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# Error characterization of SSS products using triple collocation analysis

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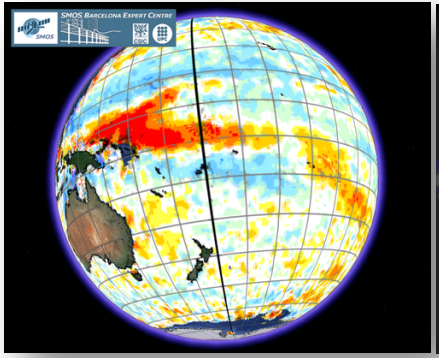
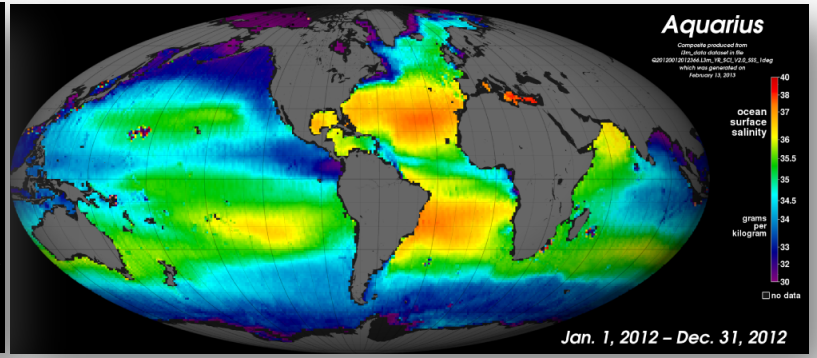
# SSS: Essential Climate Variable




More than **9 years of remote sensing SSS data** are available thanks to **satellite passive L-band missions**.

Satellite salinity measurements provide unprecedented spatio-temporal resolution/coverage as compared to any other observation system (Argo, CTD, TSG, moored buoys, etc.).

⇒ **A comprehensive error characterization** of the available SSS products is necessary.

In this study, we focus on the validation of **SMOS-BEC** and **Aquarius v4 Level 3** products.

# Limitations of direct comparison validation approach

<u>In direct comparisons, *in situ* data are assumed to be true or perfect at satellite scales</u>
=> only the **relative error** is estimated.

<u>Spatial and temporal representation</u> when comparing satellite gridded product versus in situ data:

- Vertical representation: first cm / ~5m
- Spatial representation: 0.25°/ point measurement
- Temporal representation: ~weekly / instantaneous (Argo)

=> The different spatial & temporal representation of the data will impact the direct comparisons and therefore needs to be accounted for during the validation process => ***representativeness error***

**Absolute error** estimation requires at least **3 independent** measurement systems.

=> Use of *Triple collocation Analysis*.

# Triple Collocation (Stoffelen, 1998)

- **Triple collocation** (TC) was conceived as a tool for **intercalibration** and **individual error assessment** of three different collocated WIND data sets (Stoffelen, 1998).

- Given 3 measurement systems with different spatial resolution (buoy, satellite, model), $s_i$ , $i=1,2,3$, the measurement and its error are modelled by the following linear equation:

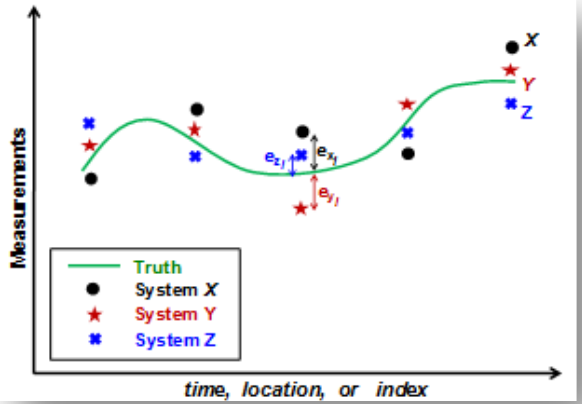
***scaling*** *calibration coef.*

*random measurement* ***error*** *(Gaussian)*

$$s_i = a_i S + b_i + \delta_i$$

***bias*** *calibration coef.*

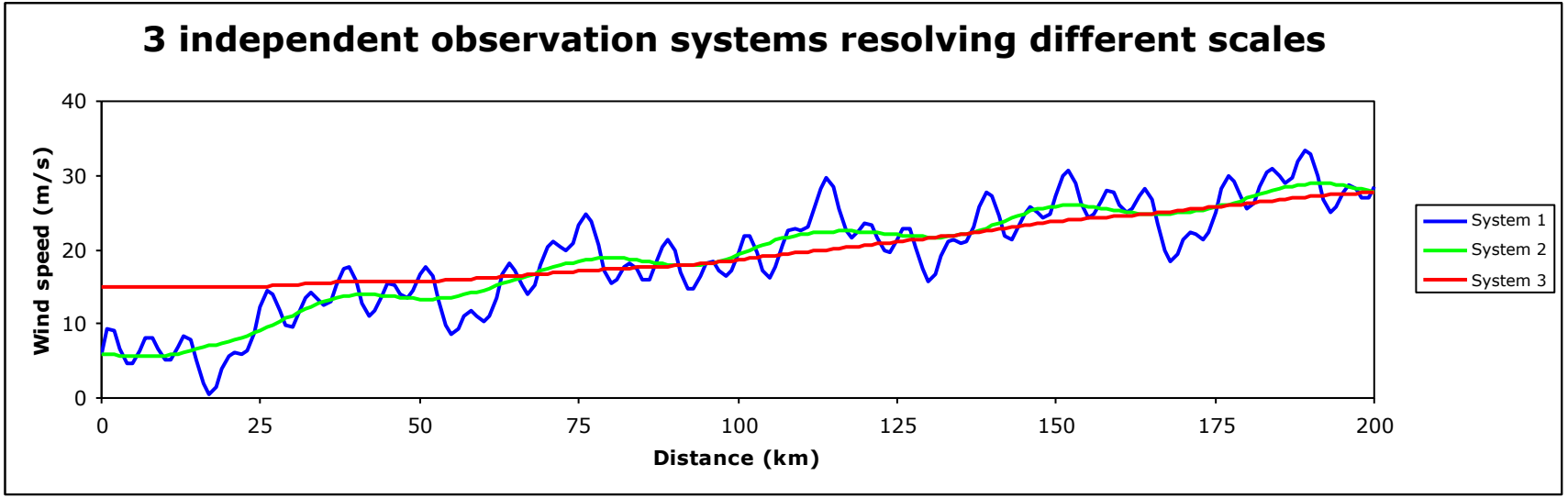
***Truth*** *at the scales commonly resolved by all 3 data sources*




TC model assumptions:

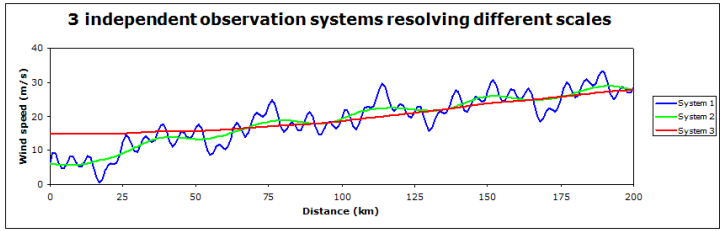
- errors are additive
- error distributions are close to Gaussian
- the collocated data sources are independent

# Triple Collocation (Stoffelen, 1998)
## Representativeness error




***Representativeness error*** ($r^2$) corresponds to the common variability resolved by Systems 1 and 2, but not resolved by system 3.

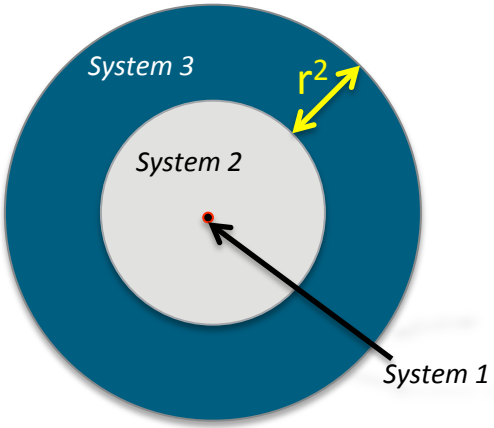
# Triple Collocation (Stoffelen, 1998)
# **Representativeness error**




- Suppose system 1 and 2 resolve **smaller turbulent** scales than system 3. The true variance common to these smaller scales is:

$$r^2 = \langle \delta_1 \delta_2 \rangle$$

which is part of the measurement errors $\delta_1$ and $\delta_2$.
=> $r^2$ is the **correlated part** of the errors of $s_1$ and $s_2$.




- Assuming that, since $s_3$ does not include these smaller scales, its measurement error $\delta_3$ is independent of $\delta_1$ and $\delta_2$, and:

$$\langle \delta_1 \ \delta_3 \rangle = \langle \delta_2 \delta_3 \rangle = 0$$

***Representativeness error*** ($r^2$) corresponds to the **common true variance** of Systems 1 and 2, not resolved by system 3.

# TC algorithm

Initialization,

$n = 0, \quad i = [1,2,3]$

$S_i^n$ = Collocated $i$-data set

$a_i^n = 1.0$

$b_i^n = 0.0$

$r^2$

**TC model**

$n = n + 1 \qquad i = [2,3]$

$$M_{ij}^n = \langle S_i^n S_j^n \rangle$$

$$a_2^n = \frac{M_{23}^n}{M_{13}^n}$$

$$b_2^n = \langle S_2^n \rangle - a_2^n \langle S_1^0 \rangle$$

$$a_3^n = \frac{M_{23}^n}{M_{12}^n - r^2}$$

$$b_3^n = \langle S_3^n \rangle - a_3^n \langle S_1^0 \rangle$$

$$S_i^{n+1} = a_i^n S_i^n + b_i^n$$

$$\frac{|a_i^n - a_i^{n-1}|}{|a_i^{n-1}|} \leq 10^{-5}$$

$$\frac{|b_i^n - b_i^{n-1}|}{|b_i^{n-1}|} \leq 10^{-5}$$

**Convergence ?**

No

Yes

***$a_3$ $\delta_1$ and $\delta_2$ depends on $r^2$***

***Errors estimated after convergence and for calibrated data***

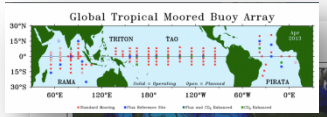
**Error Estimation (SD)**

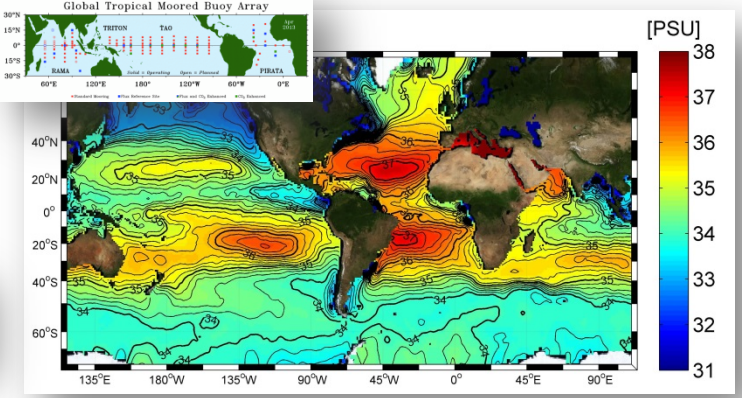
$$\varepsilon^2 = M_{12} - r^2 = M_{23} = M_{13}$$

$$\langle \delta_i^2 \rangle = M_{ii} - \varepsilon^2$$

# SSS data






| | Spatial Resolution | Temporal resolution |
|---|---|---|
| **TAO** | *Point* | *Daily average* |
| **GLORYS2V3** | *0.25°* | *Daily product* |
| **Aquarius v4** | *1°* | *7 days average* |
| **SMOS OA** | *0.25°* | *9 days average* |
| **WOA13** | *0.25°* | *Daily interpolation from monthly product* |
| **WOA09** | *1°* | *Monthly product* |

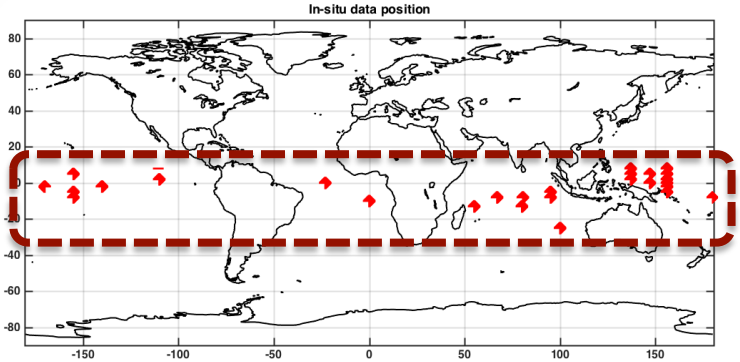
Period of study: **2013**

- all the SSS data sources are available at this period.
- 2013 is **not influenced by strong events** such as El Niño (2014-2015) or La Niña (2011-2012), which are known to be unresolved by the climatology, thus leading to strong biases in the latter.

## Collocation

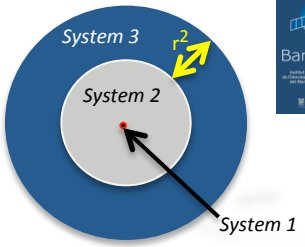
*Spatial: The* **closest grid point** *to the in-situ location is used.*
*Temporal: Collocation to the* **central day of Aquarius** *product.*

Total of **1456 collocations** with the six products are obtained over the study period of 2013, in the **Tropical band**
=> Obtained sextuplets of TAO, SMOS, Aquarius, GLORYS2V3, WOA13, WOA09 collocated data.



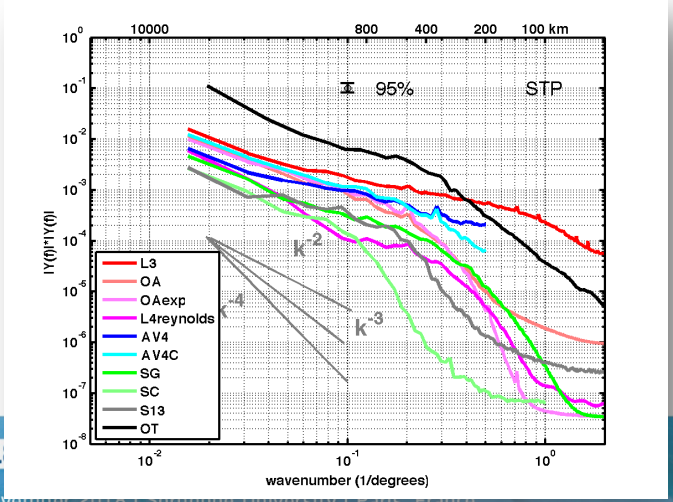

*Location (red symbols) of the TAO, PIRATA, and RAMA buoys arrays used in this study.*

# Representativeness error Estimation: method



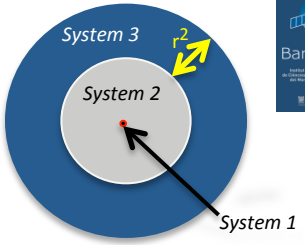

Until now, to estimate $r^2$ with sea surface wind data the methods have been based on:

- Integrating the difference between the scatterometer wind power density spectra (PDS) and those of the numerical model output (*Vogelzang et al. 2011*)
- Calculating the cumulative variance of scatterometer and model wind components (*Vogelzang et al. 2015*).




*Problem*: **SSS PDS spectral slopes** of the different products are **sensitive to the presence of noise** (*see POSTER section this afternoon, based on Hoareau et al., TGRS, 2018*).

# Representativeness error Estimation: method




***Alternative approach based on TC intercalibration assumption*** (*Lin et al., 2016*):

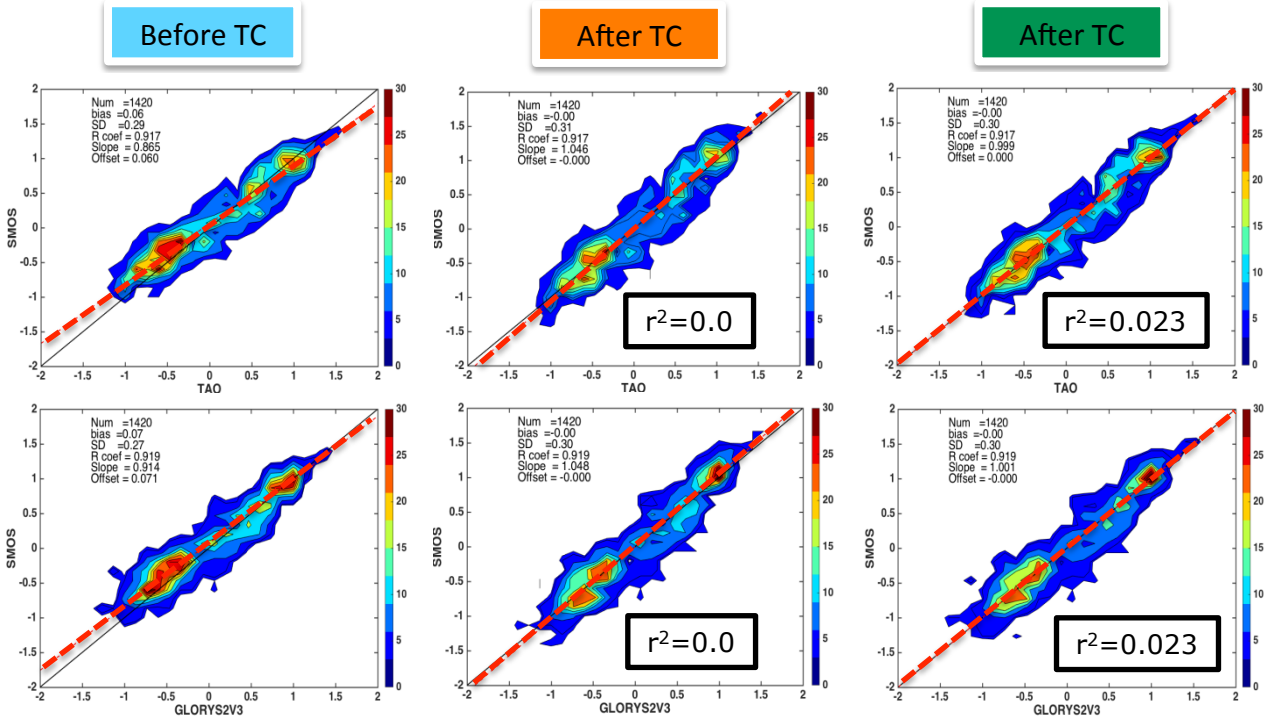
**Assumption** that a successful TC provides three data sets well intercalibrated.

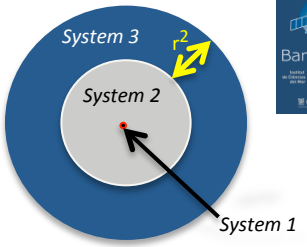
⇒ ***TC calibration coefficient $a_i$, $b_i$,*** are related to the value of $r^2$
⇒ Setting a wrong $r^2$ leads to a miscalibrated system 3 with respect to systems 1 and 2.

Therefore, an effective way of estimating $r^2$ is to repeat the TC analysis for different $r^2$ values until an optimal intercalibration of the different data sources is achieved.

***=> Check the data scatterplots after each intercalibration***

# Representativeness error Estimation



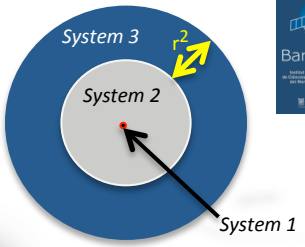




**SSS data:**
System 1 -> TAO
System 2 -> GLORYS
System 3 -> SMOS

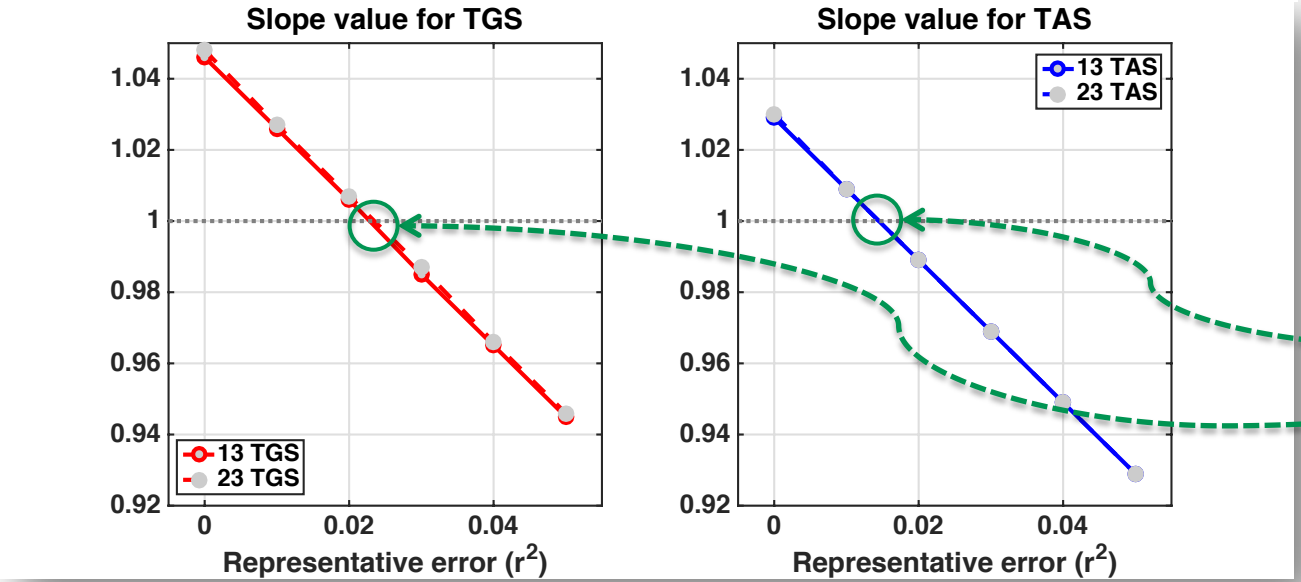
If wrong $r^2$
⇒ Not well calibrated

If correct $r^2$
=> Well calibrated

# Representativeness error Estimation: Results

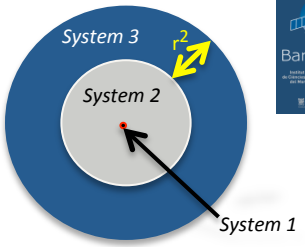



*Slope values as a function of the representativeness error ($r^2$) for the triplets (Left) TAO-GLORYS-SMOS and (Right) TAO-Aquarius-SMOS.*




Correct $r^2$ values

# Representativeness error Estimation: Results




Acronyms:
***T***-> TAO in-situ
***G***-> GLORYS model
***A***-> Aquarius satellite
***S***-> SMOS satellite
***13***-> WOA 2013 climatology
***09***-> WOA 2009 climatology

**$r^2$ estimation with sextuplets**
**=> robust TC analysis results**

$$r^2_{TGS} \approx r^2_{TGA} + r^2_{TAS}$$

$$r^2_{TA13} \approx r^2_{TAS} + r^2_{TS13}$$

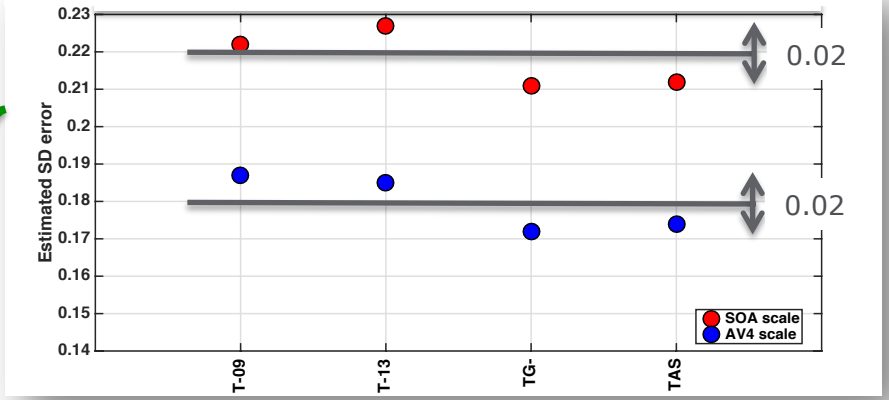
| | ***TGA*** | ***TGS*** | ***TA13*** | ***TS13*** | ***TA09*** | ***TS09*** | ***TAS*** |
|---|---|---|---|---|---|---|---|
| ***$r^2$*** | 0.009 | 0.023 | 0.027 | 0.011 | 0.034 | 0.020 | 0.015 |

*Representativeness Error ($r^2$) for the different triplets of SSS data.*

⇒ ***$r^2$*** values help to identify the systems having the finest and the coarsest effective spatiotemporal resolution:
TAO<GLORYS<Aquarius<SMOS<WOA13<WOA09

# Random Error Estimation at Satellite resolved scales

***TAO SD error** estimated by the TC algorithm at both the SMOS scale (red point) and the Aquarius scale (blue points) for different triplets.*




$$At\ system\ 2\ resolution:\ \delta_{TAO} = \sqrt{\delta_1^2 - r^2}$$

$$At\ system\ 3\ resolution:\ \delta_{TAO} = \delta_1$$

The TAO **error** variation gives an indication of the **uncertainty** of the proposed methodology **about 0.01**

*Estimated SD error of the different salinity measurements at the satellite scales*

| | TAO | GLORYS2V3 | AV4 | SMOS | WOA13 | WOA09 |
|---|---|---|---|---|---|---|
| **Aquarius scale** | 0.18±0.01 | 0.18 | 0.17±0.01 | 0.24±0.01 | 0.29 | 0.31 |
| **SMOS scale** | 0.22±0.01 | 0.21 | 0.21±0.01 | 0.20±0.01 | 0.26 | 0.29 |

# Summary & Conclusions

The **TC technique** consists of using 3 **independent**, **intercalibrated** and **collocated** data sources to provide an **estimate of their individual random error** (SD).

1) The analysis has been carried out **at the scales** resolved by the **two satellite** products: **SMOS** Objective Analysis and **Aquarius** v4 Level 3.

2) The **representative error** has been accounted for during the TC validation of **six different SSS** products along the tropical band for the year 2013 => **Sextuplets give robust TC analysis results**.

3) The **$r^2$ estimation method** is based on the analysis of the intercalibration results.

4) It has been found that the **representativeness error ($r^2$) contributes to 15% ~ 50%** of the error estimates.

5) $r^2$ values **help sorting the systems in terms of their effective spatiotemporal resolution**:
TAO < GLORYS2V3 < Aquarius v4 < SMOS OA < WOA13 < WOA09

6) The TC method developed here leads to **an uncertainty of about 0.01 in the SSS error estimates**.

# Perspectives

The validation has been carried out at the satellite-resolved spatiotemporal scales.

It has been found that the **TAO SD error** at the **Aquarius v4** and **SMOS OA** spatiotemporal scales is **0.18** and **0.22**, respectively.

=> **The error values include the contribution of the following representativeness errors:**

- the horizontal scale difference between the point-wise observation and the 0.25°-1° grid sizes of the satellite products
- the vertical mismatch between TAO measurement at 1-1.5m depth and the satellite at 1 cm depth
- the different temporal resolution of TAO (1 day) and satellite products (7-9 days).

The partition of these error contributions remains a research topic in oceanography.

# http://bec.icm.csic.es

*Hoareau N., Portabella M., Lin W., Ballabrera-Poy J., and Turiel A., "Error characterization of Sea Surface Salinity product using Triple Collocation analysis", Trans. Geosc. Rem. Sens., vol. 56 (9), pp. 5160-5168, 2018.*

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