Evaluation and intercomparison of GHRSST formatted products at a global scale

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GHRSST sciences talks

16th February 2023, online

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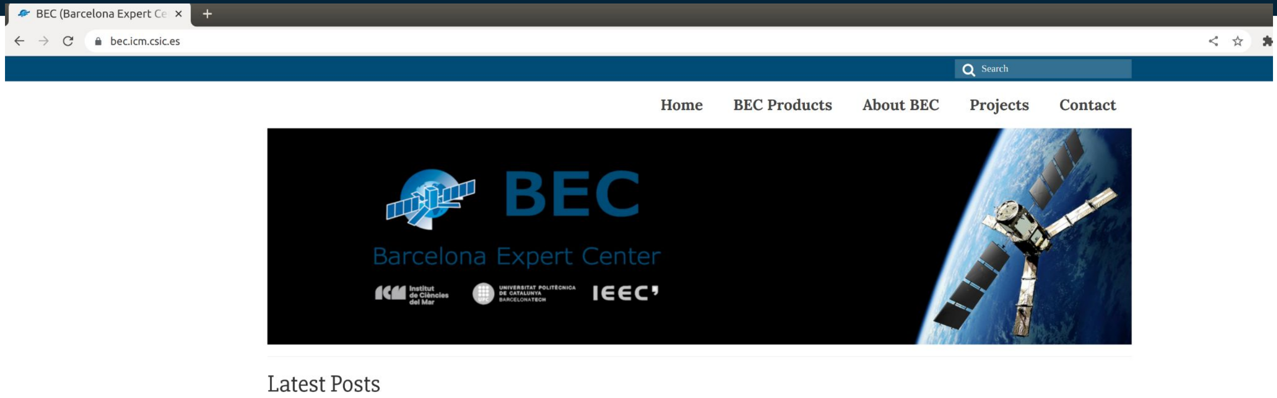

- Expert Support Laboratory for L0 and L2 of ESA Soil Moisture and Ocean Salinity (SMOS) mission
- We are currently producing and distributing:
  - Sea Surface Salinity (SSS)
    - L3 and L4 SSS products at a global scale (from L0 own production chain)
    - L3 and L4 SSS products in enclosed seas (Mediterranean, Black Sea, Baltic)
    - L3 products in cold waters (Arctic and Antarctic (on-going))
  - Soil Moisture (SM)
    - L3 products at a global scale (from ESA L2)
    - L4 SM products in the Mediterranean region

Motivation

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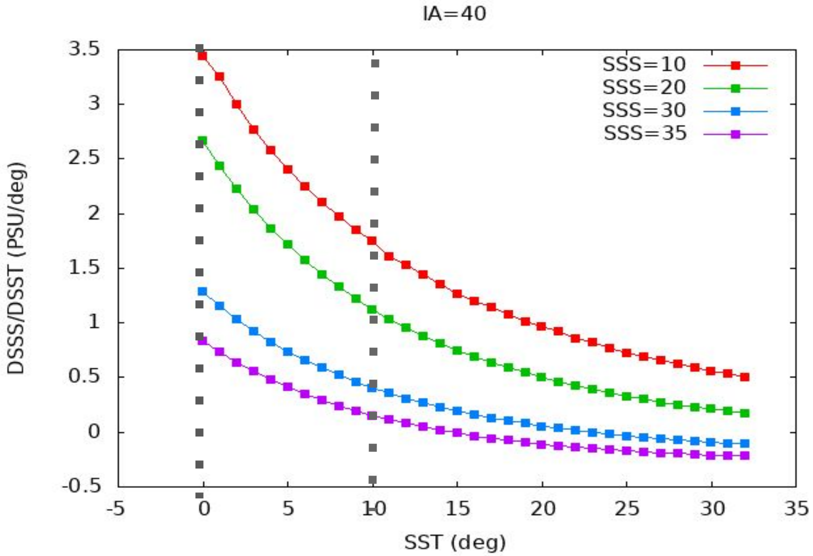
- SST plays a key role in the generation of SMOS SSS products:
  - L2/L3: as an ancillary data for the inversion of radiative models
  - L4: as a template to increase temporal and spatial resolution using multifractal fusion techniques.
- Currently, we are using SST provided by ECMWF for the SSS retrieval (L2/L3), and OSTIA SST as template for the L4 product.



High sensitivity of SSS to SST at the low SSS & low SST regions (critical for Baltic and polar regions)

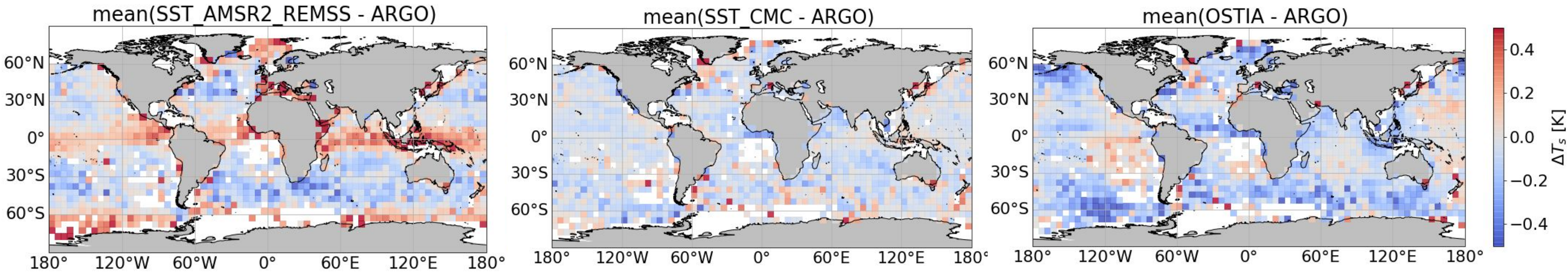
Objective

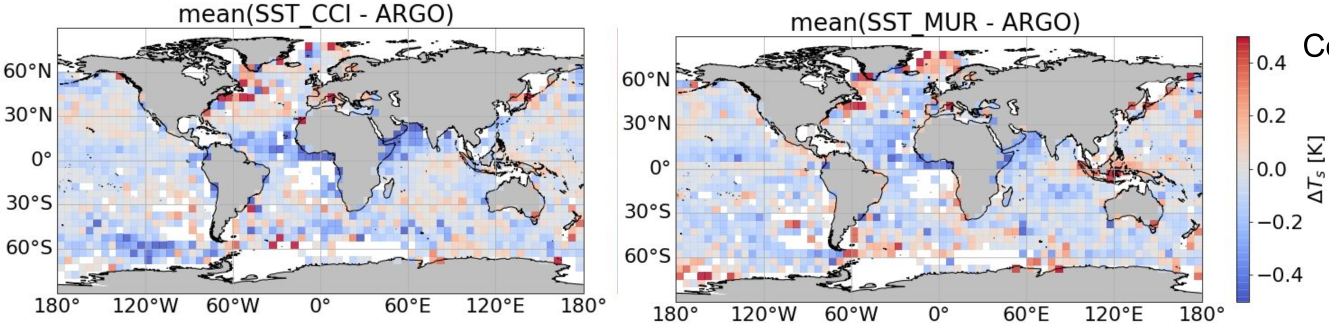
- Assessment on the best SST product, based on the following indicators:
  - Comparison with in situ data: ARGO (fiducial reference measurements)
  - Spectral analysis to assess the effective spatial resolution (feature fidelity)
  - Singularity analysis to assess the dynamical properties
  - Correlated Triple Collocation to estimate the uncertainties of the error for each product [González-Gambau et al. 2020] .

Datasets

Dataset	Spatial resolution	Source data	Sensor
AMSR2-REMSS v8.2	0.25ºx 0.25º	MW	AMSR2
CMC v3.0	0,1ºx 0,1º	MW+IR+insitu	VIIRS,AVHRR_GAC, AMSR2
OSTIA v2.0	0.05º x 0.05º	MW+IR	AVHRR, VIIRS, AMSR2, GOES_IMAGER, SEVIRI, SSMIS, SSM/I
CCI v2.1	0.05º x 0.05º	IR	ATSR, AATSR, AVHRR_GAC
MUR v4.1	0,01ºx 0,01º	MW+IR+insitu	AMSR-E, AVHRR, MODIS, SSM/I, VIIRS, in-situ
Period	daily maps for 2016		

Comparison with *in situ* data

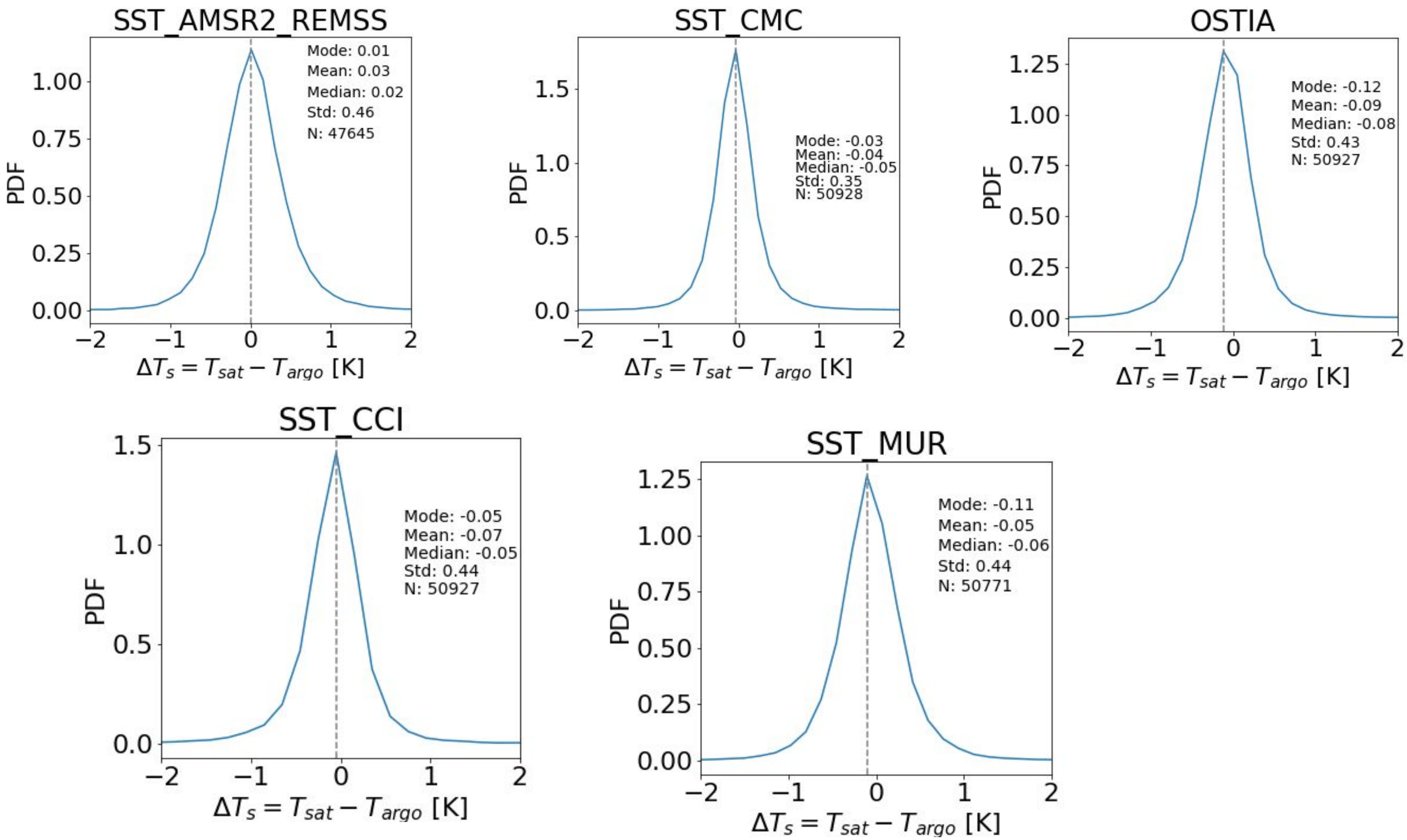




Collocation criteria:

- in situ centered (for every profile we select the closest SST pixel observation)
- 3 m < depth < 4 m

Comparison with *in situ* data



Comparison with *in situ* data (summary stats.)

Dataset	Global				
	mode	mean	median	std	N
AMSRE	0.05	0.03	0.02	0.46	47645
CMC	-0.03	-0.04	-0.05	0.35	50928
OSTIA	-0.12	-0.09	-0.08	0.43	50927
CCI	-0.05	-0.07	-0.05	0.44	50927
MUR	-0.11	-0.05	-0.06	0.44	50771

Spectral analysis

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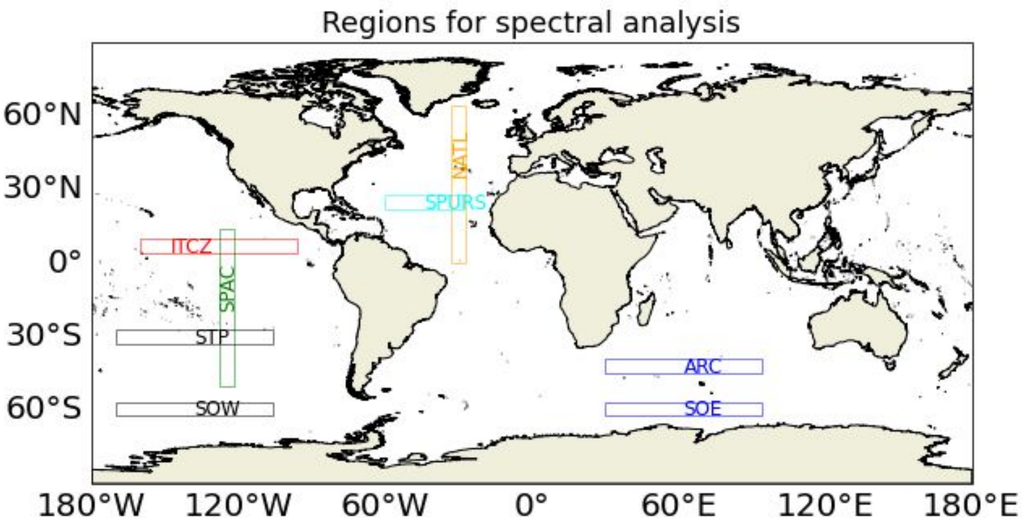
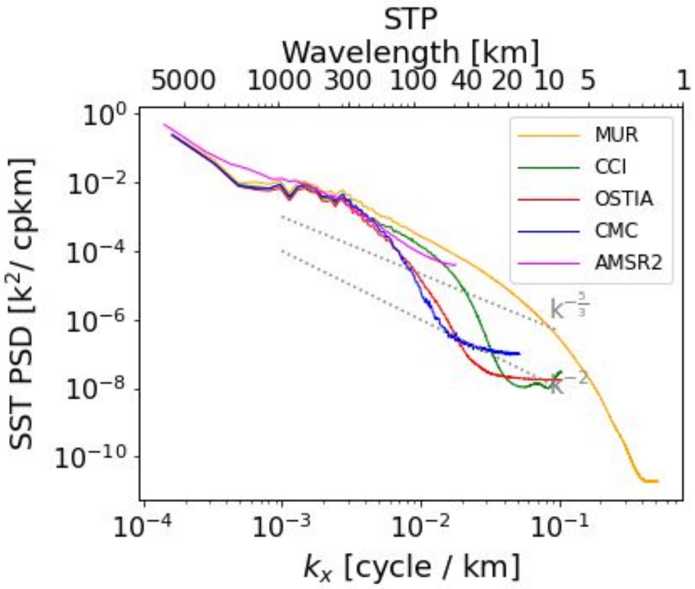
- Reynolds and Chelton (2010) showed that the grid spacing of an SST analysis is not an indicator of its feature resolution (F2T2 GHRSST Meeting 2018)

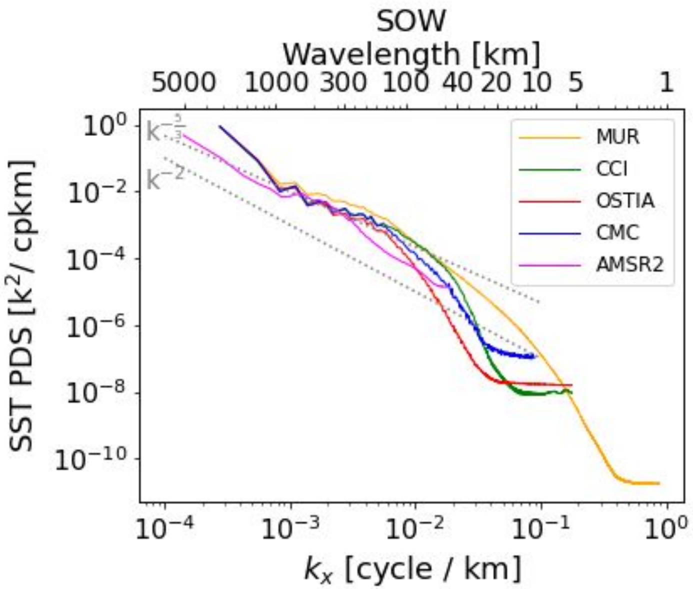
- The effective spatial resolution ($\Delta\ell$) can be estimated from the power spectral density as the λ where the energy level drops off from the expected power law ($\Delta\lambda=2\Delta\ell$)



- Just few L4 SST intercomparison works have explored spectral analysis [Reynolds et al. 2013 and Yang et al. 2021]

Spectral analysis





- CCI & MUR have the higher effective spatial resolution
- In most regions, CMC and OSTIA do not increase the effective spatial resolution of microwave observations. In SOW region MW AMSR2 drops off at larger λ.

Singularity analysis

- We propose a new metric, the **singularity spectrum**, to assess the **structural and dynamical quality** of SST products based on multifractal theory of turbulence. [Turiel et al. 2007, Isern-Fontanet et al. 2007,]
- Scale surrogate gradients, in the limit $\ell/\ell_0 \to 0$ behave as

$$\overline{|\nabla T|}_\ell(\vec{x}) \equiv \int_{\mathbb{R}^d} \ell^{-d} G(\ell^{-1}\vec{x}) |\nabla T|(\vec{x}+\vec{x}') d\vec{x}' \sim \left(\frac{\ell}{\ell_0}\right)^{h(\vec{x})}$$

- $h(\vec{x})$ is the singularity exponent. If $h(\vec{x}) \in (n, n+1)$ with n being a positive integer, $\overline{|\nabla T|}_\ell(\vec{x})$ is derivable n times but not n+1

Singularity analysis

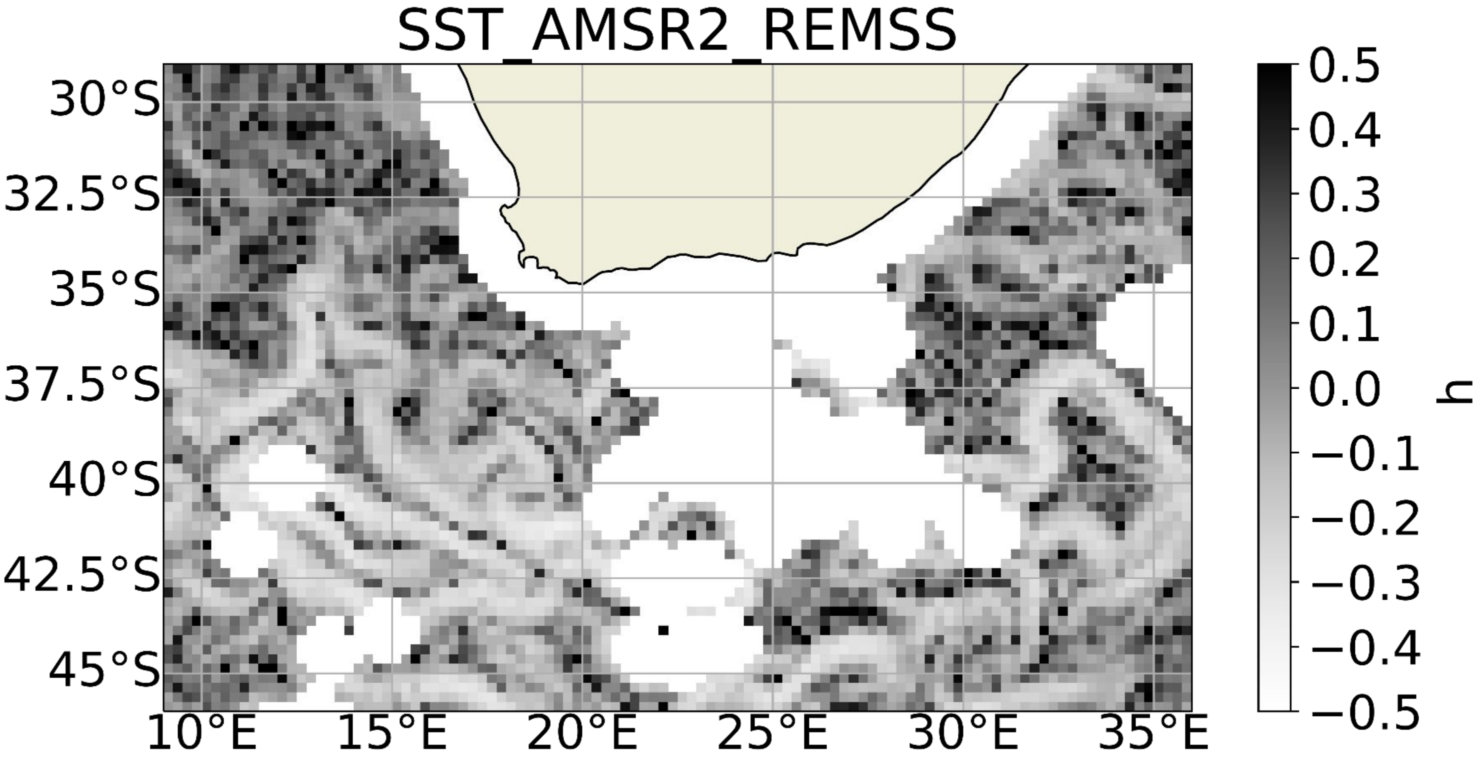
- The statistical/geometric properties of the singularity exponents are given by the **singularity spectrum**

$$D(h') \equiv d_F(\{\vec{x}|h(\vec{x} = h')\})$$

where $d_F(A)$ is the fractal dimension of a set A

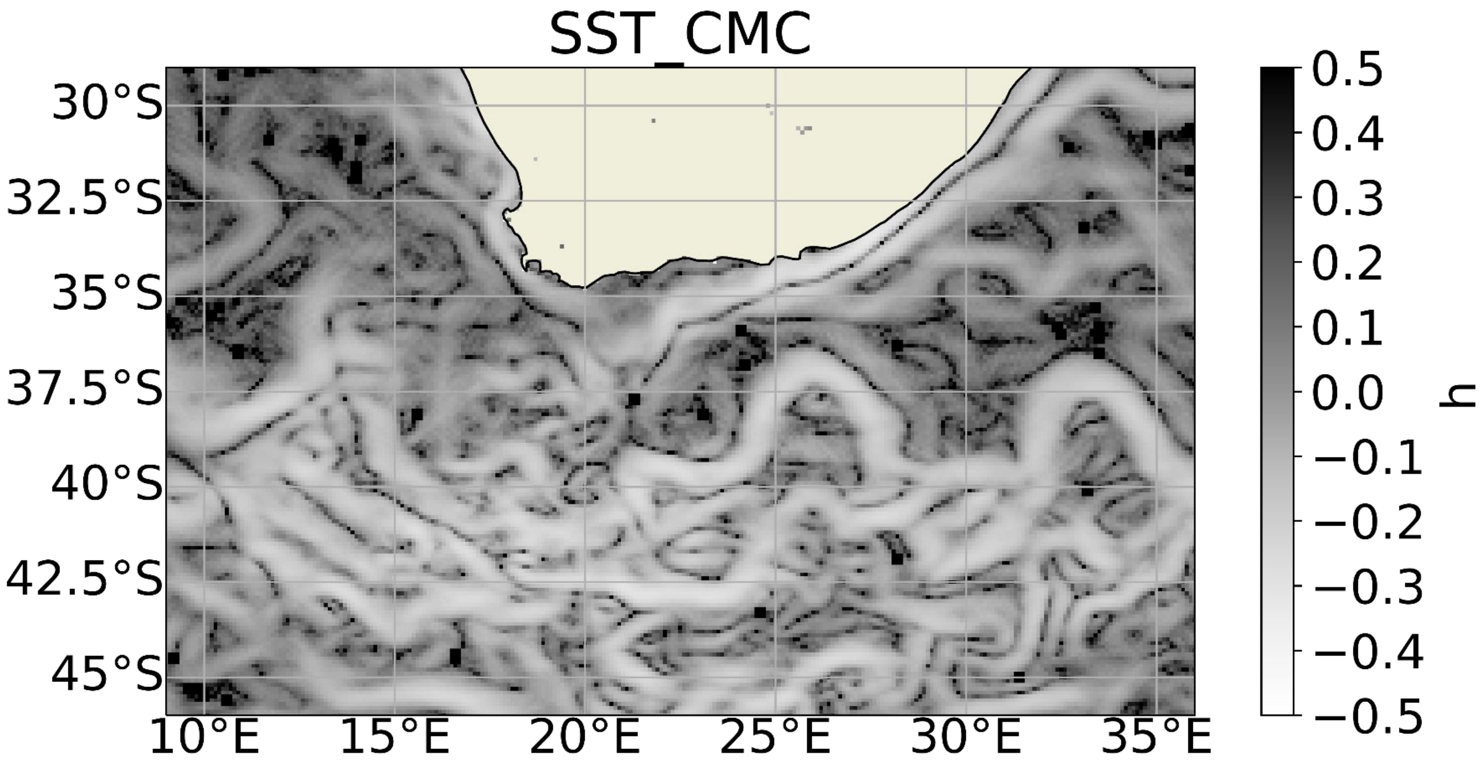
  - It can be computed from the probability density function of the singularity exponents [Pont et al. 2013]
  - D(h) is a **convex function** and it is **scale invariant**.
  - It is a representation of the turbulent cascade
  - It is the step between the canonical (statistical, structure functions) to the microcanonical formalism (geometrical, singularity exponents)

Singularity exponents



29th september 2016

Singularity exponents



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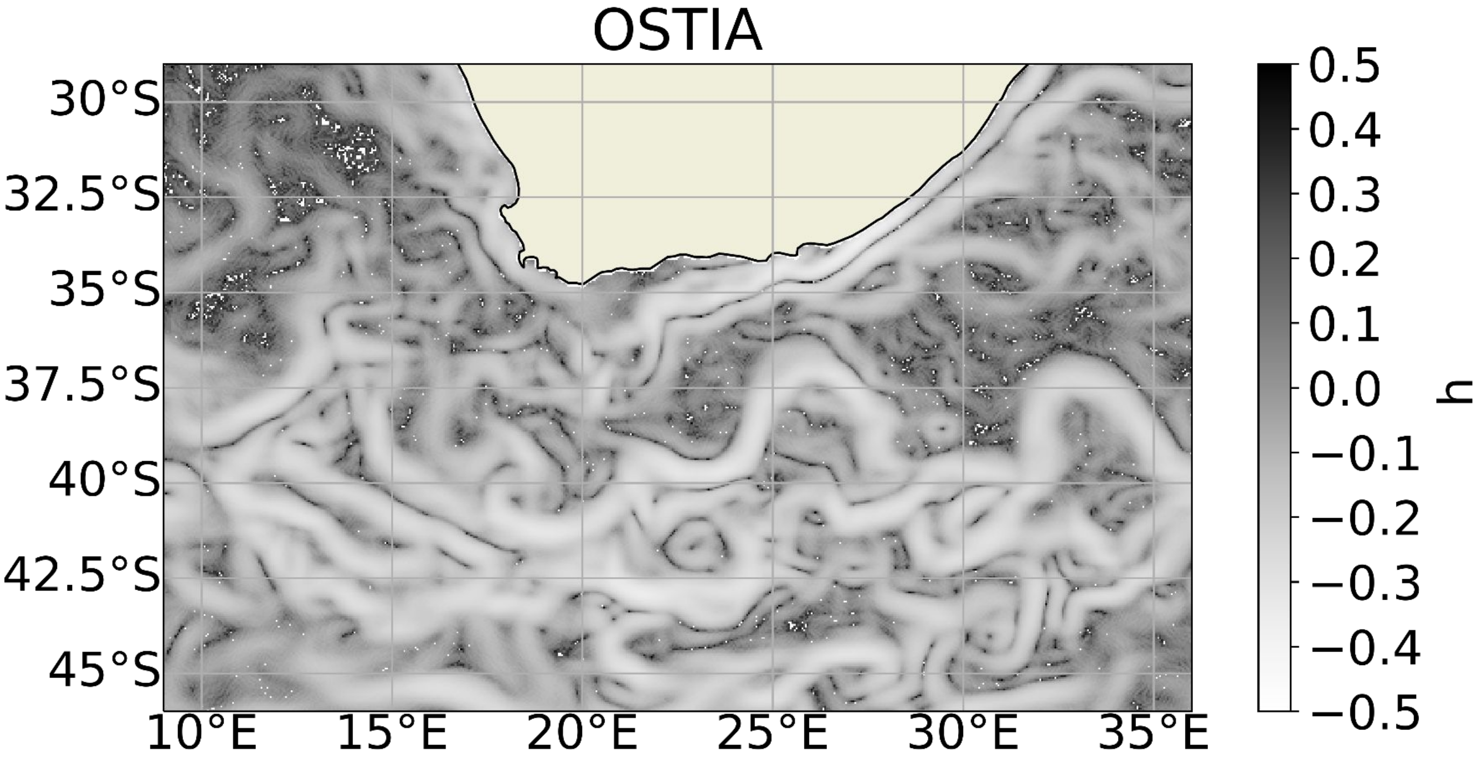
Singularity exponents



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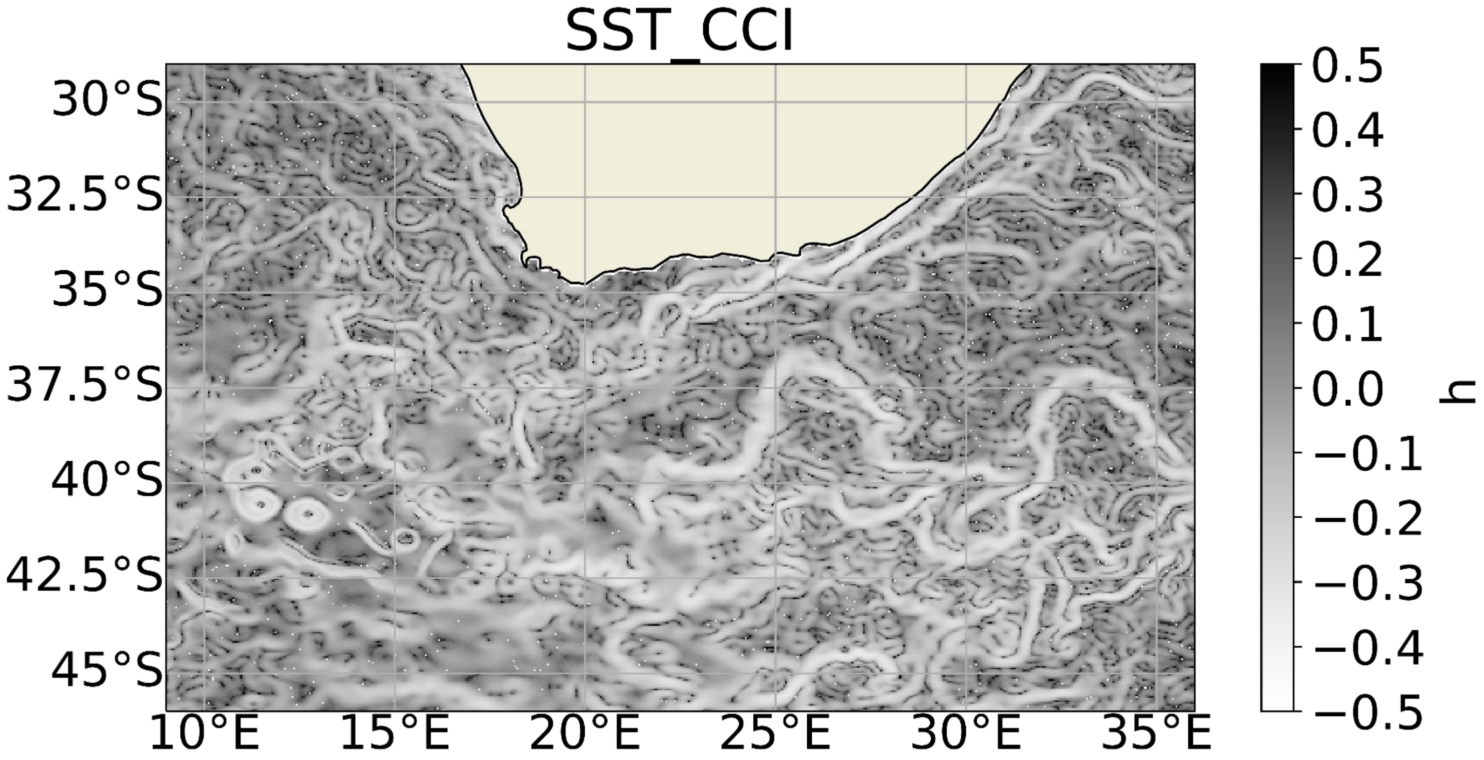
Singularity exponents



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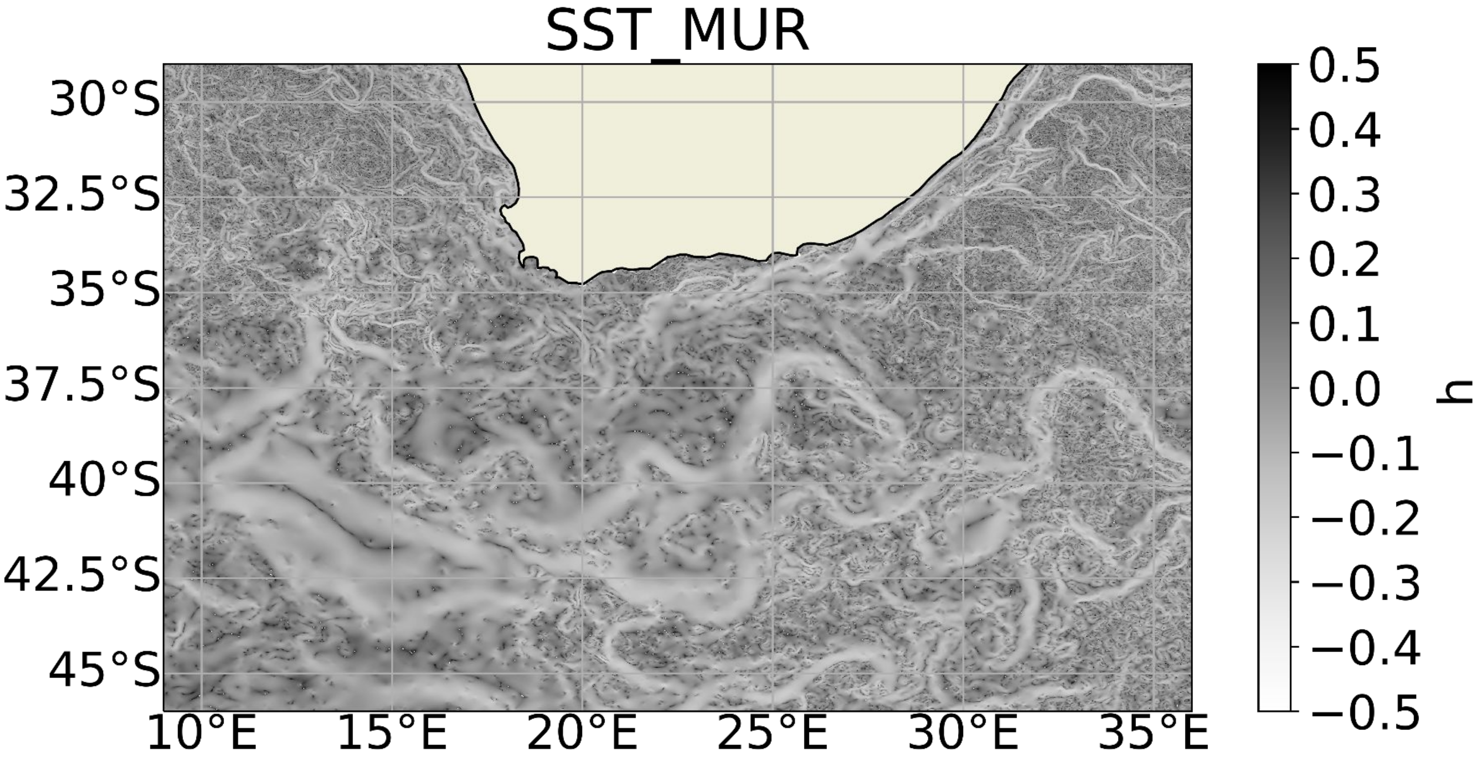
Singularity exponents



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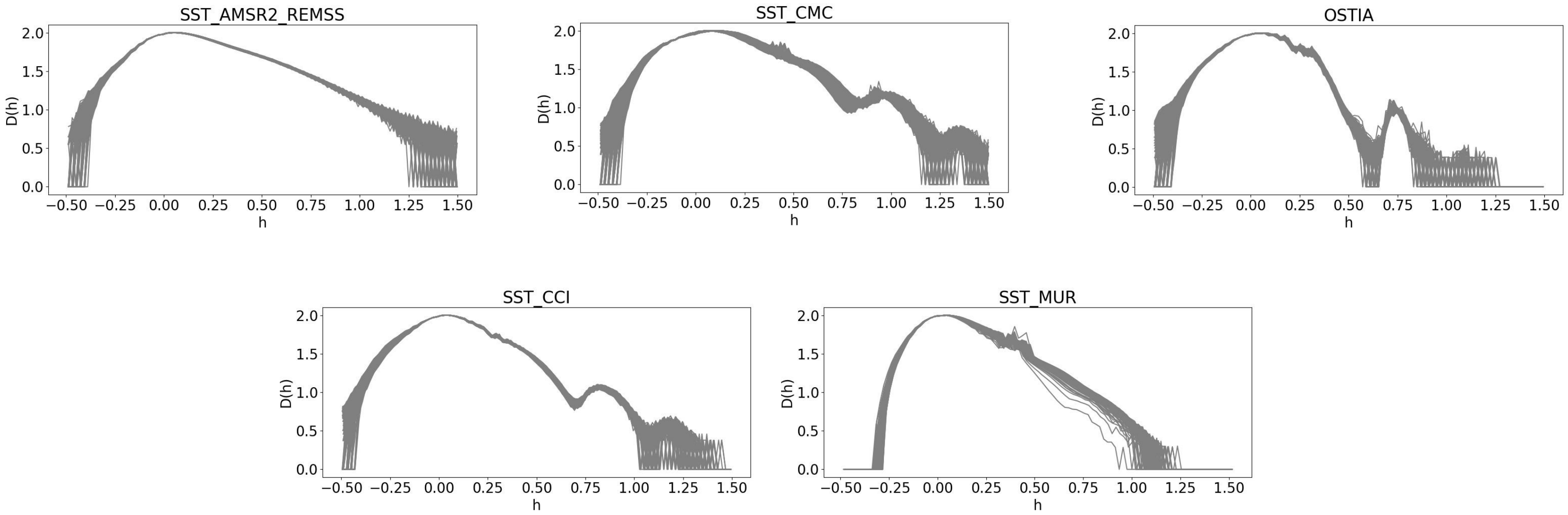
Singularity spectrum D(h)

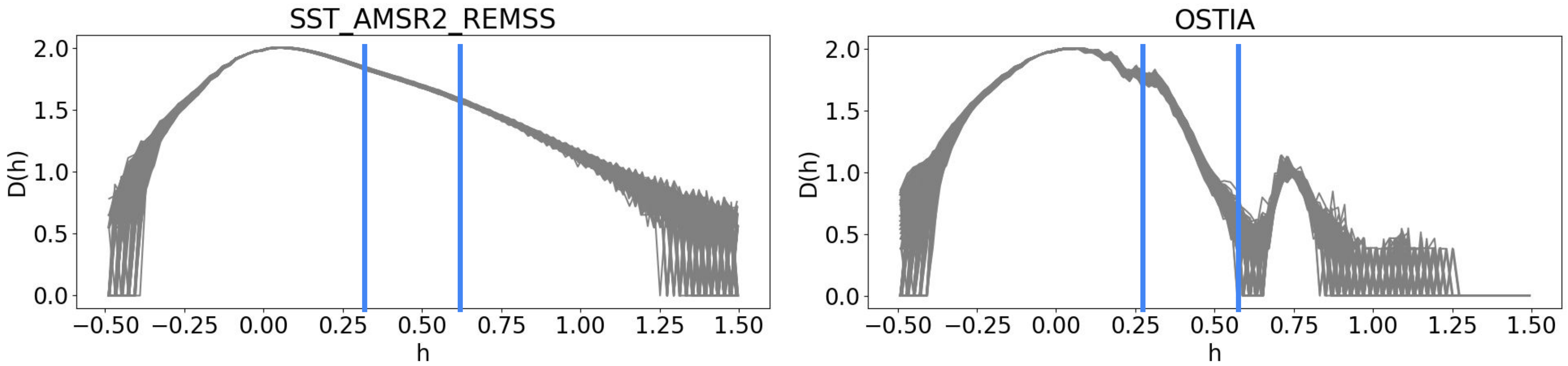
- Singularity spectrum are computed daily and at the native spatial resolution



Higher spatial resolution does not mean better dynamical representation

Singularity spectrum D(h)

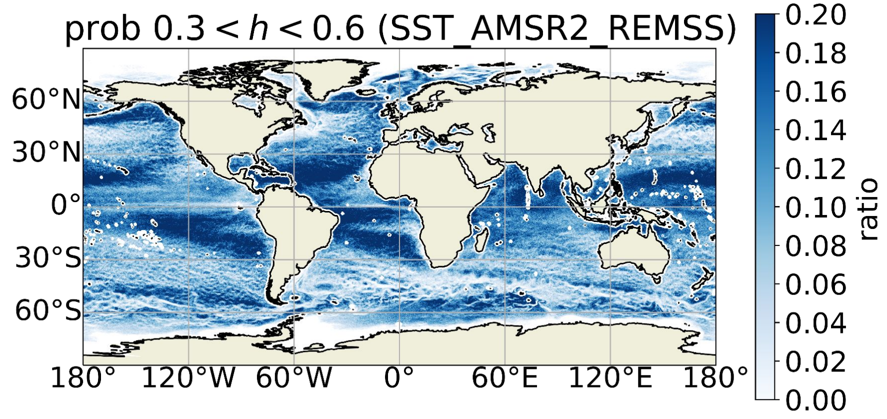
- There is a range of intermediate gradients that are being excessively smoothen. The turbulent cascade is poorly represented.

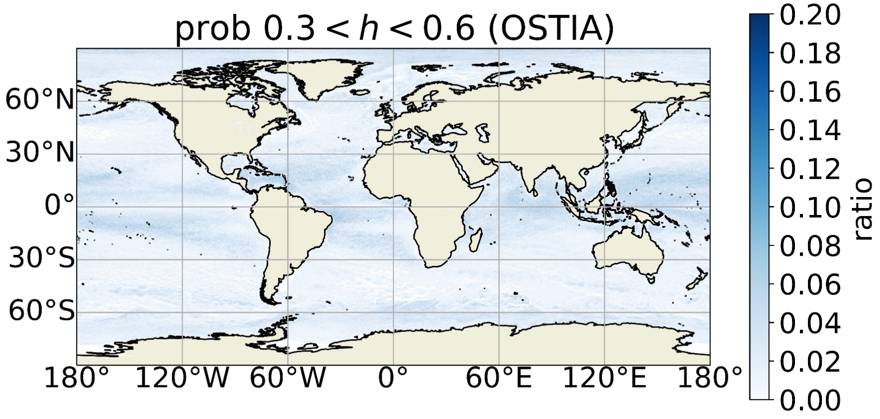


We compute the ratio of days in 2016 that present a singularity exponent within the band (0.3<h<0.6)

Singularity spectrum D(h)

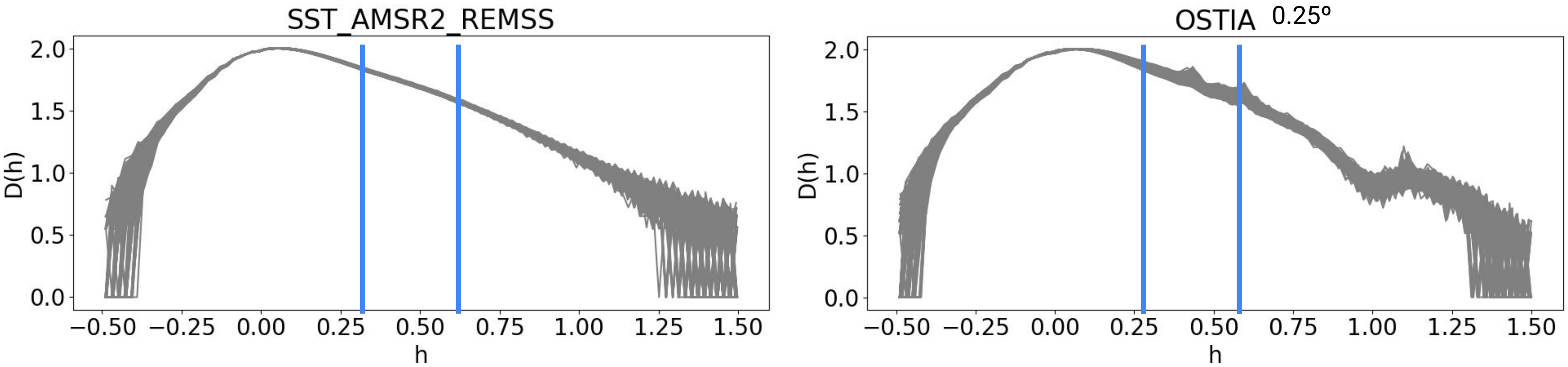
- We compute the ratio of days in 2016 that present a singularity exponent within the band (0.3<h<0.6) in order to found out the regions where the SST gradients are being smoothen





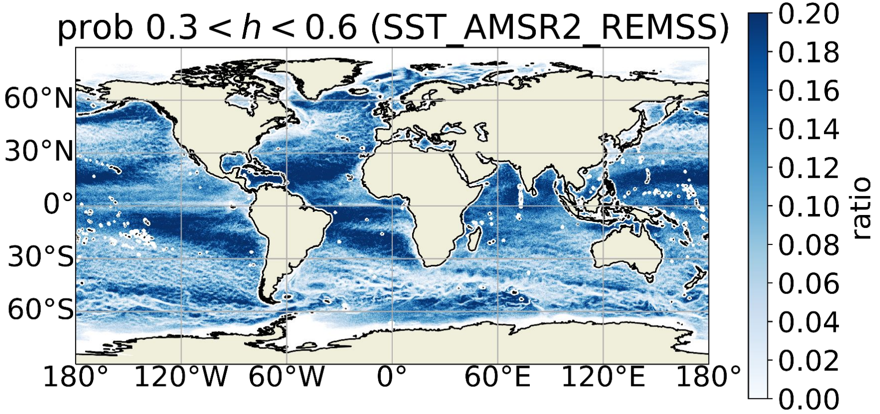
Singularity spectrum D(h)

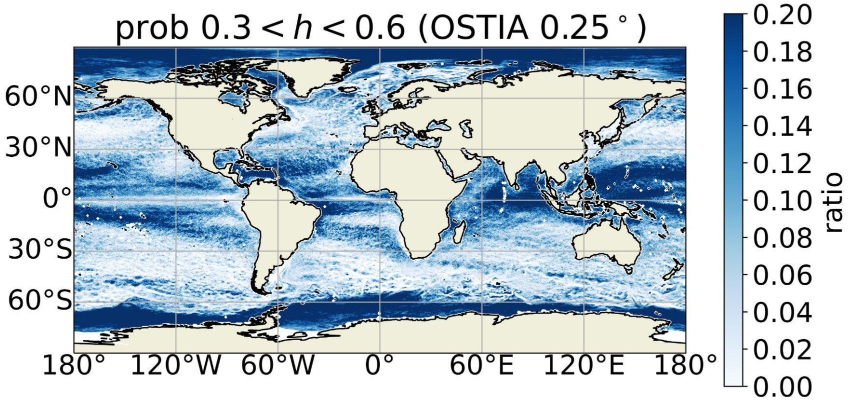
- To assess if the smoothing of intermediate gradients is caused by the L4 fusion/interpolation scheme, we interpolated OSTIA SST to a 0.25º grid, and repeat the same analysis.



Singularity spectrum D(h)

We compute the ratio of days in 2016 that have 0.3<h<0.6





Validation tool of consistency of the dynamical content of SST

Correlated triple colocation

- The triple collocation (TC) technique has been widely used to assess the quality of many geophysical variables acquired with different instruments and at different scales.

- We focus in the error characterization of remote sensing maps where having three collocated, completely independent datasets is unlikely.

- We have developed a **new formulation, the CTC (Correlated Triple Collocation)** for the case of **three datasets** that **resolve similar spatial scales,** with **two** of them being **error-correlated datasets** [González-Gambau et al. 2020].

- The **derived error maps from CTC analysis** allow us to **characterize the quality of the different datasets at each location** all over the globe.

Correlated triple colocation

- Rationale and methodology

1. We have **three series of spatially and temporally collocated measurements** x_i of the same variable θ:

$$x_i = a_i\theta + b_i + \delta_i \quad i = 1,2,3$$

2. We want to **estimate** the **standard deviation of error** δ_i, that is, $\sigma_{\delta i}$

3. **Assumptions:**

   a. Errors 1 and 2 are correlated with covariance φ_{12}, but uncorrelated with error 3.
   b. The three datasets resolve the same spatial scales, so there is no representative errors
   c. Measurements are assumed to have intercalibration factor equal to 1

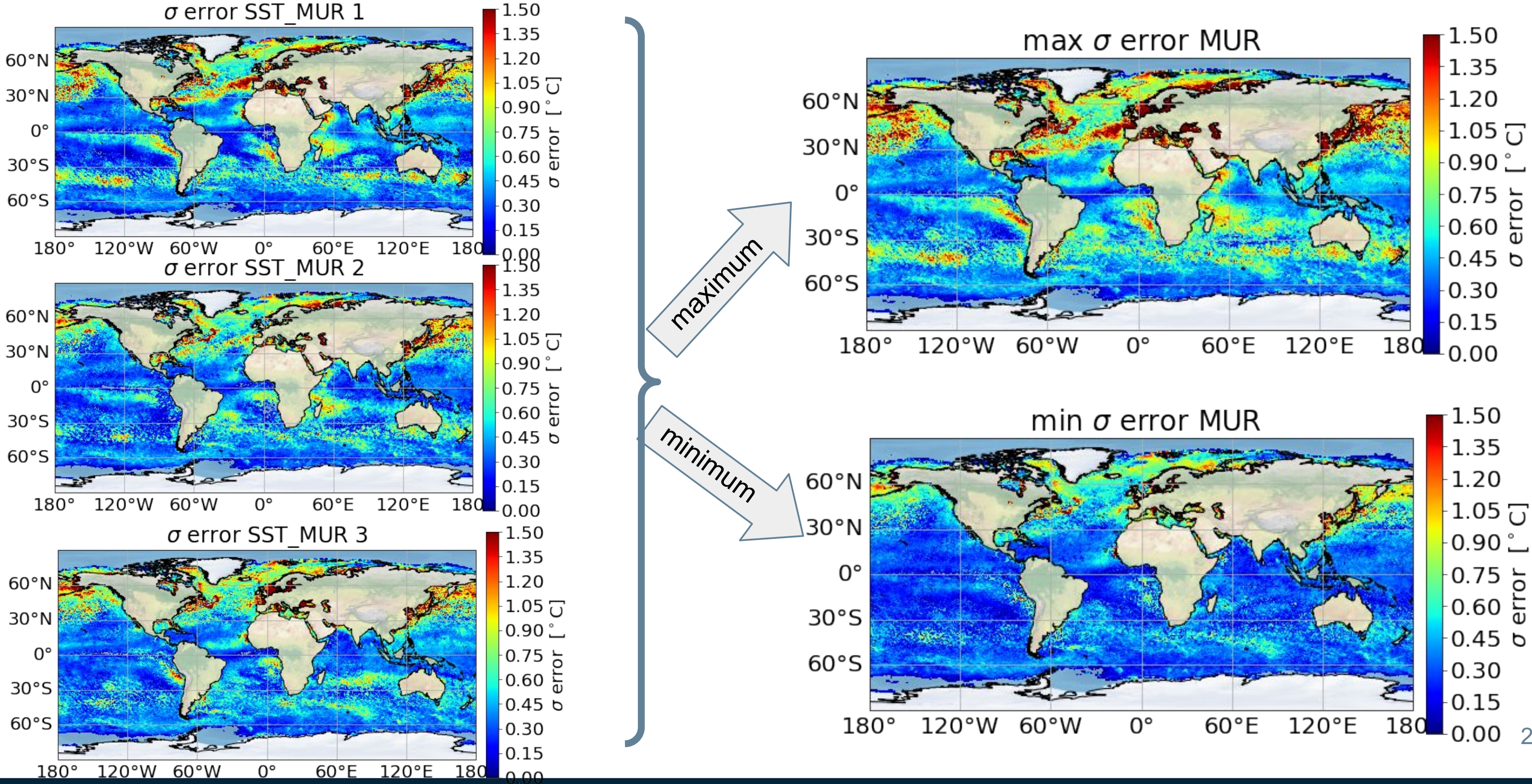
4. CTC is less sensitive to statistical fluctuations, allowing a reliable estimation of errors with scarce sampling sizes.

Correlated Triple Colocation: selecting triplets

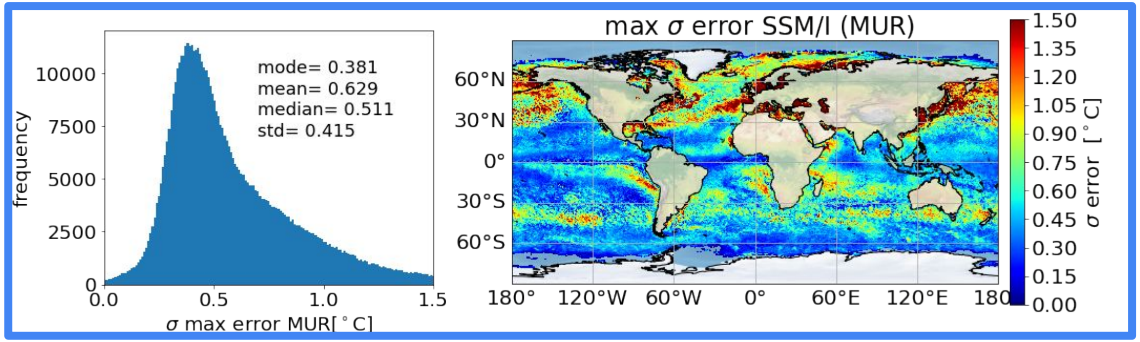
Dataset	Sensor
AMSR2-REMSS v8.2	AMSR2
CMC v3.0	VIIRS,AVHRR_GAC, AMSR2
OSTIA v2.0	AVHRR, VIIRS, AMSR2, GOES_IMAGER, SEVIRI, SSMIS, SSM/I
CCI v2.1	ATSR, AATSR, AVHRR_GAC
MUR v4.1	AMSR-E, AVHRR, MODIS, SSM/I, VIIRS, in-situ
Period	daily maps for 2016

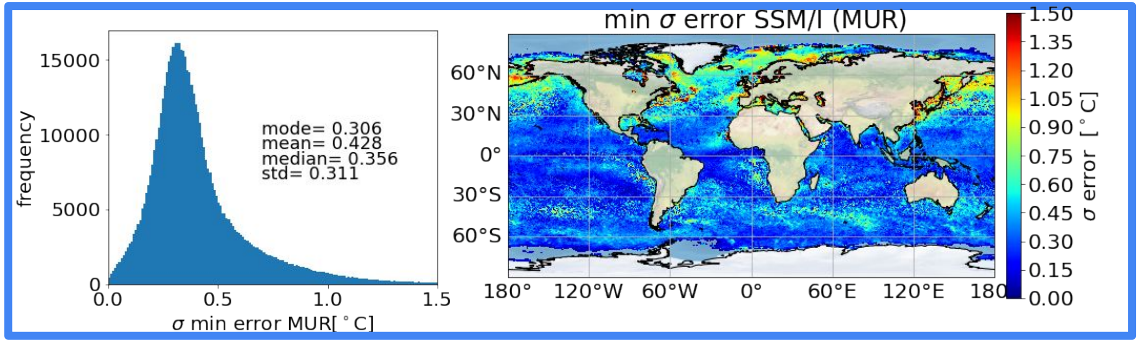
- SSM/I sensor is only present in MUR and OSTIA. We'll consider these two datasets as the one uncorrelated and perform the CTC for the triplets:
  - CCI_CMC_MUR
  - CCI_AMSR2_MUR
  - AMSR2_CMC_MUR
  - CCI_CMC_OSTIA
  - CCI_AMSR2_OSTIA
  - AMSR2_CMC_OSTIA
- The errors of the shared sensors will be consider as part of the SST variability. We obtain 3 different estimations (one per triplet) of the standard deviation of SSM/I error for each dataset (OSTIA and MUR).
- All datasets have been reinterpolated to the coarser grid (0.25º)

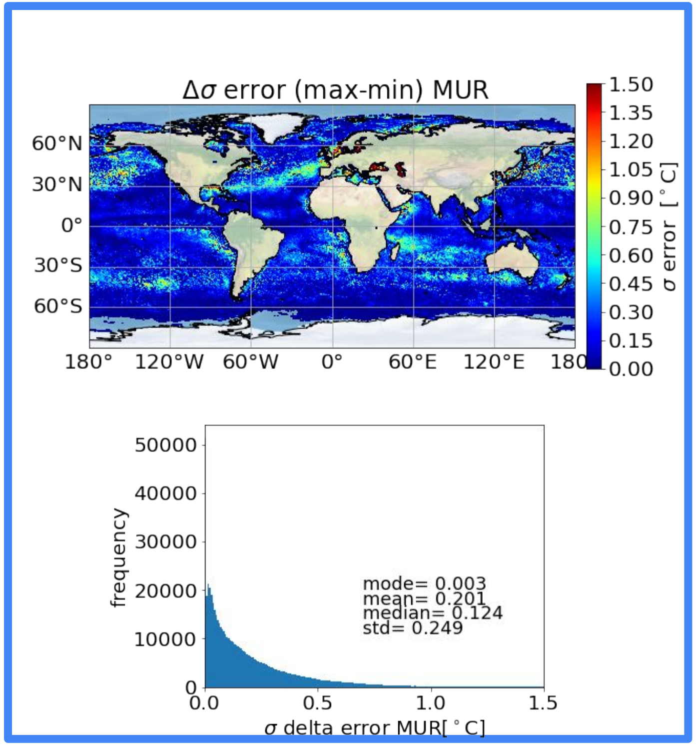
Correlated Triple Colocation MUR



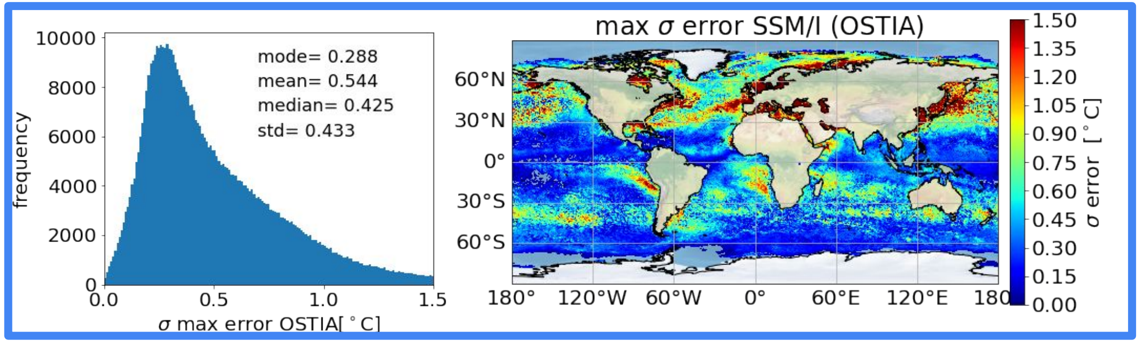
CTC MUR: SSM/I

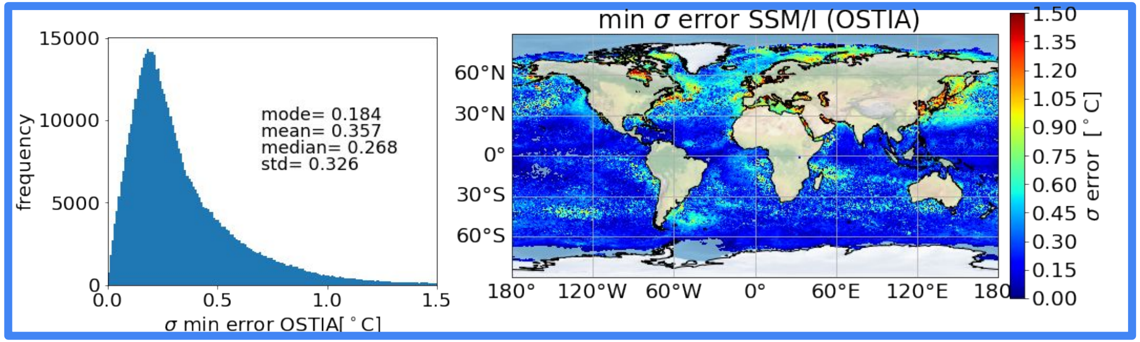

mode= 0.381
mean= 0.629
median= 0.511
std= 0.415
frequency
σ max error MUR[°C]
max σ error SSM/I (MUR)
σ error [°C]

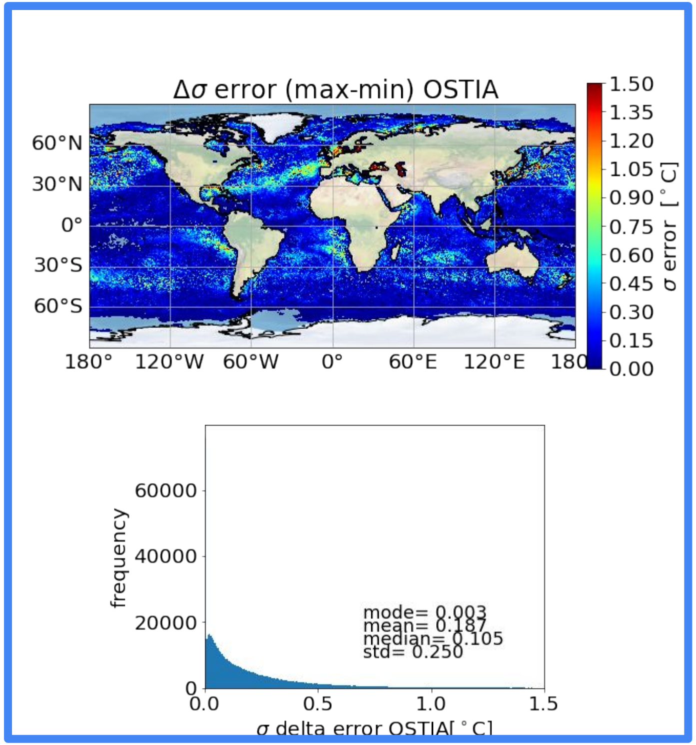

mode= 0.306
mean= 0.428
median= 0.356
std= 0.311
frequency
σ min error MUR[°C]
min σ error SSM/I (MUR)
σ error [°C]


Δσ error (max-min) MUR
σ error [°C]
mode= 0.003
mean= 0.201
median= 0.124
std= 0.249
frequency
σ delta error MUR[°C]

CTC OSTIA: SSM/I







Estimation of SSM/I error uncertainty

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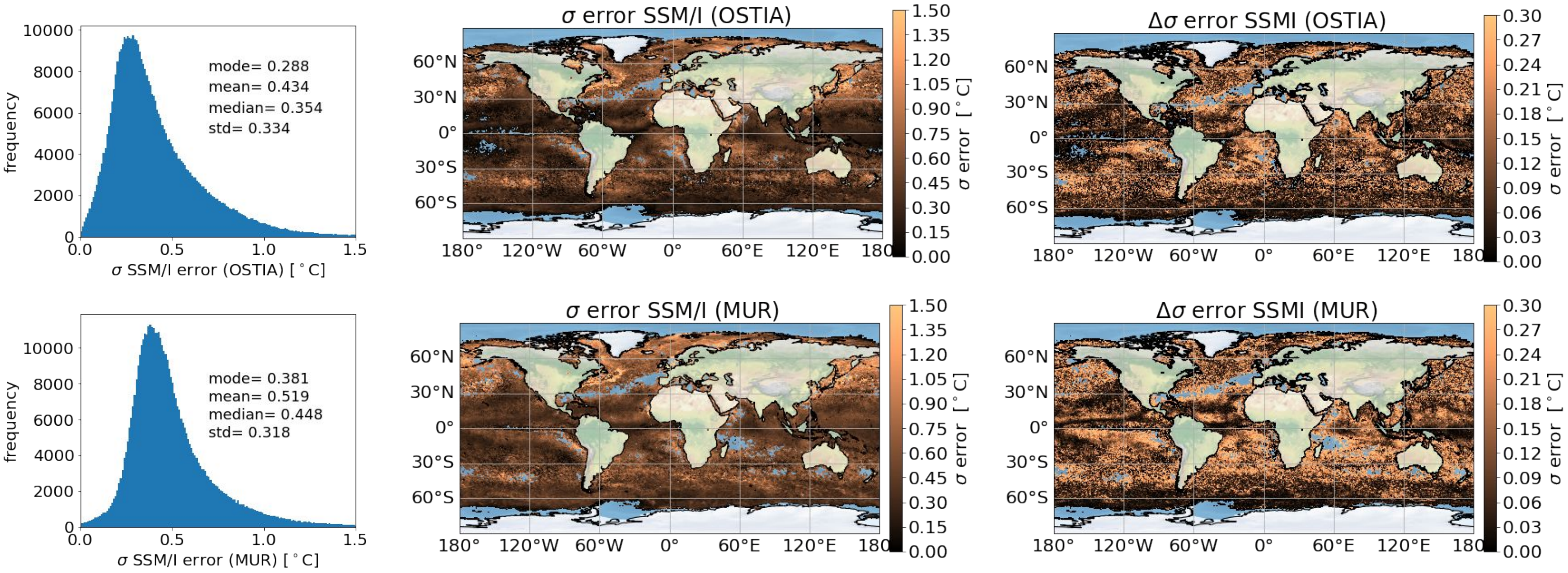

- The standard deviation of the SSM/I error is about 0.3-0.4 K, in accordance with in situ assessment
- CTC is a powerful tool for estimating the standard deviation of the errors, and providing its spatial distribution (land sea contamination, RFI, atmospheric corrections….)

Summary

- Choosing the best L4 SST analysis is not easy. GHRSST provides the users with some guidelines [Beggs 2020, GHRSST Office 2023]
- The comparison wrt in situ data does not give the "global picture".
- We proposed a new metric in order to assess SST products from a dynamical and structural perspective (the singularity spectrum) [González-Haro et al., in prep.]
- Correlated Triple Colocation is a powerful tool for estimating the standard deviation of the errors, and providing the spatial distribution of the errors (land sea contamination, RFI, atmospheric corrections….)

Summary

- Our final election: we'll use the MUR L4 SST product at its effective spatial resolution (0.1º)
  - we are currently retrieving the SSS using MUR SST at 0.1 for the regional product in the Southern Ocean
  - assessment of the impact of new SST on the retrieval (stay tuned for next GHRSST meeting)

Further work

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- Further efforts should be addressed to:
  - characterize the effective spatial resolution for smaller regions (10ºx10º) at a global scale (short/mid term)
  - use CTC at L2 to characterize the standard deviation of the errors of the different sensors (depending on available resources)
  - understand which methodological choice of producers have higher impact on not preserving the expected singularity spectrum, i.e not respecting the turbulence cascade (Feature Fidelity Task Team F2T2??)
  - improve interpolation/fusion schemes to respect the turbulence cascade

References

- [Beggs 2020] Temperature. Ch 14 in Earth observation: data, processing and applications. Volume 3B: Applications—surface waters. Cooperative Research Centre for Spatial Information (CRCSI).
- [GHRSST Office 2023] Office, G.P., Beggs, H., Karagali, I., Castro, S., 2023.Sea surface temperature: An introduction to users on the set of GHRSST formatted products. https://doi.org/10.5281/zenodo.7589540 , 10.5281/zenodo.7589540
- [González-Gambau et al. 2020] Triple Collocation Analysis for Two Error-Correlated Datasets: Application to L-Band Brightness Temperatures over Land. Remote Sens. 2020, 12, 3381. DOI: 10.3390/rs12203381
- [Isern-Fontanet et al. 2007] Isern-Fontanet, J., A., T., Garcíıa-Ladona, Font, J., 2007. Microcanonical multifractal formalism: Application to the estimation of ocean surface velocities. J. Geophys. Res. 112, C05024.
- [Pont et al. 2013] Pont, O., Turiel, A., Yahia, H., 2013. Singularity analysis of digital signals through the evaluation of their unpredictable point manifold. International Journal of Computer Mathematics 90, 1693–1707
- [Reynolds and Chelton 2010] R.W. Reynolds and D. B. Chelton, 2010: Comparisons of daily sea surface temperature analyses for 2007–08. J. Climate,23,3545–3562
- [Reynolds et al. 2013] Reynolds, R.W., Chelton, D.B., Roberts-Jones, J., Martin, M.J., Menemenlis, D., Merchant, C.J., 2013.Objective determination of feature resolution in two sea surface temperature analyses. Journal of Climate 26, 2514–2533.
- [Turiel et al. 2007] Turiel, A., Yahia, H., Pérez-Vicente, C.J., 2007. Microcanonical multifractal formalism—a geometrical approach to multifractal systems: Part I.singularity analysis.Journal of Physics A: Mathematical and Theoretical 41,015501
- [Yang et al. 2021] Yang, C., Leonelli, F.E., Marullo, S., Artale, V., Beggs, H., Nardelli, B.B., Chin, T.M., De Toma, V., Good, S., Huang, B., et al., 2021. Sea surface temperature intercomparison in the framework of the copernicus climate change service (c3s). Journal of Climate 34, 5257–5283. 18

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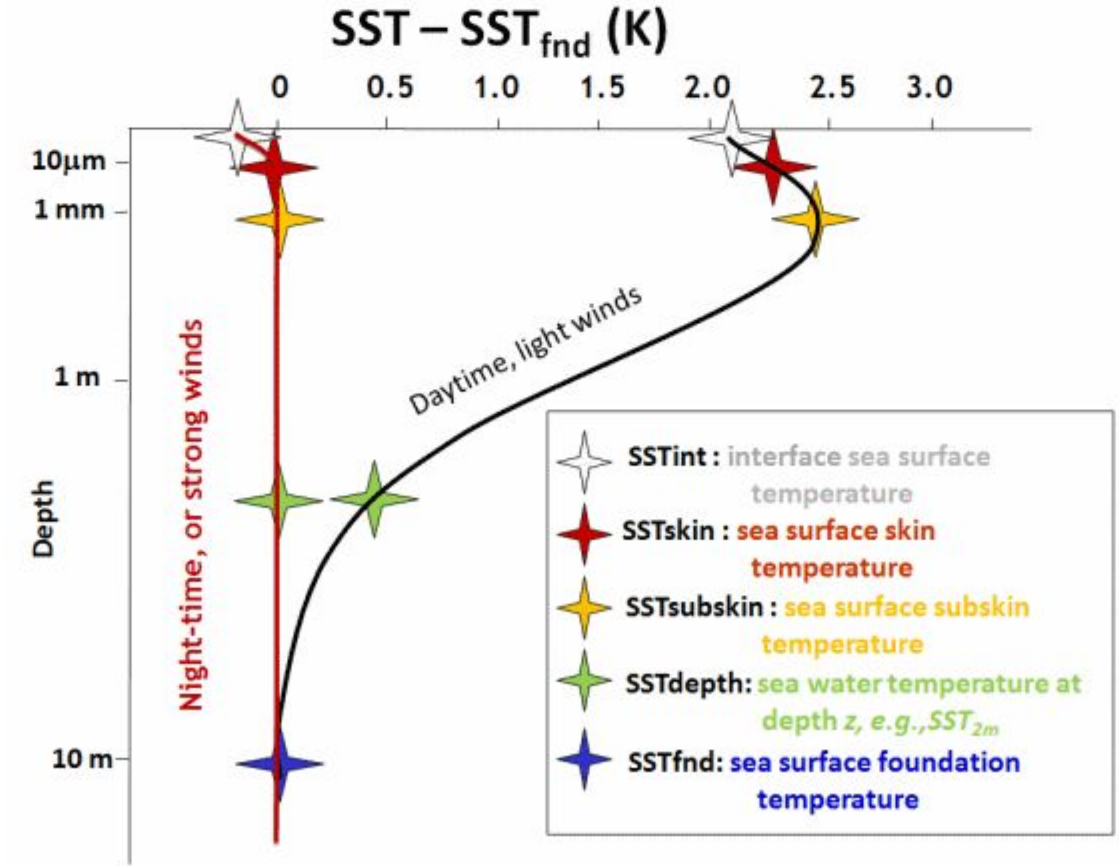
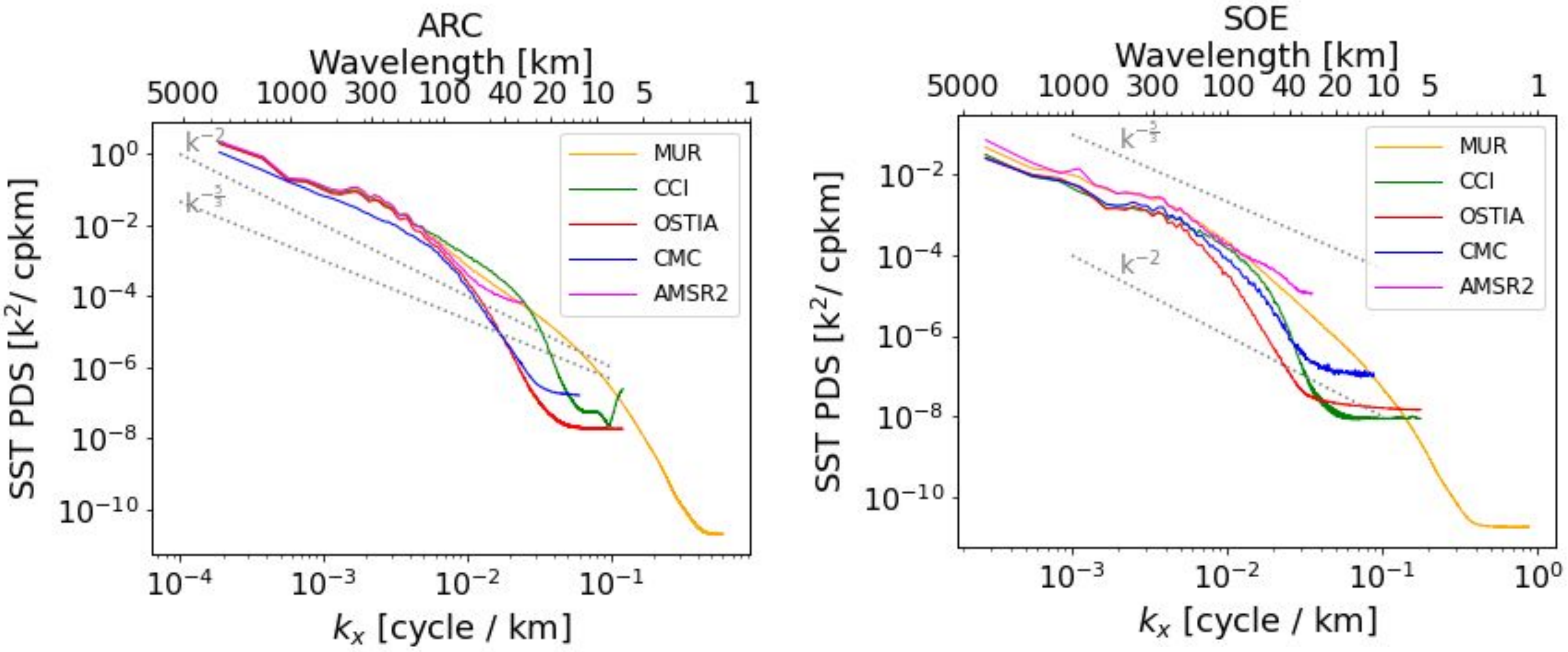
Extra Slides

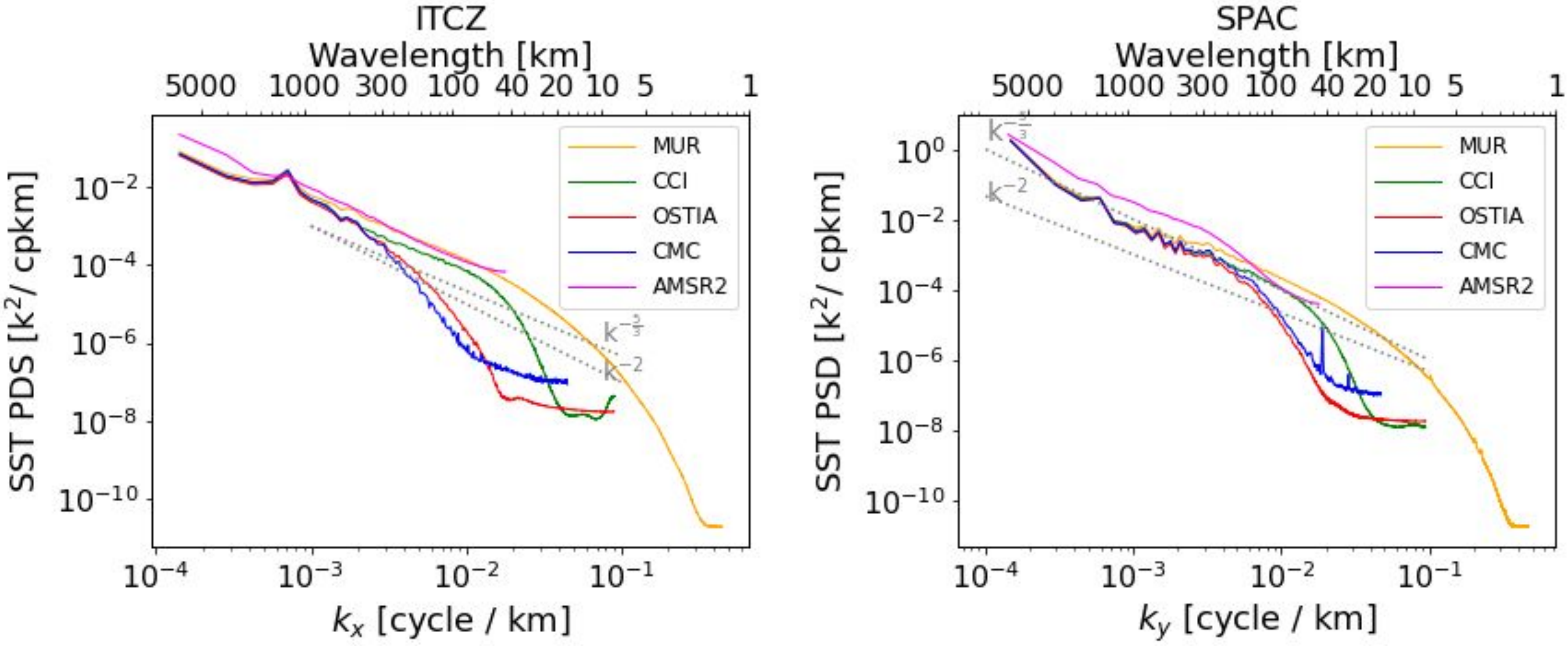
SST definitions



Spectral analysis



Spectral Analysis



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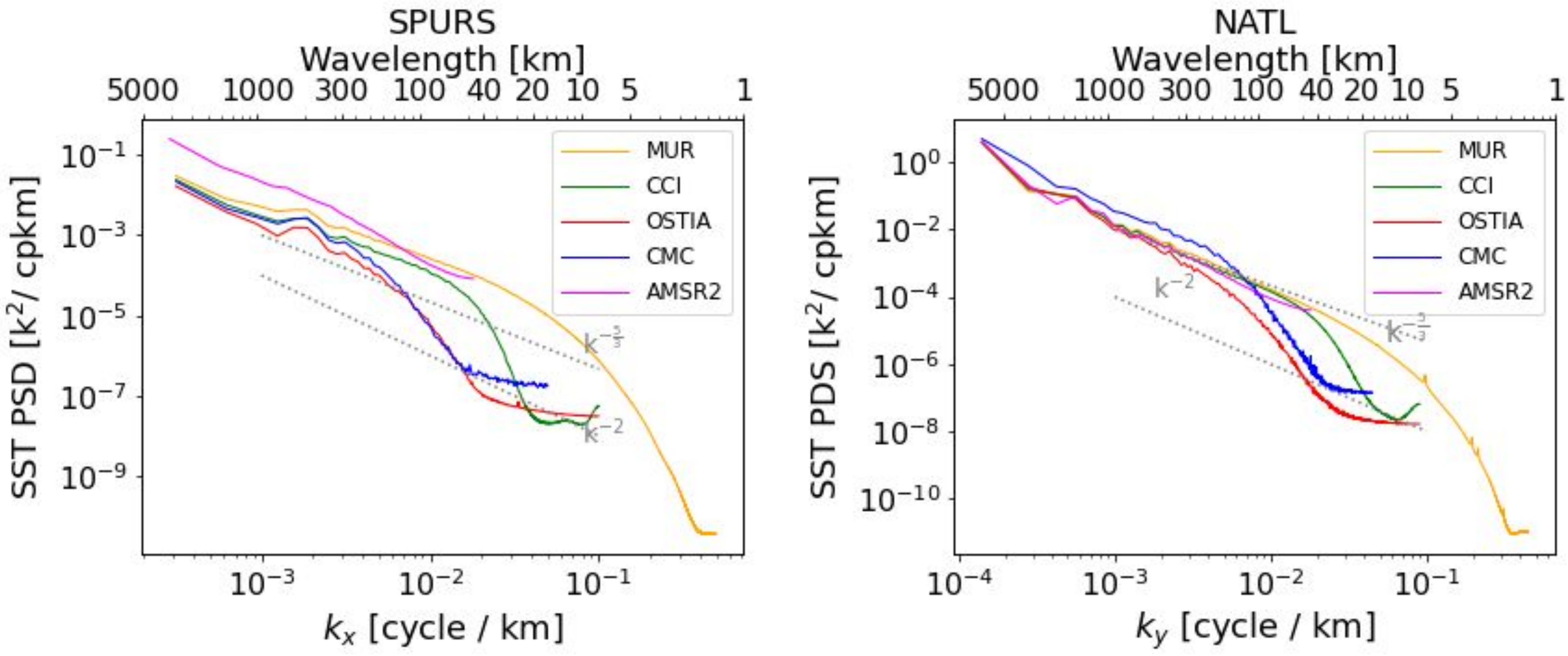
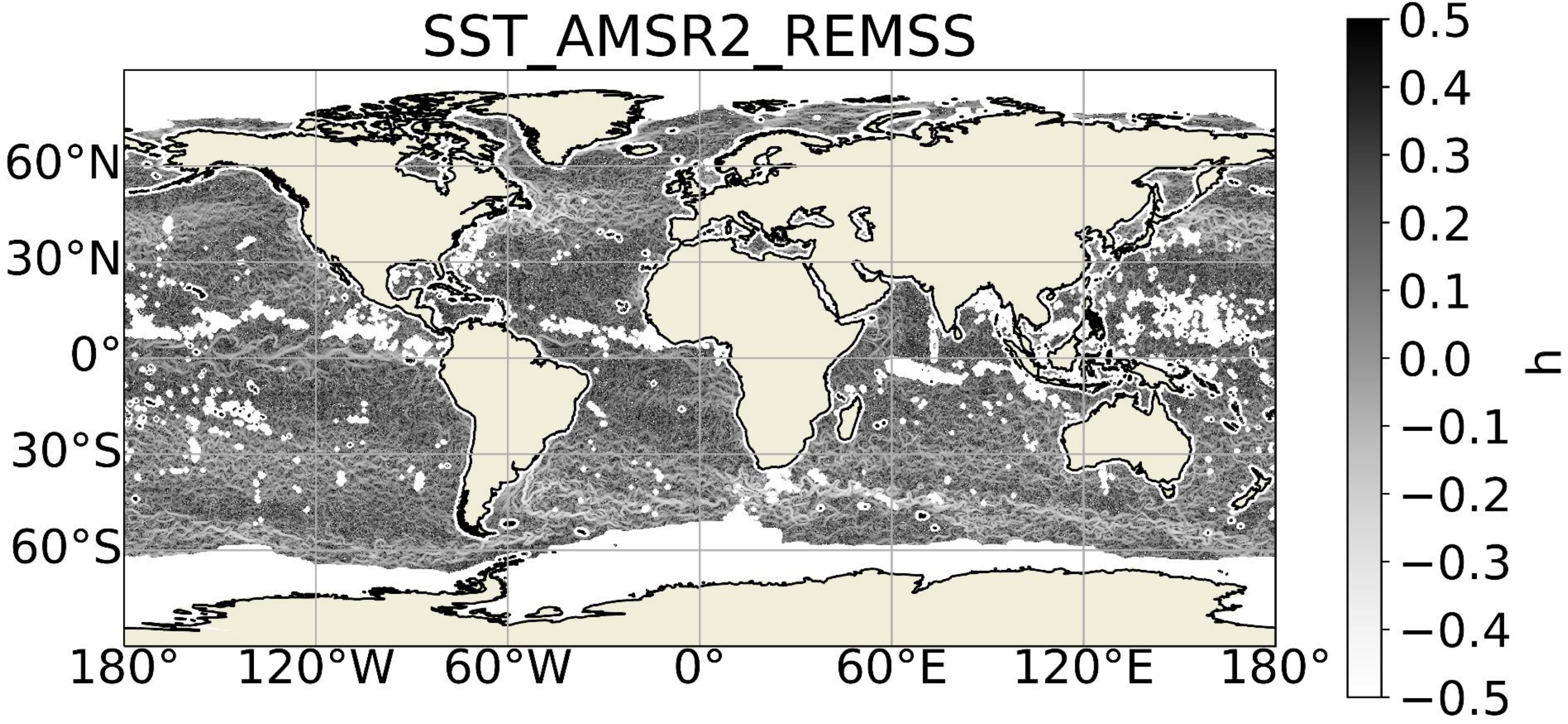


Singularity analysis



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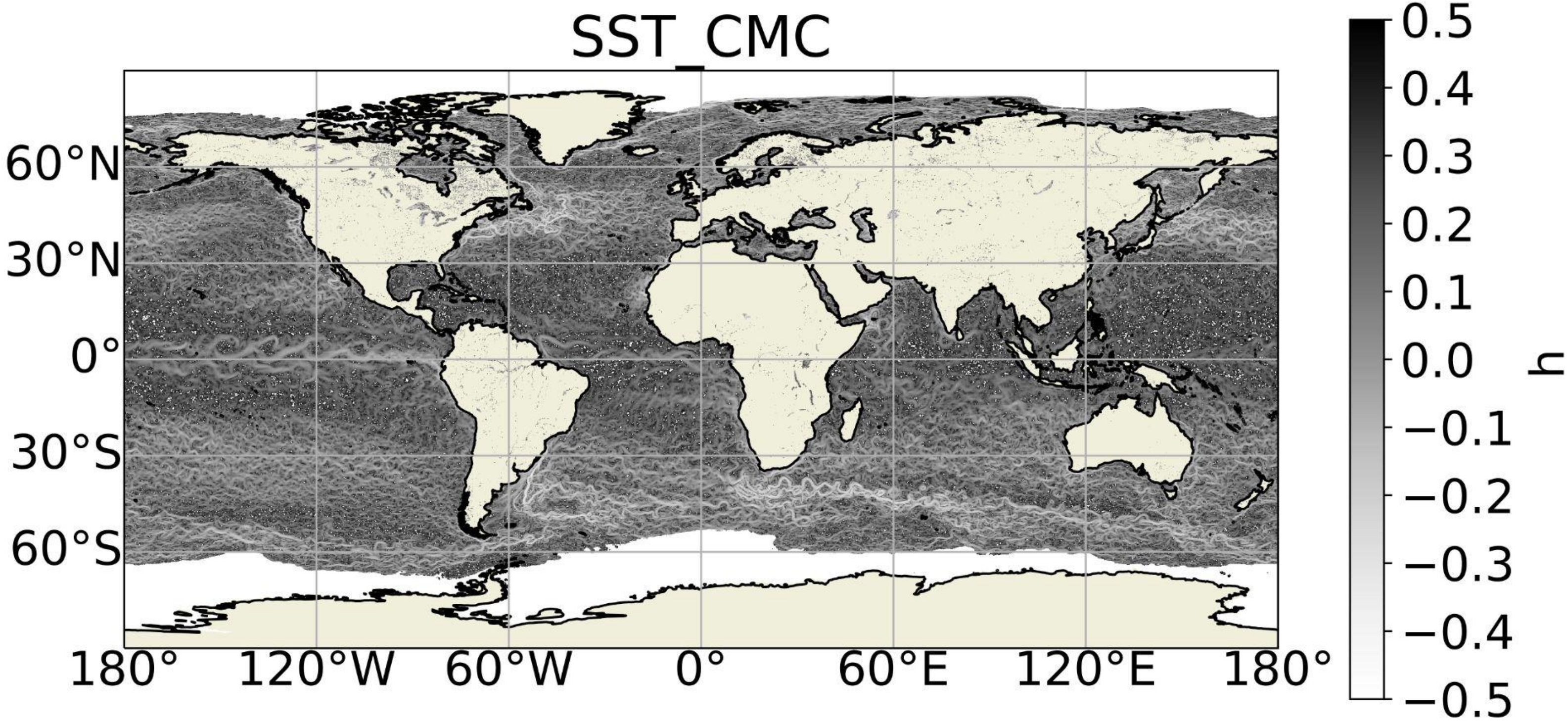

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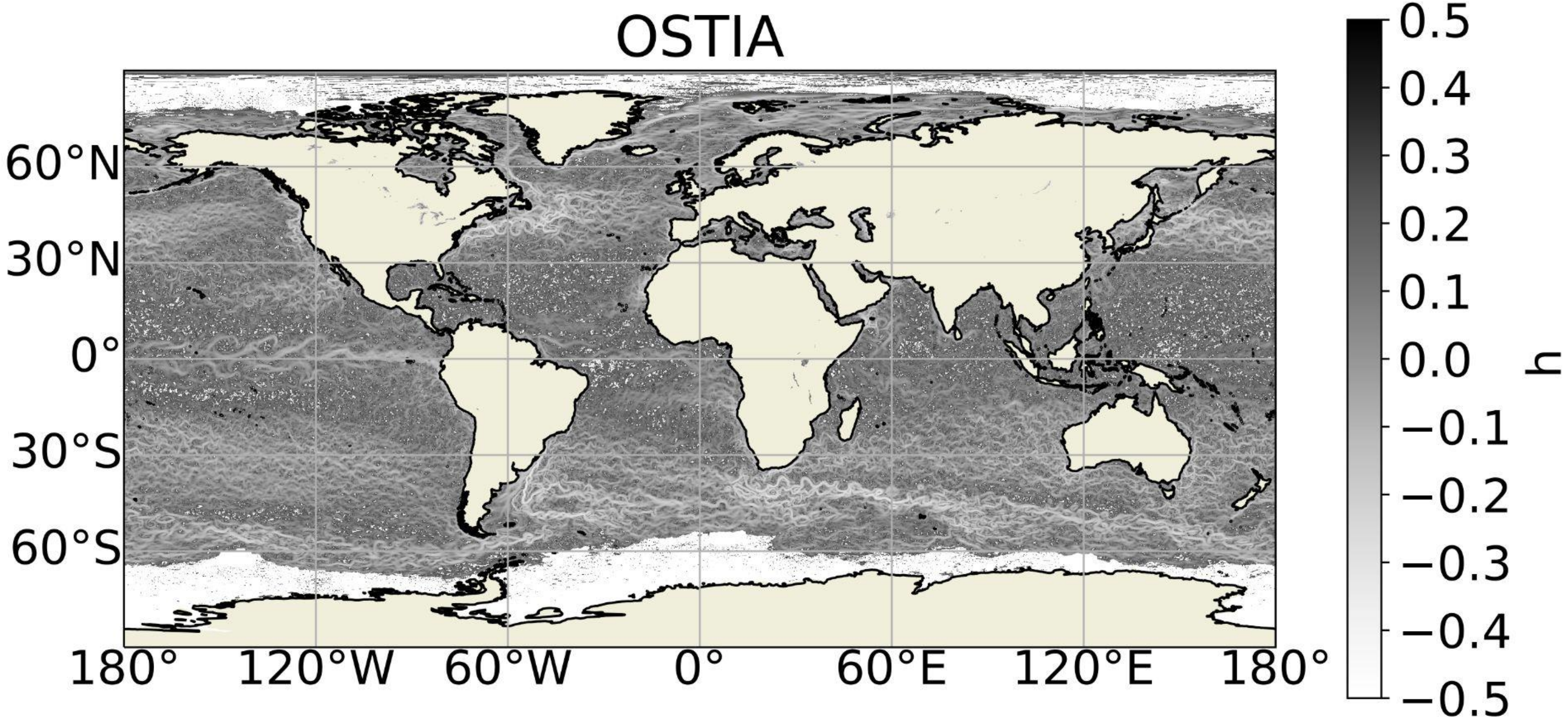

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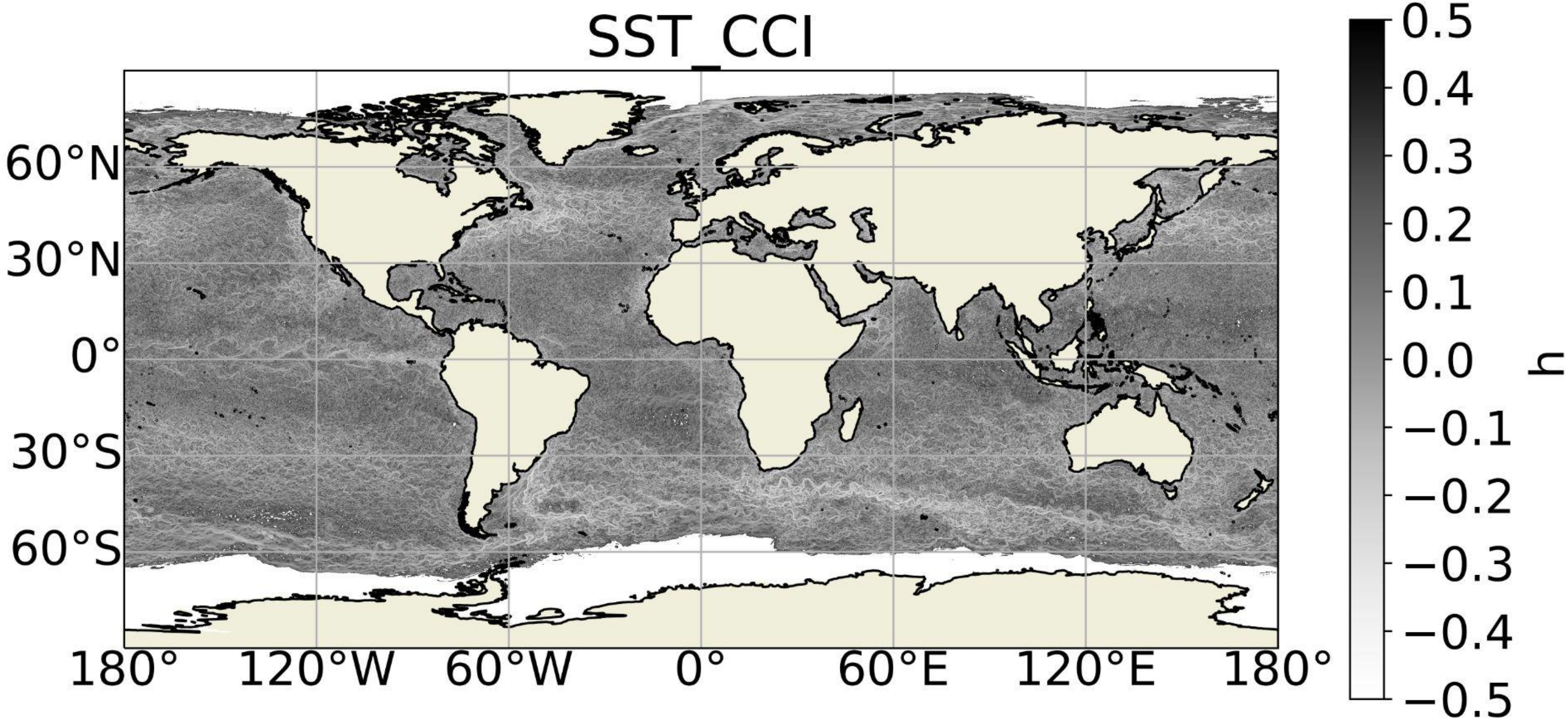
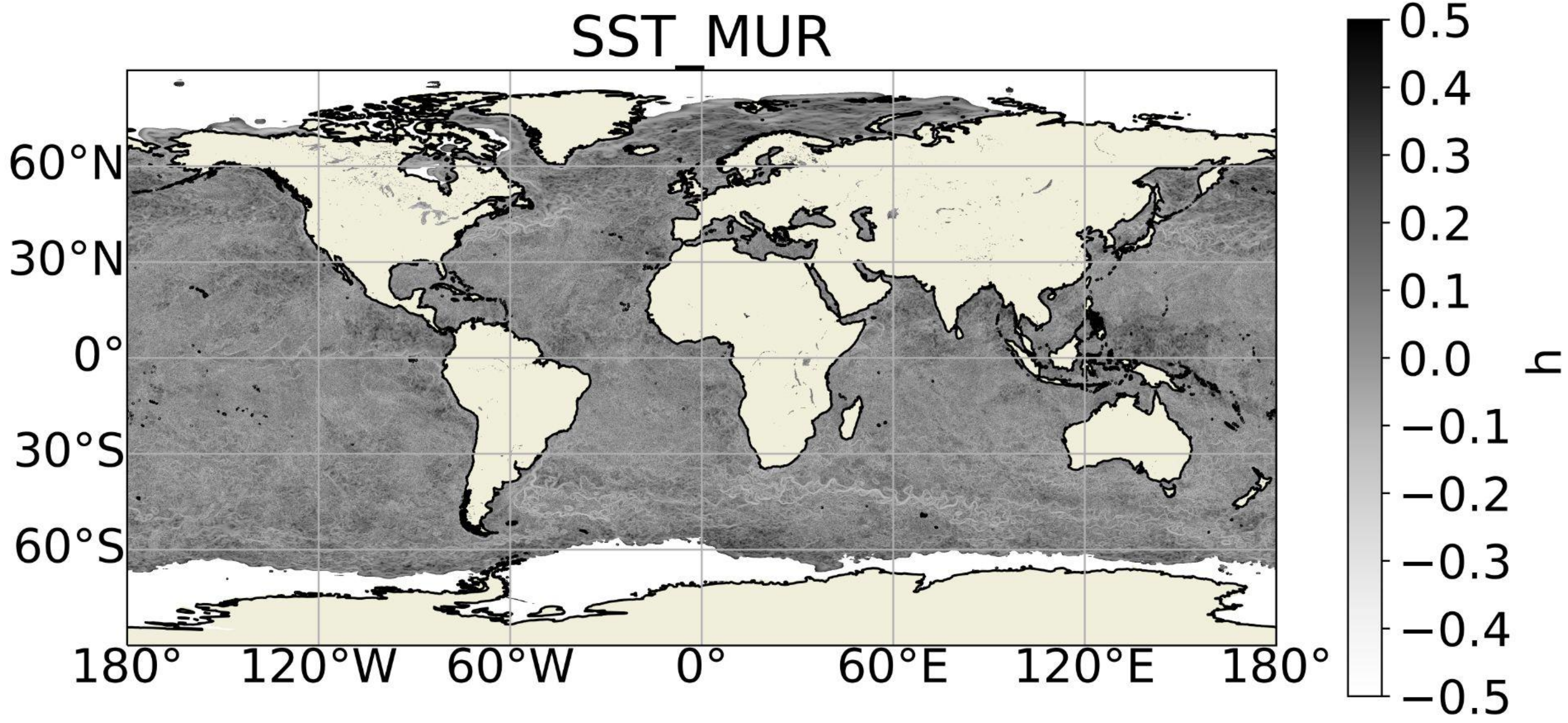


Singularity analysis



CTC: Rationale and methodology

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- We have looked for a linear transformation of x_1, x_2 into variables x_1', x_2' with errors $\delta x_1', \delta x_2'$, which are uncorrelated.

- We define the auxiliary scaling parameters u,v as:

$$u = \frac{s_2 - s_{12}}{s_1 + s_2 - 2s_{12}} \quad ; \quad v = \frac{s_1 - s_{12}}{s_1 + s_2 - 2s_{12}}$$

s_i: Variance of the measurements x_i
s_{ij}: Covariance between the measurements i, j

- The order-2 moments of the uncorrelated-error variables are defined:

- Finally, the error variances and error covariance of the original x_1, x_2 are given by:

$$\begin{cases} \sigma^2_{\delta_1} = v^2 s_1' + s_2' - s_{23}' \\ \sigma^2_{\delta_2} = u^2 s_1' + s_2' - s_{23}' \\ \sigma^2_{\delta_3} = s_3 - s_{23}' \\ \phi_{12} = -uvs_1' + s_2' - s_{23}' \end{cases}$$

V. González-Gambau et al., 2020: Triple Collocation Analysis for Two Error-Correlated Datasets: Application to L-Band Brightness Temperatures over Land. Remote Sens. 2020, 12, 3381. DOI: 10.3390/rs12203381