (Level-4) of sub-skin SST at 1/16° horizontal resolution over the Mediterranean Sea from January 2019 to 13 present. Sub-skin is the temperature at  $\sim 1$  mm depth of the ocean surface, and then potentially subject to a large diurnal cycle. 14 The product is built by combining hourly SST data from the Spinning Enhanced Visible and InfraRed Imager (SEVIRI) on 15 board Meteosat Second Generation and model analyses from the Mediterranean Forecasting System (MedFS) through optimal 16 interpolation. SEVIRI and model-MedFS (first layer) SST data are respectively used as the observation source and first-guess. 17 The choice of using a model output as first-guess represents an innovative alternative to the commonly adopted climatologies 18 or previous day analyses, providing physically consistent estimates of hourly SSTs in the absence of any observation or in situ 19 measurement. The accuracy of the MED DOISST product is assessed here by comparison against surface drifting buoy 20 measurements, covering the years 2019 and 2020. The diurnal cycle reconstructed from DOISST is in good agreement with 21 the one observed by independent drifter data, with a mean bias of  $0.041 \pm 0.001$  K and root-mean-square difference (RMSD) 22 of  $0.412 \pm 0.001$  K. The new SST product is more accurate than the input model-MedFS SST during the central warming 23 hours, when the model, on average, underestimates drifter SST by one tenth of degree. The capability of DOISST to reconstruct 24 diurnal warming events, which may reach intense amplitudes larger than 5 K in the Mediterranean Sea, is also analysed. 25 Specifically, a comparison with the OSTIA diurnal skin SST product, SEVIRI, model-MedFS and drifter data, shows that the 26 DOISST product is able to reproduce more accurately diurnal warming events larger than 1 K. This product can contribute to 27 improve the prediction capability of numerical weather forecast systems (e.g., through improved forcing/assimilation)models 28 that assimilate or correct the heat fluxes starting from Level-4 SST data, as well as the monitoring of surface heat budget 29 estimates and temperature extremes which can have significant impacts on the marine ecosystem.

The full MED DOISST product (released on 04 May 2021) is available upon free registration at <u>https://doi.org/10.48670/moi-00170https://doi.org/10.25423/CMCC/SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036</u> (Pisano et al., 2021). The reduced subset used here for validation and review purposes is openly available at <u>https://doi.org/10.5281/zenodo.5807729</u> (Pisano, 2021).

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### 36 1 Introduction

In the last decades, the development of accurate satellite-based Sea Surface Temperature (SST) products required an increasing 37 38 effort to meet an ever-growing request from scientific, operational and emerging policy needs. Indeed, infrared and/or 39 microwave satellite radiometers allow a systematic and synoptic mapping of the ocean surface temperature (under clear-sky 40 conditions for the infrared and in the absence of rain for the microwave bands) with spatial resolutions from one to few 41 kilometers and temporal sampling from hourly to daily (Minnett et al., 2019). This almost continuous coverage represents a 42 unique characteristic of satellite thermal data, which is clearly not achievable with the use of in situ measurements alone. 43 Indeed, though in situ sensors reach significantly higher accuracy than satellite sensors, with uncertainties that can reach O(10<sup>-1</sup> 44 <sup>2</sup>K), they provide pointwise seawater temperature measurements, generally characterized by a poor and non-uniform sampling 45 of the ocean surface.

46 There is a huge variety of satellite-based SST datasets, characterized by different nominal resolutions as well as temporal and 47 spatial (global or regional) coverage, and based on different processing algorithms and satellite sensors, but designed to provide 48 highly accurate SST estimates (Yang et al., 2021), Operational datasets are typically distributed in near real time (NRT). 49 delayed-mode or as reprocessed datasets, and may include different processing levels, from single satellite passes processed 50 to provide valid SST values in the original observation geometry, the so-called Level-2 (L2), to images remapped onto a regular 51 grid, also known as Level-3 (L3), up to the spatially complete Level-4 (L4), interpolated over fixed regular grids. These latter 52 are required by several applications since the lower levels are typically affected by several data voids (due to clouds, rain, land, 53 sea-ice, or other environmental factors depending on the type of sensors). The timely availability of SST data, ranging from a 54 few hours to a few days before real time, allows their use as boundary condition and/or assimilation in meteorological and 55 ocean forecasting systems (Waters et al., 2015), to improve the retrieval of ocean surface currents (Bowen et al., 2002; Rio 56 and Santoleri 2018), and monitor some weather extreme events, such as marine heatwaves (Oliver et al., 2021). The 57 reprocessing of long-term SST data records, typically covering the satellite era (1981-present), aims to provide more stable 58 and consistent datasets, complementing the NRT production, to be used to investigate climate variability and monitor changes 59 from interannual to multi-decadal timescales (Deser et al., 2010), including e.g. SST trends' estimates (Good et al., 2007; Pisano et al., 2020). The Copernicus Marine Environment Monitoring Service (CMEMS) is one of the main examples of how 60

satellite observations, including not only SST but a wide range of surface variables (e.g., sea surface salinity, sea surface
 height, ocean color, winds and waves), are exploited to derive and disseminate high-level products (Le Traon et al., 2019),

63 namely L4 data, in order to be directly usable for downstream applications.

64 The majority of the existing L4 SST datasets are provided as daily, weekly or monthly averaged fields (see e.g. Fiedler et al., 65 2019; Yang et al., 2021). Examples of well-known state-of-the-art SST daily datasets include the Global Ocean Sea Surface 66 Temperature and Sea Ice (OSTIA) dataset (Good et al., 2020), the European Space Agency (ESA) Climate Change Initiative 67 (CCI), the Copernicus Climate Change Service (C3S) Reprocessed Sea Surface Temperature Analyses (Merchant et al., 2019), 68 and the NOAA Daily Optimally Interpolated SST (OISST) v2.1 dataset, previously known/referred to as Reynolds SST 69 analysis (Huang et al., 2021). Though a daily resolution is generally sufficient to meet the requirements of many of the 70 oceanographic applications, it does not resolve the SST diurnal cycle, the typical day-night SST oscillation mainly driven by 71 solar heating. Within the oceanic thermal skin layer (few µm to 1 mm), SST is typically subject to a large potential diurnal 72 cycle (especially under low wind speed and strong solar heating conditions) reaching amplitudes up to 3 K in the world oceans 73 (Gentemann et al., 2008; Gentemann and Minnett, 2008).

74 The SST diurnal cycle has several implications on mixed layer dynamics, air-sea interaction and the modulation of the lower 75 atmosphere dynamics. The most direct consequence of the SST diurnal amplitude variability is certainly on air-sea fluxes. Clayson and Bogdanoff (2013) estimated that the diurnal SST cycle contributes approximately 5 Wm<sup>-2</sup> to the global ocean-76 77 atmosphere heat budget with peaks of about 10 Wm<sup>-2</sup> in the Tropics. The inclusion of a realistic diurnal SST cycle in 78 atmospheric numerical simulation also has a non-negligible impact on cloud dynamics. Chen and Houze (1997) have shown 79 that in the Tropical Warm Pool, where extreme localized warming events occur, the diurnal warming can contribute to 80 modulate the evolution of convective clouds and, more in general, can impact the ocean-atmosphere coupling in numerical 81 models, producing a more realistic spatial pattern of warming and precipitation (Bernie et al., 2008). Overall, the diurnal cycle 82 of SST is generally underestimated in current ocean models and the assimilation of SST at high temporal frequency has the 83 potential to improve sea surface variability and mixed layer accuracy (Storto and Oddo, 2019).

84 In principle, the best opportunity to measure the diurnal cycle comes from infrared radiometers on board geostationary 85 satellites. Their observations are sufficiently accurate and frequent to resolve the diurnal signal variability whenever cloud 86 cover is not too persistent. An example is provided by the Spinning Enhanced Visible Infra-Red Imager (SEVIRI) onboard the 87 Meteosat Second Generation (MSG) geostationary satellite covers. The operational retrieval of SST from MSG/SEVIRI 88 (managed by the European Organization for the Exploitation of Meteorological Satellites, EUMETSAT, Ocean and Sea-Ice 89 Facility, OSI-SAF) produces L3C hourly sub-skin SST products by aggregating 15 minutes (MSG/SEVIRI) observations within 1 hour. The sub-skin SST is the temperature at the base of the conductive laminar sub-layer of the ocean surface, as 90 defined by the Group of High Resolution SST (GHRSST, see e.g. Minnett et al., 2019). In practice, this is the temperature at 91

92 ~1 mm depth (see e.g., osisaf\_cdop3\_ss1\_pum\_msg\_sst\_data\_record.pdf (eumetsat.int)), and thus particularly sensitive to 93 diurnal warming.

For the global ocean, the Operational Sea surface Temperature and sea Ice Analysis (OSTIA) diurnal product (While et al., 2017) provides daily gap-free maps of hourly mean skin SST at  $0.25^{\circ} \times 0.25^{\circ}$  horizontal nominal resolution, using in situ and satellite data from infrared radiometers. The skin temperature is defined as the temperature of the ocean measured by an infrared radiometer (typically aboard satellites) and represents the temperature of the ocean within the conductive diffusiondominated sub-layer at a depth of ~10-20  $\mu$ m (GHRSST, Minnett et al., 2019). This system produces a skin SST by combining the OSTIA foundation SST analysis (Good et al., 2020) with a diurnal warm-layer temperature difference and a cool skin temperature difference derived from numerical models.

101 At regional scale, a method to reconstruct the hourly SST field over the Mediterranean Sea from SEVIRI data has been 102 proposed by Marullo et al. (2014, 2016). The reconstruction is based on a blending of satellite (SEVIRI) observations and 103 numerical model analyses (used as first-guess) using in an optimal interpolation scheme. Model analyses are provided by the 104 Mediterranean Forecasting System, MedFS (Clementi et al., 2021), and distributed through the Copernicus Marine Service 105 (hereafter referred to as Copernicus). Though model analyses by definition also assimilate observations, which could thus in 106 principle include hourly SEVIRI data, in the present configuration, MedFS they areis not able to deal with such frequent 107 updates and basically only uses one estimation of foundation SST to correct surface fluxes (see section 2.2). As such, and 108 the approach presented here represents an effective way to improve the reconstruction of SST daily cycle from high-repetition 109 satellite measurements. Previous works demonstrated the capability of SEVIRI to resolve the SST diurnal variability and to 110 reconstruct accurate L4 SST hourly fields over the Mediterranean Sea, a basin that exhibits large diurnal SST variations 111 (Buongiorno Nardelli et al., 2005; Minnett et al., 2019) that can easily exceed extreme values (~5 K) as observed in the Tropical 112 Pacific (Chen and Houze 1997), in the Atlantic Ocean and other marginal seas (Gentemann et al., 2008; Merchant et al., 2008). 113 The aim of this paper is to describe the operational implementation of a diurnal optimally interpolated SST (DOISST) product 114 for the Mediterranean Sea (MED), building on the algorithm by Marullo et al. (2014, 2016). The DOISST product routinely 115 provides hourly mean maps of sub-skin SST at 1/16° horizontal resolution over the Mediterranean Sea from January 2019 to 116 present. The assessment presented here for the DOISST product covers two complete years (2019-2020), thus extending 117 previous similar validations (Marullo et al., 2016).

#### 119 2 The data

#### 120 2.1 Satellite data

121 Input satellite SST is derived from the SEVIRI sensor onboard the Meteosat Second Generation (Meteosat-11) satellite. 122 SEVIRI has a repeat cycle of 15 minutes over the 60S-60N and 60W-60E domain: Atlantic Ocean, European Seas and western 123 Indian Ocean. The retrieval of SST from Meteosat-11/SEVIRI is managed by EUMETSAT OSI-SAF, which provides sub-124 skin SST data as aggregated (L3C) hourly products remapped onto a 0.05° regular grid. Hourly products result from 125 compositing the best SST measurements available in one hour and are made available in near real time with a timeliness of 3 126 hours (see the OSI-SAF product user manual, https://osi-saf.eumetsat.int/products/osi-206). File format follows the Data 127 Specification (GDS) version 2 from the Group for High Resolution Sea Surface Temperatures (GHRSST, https://podaac-128 tools.jpl.nasa.gov/drive/files/OceanTemperature/ghrsst/docs/GDS20r5.pdf). The computation of SST in day and night 129 conditions is based on a nonlinear split window algorithm whose coefficients are determined from brightness temperature 130 simulations on a radiosonde profile database, with an offset coefficient corrected relative to buoy measurements. A correction 131 term derived from simulated brightness temperatures with an atmospheric radiative transfer model is then applied to the 132 multispectral derived SST (OSI-SAF PUM, https://osi-saf.eumetsat.int/lml/doc/osisaf\_cdop3\_ss1\_pum\_geo\_sst.pdf). L3C 133 data are provided with additional information, including quality level and cloud flags. Such quality flags are provided at pixel level, ranging over a scale of five levels with increasing reliability: 1 (="cloudy"), 2 (="bad"), 3 (="acceptable"), 4 (="good") 134 135 to 5 (="excellent").

The accuracy of Meteosat-11 SST data has been assessed through comparison with co-located drifting buoys, for day and 136 137 night data separately covering the period from February to June 2018 (see the OSI-SAF scientific validation report, https://osi-138 saf.eumetsat.int/lml/doc/osisaf cdop2 ss1 geo sst val rep.pdf). The mean bias and standard deviation (derived from the 139 differences between SEVIRI SSTs and drifter measurements over a matchup database) during nighttime have been quantified 140 in -0.1 K and 0.53 K, respectively. During daytime, the bias remains practically unchanged (-0.09 K) and the standard deviation 141 slightly higher (0.56 K). These statistics were derived by selecting SEVIRI SST with quality flags  $\geq$  3, and it is shown that the 142 quality of SST improves when choosing higher quality levels. A similar validation procedure (Marullo et al., 2016), but 143 performed over the Mediterranean Sea by using nighttime and daytime data selected with quality flags  $\geq$  4, shows that SEVIRI SST bias and standard deviation are -0.03 K and 0.47 K, respectively. 144

For our purposes, we selected L3C SST data with quality flag  $\geq$  3, as also indicated/suggested in the OSI-SAF scientific validation report. A synthesis of the SEVIRI SST characteristics is reported in Table 1.

#### 147 2.2 Model data

- 148 The model output fields of surface temperature are derived from the <u>Mediterranean Forecasting System (MedFS)</u>, a numerical
- 149 ocean prediction system that produces analyses, reanalyses and short term forecasts for the Mediterranean Sea and the eastern

150 Atlantic ocean in the 18°W to 6°W - 31°N to 45°N box, to better resolve the exchanges at the Strait of Gibraltar, MedFS is 151 part of the Copernicus Marine Service, and provides regular and systematic information about the physical state of the 152 Mediterranean Sea (https://doi.org/10.25423/CMCC/MEDSEA\_ANALYSISFORECAST\_PHY\_006\_013\_EAS6; last access: 153 15 July 2022; Clementi et al., 2021). CMEMS Mediterranean Sea Physical Analysis and Forecasting product, and identified as 154 MEDSEA ANALYSIS FORECAST PHY 006 013 -(https://resources.marine.copernicus.eu/product-155 detail/MEDSEA\_ANALYSISFORECAST\_PHY\_006\_013/INFORMATION: 156 https://doi.org/10.25423/CMCC/MEDSEA\_ANALYSISFORECAST\_PHY\_006\_013\_EAS6; last access: 03 November 2021; 157 Clementi et al., 2021), and routinely produced by the CMEMS Mediterranean Monitoring and Forecasting Center (Med-MFC). 158 The modelling system is based on the Mediterranean Forecasting System, MFS (Pinardi et al., 2003), a coupled hydrodynamic-159 wave model implemented over the Mediterranean basin, extended into the Atlantic Sea in order to better resolve the exchanges 160 with the Atlantic Ocean at the Strait of Gibraltar, MedFS is a coupled hydrodynamic-wave model with data assimilation 161 component, with a horizontal grid resolution of 1/24° (~4 km) and 141 unevenly spaced vertical levels (Clementi et al., 2017a,b; 162 Pinardi et al., 2003)(Clementi et al., 2017). The Ocean General Circulation Model is based on the Nucleus for European 163 Modelling of the Ocean (NEMO v3.6) (Oddo et al., 2014, 2009), while the wave component is provided by Wave Watch-III. 164 The model solutions are corrected by a variational data assimilation scheme (3DVAR) of temperature and salinity vertical 165 profiles and along track satellite sea level anomaly observations (Dobricic and Pinardi 2008). The CMEMS-Copernicus 166 Mediterranean SST L4 product (https://doi.org/10.48670/moi-00172CMEMS product reference: 167 SST\_MED\_SST\_L4\_NRT\_OBSERVATIONS\_010\_004, https://resources.marine.copernicus.cu/product-168 detail/SST\_MED\_SST\_L4\_NRT\_OBSERVATIONS\_010\_004/INFORMATION; last access: 15 July 202203\_November 169  $\frac{2021}{10}$  is used for the correction of surface heat fluxes with the relaxation constant of 110 Wm<sup>-2</sup>K<sup>-1</sup> centered at midnight since 170 the product provides foundation SST (~SST at midnight).

171 The Med MFCMedFS product is produced with two different cycles: a daily cycle for the production of forecasts (i.e., ten-172 days forecast on a daily basis), and a weekly cycle for the production of analyses. For our purposes, only hourly mean SST 173 fields of sea surface temperature, which correspond to the first vertical level of the model centered at ~1 m from the surface, 174 are selected. The accuracy of SST data has been quantified via a RMSD of  $0.57 \pm 0.11$  °C and a bias of  $0.14 \pm 0.09$  °C obtained 175 comparison with satellite-based L4 SST through а data (see 176 https://catalogue.marine.copernicus.eu/documents/QUID/CMEMS-MED-QUID-006-013.pdf). A synthesis of the model-177 derived SST characteristics is reported in Table 1.

#### 178 2.3 In situ data

Surface drifting buoys have been used for validation purposes (Section 4). Since there are no in situ instruments able to routinely measure skin/sub-skin SSTs, the commonly adopted validation procedure is to use drifters' data, also due to their high accuracy and closeness to the sea surface (their representative depth attains around ~20 cm; Reverdin et al., 2010), and to their abundance compared to other in situ instruments, which allows to achieve a more consistent and homogeneous temporal
 and spatial coverage. Of course, these observations are affected by a representativeness error when compared to sub-skin SSTs,
 which is typically quantified in terms of a bias between the two estimates.

Drifter data have been obtained from the <u>CMEMS</u><u>Copernicus</u>IN SITU (INS) TAC (identified <u>as</u><u>through</u> <u>https://doi.org/10.48670/moi-00044</u> for the <u>Mediterranean Sea</u><u>INSITU\_MED\_NRT\_OBSERVATIONS\_013\_035</u>, <u>https://resources.marine.copernicus.eu/product\_detail/INSITU\_MED\_NRT\_OBSERVATIONS\_013\_035/INFORMATION</u>; and <u>https://doi.org/10.48670/moi-00043</u> for the Northeastern Atlantic ocean<u>INSITU\_IBL\_NRT\_OBSERVATIONS\_013\_033/INFORMATION</u>; <u>https://resources.marine.copernicus.eu/product\_detail/INSITU\_IBL\_NRT\_OBSERVATIONS\_013\_033/INFORMATION</u>; last access: <u>15 July 202203 November 2021</u>), which collects and distributes a variety of physical and biogeochemical seawater measurements, provided with the same homogeneous file format . Each in situ measurement, including drifters, undergoes

automated quality controls before its distribution. The quality of the data is expressed by control flags indexed from 0 to 9, with the value of 1 indicating best quality. Drifter data have been used to compile an hourly matchup database (section 4.1) over which validation statistics have been produced of co-located (in space and time) diurnal optimally interpolated SST (DOISST) values and model outputs (Section 4.1), and validation statistics are based on the comparison among DOISST, model SST and drifting buoy measurements over the matchup database (section 4.2). A synthesis of the drifter SST characteristics is reported in Table 1.

#### 198 2.4 OSTIA diurnal

199 The OSTIA diurnal skin SST product (While et al., 2017) provides gap-free global maps of hourly mean skin SST at 0.25° x 200 0.25° horizontal resolution, obtained by combining in situ and infrared satellite data. This product is operationally produced 201 by the Met Office within the Copernicus Marine Service (https://doi.org/10.48670/moi-00167identified as 202 SST GLO SST L4 NRT OBSERVATIONS 010 014, https://resources.marine.copernicus.eu/product-203 detail/SST\_GLO\_SST\_L4\_NRT\_OBSERVATIONS\_010\_014/INFORMATION; last access: 15 July 202202 May 2022), and 204 created using the Operational Sea surface Temperature and Ice Analysis (OSTIA) system (Good et al., 2020). The OSTIA 205 system also produces a global daily average foundation SST L4 product (https://doi.org/10.48670/moi-00165identified as 206 SST\_GLO\_SST\_L4\_NRT\_OBSERVATIONS\_010\_001, https://resources.marine.copernicus.eu/product-207 detail/SST\_GLO\_SST\_L4\_NRT\_OBSERVATIONS\_010\_001/INFORMATION: last access: 15 July 202202\_May 2022). 208 Since the skin SST can be considered as the sum of three components, namely the foundation SST, the warm layer and the 209 cool skin, the OSTIA diurnal product is created by adjusting the OSTIA foundation SST analysis with a modelled diurnal 210 warm layer analysis (which assimilates satellite observations) and a cool skin model, based respectively on the Takaya (Takaya 211 et al., 2010) and Artale models (Artale et al., 2002). Assimilation into the warm layer model makes use of SEVIRI, GOES-W 212 and MTSAT-2 geostationary infrared sensors, and of the polar orbiting VIIRS radiometer. Further details on the method can 213 also be found in Copernicus PUM (https://catalogue.marine.copernicus.eu/documents/PUM/CMEMS-SST-PUM-010214 014.pdf)https://catalogue.marine.copernicus.eu/documents/PUM/CMEMS\_SST\_PUM-010-014.pdf). A synthesis of the

215 OSTIA diurnal SST characteristics is reported in Table 1.

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SST								
Source	Definition	Vertical level	Spatial res.	Temporal res.	Spatial coverage	Temporal coverage	Processing level	
ModelMedFS	Depth SST	1 m (first model layer)	0.042°x0.042°	Hourly	17.3°W– 36.3°E, 30.2°N–46°N	2019- Present	Model output	
SEVIRI	Sub-skin SST	~1 mm (surface only)	0.05°x0.05°	Hourly	60°W–60°E, 60°S–60°N	2015- Present	L3C	
OSTIA diurnal	Skin SST	~10-20 μm (surface only)	0.25°x0.25°	Hourly	Global	2015- Present	L4	
Surface Drifting Buoys	Depth SST	~20 cm (surface only)	Not applicable	Hourly	30°W-36.5°E, 20°N-55°N	2010- Present	L2	

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 Table 1. Summary of the SST products used to produce (Model\_MedFS and SEVIRI), validate (surface drifting buoys), and

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 intercompare (all) the DOISST product. The SST nomenclature (skin, sub-skin, and depth) follows the Group for High

 220
 Resolution
 Sea
 Surface
 Temperatures
 (GHRSST)
 definitions
 (https://podaac 

 221
 tools.jpl.nasa.gov/drive/files/OceanTemperature/ghrsst/docs/GDS20r5.pdf).

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## 223 3 The Mediterranean diurnal optimally interpolated SST product

## 224 3.1 Product overview

225 The Mediterranean diurnal optimally interpolated SST (hereafter referred to as MED DOISST) operational product consists 226 of hourly mean gap-free (L4) satellite-based estimates of the sub-skin SST over the Mediterranean Sea (plus the adjacent 227 Eastern Atlantic box, see Section 2.2) at 0.0625° x 0.0625° grid resolution, from 1st January 2019 to near real time. 228 Specifically, the product is updated daily and provides 24 hourly mean data of the previous day, centered at 00:00, 01:00, 229 02:00,...,23:00 UTC. The MED DOISST product is published on the CMEMS Copernicus on line catalogue and identified as 230 SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036 (CMEMS product reference) and cmems\_obs-sst\_med\_phy-231 sst\_nrt\_diurnal-oi-0.0625deg\_PT1H-m (CMEMS-dataset reference). Further details on the product characteristics are provided 232 in Table 2. 233 DOISST is the result of a blending of SEVIRI sub-skin SSTs and modelled-MedFS SSTs (as detailed in the next section 3.2),

the former representative of a depth of 1 mm and the latter of 1 m. Then, the DOISST effective depth does, in principle, vary

235	between 1 mm up to 1 m, depending on how the relative amount of satellite observationsmany satellite observations enter used
236	in the interpolation. However, As-diurnal warming is significantly reduced under cloudy conditions (when SEVIRI data are
237	not available), so that, in those cases, however, the difference between the SST at 1 m and the sub-skin SST will be much
238	smaller when SEVIRI observations are not presentis small. Under clear sky conditions, SEVIRI observations will dominate
239	the retrieved SST, so the For this reason, we can define the DOISST product can be safely defined as representative of sub-

skin values.

## CMEMS-Copernicus Marine Service Product ID: SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036 CMEMS-Dataset ID: cmems\_obs-sst\_med\_phy-sst\_nrt\_diurnal-oi-0.0625deg\_PT1H-m

 

 General description
 The <u>CMEMS Copernicus</u> Mediterranean diurnal product provides near-real-time, hourly mean, gap-free (L4) sub-skin SST fields over the Mediterranean Sea and the adjacent Atlantic box over a 0.0625°x0.0625° regular grid, covering the period from 2019 to present (one day before real time). This product is built from optimal interpolating the Level-3C (merged single-sensor, L3C) SEVIRI data as observations and the <u>CMEMS Copernicus</u> Mediterranean <u>model MedFS</u> analyses as first-guess.



0.0625° x 0.0625° (1/16°) degrees [871x253]		
Hourly		
Mediterranean Sea + adjacent North Atlantic box		
(W=-18.1250, E=36.2500, S=30.2500, N=46.0000)		
2019/01/01 - near real time (-14H)		
~1 mm (surface only)		
Sub-skin SST (K)		
Analysis Error (%)		
NetCDF - CF-1.4 convention compliant		
https://doi.org/10.48670/moi-		
00170https://doi.org/10.25423/CMCC/SST_MED_PHY_SUBSKIN_L4_NRT_01		
<u>0_036</u>		

Eventual updates of this product will be described in the corresponding Product User Manual (PUM) and Quality Information Document (QUID) available on the <u>CMEMS-Copernicus Marine Service</u> on line catalogue.

(1)

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243 Table 2. The CMEMS-Copernicus Marine Service MED DOISST product description synthesis.

#### 244 3.2 Background

Comments

The reconstruction of gap-free hourly mean SST fields is based on a blending of <u>SEVIRI</u> (satellite) observations and <u>MedFS</u> (model) analyses (used as first-guess/background) using optimal interpolation (OI), following the approach proposed by Marullo et al. (2014). The OI method determines the optimal solution to the interpolation of a spatially and temporally variable field with data voids, where "optimal" is intended in a least square sense (see e.g. Bretherton et al., 1976). The optimally interpolated variable, or analysis ( $F_a$ ), is obtained as follows:

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 $F_{a}(x,t) = F_{b}(x,t) + \sum_{i,i=1}^{n} W_{i,i}(F_{obs,i}(x,t) - F_{b}(x,t))$ 

In practice, the analysis  $F_a(x, t)$  at a particular location in space and time (x, t) is obtained as a correction to a background field  $(F_b(x, t))$ . The correction is estimated as a linear combination of the observation anomalies  $(F_{obs} - F_b)$ , where the coefficients  $W_{i,i}$  are obtained by minimizing the analysis error variance.

256 The choice of using a model outputMedFS SST as first-guess represents the best alternative to the use of climatologies or 257 previous day analyses, as usually done by other schemes to produce daily SST L4 maps, since the model provides physically 258 consistent estimates of hourly SSTs in the absence of any observation or in situ measurement (Marullo et al., 2014). In fact, 259 the model takes into account the effect of air-sea interactions by imposing external forcings that drive momentum and heat 260 exchanges at the upper boundary. As such, it is able to reproduce at least part of the diurnal warming effects, that are driven 261 by the forcing diagnosed from atmospheric model analyses. Using the model outputMedFS SST as a first-guess means we are 262 treating the hourly satellite data as corrections to the hourly model data. These observation anomalies are generally small and 263 mostly drive corrections to the spatial patterns, while displaying a reduced diurnal cycle. Anomaly data from different times 264 of the day can thus be more "safely" used to build the interpolated field at each reference time (with different weights). 265 Unfortunately, the first MedFS model layer is at 1 m depth, which means that it will generally underestimate the diurnal cycle 266 anyway. While 1D models could in principle be used to better reproduce sub-skin SST from model data, the approach presented 267 here is focusing on providing estimates that are as close as possible to the original satellite data, avoiding the complications of 268 setting up an additional preprocessing step just to improve the first-guess.

#### 270 3.3 Processing chain

The DOISST system ingests merged single-sensor (L3C) SEVIRI data-<u>SST</u> as the observation source, and the <u>CMEMS</u>
 Mediterranean Sea model outputsMedFS SST (first layer) as first-guess.

273 The data sub-sampling strategy, inversion technique and numerical implementation of the optimal interpolation scheme are

based on the CMEMS Copernicus NRT MED SST processing chain (Buongiorno Nardelli et al., 2013), which provides daily

page 275 mean fields of foundation SST over the Mediterranean Sea (https://doi.org/10.48670/moi-00172CMEMS product reference:

276 SST\_MED\_SST\_L4\_NRT\_OBSERVATIONS\_010\_004, https://resources.marine.copernicus.eu/product-

277 detail/SST\_MED\_SST\_L4\_NRT\_OBSERVATIONS\_010\_004/INFORMATION; last access: 15\_July\_202203\_November

278 2021). Here, the diurnal SST chain is organized in three main modules (Fig. 1).





Formattato: Allineato al centro

280

Figure 1. Schematic diagram of the processing chain used for the MED DOISST SST product.

282

Module M1 manages the external interfaces to get both upstream L3C <u>SST</u> and model data: hourly mean L3C sub-skin SST data at 0.05° grid resolution are downloaded from OSI-SAF while hourly MedFS SST data at 1.0182 meter (first level) at

285 0.042° grid resolution from the Copernicus Marine Service.; hourly seawater potential temperatures at 1.0182 meter are

286 obtained from the CMEMS Mediterranean Sea model outputs, provided on a 0.042° regular grid.

Module M2 extracts and regrids (through bilinear interpolation) <u>both SEVIRI L3C L3C data and model outputsMedFS SST</u>
 <u>data</u> over the <u>CMEMS Mediterranean SeaDOISST</u> geographical area domain at 1/16° grid resolution (see Table 2). A selection
 over SEVIRI is performed by flagging the pixels with quality flag < 3.</li>

Module M3 performs a space-time optimal interpolation (OI) algorithm. L4 data are obtained as a linear combination of the SST anomalies, weighted directly with their correlation to the interpolation point and inversely with their cross-correlation and error (Eq. 1). Correlations are typically expressed through analytical functions with predefined spatial and temporal decorrelation lengths. Here, the covariance function  $f(r, \Delta t)$  is the one defined in Marullo et al. (2014), and given as the product of a spatial and temporal component:

, d

(2)

$$f(r,\Delta t) = \left[\alpha. e^{-\frac{r}{R}} + \frac{1-\alpha}{(1+r)^c}\right] \cdot e^{-\left(\frac{\Delta t}{T}\right)^{\alpha}}$$

where r is the distance (in km) between the observation and the interpolation point;  $\Delta t$  is the temporal difference (in hours) between the observation and the interpolation point; R = 200 km is the decorrelation spatial length; T = 36 h is the decorrelation time length; the other parameters are set as follows: a = 0.70, c = 0.26, d = 0.4. All these parameters have been derived in Marullo et al. (2014), deduced from a nonlinear least square fit between the estimated temporal and spatial correlations In practice, the weights in expression (1) are computed directly from the analytical function (2).

The input data are selected only within a limited sub-domain (within a given space-time interval, also called "influential" radius), with a temporal window of  $\pm 24$  h (this the result of several trials over a large variety of environmental conditions; Marullo et al., 2014) and a spatial search radius of about 700 km (Buongiorno Nardelli et al., 2013). A check to avoid data propagation across land is performed between each pixel within the sub-domain and the given interpolation point (eventually discarded if there are land pixels between the straight line connecting the two points).

The interpolation error (analysis\_error field in the L4 file, Table 2) is obtained from the formal definition of the error variance derived from optimal interpolation theory (e.g., Bretherton et al., 1976). This error ranges between 0-100%, meaning that the error is almost zero when an optimal number of observations is present within the space-time influential radius, while only first-guess data are used (i.e. no observations are found within the search radius) when the error is 100%.

The optimal interpolation algorithm is synthetized as follows. For clarity, in order to interpolate an SST map on a given day at 12:00 UTC the following steps have to be done:

ł	313	•	Download of $\pm 24$ hourly SEVIRI L3C and MedFS (first layer) SST fields (in their native spatial resolution) centered
	314		with respect to the interpolation time;
	315	•	Extract and regrid over the DOISST geographical domain at 1/16°;
	316	•	Retain only SEVIRI data with quality flag $\geq$ 3;
	317	•	Subctract hourly MedFS SSTs from valid SEVIRI SSTs to produce SST anomalies;
-	318	•	Use SST anomalies as data input for the optimal interpolation analysis;

319	Collect anomalies in a space/time window of 700 km/ ±24 h with respect to the interpolation position/time;
320	Run Optimal interpolation using the covariance function defined above;
321	• Add the hourly (at 12:00 UTC) MedFS SST field to the optimally interpolated output again.
322	
323	Obviously, the symmetric temporal window (±24 hourly) can be applied only for reprocessing. During near-real-time DOISST
324	processing, the input data are collected starting from 24 h before the interpolation time up to the last available SEVIRI hourly
325	SST field.
326	Finally, the main difference with the original method is that all the input observations are interpolated, while in Marullo et al.
327	(2014) valid SST observations are left unchanged (not interpolated).
328	The optimal interpolation algorithm is synthetized as follows:
329 330	<ul> <li>Hourly SEVIRI and model SSTs in a space/time window of 700 km/ ±24 h around the interpolation position/time are ingested;</li> </ul>
331	• SEVIRI data with quality flag $\geq$ 3 are retained;
332	Regridding over the Mediterranean Sea;
333	<ul> <li>Hourly model SSTs are subtracted from valid SSTs producing SST anomalies;</li> </ul>
334	<ul> <li>SST anomalies are used as data input for the optimal interpolation analysis;</li> </ul>
335	<ul> <li>Optimal interpolation is run using the covariance function defined above;</li> </ul>
336	<ul> <li>The model SST is added to the optimally interpolated output again.</li> </ul>
337	
338	The only difference with the original method is that all the input observations are interpolated, while in Marullo et al. (2014)
339	valid SST observations are left unchanged (not interpolated).

#### 340 4 Validation of diurnal product

#### 341 4.1 Validation framework

The accuracy of the MED DOISST product has been assessed through comparison with independent co-located (in space and 342 343 time) surface drifting buoy data (matchups). The relative and absolute validation framework is thus based on the compilation 344 of a matchup database between DOISST, SEVIRIL3C, MedFS (all available at 1/16° as described in section 3.3), and OSTIA 345 diurnal (kept at its original <sup>1</sup>/<sub>4</sub>° resolution), and drifters measurements covering the full years 2019 and 2020. The large number 346 of drifters provides a rather homogeneous and continuous spatial and temporal coverage over the whole period (Fig. 2) allowing 347 a robust statistical approach.

348 Firstly, a pre-selection of high-quality drifter data is performed, retaining only temperatures with quality flag equal to 1 (good) 349 or 2 (probably good) (see section 2.3). Then, the co-location is carried out on hourly basis, building a matchup database by 350 collecting the closest (in spacenearest neighbour) SST grid point to the in situ measurement within a symmetric temporal 351 window of 30 minutes with respect to the beginning of each hour. A final quality outlier detection check is carried out by 352 identifying drifter data for which the module of the difference with respect to satellite observations exceeds n-times the 353 standard deviation  $\sigma$  of the distribution of the differences ( $\delta$ ). At each step n decreases-, and data that fall out of the interval 354  $I = [mean(\delta) - n \cdot \sigma, mean(\delta) + n \cdot \sigma]$  are flagged as outliers and removed. For each n, the selected outliers are eliminated 355 and the process is repeated for the same value of n until no more outliers are detected. Then the system moves to n-1. The 356 process starts for n=10 and stops at n=3, and removes  $\sim 1\%$  of the total original sampling (as expected from a gaussian 357 distribution) of drifter data that clearly revealed anomalous temperature values.

The main validation statistics are quantified in terms of mean bias and Root-Mean-Square Difference (RMSD) from matchup temperature differences (namely, SST minus drifter). Each statistical parameter is associated with a 95% confidence interval computed through a bootstrap procedure (Efron 1994).

361 In order to evaluate the DOISST performance with respect to the model, the same validation procedure has been applied to the 362 modelled SST.

363

#### 364 4.2 Comparison with drifters

#### 365 4.2.1 The mean diurnal cycle

The spatial distribution of DOISST and drifter matchups over the 2019-2020 period, along with their pointwise difference (i.e., DOISST minus drifter measurement) shows a rather homogeneous coverage over the most of the <u>CMEMS MEDDOISST</u> geographical domain (Fig. 2), although some areas are characterized by quite low coverage, such as the North Adriatic Sea or North Aegean Sea. The spatial distribution also evidences the predominance of a positive bias, indicating that DOISSTs are warmer than drifters' temperatures on average.





The DOISST product shows effectively an overall small positive mean bias of  $0.041 \pm 0.001$  K and a RMSD of  $0.412 \pm 0.001$ K (Table 2). A negative bias of -0.100 ± 0.001 K and slightly larger RMSD -of 0.467 ± 0.001 K characterize model-MedFS SSTs. Both DOISST and the modelMedFS show high and comparable correlation coefficients (more than 0.99).

CMEMS Mediterranean DOISST geographical domain from 2019/01/01 to 2020/12/31.

	Period	Mean bias (K)	RMSD (K)	Correlation coeff.	Matchups
DOISST	2019-01-01 to 2020-12-31	$0.041\pm0.001$	$0.412\pm0.001$	0.992	548959
Model	2019-01-01 to 2020-12-31	$-0.100 \pm 0.001$	$0.467\pm0.001$	0.991	548959
MedFS					

Table 3. Summary statistics of DOISST and model-MedFS outputsSST. Mean bias (K), RMSD (K), and correlation coefficient are derived from temperature differences against drifters' data over the period 2019-2020. Each statistical parameter is associated with a 95% confidence interval computed through a bootstrap procedure (Efron 1994).

The hourly mean bias of DOISST and model-MedFS\_shows similar but opposite behaviour (Fig. 3a, and Table 4). In both 389 390 cases, the bias clearly exhibits a diurnal oscillation during the 24 hours but, while the bias of DOISST increases positively 391 during the central diurnal warming hours, the one of the model MedFS increases negatively. The DOISST mean bias is 392 practically null between 17:00 to 06:00 local time, ranging between -0.001 and 0.03 K, and highest (~0.1 K) between 10:00 393 and 13:00 local time. The MedFS bias of the model oscillates around ~-0.07 K between 23:00 and 07:00 local time. Then, it 394 increases (in absolute value) reaching the peak of ~-0.16 K between 11:00 and 14:00 and decreases successively. Similar 395 results are obtained for the RMSD, which increases with diurnal warming (Fig. 3b, Table 4). However, the RMSD of DOISST 396 is less impacted by diurnal variations, characterized by an amplitude of ~0.04 K against ~0.14 K of the modelMedFS.



<u>(a)</u>

<u>(b)</u>



Figure 3. (a) Mean bias (K) and (b) RMSD (K) relative to MED DOISST (blue line) and model-MedFS (purple line) based on

the differences against drifters' data. Mean bias and RMSD are given as hourly mean over the period 2019-2020.

Hour	Mean BIAS	RMSD (K)	BUOY-AVAIL	Mean BIAS (K)	RMSD (K)
(local	(K)	(DOISST)		(ModelMedFS)	(ModelMedFS)
time)	(DOISST)				
HH: 00	$0.001\pm0.005$	$0.398 \pm 0.004$	22807	$-0.076 \pm 0.006$	$0.431\pm0.006$
HH: 01	$0.009\pm0.005$	$0.399 \pm 0.004$	23004	$-0.072 \pm 0.006$	$0.431\pm0.006$
HH: 02	$0.014\pm0.005$	$0.396 \pm 0.004$	22798	$-0.073 \pm 0.005$	$0.431\pm0.006$
HH: 03	$0.015\pm0.005$	$0.396\pm0.004$	23078	$-0.068 \pm 0.006$	$0.427\pm0.006$
HH: 04	$0.008\pm0.005$	$0.392\pm0.004$	22857	$-0.070 \pm 0.005$	$0.425\pm0.006$
HH: 05	$0.017\pm0.005$	$0.395\pm0.004$	22806	$-0.070 \pm 0.005$	$0.425\pm0.006$
HH: 06	$0.029\pm0.005$	$0.403\pm0.004$	22819	$-0.069 \pm 0.006$	$0.425\pm0.006$
HH: 07	$0.053\pm0.005$	$0.407\pm0.004$	23379	$-0.067 \pm 0.005$	$0.419\pm0.006$
HH: 08	$0.076\pm0.005$	$0.415\pm0.004$	23501	$-0.078 \pm 0.006$	$0.423 \pm 0.006$
HH: 09	$0.094\pm0.005$	$0.423 \pm 0.004$	23481	$-0.100 \pm 0.006$	$0.436\pm0.006$
HH: 10	$0.099\pm0.006$	$0.435\pm0.004$	23270	$-0.125 \pm 0.006$	$0.473\pm0.007$
HH: 11	$0.101\pm0.006$	$0.442\pm0.004$	23311	$-0.147 \pm 0.006$	$0.510\pm0.007$
HH: 12	$0.098\pm0.006$	$0.442\pm0.004$	23129	$-0.159 \pm 0.007$	$0.546\pm0.009$
HH: 13	$0.091 \pm 0.006$	$0.440\pm0.005$	22836	$-0.161 \pm 0.007$	$0.560\pm0.009$
HH: 14	$0.070\pm0.006$	$0.436 \pm 0.004$	22673	$-0.157 \pm 0.007$	$0.563\pm0.011$
HH: 15	$0.062\pm0.006$	$0.431 \pm 0.004$	22418	$-0.139 \pm 0.007$	$0.540\pm0.009$
HH: 16	$0.051 \pm 0.006$	$0.424\pm0.004$	22368	$-0.123 \pm 0.007$	$0.515\pm0.008$
HH: 17	$0.032\pm0.006$	$0.417\pm0.004$	22019	$-0.111 \pm 0.006$	$0.491 \pm 0.007$
HH: 18	$0.014\pm0.006$	$0.410\pm0.004$	21916	$-0.100 \pm 0.006$	$0.469\pm0.007$
HH: 19	$-0.001 \pm 0.005$	$0.399\pm0.004$	22117	$-0.095 \pm 0.006$	$0.458\pm0.007$
HH: 20	$0.001\pm0.005$	$0.393 \pm 0.004$	22458	$-0.090 \pm 0.006$	$0.448\pm0.006$
HH: 21	$0.014\pm0.005$	$0.391\pm0.004$	23229	$-0.083 \pm 0.005$	$0.436\pm0.006$
HH: 22	$0.011\pm0.005$	$0.392\pm0.004$	23272	$-0.084 \pm 0.006$	$0.428\pm0.006$
HH: 23	$0.006\pm0.005$	$0.399 \pm 0.004$	23413	$-0.078 \pm 0.006$	$0.429 \pm 0.006$

401

Table 4. Summary statistics of MED DOISST and model MedFS products based on the differences against drifters' data over 402 the matchup points. Mean bias (K), RMSD (K) and number of matchups are given as hourly mean over the period 2019-2020. 403 Each statistical parameter is associated with a 95% confidence interval computed through a bootstrap procedure (Efron 1994). 404

405 The mean diurnal cycle of DOISST (namely, the 24-hour mean SSTs estimated over the matchup dataset) is in very good 406 agreement, within the error confidence interval, with the SST cycle reconstructed from drifters (Fig. 4). The two diurnal cycles 407 are practically unbiased between 17:00 and 06:00, while they are biased by ~0.1 K between sunrise and 16:00, coherently with 408 the DOISST bias oscillation (Fig. 3a). This bias could be related to skin SST getting warmerwarming faster than the 409 temperature at 20 cm depth. The diurnal cycle of model-MedFS\_SST maintains always below that of in situ temperatures,

- 410 evidencing larger differences during the central diurnal warming hours (Fig. 4). However, apart from the biases likely induced
- 411 by the different depths, the SST amplitude as estimated from the DOISST and the model MedFS is ~2.3% larger and ~16%
- smaller than that of drifters, respectively, suggesting that the model tends to underestimate diurnal variations.





Figure 4. Mean diurnal cycle for MED DOISST (blue line), model MedFS (purple line) and drifters (red line) computed over the matchups from 2019 to 2020.

417
418 A delay of ~1 hour of the modelMcdFS with respect to DOISST and in situ on the onset of diurnal warming and in reaching
419 the maximum is also evident. This delay could be explained as the physical result of delayed solar heating of the skin layer
420 sensed by the satellite and of the first model layer. This may also be a consequence of the different packaging of the SEVIRI
421 and model McdFS SST data into the hourly files: model McdFS hourly SST fieldsones are centered at half of every hour (e.g.,
422 12:30), while SEVIRI L3C at the beginning of each hour (e.g., 12:00) and obtained from collating data within one hour (from
423 11.30 to 12:29).

The capability of DOISST to capture and realistically reproduce diurnal variability is further investigated by analysing the seasonally averaged SST diurnal cycle (Fig. 5), computed as for the mean diurnal cycle (by using the matchup dataset) but







<u>(a)</u>

433

<u>(b)</u>





Figure 5. Seasonal mean diurnal cycle over the period 2019-2020 for MED DOISST (blue line), model-MedFS (purple line) 436 437 and in situ (red line). (a) Winter (December to February); (b) Spring (March to May); (c) Summer (June to August); and (d) Autumn (September to November).

	Period	Mean bias (K)	RMSD (K)	Matchups
	DOISST	$0.045\pm0.003$	$0.428\pm0.002$	
D-J-FWinter	MedFSModel	$-0.084 \pm 0.004$	$0.563 \pm 0.003$	90247
MAMEnning	DOISST	$0.036 \pm 0.001$	$0.383 \pm 0.001$	200440
M-A-MSpring	MedFSModel	$-0.101 \pm 0.001$	$0.389 \pm 0.002$	308448

	DOISST	$0.012\pm0.003$	$0.483 \pm 0.002$	74107
J-J-A <u>Summer</u>	MedFSModel	$-0.117 \pm 0.003$	$-0.117 \pm 0.003 \qquad \qquad 0.486 \pm 0.004$	
	DOISST	$0.079 \pm 0.003$	$0.429 \pm 0.002$	2/1/2
<u>S-O-NAutumn</u>	MedFSModel	$-0.098 \pm 0.004$	$0.590 \pm 0.004$	76157

Table 5. Summary statistics of DOISST and model MedFS outputsSSTs. Mean bias (K) and RMSD (K) are derived from temperature differences against drifters' data during winter (D-J-F), spring (M-A-M), summer (J-J-A) and autumn (S-O-N) over the period 2019-2020. Each statistical parameter is associated with a 95% confidence interval computed through a bootstrap procedure (Efron 1994).

446 The capability of DOISST to reproduce diurnal warming events is analysed in the following section.

## 447

445

#### 448 4.2.2 Diurnal warming events

Diurnal warming (DW) can be defined as the difference between the SST at a given time of the day and the foundation SST (see e.g. Minnett et al., 2019), i.e. the water temperature at a depth such that the daily variability induced by the solar irradiance is negligible. In many cases, the foundation SST coincides with the night minimum SST, namely the temperature that is recorded just before sunrise.

453 The capability of DOISST to describe diurnal warming events is analysed here in comparison with SEVIRI L3C, OSTIA 454 diurnal, MedFS model and drifter data. The evaluation is carried out by computing daily Diurnal Warming Amplitudes 455 (DWAs) from drifters and building a matchup dataset of DWAs as estimated from DOISST, SEVIRI L3C, OSTIA and MedFS 456 model data. The inclusion of SEVIRI data is mainly aimed at evaluating the impact of optimal interpolation on the input 457 SEVIRI SSTs, while OSTIA diurnal is used as an intercomparison product. The DWA is estimated here as a difference between 458 the maximum occurred during daytime (10:00-18:00 local time) and the minimum during nighttime (00:00-06:00 local time) 459 (see also Takaya et al., 2010; While et al., 2017). Explicitly, for each day (from 2019 to 2020+) and for each drifter the two 460 positions and times relative to the minimum and maximum temperature are stored; over the same times and nearest positions, 461 the temperatures of the other datasets are stored too. The grid resolution of OSTIA diurnal (namely, 0.25° deg.) has been left 462 unchanged since what is needed is just the SST value at a given position, the nearest to the drifter's one.

The scatter plots of DOISST, SEVIRI, OSTIA, and <u>MedFS model</u> vs in situ-measured DWA have been computed for the years 2019-2020 (Fig. 6) and organized during spring-summer and winter-autumn seasons (Fig. 7). This choice is aimed at comparing the behaviour of the four products as a function of the seasons, since larger DWA intensities are expected in the spring-summer period. 467 Overall, there is a good agreement between DOISST and drifter DWAs (Fig. 6a) as confirmed by an almost null mean bias (-468 0.02 K), low RMSD (0.38 K) and high correlation coefficient (0.82). The largest DW amplitudes reach values as high as 4 K 469 in both DOISST and drifter data. SEVIRI (Fig. 6b) shows the same bias (-0.02 K) of DOISST in reconstructing DWAs but 470 higher RMSD (0.49 K) and lower correlation (0.74). It is relevant to note that the spread of SEVIRI DWAs around the line of 471 perfect agreement is reduced in DOISST, which coherently has a lower RMSD. The modelMedFS (Fig. 6c) clearly 472 underestimates diurnal amplitudes larger than 1 K, and it is characterized by a high mean bias (-0.23 K) and RMSD (0.55 K), 473 and lowest correlation coefficient (0.66). Similarly, OSTIA diurnal (Fig. 6d) underestimates DWAs larger than 1 K, and it is 474 characterized by the highest mean bias (-0.28 K), RMSD of 0.54 K but shows less dispersion than the modelMedFS around 475 the line of perfect agreement (correlation of 0.72).

476 The majority of DWA events lie between 0-1 K all over the year, but higher values are effectively reached during spring and 477 summer (Fig. 7). During these seasons, it appears more evident the capability of DOISST to better describe DWAs larger than 478 1 K (mean bias = -0.04 K; RMSD = 0.42 K; corr. = 0.83) compared to SEVIRI (mean bias = -0.05 K; RMSD = 0.53 K; corr. 479 = 0.76) and especially to the modelMedFS (mean bias = -0.27 K; RMSD = 0.65 K; corr. = 0.63) and OSTIA diurnal (mean bias = -0.39 K; RMSD = 0.66 K; corr. = 0.71). During winter and autumn, the overall statistics of the four products get better, 480 481 clearly due to the fact that the majority of DWA events range between 0-0.5 K. However, DWA events exceeding 1 K are also 482 observed, and such intense amplitudes are not found in the model-derived and OSTIA DWAs. Additionally, the good 483 agreement between DOISST and drifters still confirms that interpolated data do not suffer from the increased cloud cover 484 during winter and autumn periods.

(a)





(c)



Figure 6. DWA scatter plots for (a) DOISST, (b) SEVIRI L3C, (c) model<u>MedFS</u>, and (d) OSTIA diurnal vs drifters over
 the period 2019-2020.









490 Figure 7, DWA scatter plots for DOISST (a,b), SEVIRI L3C (c,d), model MedFS (e,f), and OSTIA diurnal (g,h) vs drifters 491 during Spring (M-A-M) and Summer (J-J-A), and Winter (D-J-F) - Autumn (S-O-N), over the period 2019-2020. 492

493 Having demonstrated the reliability of DOISST in the DWA estimate, we analyze its capability to reproduce the typical spatial 494 variability and intensity of DW events in the Mediterranean Sea, a basin characterized by a frequent occurrence of intense DW 495 events (Böhm et al., 1991; Buongiorno Nardelli et al., 2005; Gentemann et al., 2008; Merchant et al., 2008). In our investigation 496 area, the 2019-2020 mean DWA ranges from a minimum of 0.4 K in the Atlantic Ocean box off the Strait of 497 Gibraltar, to a maximum of 1.2 K in several regions of the Mediterranean Sea (Fig. 8a) where individual diurnal warming 498 events exceeding 1 or even more than 2 K are quite frequent. The largest DWA were observed in the Levantine Basin, in the 499 North Adriatic Sea and in correspondence with the Alboran Gyre. Less intense, though still remarkable, mean DWA patches 500 reaching 0.9 K are found around the southern tip of the Italian Peninsula as well as in the coastal Ligurian Sea. In the same 501 areas, it is found that the frequency of DW events larger than 1 K and 2 K can reach up to 55% and 10% of the analyzed time 502 series, respectively (bearing in mind that our time series is given by the total number of days in -2019 and 2020) (Fig. 8b-c). 503 The spatial variability and magnitude of the DWA described by the DOISST product are consistent with past and recent studies 504 on the SST diurnal variability in the Mediterranean Area (Minnet et al. 2019; Marullo et al. 2016; Marullo et al. 2014).

505 The magnitude of the maximum SST diurnal oscillation is also investigated. The spatial distribution of the maximum DWA observed through 2019-2020 in the Mediterranean Sea (6°W to 36°E and 30°N to 46°N) (Fig. 8d) shows that the largest 506 507 amplitudes reach and exceed 3 K in 98% of the basin and local DWA patches exceeding 6 K are also ubiquitous, confirming that the Mediterranean is one of the areas with the largest DWs of the global ocean (Minnet et al. 2019, and references therein). 508

a)

c)







509

Figure 8. a) Mean diurnal warming amplitude (DWA) derived from DOISST; b) Percentage (over the total number of days in the 2019-2020 period) of DOISST DWA larger than 1 K; c) Percentage of DOISST DWA larger than 2 K; d) Maximum observed DOISST DWA. All the maps refer to the 2019-2020 period.

When compared to the model, DOISST exhibits mean DWAs with larger intensity than model outputs<u>MedFS ones</u> in all the
locations of the study area (Fig. 9). The ΔDWA, defined as DWA <sub>DOISST</sub> minus <u>DWA<sub>Model</sub>DWA<sub>MedFS</sub></u>, is always larger than 0.2
K and locally reaches extreme values of ~1 K. The extent of the ΔDWA generally increases in areas where the DOISST mean
DWA is larger, such as in the Alboran Sea, Ligurian Sea, Levantine Basin and Southern Tyrrhenian, suggesting a tendency of
the model to underestimate the largest DW events.





Figure 9. Mean amplitude of the SST DW. Differences between the mean DWA seen by the DOISST product and the model outputsMedFS. (first layer).

## 523

#### 524 5 Data availability

525 The Mediterranean diurnal optimal interpolated SST product is distributed as part of the CMEMS-Copernicus Marine Service 526 catalogue, and identified as SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036 (CMEMS-Copernicus product reference) and 527 cmems obs-sst med phy-sst nrt diurnal-oi-0.0625deg PT1H-m (CMEMS Copernicus dataset reference) 528 (https://doi.org/10.48670/moi-00170https://resources.marine.copernicus.eu/product-529 detail/SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036/INFORMATION, last access: 03 November 2021, 530 https://doi.org/10.25423/CMCC/SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036; last access: 15 July 2022; Pisano et al, 531 2021). Access to the product is granted after free registration as a user of CMEMS-the Copernicus Marine Service at 532 https://resources.marine.copernicus.eu/registration-form (last access: 15 July 202203 November 2021). Once registered, users 533 can download the product through a number of different tools and services, including the web portal Subsetter, Direct-GetFile 534 (DGF) and FTP. A Product User Manual (PUM) and QUality Information Document (QUID) are also available as part of the 535 CMEMS -Copernicus documentation (https://resources.marine.copernicus.eu/product-536 detail/SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036/DOCU MENTATION, last access: 15 July 202203 November 2021). 537 Eventual updates of the product will be reflected in these documents. The basic characteristics of the DOISST product are 538 summarized in Table 2. The reduced subset used here for validation and review purposes is openly available at 539 https://doi.org/10.5281/zenodo.5807729 (Pisano, 2021).

#### 541 6 Summary and conclusions

542 A new operational Mediterranean diurnally varying SST product has been released (May 2021) within the Copernicus Marine 543 Environment Monitoring Service (CMEMS). This dataset provides optimally interpolated (L4) hourly mean maps of sub-skin 544 SST over the Mediterranean Sea at 1/16° horizontal resolution, covering the period from 1<sup>st</sup> January 2019 to near real time (1 545 day before real time) (Pisano et al., 2021). The diurnal optimal interpolated SST (DOISST) product is obtained from a blending 546 of hourly satellite (SEVIRI) data and model (MedFS) outputs SSTs via optimal interpolation, where the former are used as the 547 observation source and the latter as background. This method has been firstly proposed by Marullo et al. (2014), validated over 548 one year (2013) in Marullo et al. (2016), and implemented here operationally. The validation of the operational product was 549 also extended over two years (2019-2020) and based on a direct comparison with in situ drifting buoys data.

In an ideal case, all data (satellite, model and in situ) would be generated and comparedavailable at the same depth. Unfortunately, the first MedFS model layer is centered at 1 m depth, while sub-skin SST is, by definition, representative of a depth of ~1 mm. In principle, it could be possible to correct all the data, bringing them all to the same depth before any comparison or merging, by applying some model (see e.g. Zeng et al., 1999). However, any correction algorithm would have added potential uncontrolled error sources (e.g., related to ancillary data and/or to model assumptions) and implied significant additional operational efforts. For these reasons, rather than trying to correct the first-guess bias, we preferred to leave it uncorrected, and focus on optimising the corrections driven by available hourly satellite data.

557 DOISST proved to be rather accurate when compared to drifter measurements, and correctly reproduced the diurnal variability 558 in the Mediterranean Sea. The accuracy of DOISST results in an overall, almost null, mean bias of ~0.04 K and RMSD of 559 ~0.41 K (Table 3). This product is also more accurate than the input modelMedFS, which shows a mean bias of ~-0.1 K and 560 RMSD of ~0.47 K. A warm (positive) and cold (negative) bias characterizes the DOISST and the modelMedFS, respectively, 561 also during seasons (Fig. 5). These opposite biases are likely related to the different nature of the SST provided by DOISST, 562 model and drifter data, i.e. sub-skin (~1 mm from the surface), averaged 1 m depth and 20 cm depth, respectively, and then 563 consistent with the physical consequence of a reduction of the temperature with depth due to the vertical heat transfer-heat 564 process. The DOISST RSMD generally keeps lower values compared to the modelMedFS, ranging from a minimum of ~0.40 565 K (vs ~0.42 K for the model MedFS) to a maximum of ~0.44 K (vs ~0.56 K for the model MedFS). These results also confirm 566 the robustness of this blending algorithm that, even if based on model analyses used as first-guess, it successfully brings 567 DOISST closer to the in situ measured SST than the MedFS estimates.

568 Compared to its native version (Marullo et al., 2016), the DOISST product maintains the same RMSD (estimated in 0.42 K) 569 but displays a lower mean bias (estimated as -0.10 K). The reduced bias could be ascribed to the fact that valid SEVIRI SST values are always interpolated in DOISST, while they are left unchanged (not interpolated, see section 3.3) in the original method. Additionally, the DOISST bias is comparable with that estimated for SEVIRI over the Mediterranean Sea (-0.03 K; Marullo et al. 2016), while the DOISST RMSD is rather lower than SEVIRI one (0.47 K; Marullo et al. 2016). The DOISST bias is also lower than that of the OSTIA diurnal product, which produces gap-free hourly mean fields of skin SST for the global ocean, and has been found to underestimate the diurnal range of skin SST by 0.1-0.3 °C (While et al., 2017).

The analysis of the SST diurnal cycle as estimated from both DOISST, model-MedFS and drifter data shows that the diurnal 575 576 oscillation in SST is well reconstructed by the DOISST while the modelMedFS tends to underestimate this amplitude mainly 577 during the central warming hours (Fig. 4), and during spring and summer (Fig. 5b, c). Specifically, DOISST overestimates the 578 mean diurnal amplitude by ~2.3% compared to that of drifters, while the modelMedFS underestimates it by ~16%. This is 579 particularly evident in the analysis of diurnal warming (DW) events, where diurnal warming amplitudes (DWAs) as estimated 580 by DOISST, modelMedFS, SEVIRI, and OSTIA diurnal data are compared vs drifter-derived DWAs. This analysis shows that 581 amplitudes exceeding 1 K, as measured by drifters, are well reconstructed by DOISST (Fig. 6a) with a mean bias of ~-0.02 K 582 and RMSD of ~0.38 K. The comparison with reconstructed SEVIRI DWAs (Fig. 6b) demonstrates that optimal interpolation does not change the SEVIRI bias, which is practically null for both SEVIRI and DOISST (~-0.02 K), while it reduces the 583 584 SEVIRI RMSD, from ~0.49 K (SEVIRI) to ~0.38 K (DOISST). This is also evident in the reduction of the spread of SEVIRI 585 DWAs around the line of perfect agreement (Fig. 6b). Both the modelMedFS and OSTIA diurnal underestimate DWAs when 586 exceeding 1 K with a mean bias of ~-0.23 K (modelMedFS, Fig. 6c) and ~-0.28 K (OSTIA, Fig. 6d), and RMSD of ~0.55 K 587 for both products.- This underestimation could be related to several factors, such as that the vertical resolution of the 588 modelMedFS does not resolve the vertical temperature profile within the warm layer. Yet, the physics and atmospheric forcing 589 and/or the assimilation implemented in the modelMedFS and OSTIA, though different, are only partially able to resolve diurnal 590 variations larger than 1 K. In any case, we can argue that the tendency of the model MedFS to underestimate DWAs, mainly 591 for amplitudes > 1 K, does not strongly impact the performance of DOISST in reconstructing these amplitudes. This is likely 592 due to two concurrent factors, the high accuracy of SEVIRI SST data and that the Mediterranean area is particularly advantageous in terms of clear sky conditions. 593

Finally, the seasonal analysis also reveals that DOISST is not impacted by the different environmental conditions in the Mediterranean Sea, in particular from the much frequent cloudiness during winter and autumn periods.

596 Overall, the DOISST product is able to accurately reconstruct the SST diurnal cycle, including diurnal warming events, for the 597 Mediterranean Sea and can thus represent a valuable dataset to improve the study of those processes that require sub-daily 598 frequency.

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