Comparisons & Metrological Compatibility

IOCCG Training

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European Commission

Vocabulary (1)

- **measurand**: well-defined physical quantity that is to be measured
- **uncertainty of a measurement**: a parameter, associated with the result of a measurement that characterizes the dispersion of the values that could reasonably be attributed to the measurand
- **error:** difference between the measurement and the true value of the measurand (or a reference quantity value, assumed to have negligible uncertainty)
- **compatibility***:*

property of a set of measurement results, such that the absolute value of the difference of any pair of measured quantity values from two different measurement results is smaller than some chosen multiple of the standard measurement uncertainty of that difference
i.e., **agreement of 2 data sets within their stated uncertainties**

Vocabulary(2)

Uncertainty associated between X_A and X_B:

$$\boldsymbol{u^2(X_B - X_A) = u^2(X_A) + u^2(X_B) - 2u(X_A)u(X_B)r(e(X_A), e(X_B))}$$

Compatibility: the difference of any pair of **measured quantity values** from two different measurement results is smaller than some chosen multiple *k* of the **standard measurement uncertainty** of that difference

VIM 2012

$$\boldsymbol{|X_B - X_A| < k\sqrt{u^2(X_A) + u^2(X_B) - 2u(X_A)u(X_B)r(e(X_A), e(X_B))}}$$

should be true for 68% of cases (*k*=1) with a normal hypothesis

Comparisons of Field Data

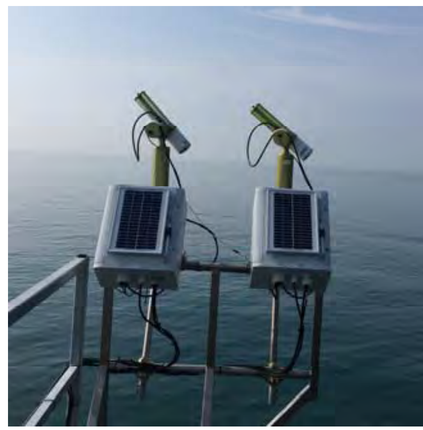
Example with R_{RS} data

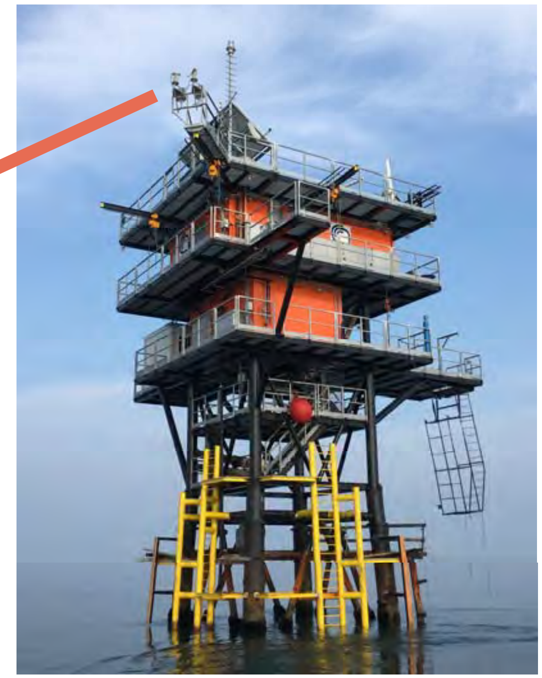
Comparison of Field Data: Example at AAOT (1)

AAOT: Acqua Oceanographic Tower

Operations of 2 SeaPRISM systems over 2017-2023

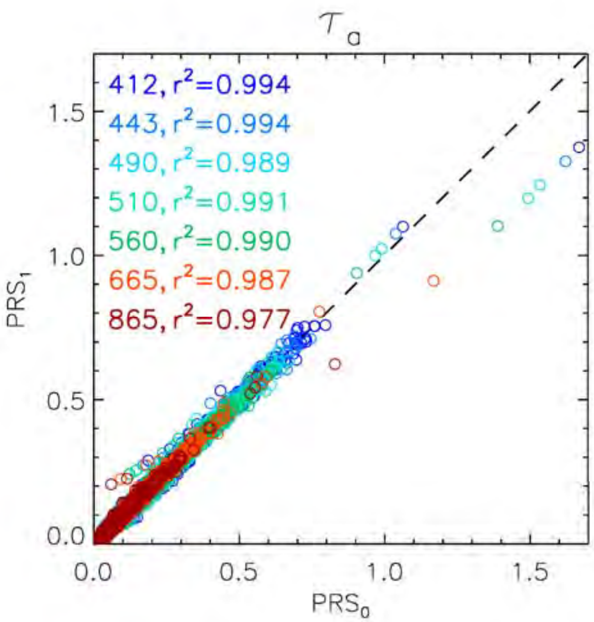
4449 pairs of coincident (Δt<10’) measurements over 659 days of data acquisitions



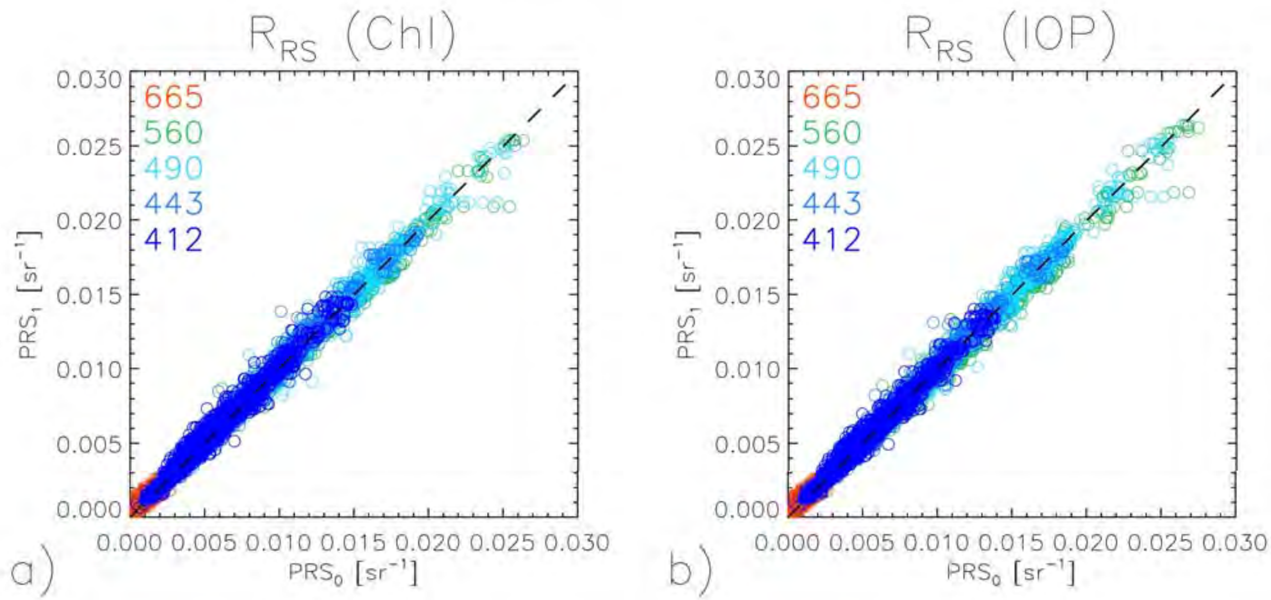


Comparison of Field Data: Example at AAOT (2)

aerosol optical thickness



remote sensing reflectance



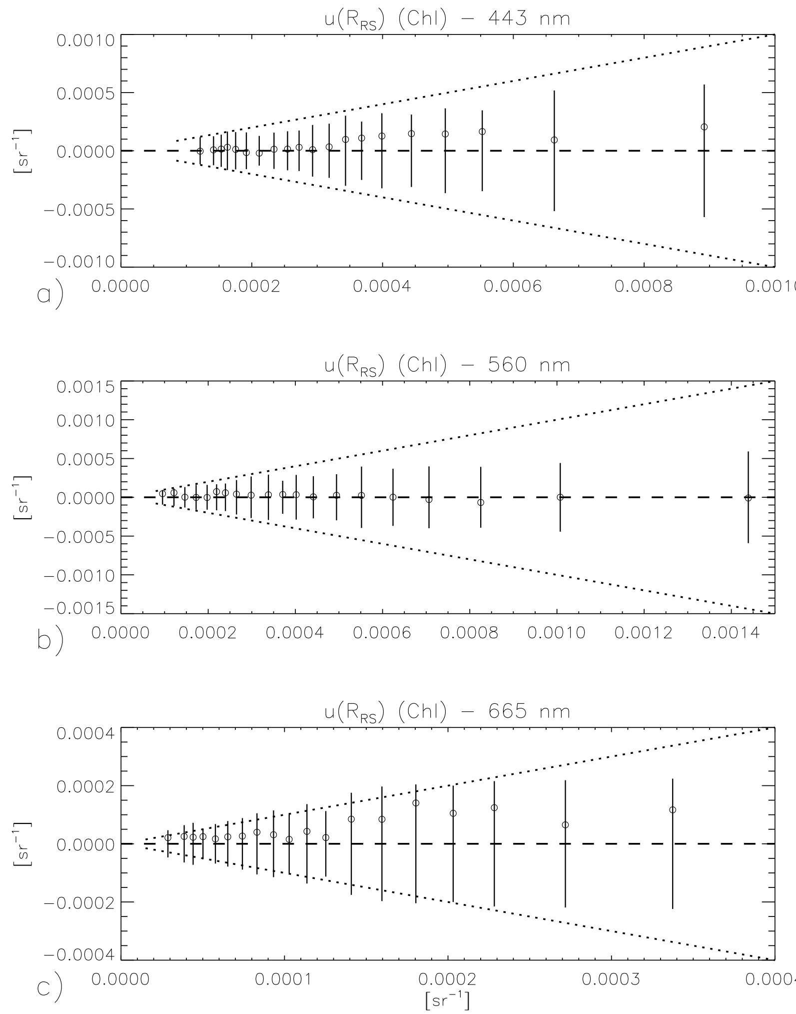
Mélin et al. *FRS* 2024

Comparison of Field Data: Example at AAOT (3)

$$u^2(X_2 - X_1) = u^2(X_1) + u^2(X_2) - 2u(X_1)u(X_2)r(e(X_1), e(X_2))$$

$$|R_{RS,1} - R_{RS,0}| < k\sqrt{u^2(R_{RS,0}) + u^2(R_{RS,1}) - 2r_\varepsilon u(R_{RS,0})u(R_{RS,1})}$$

% (*k*=1)	412	443	490	560	665
R_{RS}^{Chl}, r_ε=0	89	92	94	93	81
R_{RS}^{Chl}, r_ε=0.5	78	82	86	83	70
R_{RS}^{IOP}, r_ε=0	87	90	93	81	67
R_{RS}^{IOP}, r_ε=0.5	74	80	85	65	55



Data from the two systems appear generally consistent with their stated uncertainties, indicating that they are metrologically compatible

Mélin et al. *FRS* 2024

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Comparisons of EO data

What we know

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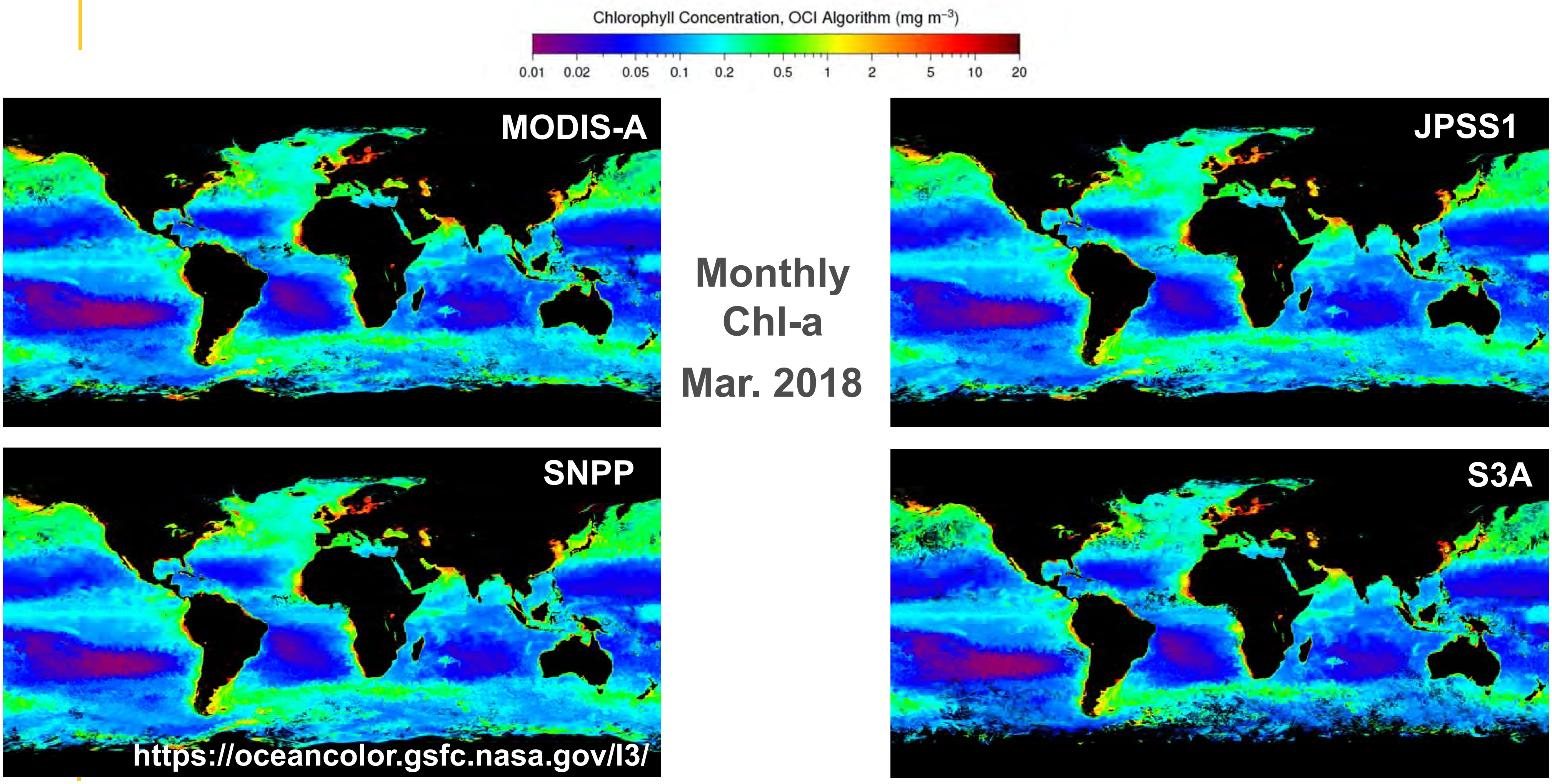
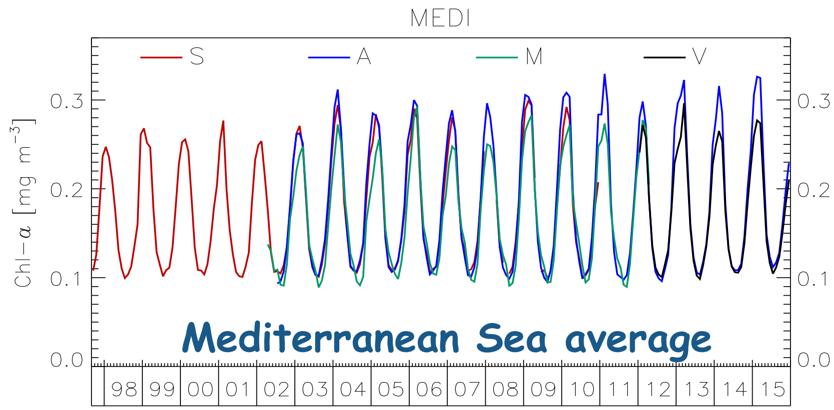
General consistency between missions (1)

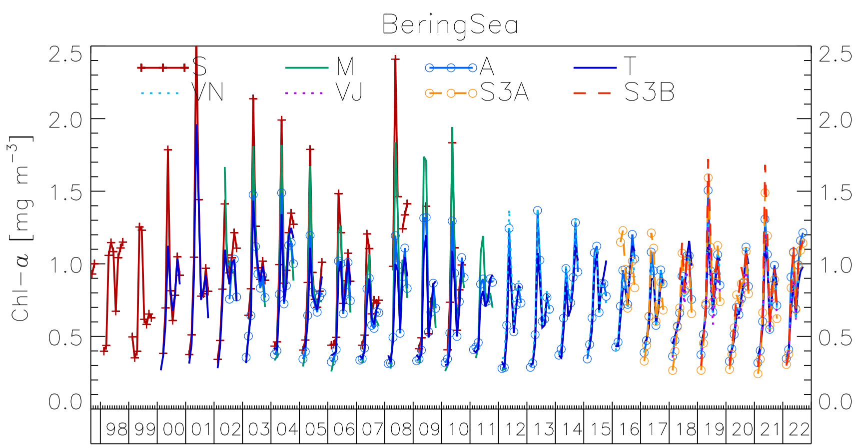


General consistency between missions (2)

NASA products:
- SeaWiFS
- MERIS
- MODIS-Aqua
- VIIRS



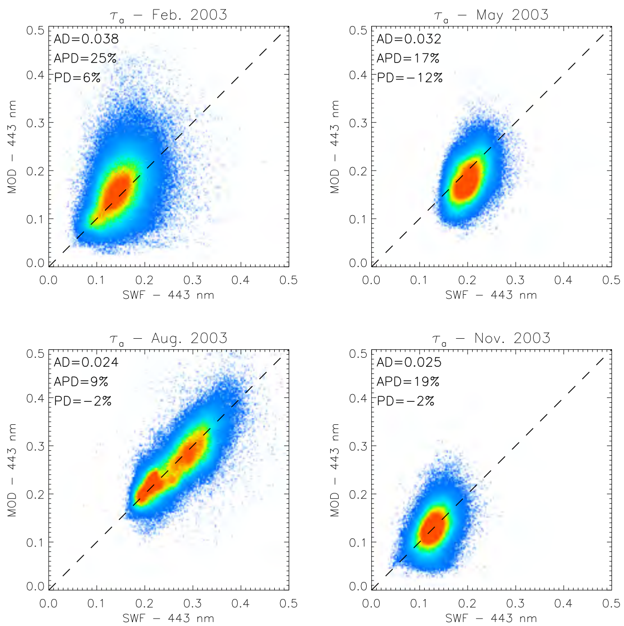
- S: SeaWiFS
- M: MERIS
- A: MODIA-Aqua
- T: MODIS-Terra
- VN: VIIRS-SNPP
- VJ: VIIRS-JPSS1
- S3A: OLCI S-3A
- S3B: OLCI S-3B



General consistency between missions (3)

MODIS-A vs SeaWiFS

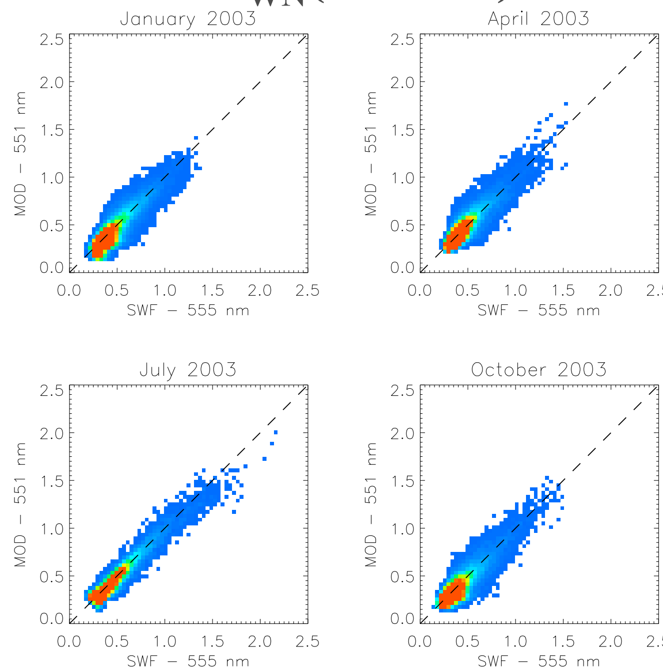
$\tau_a(443)$



Mediterranean Sea

Mélin et al., *RSE* 2007

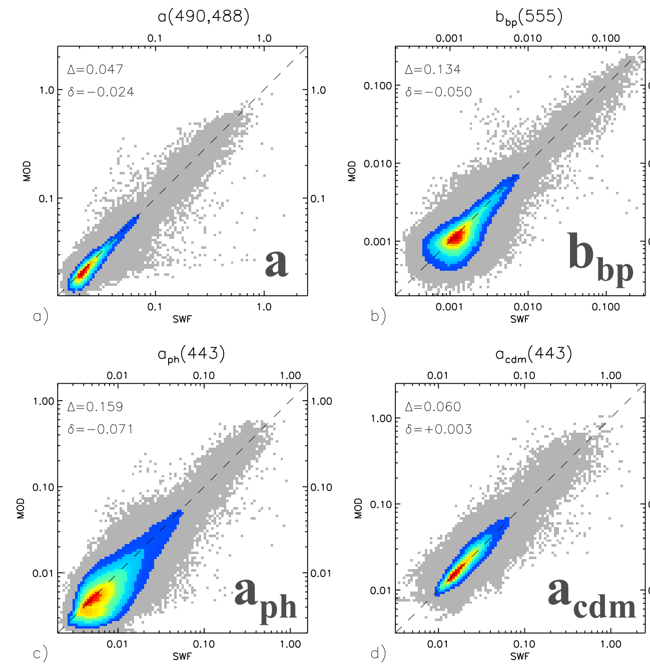
$L_{WN}(551/555)$



Mediterranean Sea

Mélin et al., *ASR* 2009

IOPs



Adriatic Sea

Mélin et al., *OS* 2011

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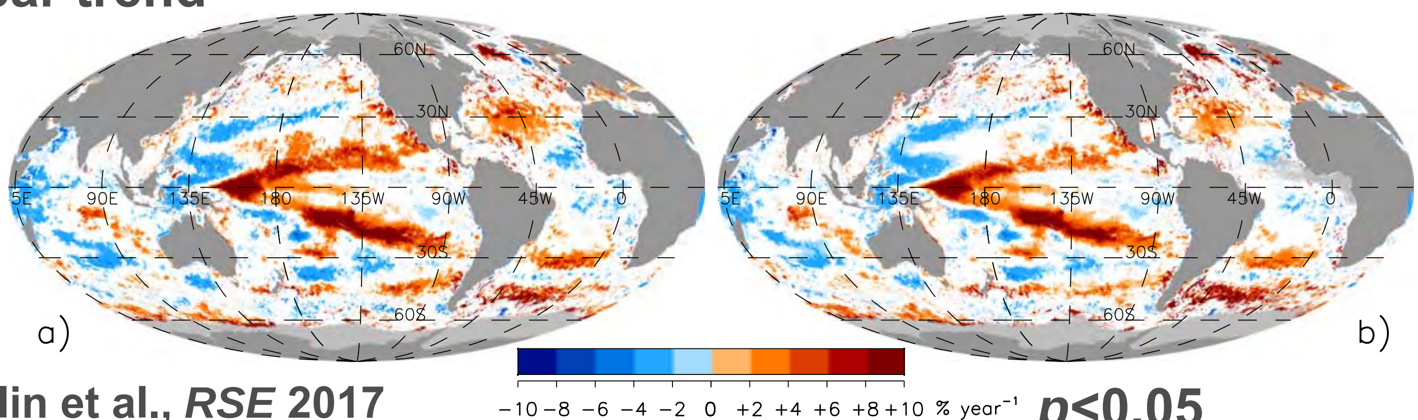
General consistency between missions (4)

Chl-a 10-year trend
Aug. 2002
Jul. 2011

MODIS-A



MERIS

Mélin et al., *RSE* 2017

p<0.05

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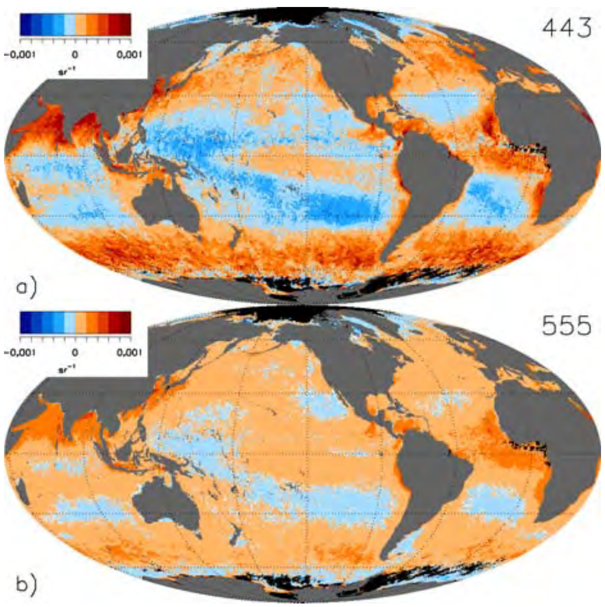
Ocean Color products (R_{RS}, IOPs, Chl-a) from various missions show differences varying:

in space



SeaWiFS-MODIS

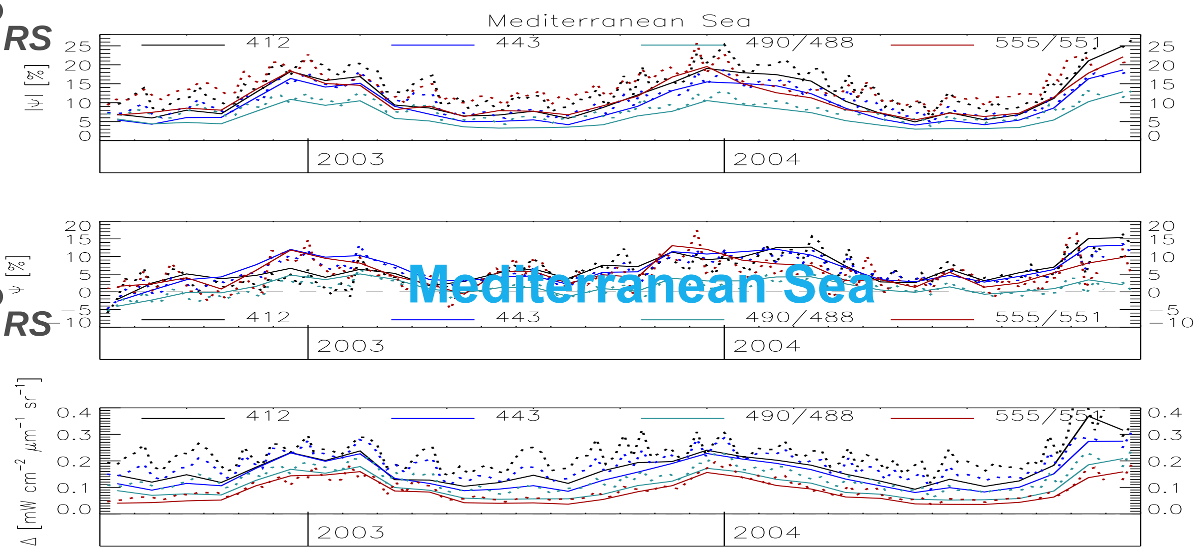
$$\delta = \sum_{i=1}^{N} (y_i - x_i)$$

Mélin et al., *RSE* 2016

in time

R_{RS}

R_{RS}



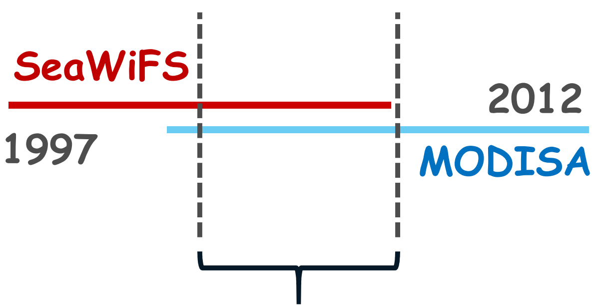
$$|\psi| = \sum_{i=1}^{N} \frac{2|y_i - x_i|}{x_i + y_i} \qquad \psi = \sum_{i=1}^{N} \frac{2(y_i - x_i)}{x_i + y_i}$$

Mélin et al., *ASR* 2009

Small systematic inter-mission differences are sufficient to introduce spurious trends

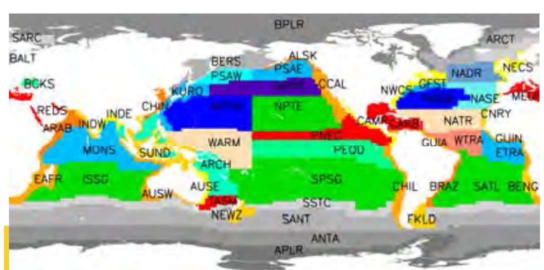
Comparing **trend slopes** of merged products affected by a bias wrt those obtained for a series of reference

p: level of significance (*t*-test) quantifying the degree to which 2 trends differ

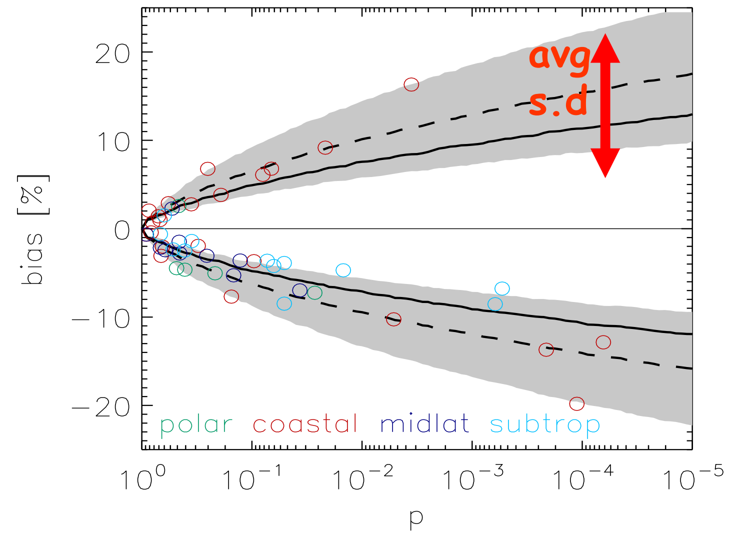


$$x_{MRG}(m) = \tfrac{1}{2}[x_S(m)+(1 + \%bias/100)\, x_{A,corr}(m)]$$

$\%bias$: [-50% to +50%]



Mélin, *IJRS* 2016



50% 90% 99% ***p***

differences of 5-6%

significant differences in slopes ($p<0.05$)

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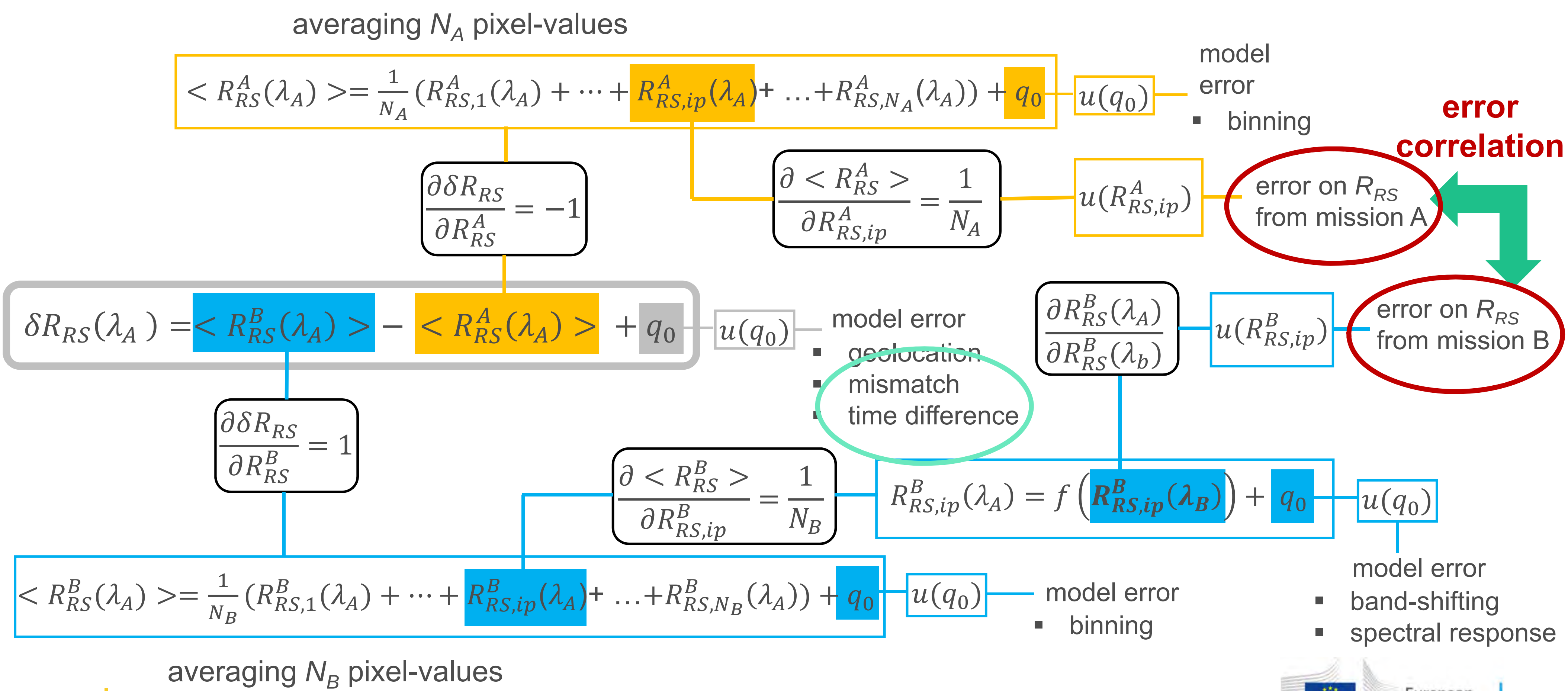
Framework to characterize differences between products (e.g., R_{RS})



The Case of Composites

$$\delta R_{RS}(\lambda_A) = < R_{RS}^{B}(\lambda_A) > - < R_{RS}^{A}(\lambda_A) > + q_0$$

$u(q_0)$

model error

- geolocation
- mismatch
- time difference

- Different times of the day for a daily datum (polar-orbiting)
- Grid points incompletely/variably filled
- Different days for a time composite

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Comparisons of EO data

Examples with R_{RS} at validation sites (AERONET-OC)

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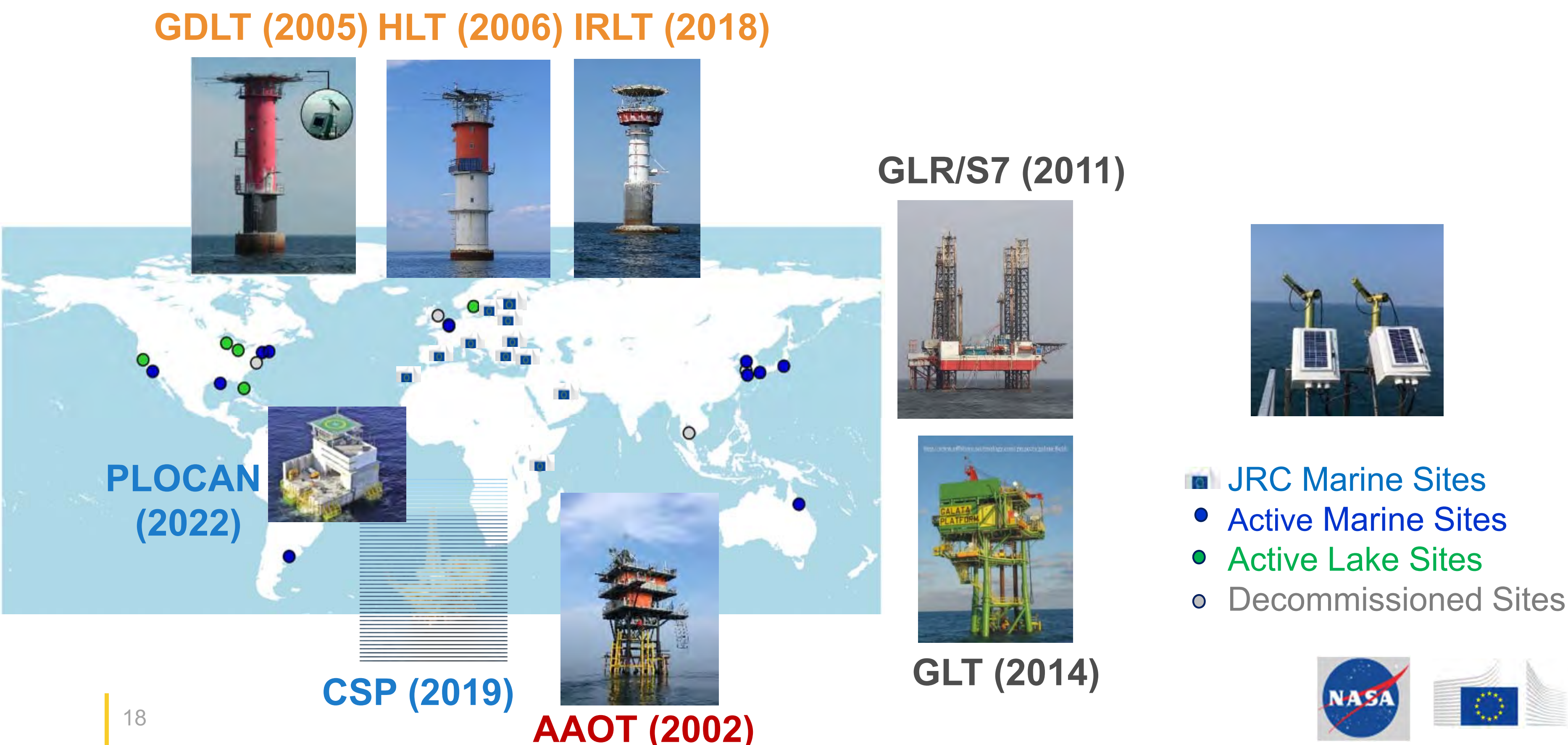
Source of field R_{RS} data: AERONET-OC



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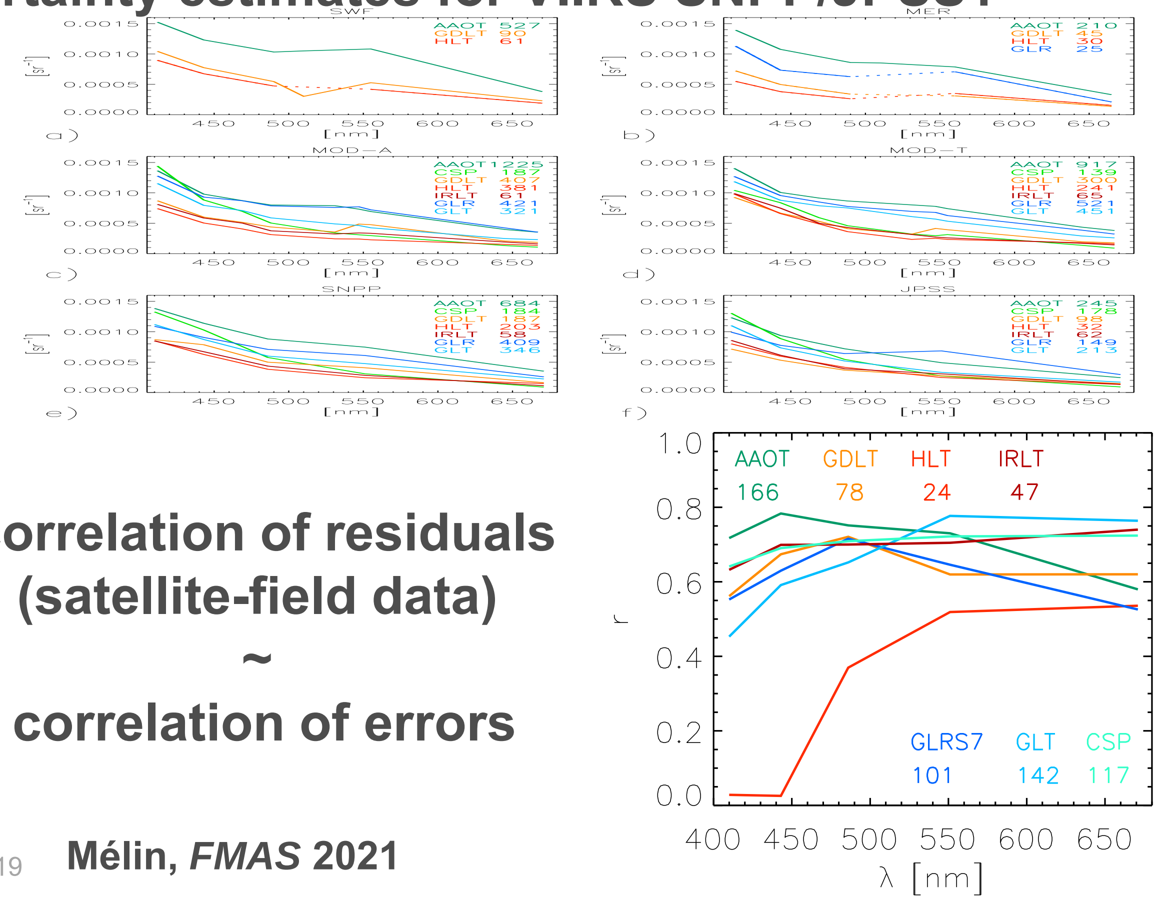
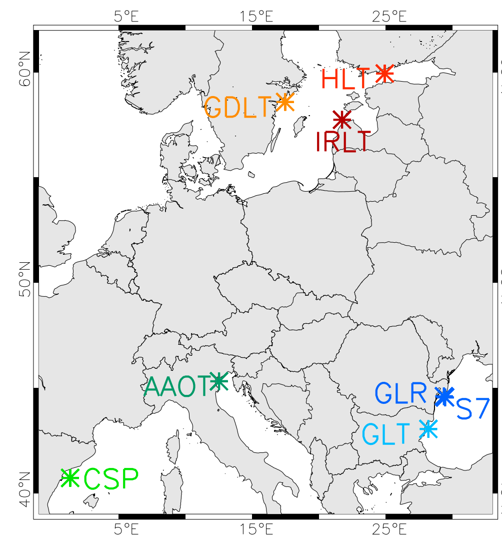
Comparison of EO Data: Example with VIIRS (1)

Uncertainty estimates for VIIRS SNPP/JPSS1





correlation of residuals (satellite-field data)

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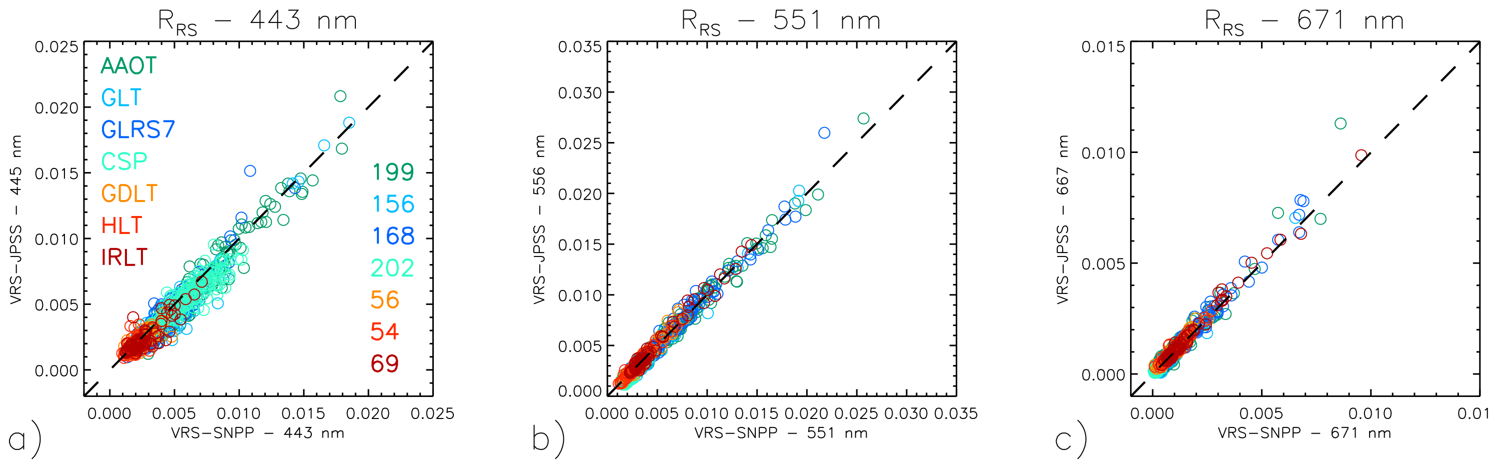
correlation of errors

Mélin, *FMAS* 2021

Comparison of EO Data: Example with VIIRS (2)

SNPP vs JPSS1



Fraction of data verifying (*k*=1) (no representation error):

$$\left|R_{RS}^{B} - R_{RS}^{A}\right| < k\sqrt{u^2\left(R_{RS}^{A}\right) + u^2\left(R_{RS}^{B}\right) - 2u\left(R_{RS}^{A}\right)u\left(R_{RS}^{B}\right)r\left(e\left(R_{RS}^{A}\right), e\left(R_{RS}^{B}\right)\right)}$$

AAOT	410	443	486	551	671
r=0 (%)	93	90	93	92	95
r≠0 (%)	69	*60*	70	76	89

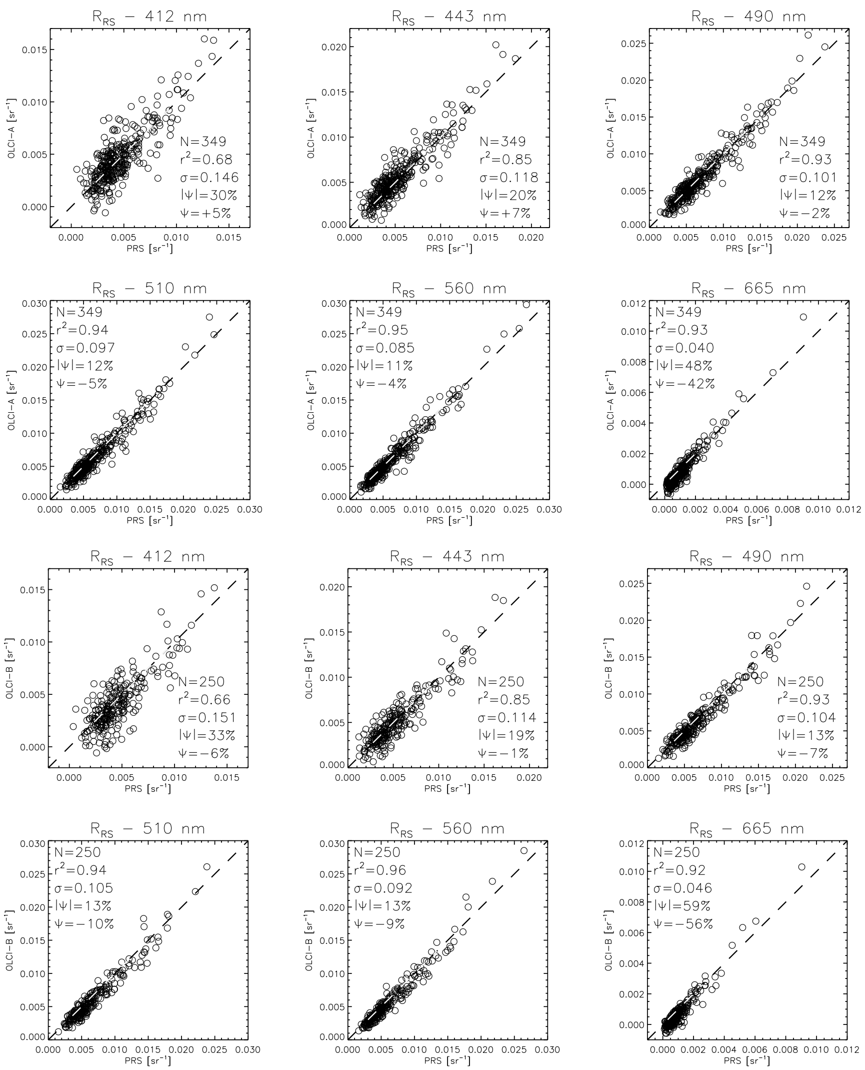
GLT	410	443	486	551	671
r=0 (%)	91	87	87	90	95
r≠0 (%)	85	*67*	71	*67*	81

Mélin, *FMAS* 2021

Comparison of EO Data: Example with OLCI (1)

S3A

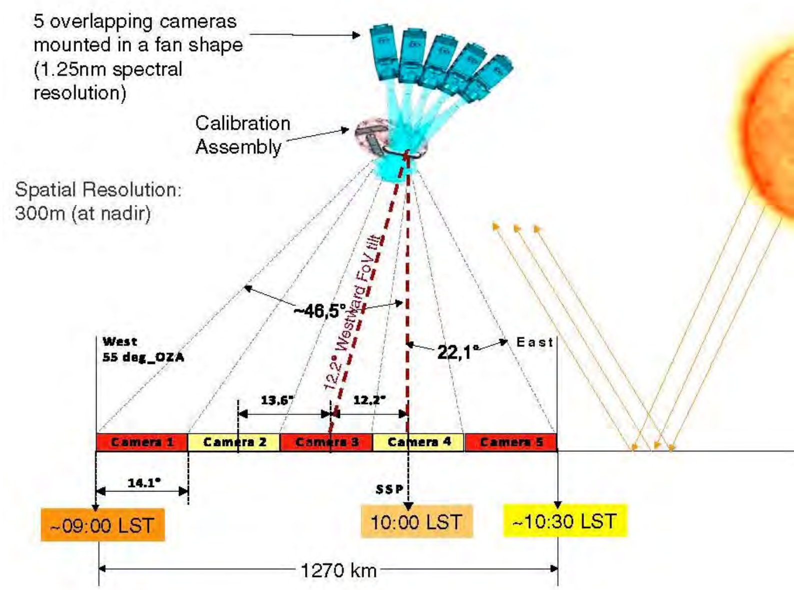
S3B



Cam.	1	2	3	4	5	
S3A	24%	26%	15%	21%	13%	N=349
S3B	30%	20%	16%	20%	13%	N=220

(out of tandem)

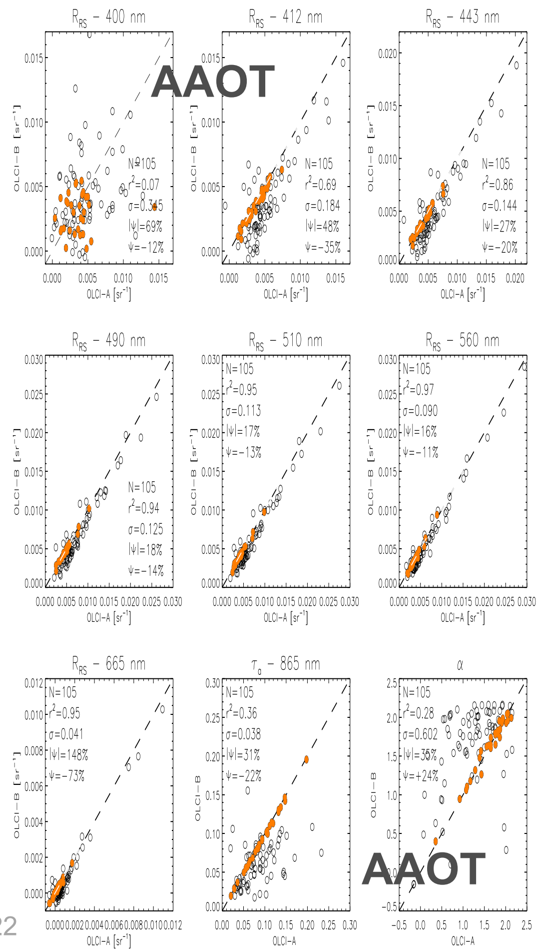
Donlon et al. *RSE* (2012)



 OLCI validation results at AAOT (*l2gen*)

Comparison of EO Data: Example with OLCI (2)

OLCI S3A vs S3B



Orange: tandem phase

		S3A				
	Cam.	**1**	**2**	**3**	**4**	**5**
S3B	**1**			5.5%	46.6%	23.2%
	2		1.4%			11.0%
	3					
	4				2.7%	
	5	8.2%				1.4%

=75%

Beware of conditions represented by the comparison data set before reaching conclusions

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Collocation Statistics

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Collocation (1): with Reference Data

For i=1,N validation points:

$$\begin{cases} x_i = r_i + \gamma_i \\ y_i = \beta\, r_i + \delta + \varepsilon_i \end{cases}$$

r: reference values ("truth")
x: in-situ measurements with σ_γ known
γ: associated random error term (mean=0, un-correlated)
y: satellite values, with σ_ε unknown
ε: associated random error term (mean=0, un-correlated)
δ: additive bias
β: multiplicative bias

$$\Rightarrow \quad \sigma_\varepsilon^2 = \sigma_y^2 - \frac{\sigma_{xy}^2}{\sigma_x^2 - \sigma_\gamma^2}$$

(δ and β can also be computed)

Mélin et al. *RSE* 2016; Mélin, *FMAS* 2021; Mélin *RSE* 2022

Collocation (2): with 2 Similar Data Sets

For i=1,N comparison points:

$$\begin{cases} x_i = r_i + \gamma_i \\ y_i = \beta\, r_i + \delta + \varepsilon_i \end{cases}$$

$$\eta = \frac{\sigma_\varepsilon}{\sigma_\gamma}$$

r: reference values ("truth")
x: in-situ measurements with σ_γ unknown
γ: associated random error term (mean=0, un-correlated)
y: satellite values, with σ_ε unknown
ε: associated random error term (mean=0, un-correlated)
δ: additive bias
β: multiplicative bias

$$\beta = \frac{-\eta^2\sigma_x^2 + \sigma_y^2 + \sqrt{(\sigma_y^2 - \eta^2\sigma_x^2)^2 + 4\sigma_{xy}^2\eta^2}}{2\sigma_{xy}}$$

Slope of Model II linear regression
Legendre & Legendre (1998)

$$\begin{cases} \sigma_\gamma^2 = \frac{1}{2}\left[\sigma_x^2 + \frac{\sigma_y^2}{\eta^2} - \sqrt{\left(\frac{\sigma_y^2}{\eta^2} - \sigma_x^2\right)^2 + 4\sigma_{xy}^2/\eta^2}\right] \\ \sigma_\varepsilon^2 = \frac{1}{2}\left[\eta^2\sigma_x^2 + \sigma_y^2 - \sqrt{(\sigma_y^2 - \eta^2\sigma_x^2)^2 + 4\sigma_{xy}^2\eta^2}\right] \end{cases}$$

Mélin, *FMAS* 2021; Mélin *RSE* 2022

Collocation (3): with 2 Similar Data Sets

By the way:

$$\Delta_c^2 = \sigma_x^2 + \sigma_y^2 - 2\sigma_{xy}$$

$$\Delta_c^2 = (\beta - 1)^2\sigma_x^2 + \beta(2 - \beta)\sigma_\gamma^2 + \sigma_\varepsilon^2 \longrightarrow \sigma_\gamma^2 + \sigma_\varepsilon^2$$

if $\beta \longrightarrow 1$

Comparison is the 3rd principle of metrology

Shift to variable-centric view (consistent multi-mission data records) is still a challenge

Comparison of data has enormous potential (partly untapped)

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Bonus on Collocation Statistics

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Collocation : with 2 Similar Data Sets, with error correlation

For i=1,N comparison points:

$$\begin{cases} x_i = r_i + \gamma_i \\ y_i = \beta\, r_i + \delta + \varepsilon_i \end{cases}$$

$$\eta = \frac{\sigma_\varepsilon}{\sigma_\gamma}$$

r: reference values ("truth")
x: in-situ measurements with σ_γ unknown
γ: associated random error term (mean=0, correlated)
y: satellite values, with σ_ε unknown
ε: associated random error term (mean=0, correlated)
δ: additive bias
β: multiplicative bias

$$\beta = \frac{\sigma_y^2 - \eta^2\sigma_x^2 + \sqrt{(\sigma_y^2 - \eta^2\sigma_x^2)^2 + 4(\sigma_{xy} - r_{\varepsilon\gamma}\eta\sigma_x^2)(\eta^2\sigma_{xy} - r_{\varepsilon\gamma}\eta\sigma_y^2)}}{2(\sigma_{xy} - r_{\varepsilon\gamma}\eta\sigma_x^2)}$$

$r_{\varepsilon\gamma}$ **: Correlation between ε_i and γ_i**

Mélin, *FRS* 2024

Collocation : with 2 Similar Data Sets, with error correlation

$$\begin{cases} \sigma_\gamma^2 = \dfrac{\beta\sigma_x^2 - \sigma_{xy}}{\beta - \eta r_{\varepsilon\gamma}} \\ \\ \sigma_\varepsilon^2 = \dfrac{\sigma_y^2 - \beta\sigma_{xy}}{1 - \beta r_{\varepsilon\gamma}/\eta} \end{cases}$$

$$\Delta_c^2 = (\beta - 1)^2 + \left[\beta(2-\beta) + \eta^2 - 2\eta r_{\varepsilon\gamma}\right]\sigma_\gamma^2$$

$\longrightarrow \sigma_\gamma^2(1 + \eta^2 - 2\eta r_{\varepsilon\gamma})$ **if** $\beta \longrightarrow$ **1**

$\longrightarrow \sigma_\gamma^2(2 - 2r_{\varepsilon\gamma})$ **if** $\beta \longrightarrow$ **1 and** $\eta = 1$

Mélin, *FRS* 2024

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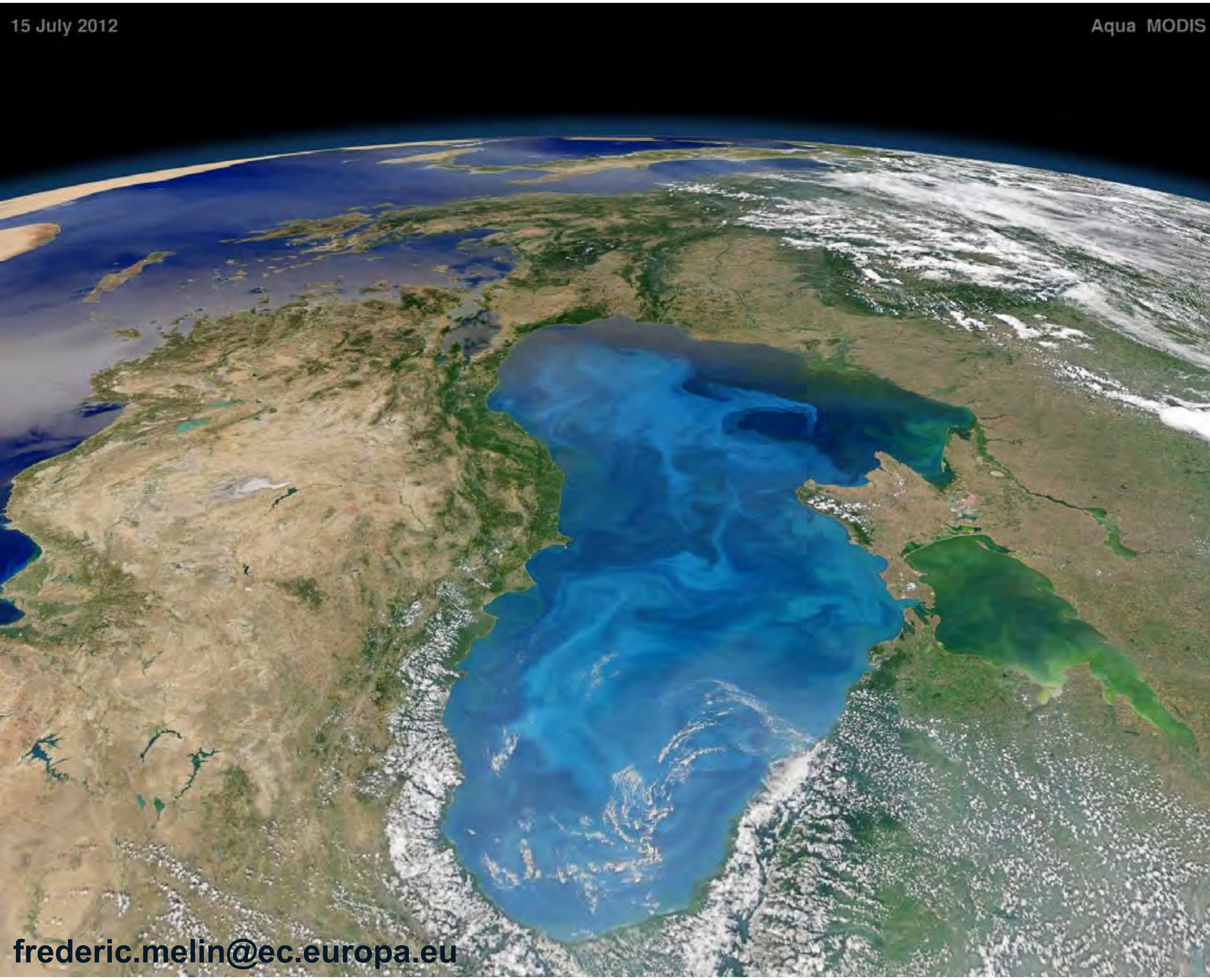

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Thank you!

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