Validation of inferred high resolution ocean pCO_2 and air-sea fluxes with in-situ and remote sensing data.

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STSE ESA OceanFlux - Theme 3 : Upwelling

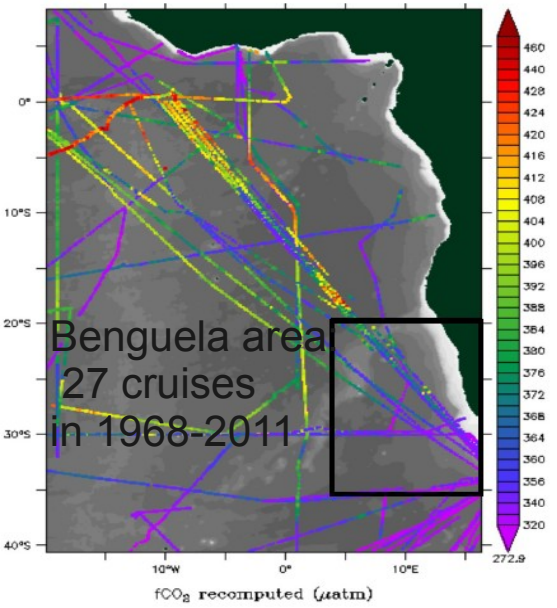
oceanflux
support to science element

Why this work?

- Importance of submesoscale features.

- Scarcity of oceanographic cruises and lack of available satellite products.

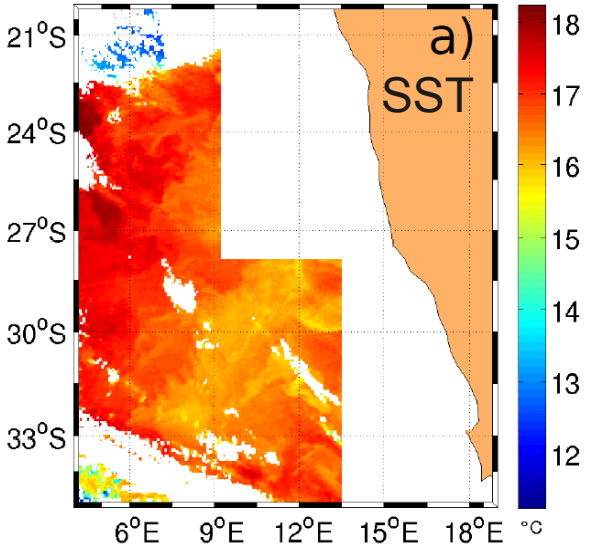
Surface water fCO_2 (µatm) from SOCAT. version 2



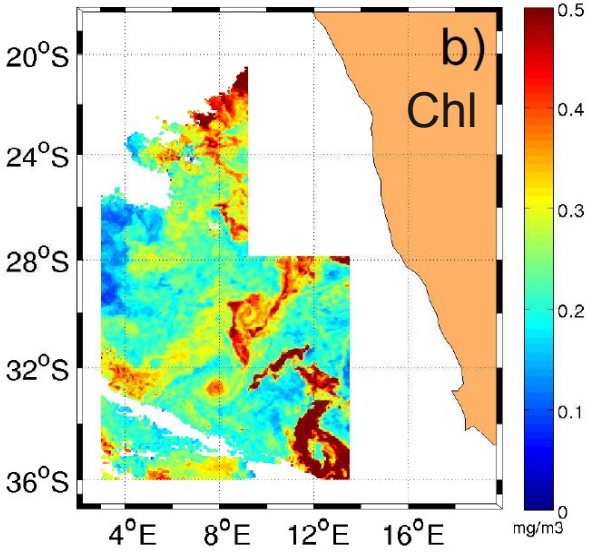
- GOAL: To obtain an assesment of spatial variability of GHGs concentrations at small scales (~4 km) from satellite images in the EBUS.

The idea

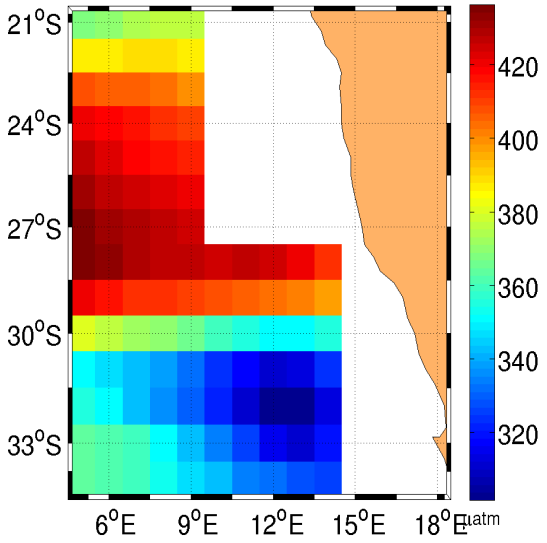
Spatial resolution ~ 4 km



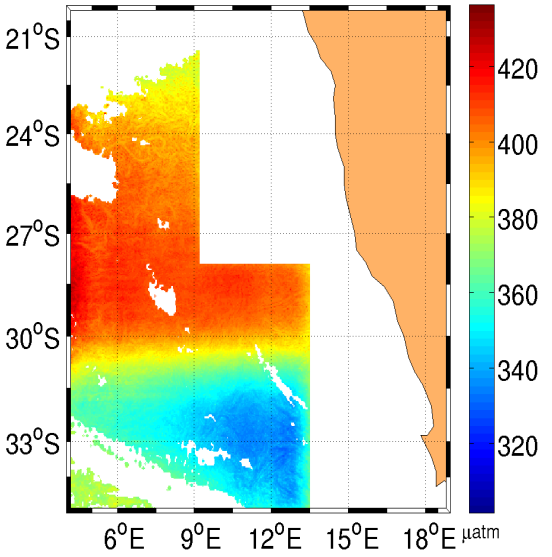
+



pCO_2 from CarbonTracker
Spatial resolution ~ 110 km



Inferred pCO_2
Spatial resolution ~ 4 km



Variations in phytoplankton (carbon cycling), Variations in temperature (solubility) → Variations in CO2

How to do it?

1. How to obtain the small scale information?

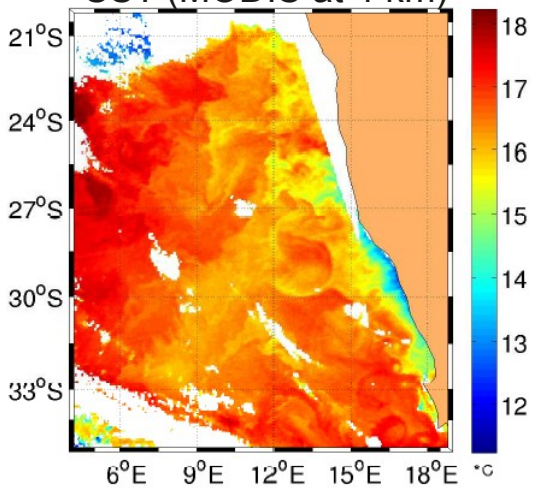
Turbulence → energy cascades → multifractal hierarchy
→ scale invariant behaviour → power-laws → scaling exponents h

Microcanonical Multiscale Formalism:
Set of scaling exponents obtained as sets of geometrically localized singularity exponents.

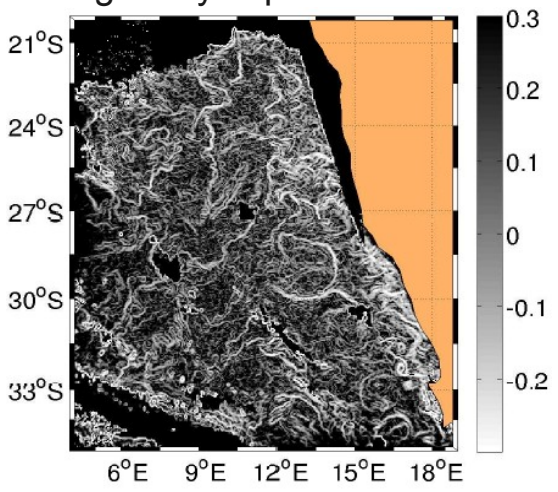
$$\mathcal{F}_h = \{\mathbf{x} \ : \ h(\mathbf{x}) = h\}$$

$$\left.\begin{array}{l} \frac{1}{r}|s(\mathbf{x}+\mathbf{r}) - s(\mathbf{x})| \sim r^{h(\mathbf{x})} \\ \mathcal{T}_\psi|\nabla s|(\mathbf{x},r) = \alpha(\mathbf{x}) r^{h(\mathbf{x})+d} + o\left(r^{h(\mathbf{x})+d}\right) \ (r \longrightarrow 0) \end{array}\right\} h(x) = \frac{\log(\mathcal{T}_\psi|\nabla s|(\mathbf{x},r_0)/\langle \mathcal{T}_\psi|\nabla s|(\cdot,r_0)\rangle)}{\log r_0} + o\left(\frac{1}{\log r_0}\right)$$

SST (MODIS at 4 km)



Singularity exponents of SST

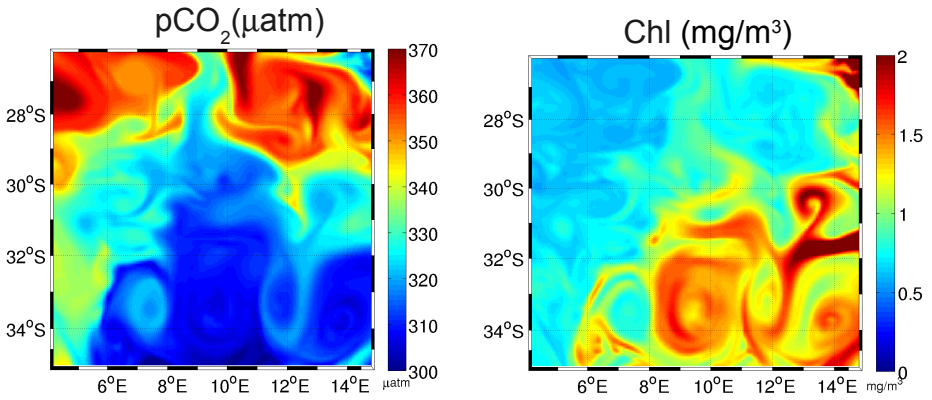


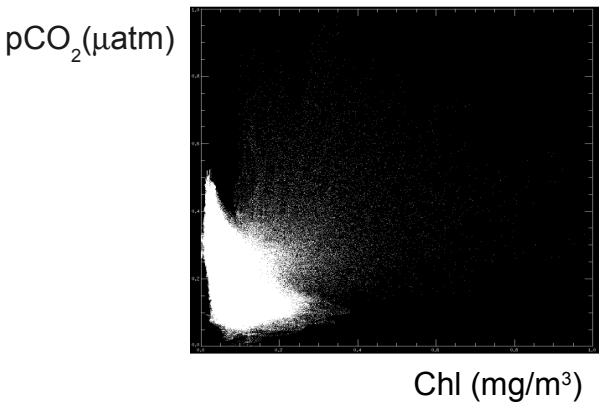
- Measure of the degree of regularity of the image, associated to transitions

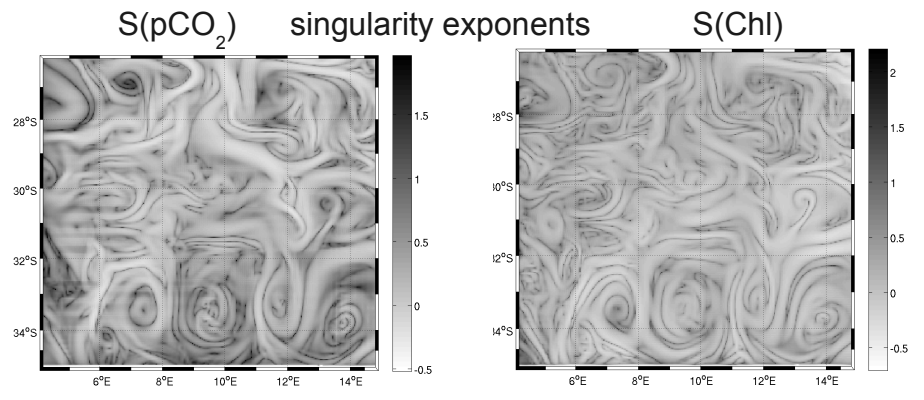
(*Turiel et al 2008* ; *Yahia et al. 2010*)

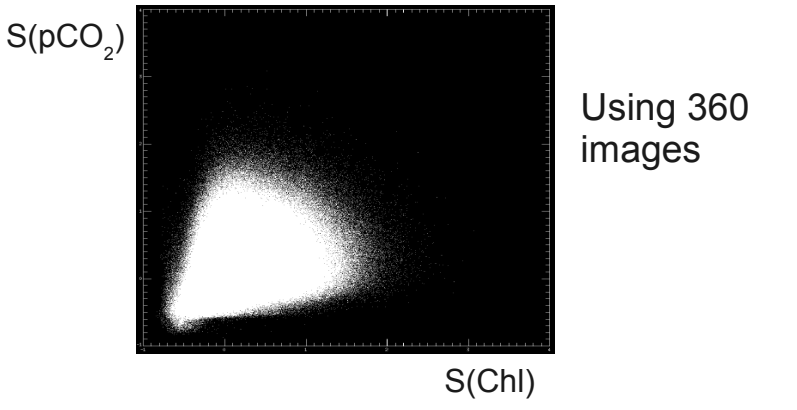
2. How to connect different tracer images?

ROMS-BIOEBUS model in the Benguela upwelling system









pCO2≠pCO2(SST,CHL)

S(pCO2)=S(pCO2)(S(SST),S(CHL))

Proxy of $S(pCO_2)$ at high resolution:

$$\mathcal{S}(pCO_2)(\mathbf{x}) = a(\mathbf{x})\mathcal{S}(SST)(\mathbf{x}) + b(\mathbf{x})\mathcal{S}(Chl-a)(\mathbf{x}) + c(\mathbf{x})\mathcal{S}(pCO_2{}^{LR})(\mathbf{x}) + d(\mathbf{x})$$

Regression coefficients a(x),b(x),c(x),d(x) are estimated from ROMS-BIOEBUS output data

3. Cross-scale inference of pCO_2 data

Multiresolution analysis on signal S(pCO_2) (proxy of pCO_2 at high resolution)

Decomposition of the signal at different scales: Wavelet projections

$$\mathcal{T}_\psi \mathcal{S}(pCO_2)(\mathbf{x}, \mathbf{r}_j) = \sum_{n \in \mathbb{Z}} \langle \mathcal{S}(pCO_2) | \psi_{x_n, r_j} \rangle \psi_{x_n, r_j}(u)$$

$\boldsymbol{A_j}$ orthogonal projection of $\boldsymbol{V_j}$ (approximation space)
$\boldsymbol{P_j}$ orthogonal projection of $\boldsymbol{W_j}$ (detail space)

Reconstruction formula:

$$A_{j-1} pCO_2 = A_j pCO_2 + P_j h$$

Sudre et al. 2014

Input Data

- **CarbonTracker air-sea fluxes at low resolution: 1° ~ 110 km**

Temporal evolution of a tracer c in the atmosphere :

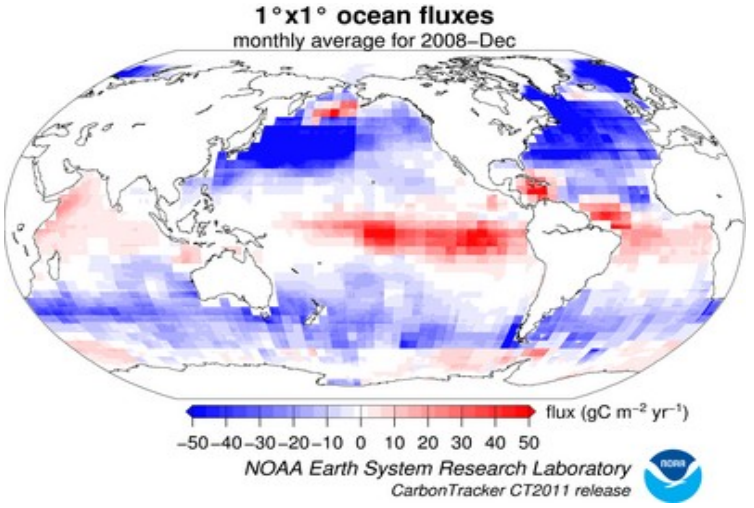
$$\frac{\partial c}{\partial t} = -u\nabla c + \frac{1}{\rho}\nabla(\rho T_d \nabla c) + \frac{1}{\rho}g + F$$

F, net flux at the interface

Atmospheric CO_2 data provided by SCIAMACHY and GOSAT. (*Garbe et al. 2007, 2014*)

Air-sea CO_2 fluxes from CarbonTracker (1° x 1° spatial resolution)

(*Peters et al. 2007*)



Relation between net air-sea flux and pCO_2

$$F = \alpha K(p^{air}_{CO_2} - p^{ocean}_{CO_2})$$

- $p^{ocean}_{CO_2}$ obtained from inverse modeling and satellite data at resolution of CarbonTracker .

Input Data

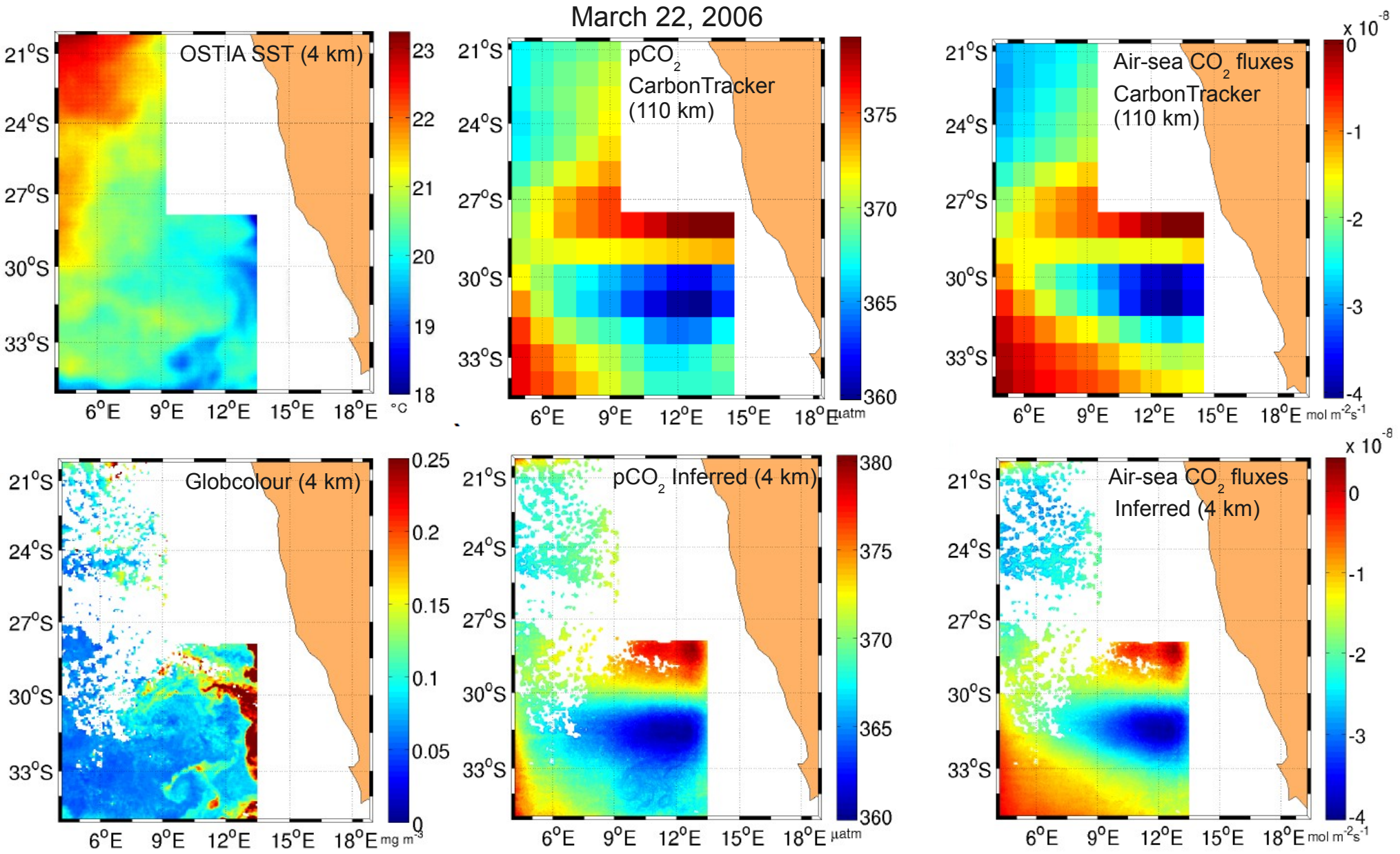
- **SST and Chl-a from Satellite at high resolution: ~ 4 km**

Name reference	Parameter	Instruments	Satellites	Resolution
OSTIA	SST	Optimal interpolation		5 km / daily
MODIS	SST	MODIS	AQUA	4 km / daily
MERIS	Chl-a	MERIS	ENVISAT	4 km / daily
Globcolour	Chl-a	MODIS/MERIS/SeaWiFS (Merged globcolour)	AQUA/ENVISAT	4 km / daily

Three combinations of Chl-a and SST products:

- MERIS-OSTIA
- Globcolour-OSTIA
- Globcolour-MODIS

Super-resolution pCO_2 in the Benguela Upwelling System



The cascade of information across the scales enhances gradients in the field of pCO2

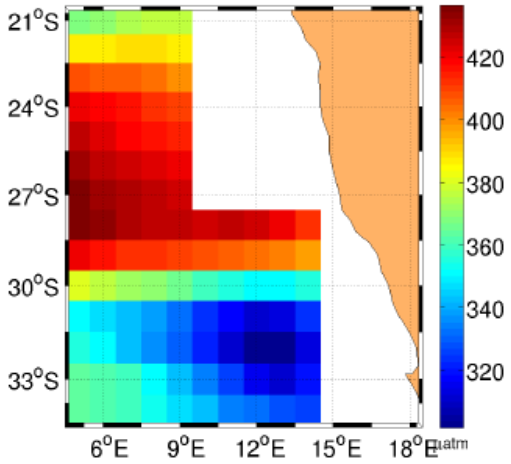
Evaluation analysis of using different satellite data combinations:

- Number of valid points yielded in the inferred pCO_2 field

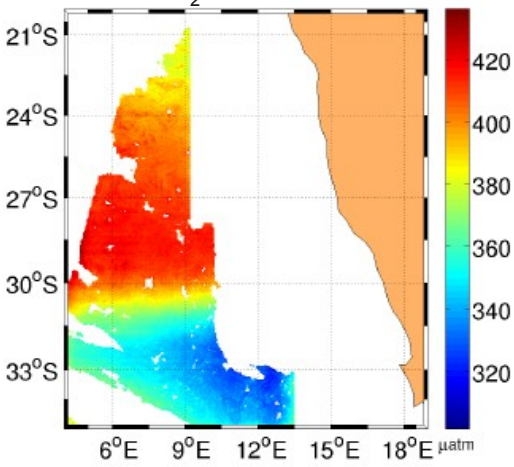
- Degradation of the information contained in the transition fronts

Septembre 21, 2006

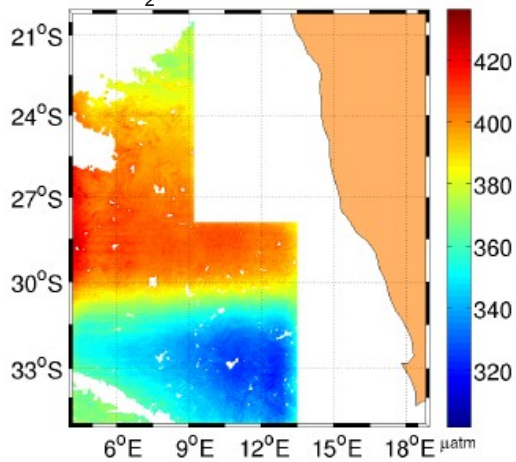
pCO_2 from CarbonTracker (110 km)



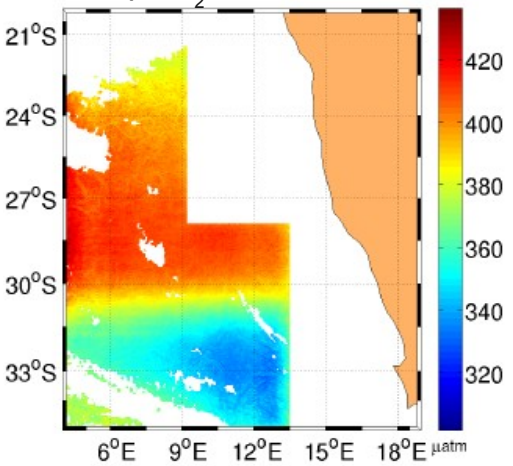
Inferred pCO_2 from MERIS-OSTIA (4 km)



Inferred pCO_2 from Globcolour-OSTIA (4 km)



Inferred pCO_2 from Globcolour-MODIS (4 km)



Hernandez-Carrasco et al. submitted

- Number of valid points yielded in the inferred pCO2 field

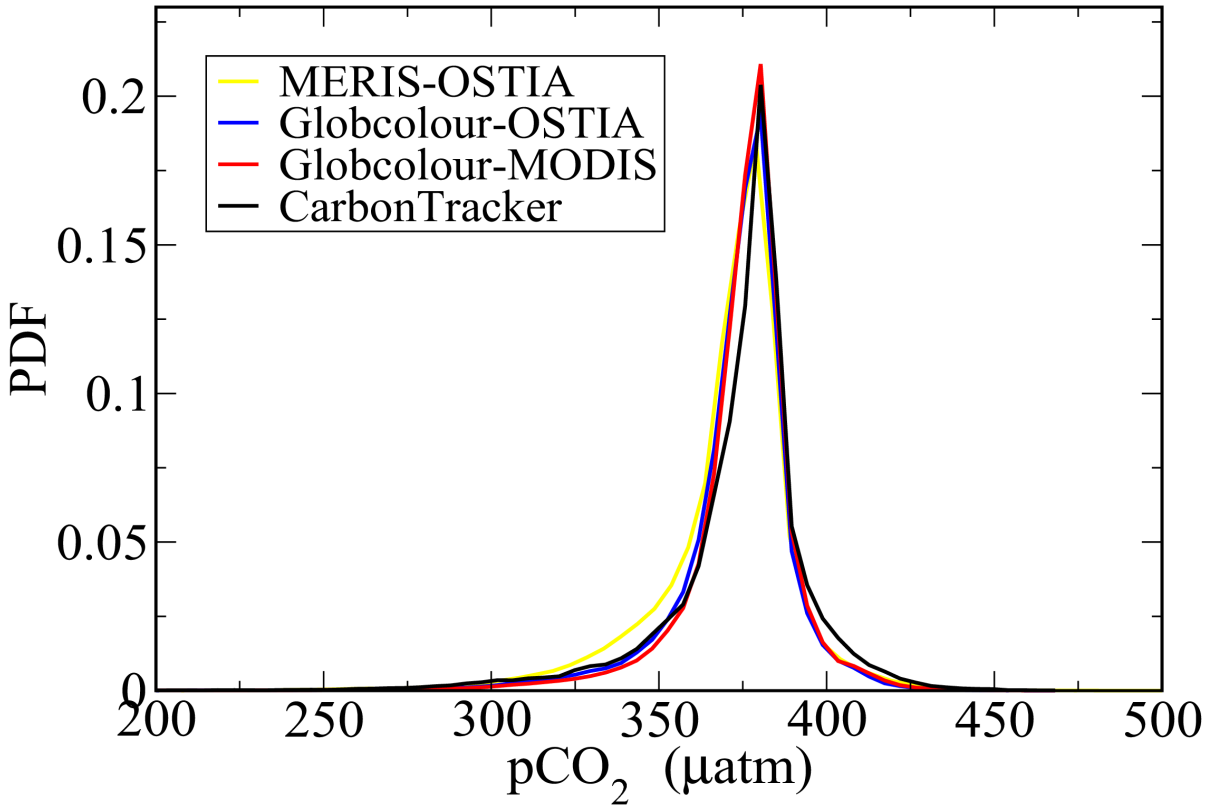
Valid Points in the inferred pCO_2 fields: 2006/2008	
N° total pixels domain	55711378
N° Points OSTIA-MERIS	9800776
N° Points OSTIA-GLOBCOLOUR(AVW)	26382072
N° Points OSTIA-GLOBCOLOUR(GSM)	27313043
N° Points MODIS-GLOBCOLOUR(GSM)	20397047
Proportion OSTIA-GSM/OSTIA-MERIS	2.78
Proportion OSTIA-GSM/MODIS-GSM	1.33
Proportion MODIS-GSM-/OSTIA-MERIS	1.08
LP_{OM}	82%
LP_{OG}(AVW)	53%
LP_{OG}(GSM)	51%
LP_{MG}	63%

- loss of valid points: $$LP_x = \frac{N_p - N_x}{N_p} 100\%$$

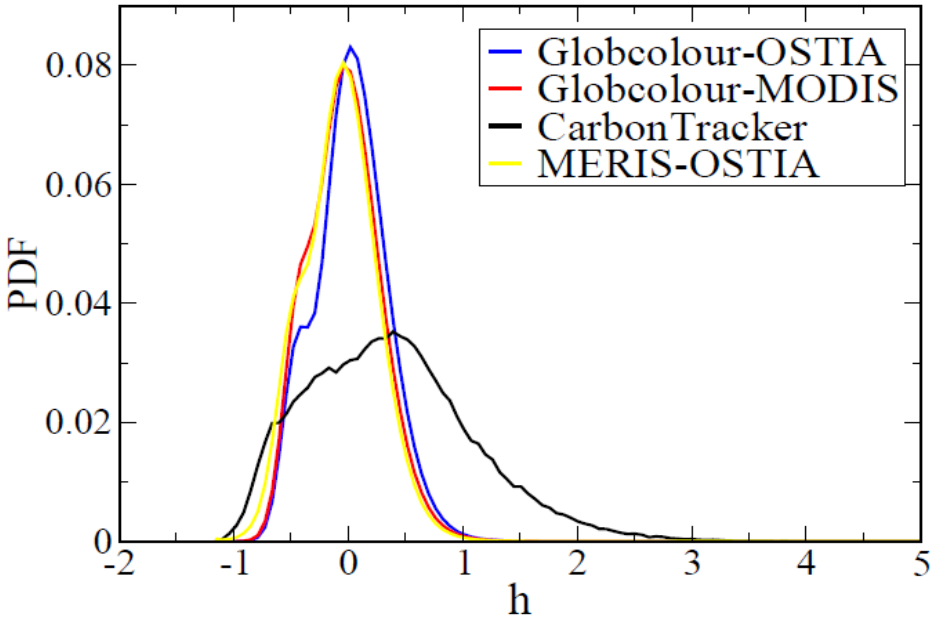
Np = 557711378, total number of pixels removing the pixels of the CarbonTracker mask
Nx = number of valid points in the inferred pCO2 for each product combination.

Analysis of degradation of the realism of the transition fronts

- analysis of probability distribution functions (PDFs) of pCO_2 values



- analysis of PDFs of singularity exponents of pCO2

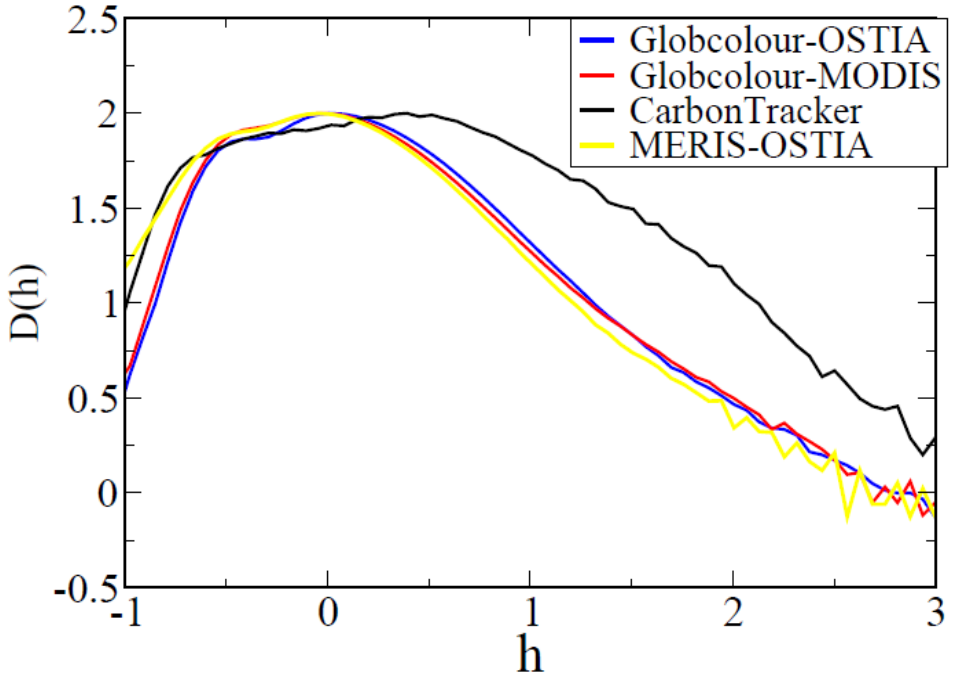


- Scale dependent of PDFs

$$\rho_{r_0}(h) = A_0 r_0^{d-D(h)}$$

- Multifractal character

- analysis of singularity spectra

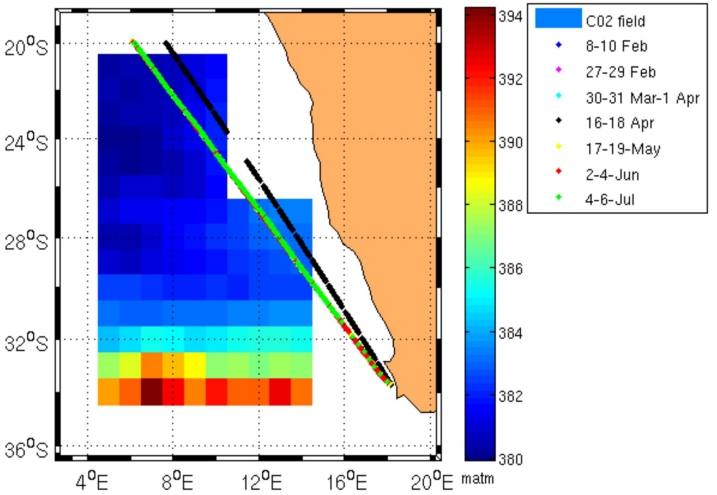


$$D(h) = d - \frac{\log\left(\rho_{r_0}(h)/\rho_{r_0}^M\right)}{\log r_0} \qquad \rho_{r_0}^M = \max_h\{\rho_{r_0}(h)\}$$

Validation with in-situ measurements

Available cruise data from SOCAT (Surface Ocean CO2 Atlas) in the Benguela upwelling region

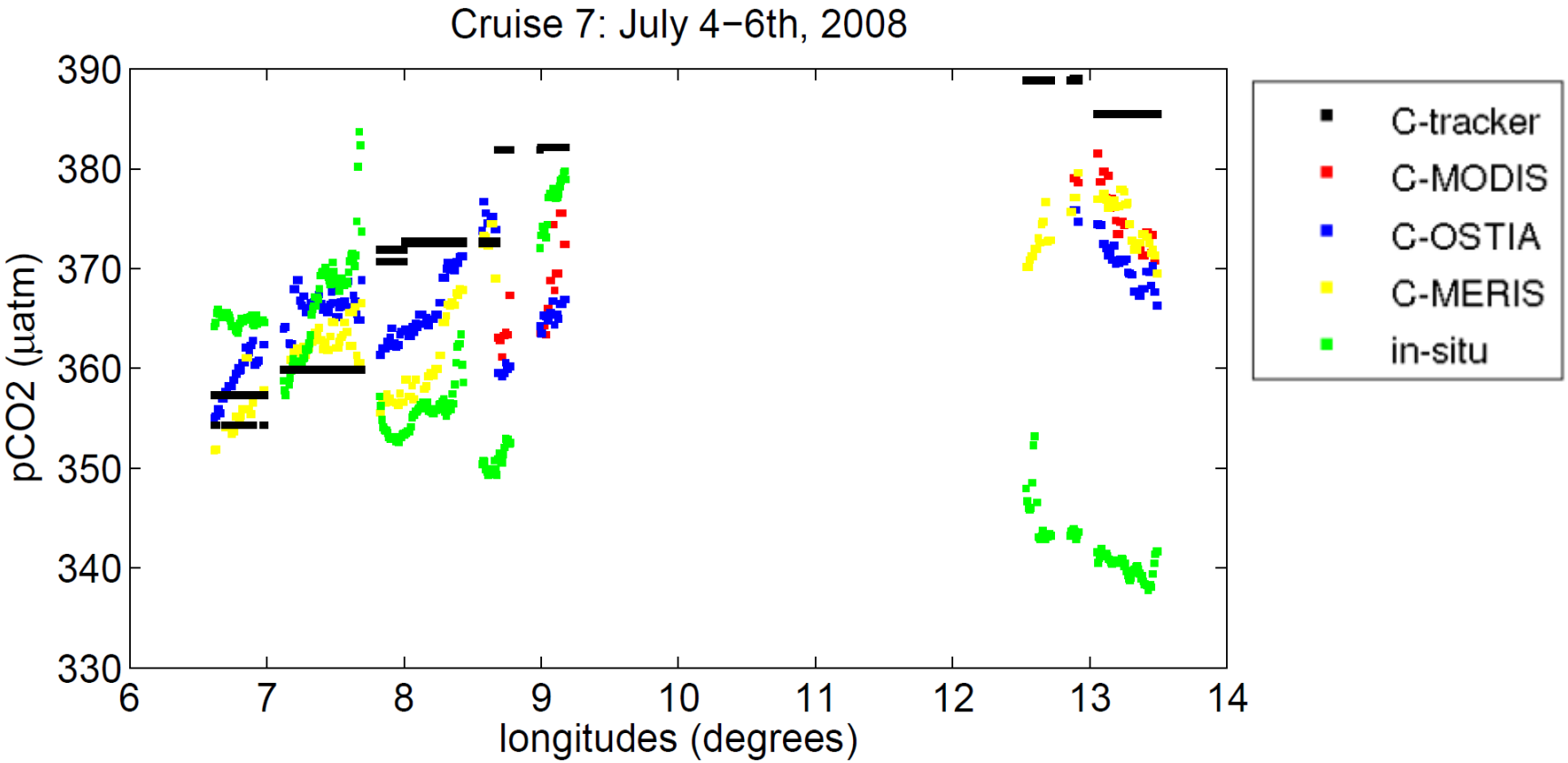
- **2000**, one cruise: *ANT-18-1*
- **2004**, one cruise: *0404SFC-PRT*
- **2005**, five cruises: *QUIMA2005-0804*, *QUIMA2005-0821*, *QUIMA2005-0922*, *QUIMA2005-1202*, *QUIMA2005-1220*
- **2006**, eight cruises: *QUIMA2006-0326*, *QUIMA2006-0426*, *QUIMA2006-0514*, *QUIMA2006-0803*, *QUIMA2006-0821*, *QUIMA2006-0921*, *QUIMA2006-1013*, *QUIMA2006-1124*
- **2008**, seven cruises: *QUIMAVOS2008-1*, *QUIMAVOS2008-2*, *QUIMAVOS2008-3*, *QUIMAVOS2008-4*, *QUIMAVOS2008-5*, *QUIMAVOS2008-6*, *QUIMAVOS2008-7*
- **2010**, one cruise: *ANT27-1*



24 cruises in 2000-2010

We use QUIMA cruises in 2005, 2006, 2008 (20 cruises)

Values of pCO2 at the intersections: inferred field - in-situ measurement



Inferred pCO_2 values show small scale variability in the zonal direction

At all valid intersections points in each SST-OC combination

Statistical computations QUIMAVOS2006/2008			
	MERIS - OSTIA	Globcolour - OSTIA	Globcolour - MODIS
Number of valid intersections	747	1928	1460
Mean Error carbontracker-insitu (μatm)	2.97	8.83	14.93
Mean Error inferred-insitu (μatm)	-0.15	3.42	8.42
Mean Absolute Error carbontracker-insitu (μatm)	21.34	22.08	22.07
Mean Absolute Error inferred-insitu (μatm)	17.77	16.47	16.62
Mean Relative Error carbontracker-insitu	0.059	0.060	0.061
Mean Relative Error inferred-insitu	0.048	0.045	0.046

At the same valid intersections points in the three SST-OC combinations

Statistical computations QUIMAVOS2006-2008			
	MERIS - OSTIA	Globcolour - OSTIA	Globcolour - MODIS
Number of valid intersections	458	458	458
Mean Error carbontracker-insitu (μatm)	7.60	8.01	8.01
Mean Error inferred-insitu (μatm)	4.37	1.62	3.32
Mean Absolute Error carbontracker-insitu (μatm)	23.63	23.23	23.23
Mean Absolute Error inferred-insitu (μatm)	19.92	16.31	18.85
Mean Relative Error carbontracker-insitu	0.065	0.065	0.064
Mean Relative Error inferred-insitu	0.055	0.045	0.051

Summing-up

- Novel method to reconstruct maps of ocean CO_2 fluxes at super resolution (~4km) from CarbonTracker CO_2 fluxes data at low resolution (~110 km).
- Inferred representation of pCO_2 improves the description provided by CarbonTracker.
- Merged products (Globcolour) improve the number of valid points in the pCO_2 field and the number of intersections for validation.
- Transitions fronts are well represented in the inferred pCO2 using merged products.
- Mean absolute error with respect to *in-situ* measurements is smaller for the inferred pCO_2 than for CarbonTracker (16.3 and 23.2 µatm, respectively).

What's the next

- Introduce seasonal and coefficients a(x), b(x), c(x) and d(x) of the multiple linear regression computed with a ROMS/BIOEBUS simulation.

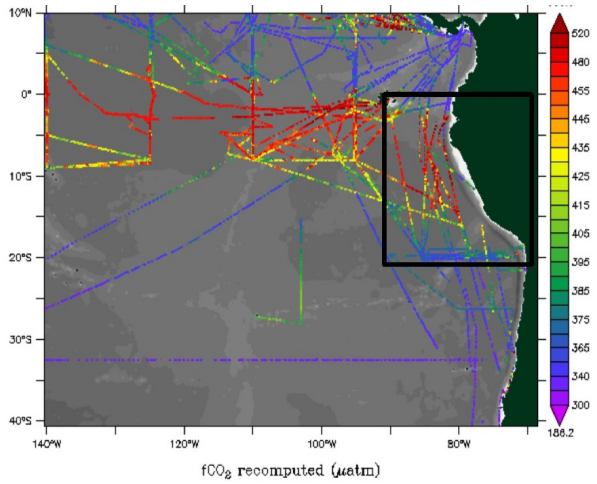
$$\mathcal{S}(pCO_2^{ocean})(x) = a(x)\mathcal{S}(SST)(x) + b(x)\mathcal{S}(Chl\_a)(x) + c(x)\mathcal{S}(pCO_{2LR}^{ocean}) + d(x)$$

- Add the salinity parameter (Level 3 SMOS) in the inference of pCO_2 as a new parameter in the multiple linear regression analysis.

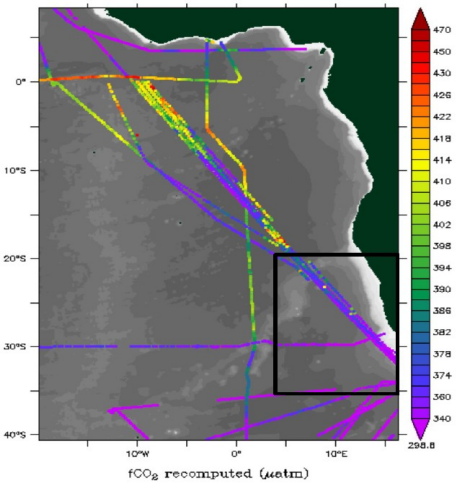
$$\mathcal{S}(pCO_2^{ocean})(x) = a(x)\mathcal{S}(SST)(x) + b(x)\mathcal{S}(Chl\_a)(x) + c(x)\mathcal{S}(pCO_{2LR}^{ocean}) + d(x)\mathcal{S}(SSS) + e(x)$$

- Extend the estimations of inferred pCO_2 to regions in the interior of ocean basins where more in-situ data are available, thereby improving the validation of the method.

Peru and Eastern South Pacific

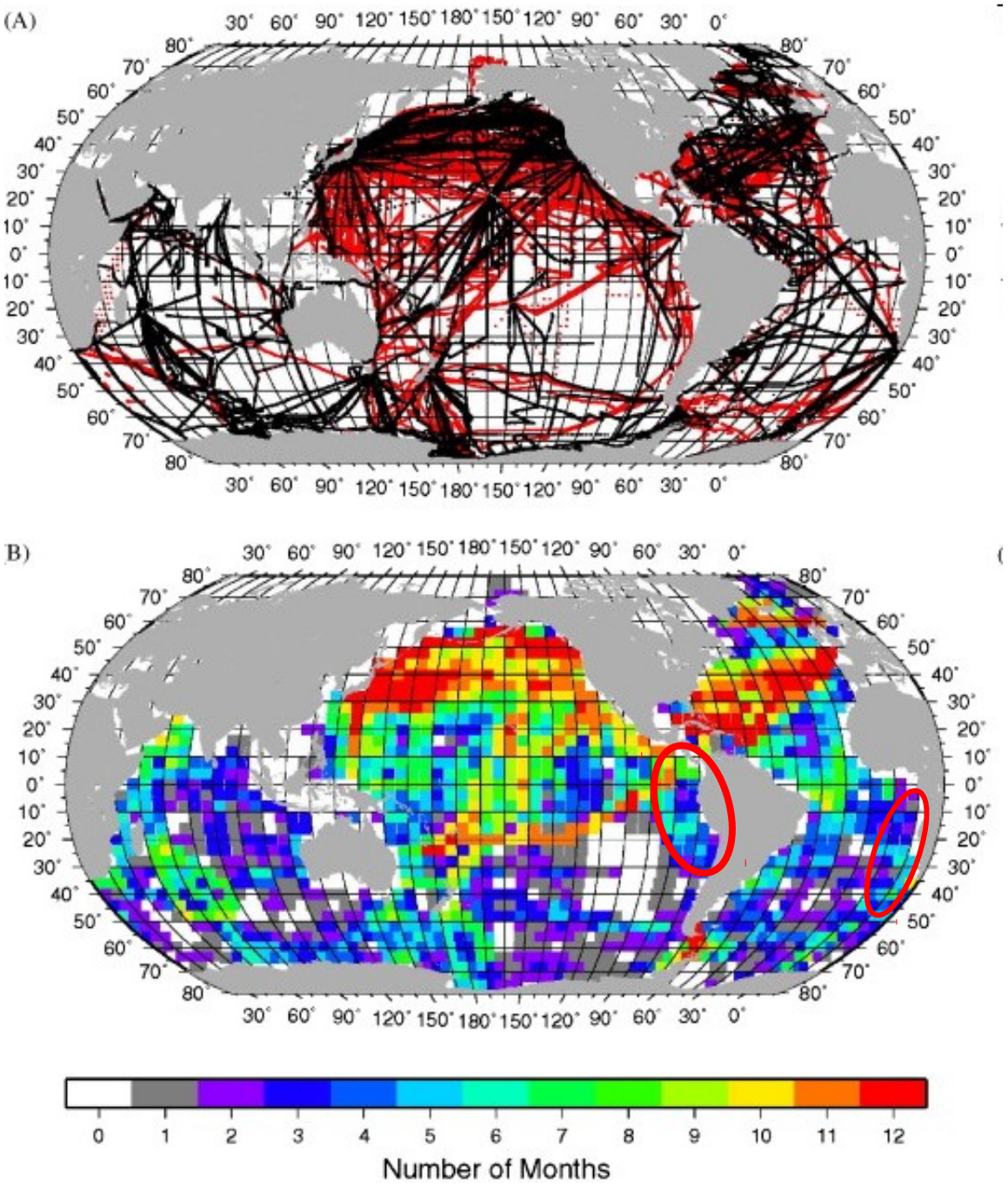


Benguela and Eastern South Atlantic



SOCAT version 2
(2000-2010)

Thank you for your attention !!



Red tracks: new data since Takahashi et al., 2002

Number of months in each 4°x5° box with at least one pCO_2 measurement since early 70's

How to do it?

Microcanonical Multiscale Formalism: geometrical assessment of turbulent systems

1. How to extract the small structure information ? Singularity Exponents

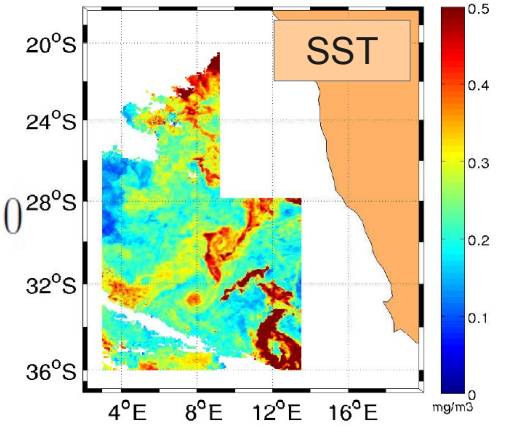
- Measure of the degree of regularity of the image, asociated to transitions: Limiting behaviour of gradients

$$\mathbb{T}_r s(x) = \int\int_{\mathcal{B}(x,r)} \|\nabla s\|(y)\mathrm{d}y$$

$$\mathbb{T}_r s(x) = \alpha(x) r^{h(x)+2} + o\left(r^{h(x)+2}\right) \; (r \longrightarrow 0$$

- Measure of the reconstructibility of a signal: Most Singular Components,

$$\mathcal{F}_h = \{\mathbf{x} : h(\mathbf{x}) = h\}$$

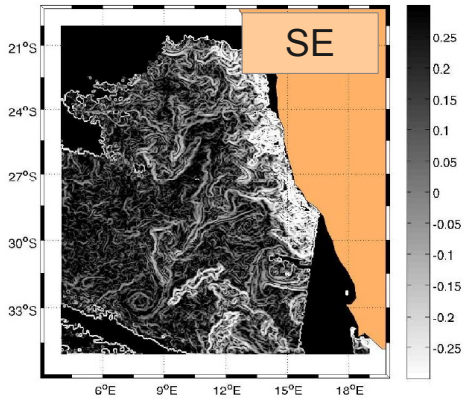


2. How to connect different tracer images?

- Functional dependencies : pCO2⇏pCO2(SST,CHL) ⟶ Multilinear regresion
  SE(pCO2)=SE(pCO2)(SE(SST),SE(CHL))

$$SE(p_{CO_2}^{ocean})(x) = a(x)SE(SST)(x) + b(x)SE(Chl_a)(x) + c(x)SE(p_{CO2}^{ocean}(LR)) + d(x)$$

Regresion coefficients a(x),b(x),c(x) estimated from ROMS simulations data



3. How to propagated the information across scales?

Optimal Wavelet decomposition of the signals at different scales in order to obtain the local variable transferring information.

$$WS(p_{CO_2}^{ocean})(u,r_1) = \eta_{r_1/r_2}(x) WS(p_{CO_2}^{ocean})(u,r_2) \longrightarrow \eta_{r_1/r_2}(x) = \frac{\alpha_p(x)}{\alpha_c(x)}$$

Cascade coefficients

3. Cross-scale inference of pCO_2 data

Decomposition of the signals at different scales: Wavelet projections

Optimal Wavelets: The set of points the **Most Singular Manifold** (smallest values of h)

$$\mathcal{F}_\infty = \{\mathbf{x} \,:\, h(\mathbf{x}) = h_\infty = min(h(\mathbf{x}))\}$$

Most Singular Manifold: - Geometrical place where the transitions are the strongest.
- Associatted with the highest frequencies in a turbulent signal where the multifractal hierarchy F_h converges.

→ Multifractal hierarchy correspond to a description of the detail spaces of a multiresolution analysis performed on a turbulent signal.

$\boldsymbol{A}_j$ ortogonal projection of $\boldsymbol{V}_j$ (approximation space)
$\boldsymbol{P}_j$ ortogonal projection of $\boldsymbol{W}_j$ (detail space)

→ Reconstruction formula

$$A_{j-1}pCO_2 = A_j pCO_2 + P_j h$$

Sudre et al. 2014

Using reconstruction formula, the multiresolution analysis on signal S(pCO_2)(proxy) and the cross-scale inference on physical variable pCO_2 at low-resolution we can derive the pCO_2 at super-resolution of SST and Chl-a.

Input Data

- **CarbonTracker air-sea fluxes at low resolution: 1° ~ 100 km**

Temporal evolution of a tracer c in the atmosphere :

$$\frac{\partial c}{\partial t} = -u\nabla c + \frac{1}{\rho}\nabla(\rho T_d \nabla c) + \frac{1}{\rho}g + F$$

F, net flux at the interface

- *F* can be estimated using optimal control and inverse problem modeling from atmospheric CO_2 data provided by SCIAMACHY and GOSAT. (*Garbe et al. 2007, 2014*)

- Since SCIAMACHY and GOSAT sampling is not dense enough in Benguela we use data of CO2 fluxes from CarbonTracker (*Peters et al. 2007*)

Relation between net air-sea flux and pCO_2

$$F = \alpha K (p^{air}_{CO_2} - p^{ocean}_{CO_2})$$

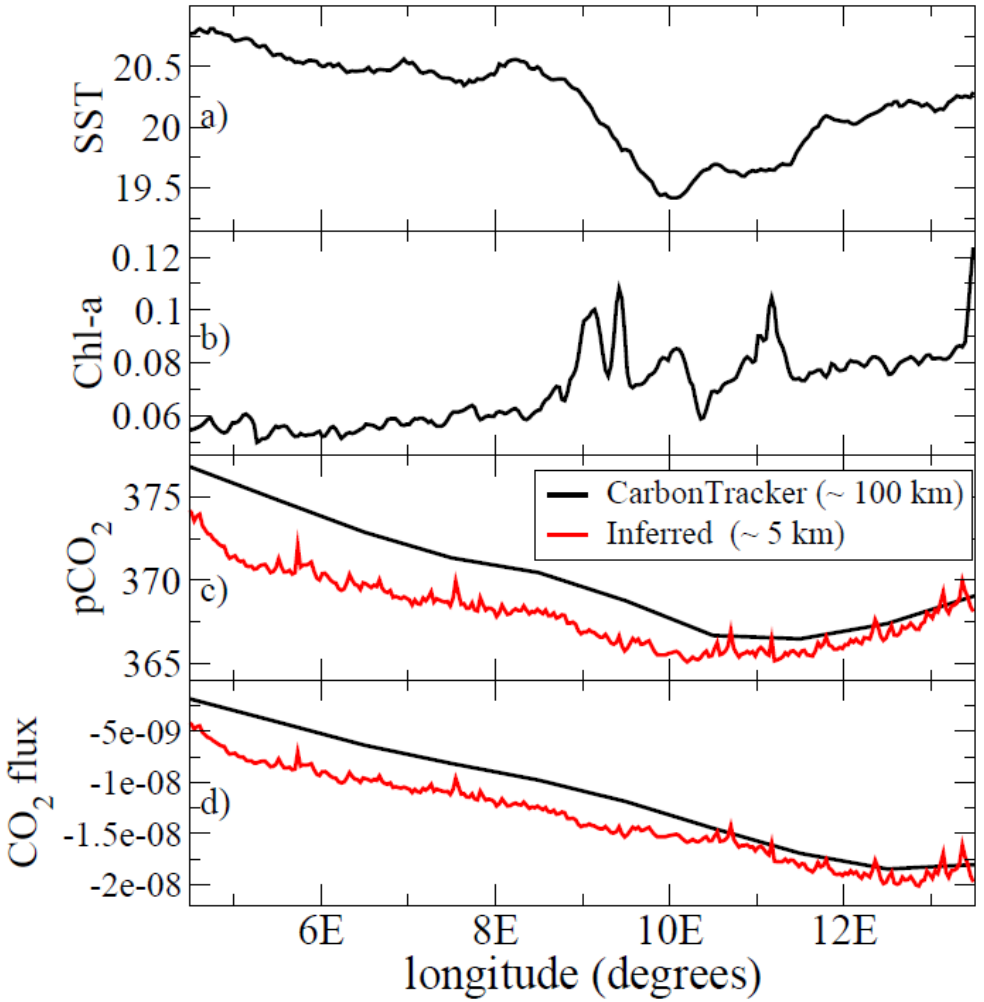
- ***α***, gas solubility: ***α***=***α***(SST, salinity)
- ***K***, gas transfer velocity: ***K***=***K***(wind,S,T^a, sea state) ontained from EO data and parameterization developed by Sweeney et al. 2007.
- p^{air}_{CO2} assumed constant over the upwelling region under study (Ascension Island station)

- So p^{ocean}_{CO2} obtained from inverse modeling and satellite data at resolution of CarbonTracker .

- **SST and Chl-a from Satellite at high resolution: ~ 4 km**

Name reference	Parameter	Instruments	Satellites	Resolution
OSTIA	SST	OSTIA (Optimal interpolation)	GHRSST	5 km / daily
MODIS	SST	MODIS	AQUA	4 km / daily
MERIS	Chl-a	MERIS	ENVISAT	4 km / daily
Globcolour	Chl-a	MODIS/MERIS/SeaWiFS (Merged globcolour)	AQUA/ENVISAT	4 km / daily

Longitudinal profiles at 33.5°S

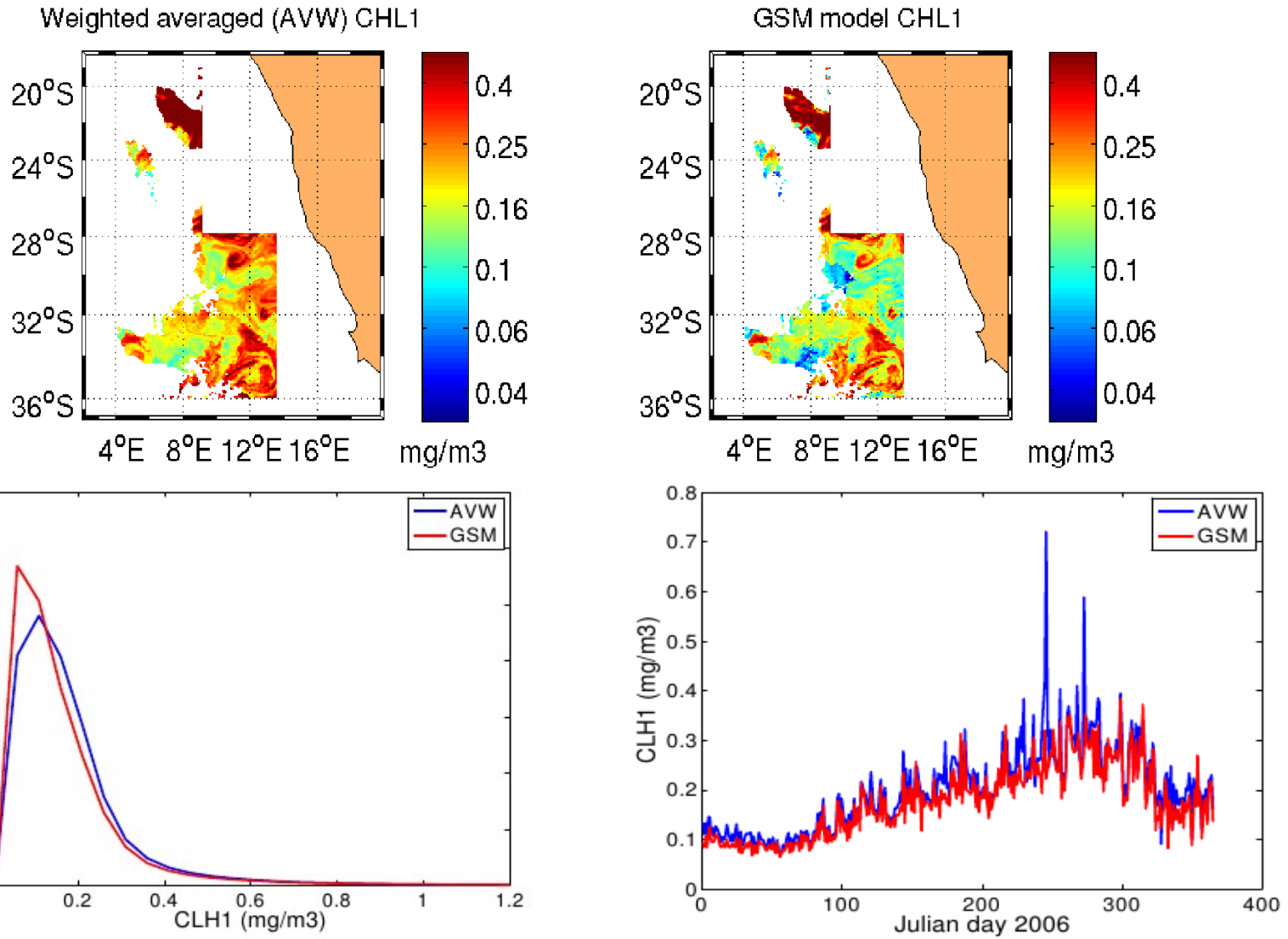


Small spatial scale variability and large spatial scale variability (different shape of profile between CarbonTracker and Inferred pCO2)

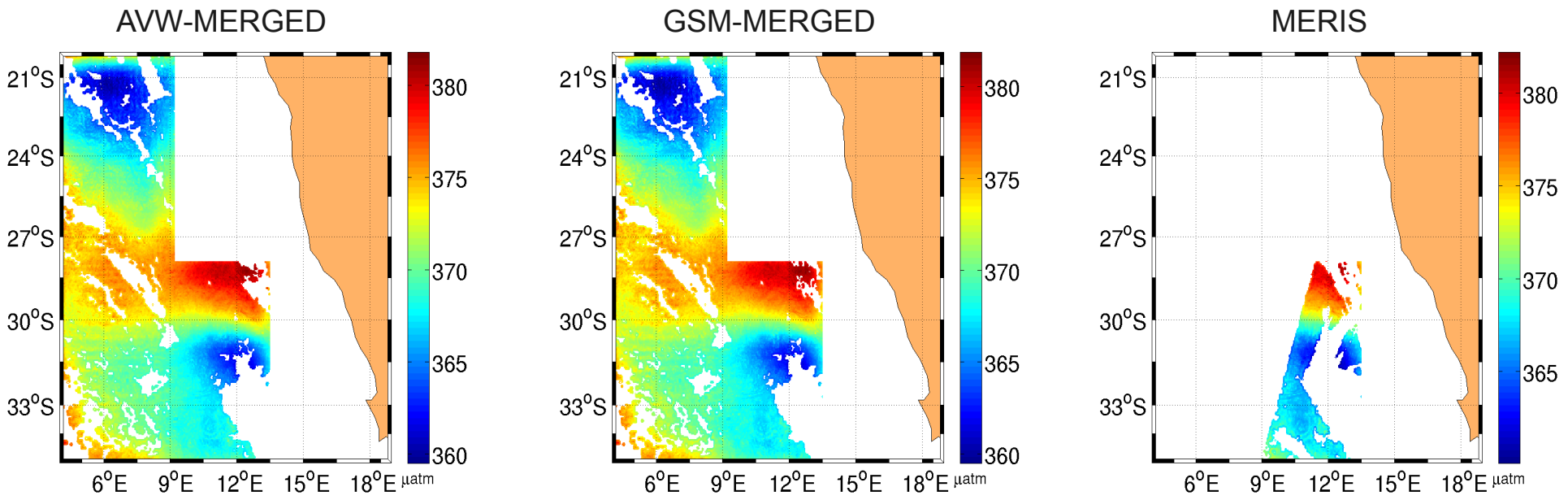
Globcolour merged products

AVW (Weighted Average Value): Values of chl_a are weighted by the relative error for each sensor on the simple averaging.

GSM (Garver, Siegel, Maritorena Model): fully normalized water leaving radiances



Inferred pCO2 using AVW and GSM merged products for ocean color



Comparison of number of points in the pCO2 fields

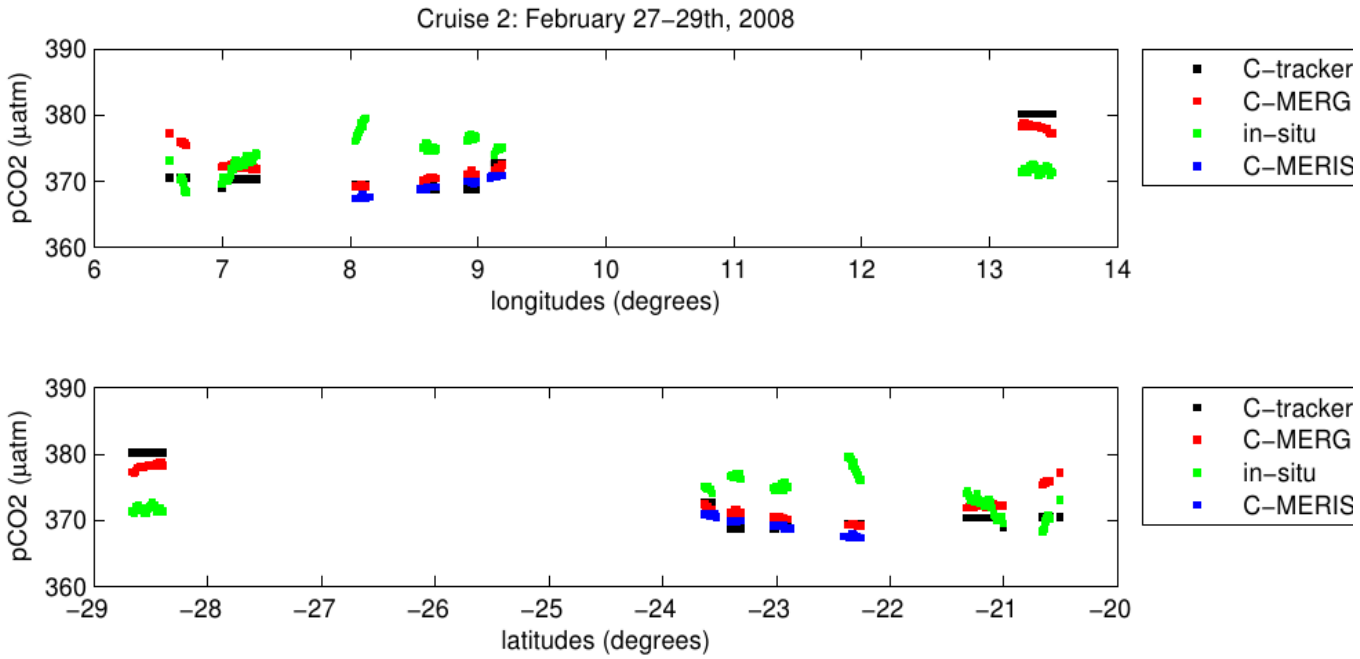
Number of points in the pCO2 fields			
	2006	2008	**2006+2008**
N° Points MERIS	4306877	5493899	**9800776**
N° Points AVW-MERGED	13500676	12881396	**26382072**
N° Points GSM-MERGED	14000396	13312647	**27313043**
Proportion AVW-MERGED/MERIS	3.14	2.34	**2.69**
Proportion GSM-MERGED/MERIS	3.25	2.42	**2.78**
Proportion AVW-MERGED/GSM-MERGED	1.03	1.03	**1.03**

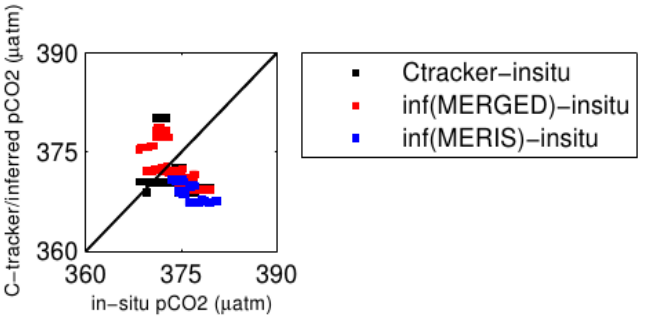
The number of points is **2.69** and **2.78** times larger when we used AVW and GSM MERGED products as compared with MERIS

Validation of CarbonTracker and inferred super-resolution pCO2 using in-situ measurements

- AVW-MERGED 2008

All intersection points

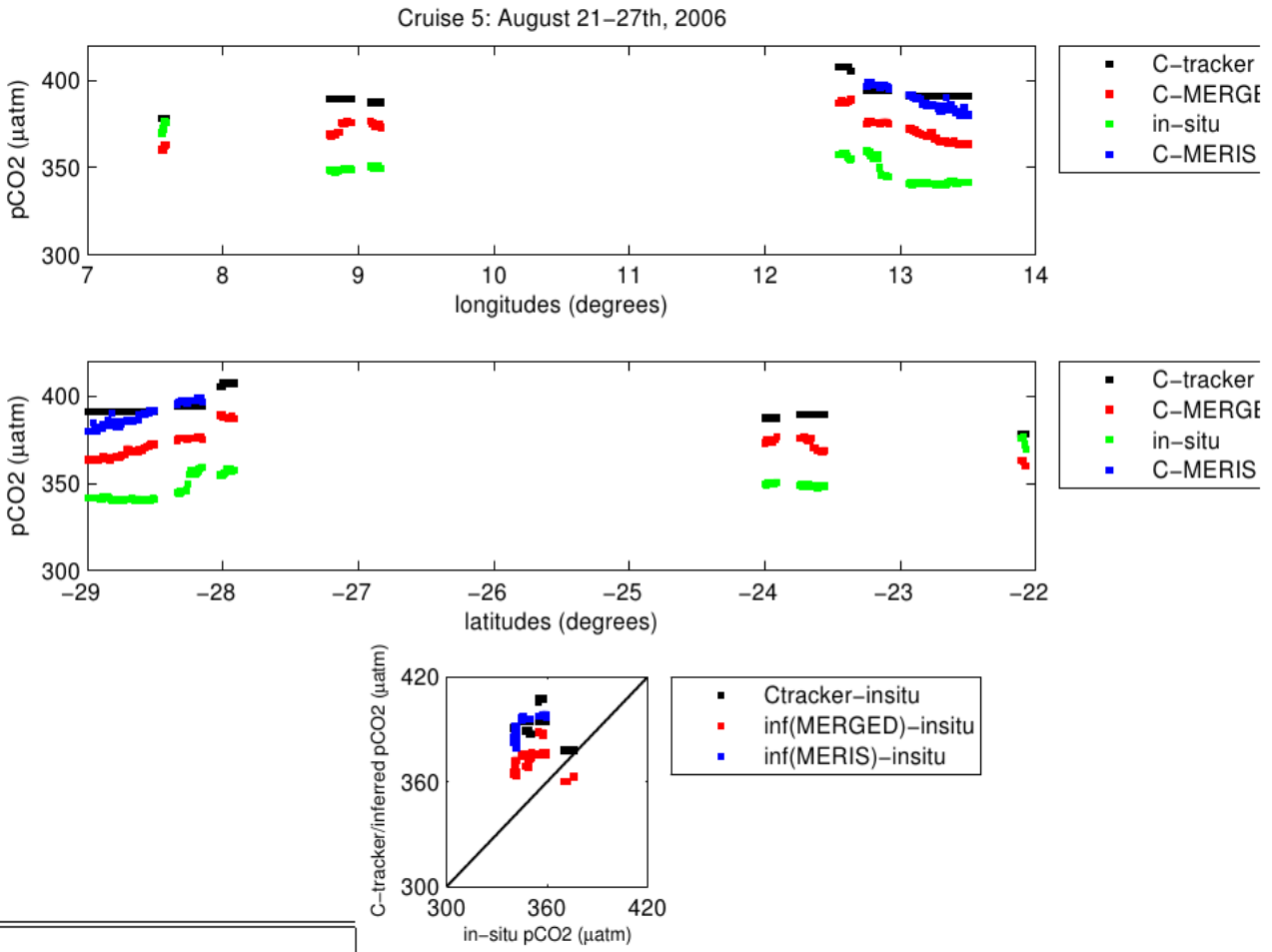




Statistical computations		
	MERIS	MERGED
N intersections	510	819
Mean Error carbontracker-insitu (μatm)	-3.6202	-6.2576
Mean Error inferred-insitu (μatm)	-6.6144	-8.2747
Mean Absolut Error carbontracker-insitu (μatm)	20.2404	19.9042
Mean Absolut Error inferred-insitu (μatm)	17.6495	18.2203
Mean Relative error carbontracker-insitu	0.0543	0.0523
Mean Relative error inferred-insitu	0.0467	0.0474

- AVW-MERGED 2006

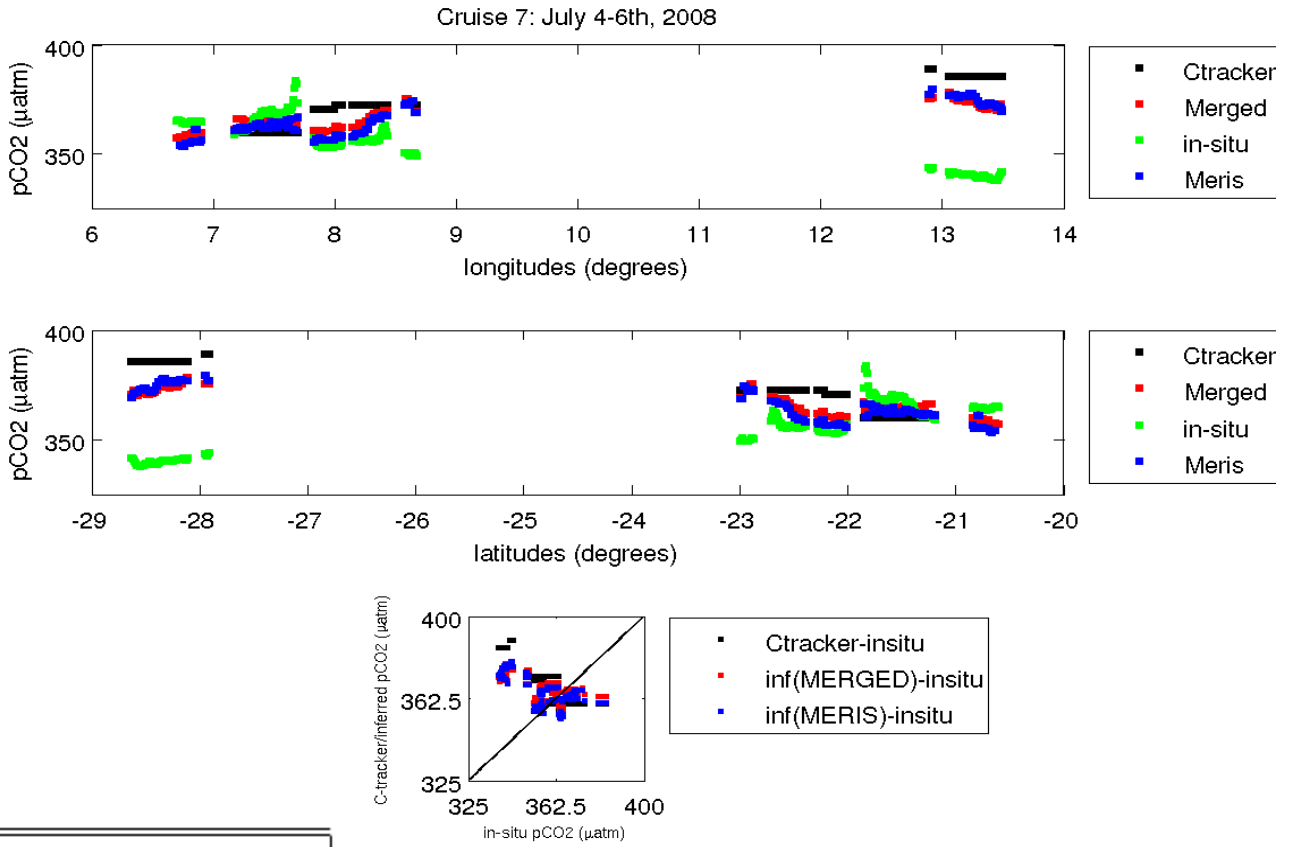
All intersection points



Statistical computations		
	MERIS	Globcolour Merged (Weighted Average)
Number of valid intersections	237	1047
Mean Error carbontracker-insitu (μatm)	17.14	21.16
Mean Error inferred-insitu (μatm)	13.86	12.84
Mean Absolute Error carbontracker-insitu (μatm)	23.71	24.57
Mean Absolute Error inferred-insitu (μatm)	18.03	15.68
Mean Relative Error carbontracker-insitu	0.068	0.069
Mean Relative Error inferred-insitu	0.051	0.044

- AVW-MERGED 2008

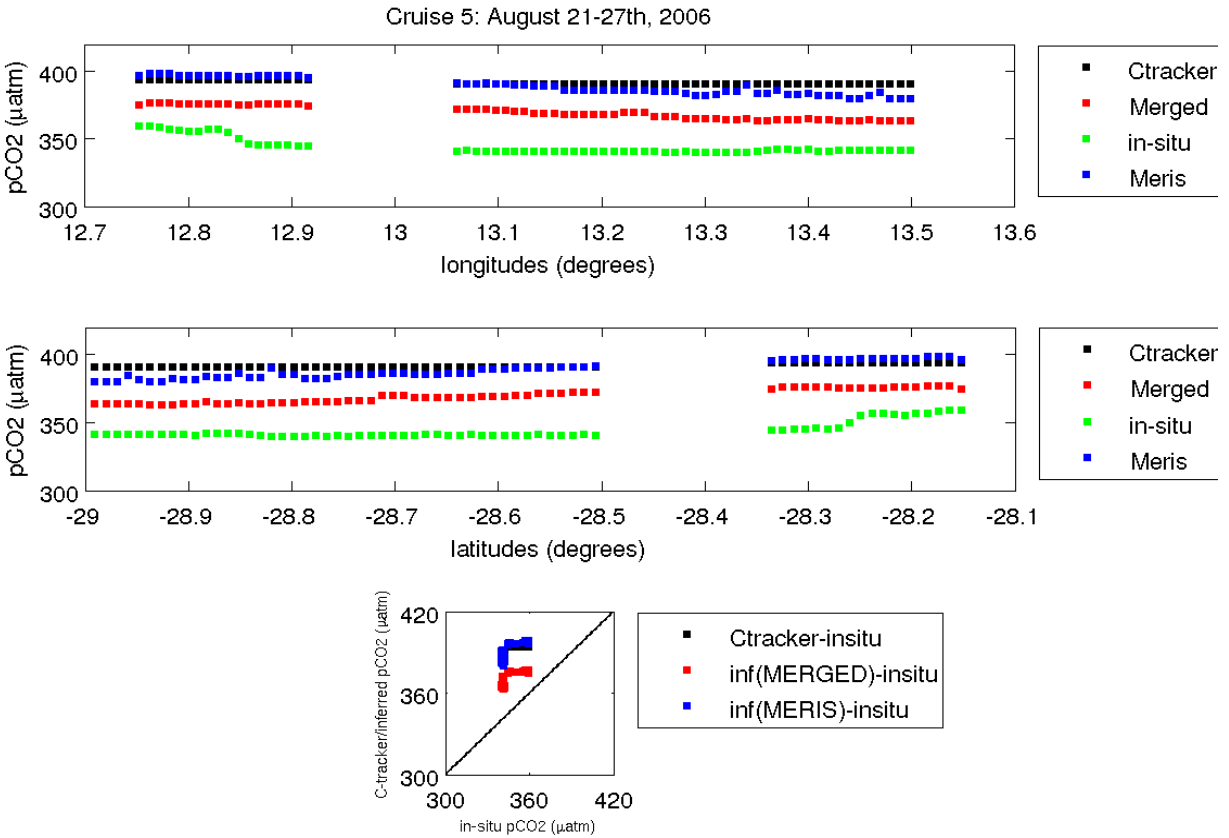
At same points meris-merged



Statistical computations		
	MERIS	MERGED
N intersections	486	486
Mean Error carbontracker-insitu (μatm)	-3.73	-3.03
Mean Error inferred-insitu (μatm)	-6.62	-5.41
Mean Absolut Error carbontracker-insitu (μatm)	20.65	19.93
Mean Absolut Error inferred-insitu (μatm)	18.11	17.82
Mean Relative error carbontracker-insitu	0.055	0.053
Mean Relative error inferred-insitu	0.048	0.047

- AVW-MERGED 2006

At same points meris-merged



Statistical computations		
	MERIS	Globcolour Merged (Weighted Average)
Number of valid intersections	236	236
Mean Error carbontracker-insitu (μatm)	17.14	17.21
Mean Error inferred-insitu (μatm)	13.86	9.64
Mean Absolute Error carbontracker-insitu (μatm)	23.72	23.81
Mean Absolute Error inferred-insitu (μatm)	18.03	13.37
Mean Relative Error carbontracker-insitu	0.068	0.068
Mean Relative Error inferred-insitu	0.0515	0.038

Global statistics

All intersections

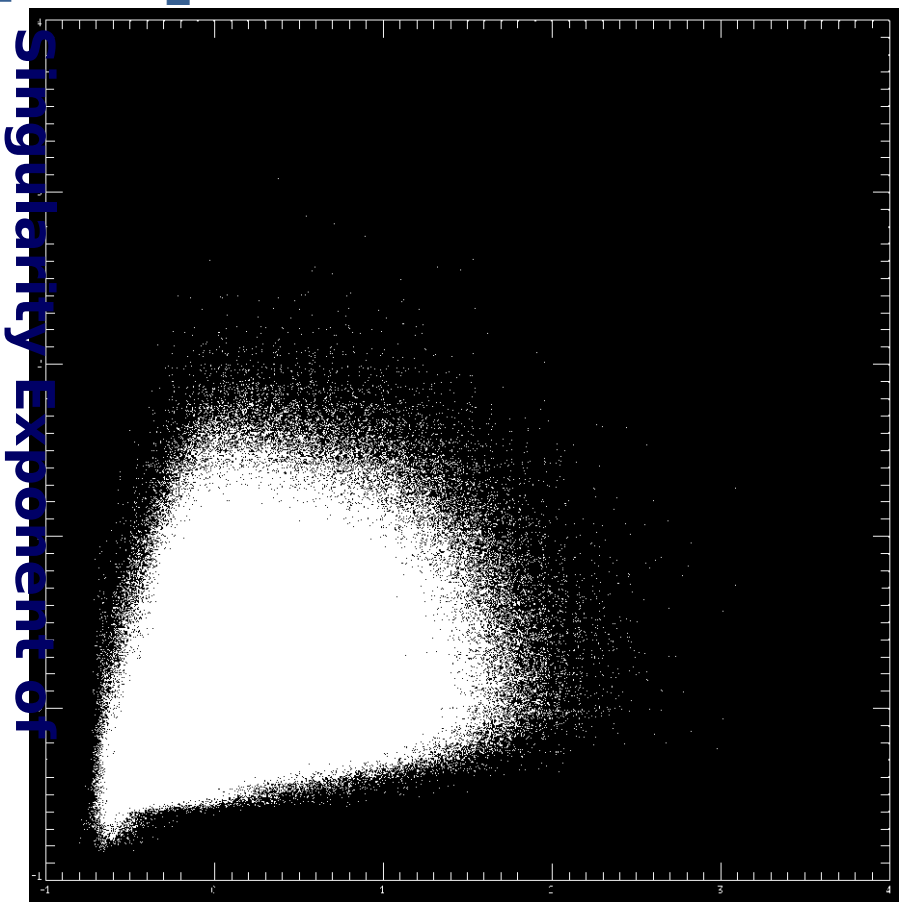
Statistical computations all cruises QUIMA2006/2008				
	MERIS	Globcolour merged (weighted average)	MERIS	Globcolour merged (GSM)
Number of valid intersections	747	1866	747	1928
Mean Error carbontracker-insitu (μatm)	2.97	9.12	2.97	8.83
Mean Error inferred-insitu (μatm)	-0.12	3.57	-0.15	3.42
Mean Absolute Error carbontracker-insitu (μatm)	21.34	22.52	21.34	22.08
Mean Absolute Error inferred-insitu (μatm)	17.77	16.79	17.77	16.47
Mean Relative Error carbontracker-insitu	0.059	0.062	0.059	0.060
Mean Relative Error inferred-insitu	0.048	0.045	0.048	0.044

At same points meris-merged

Statistical computations all cruises QUIMA2006/2008				
	MERIS	Globcolour merged (weighted average)	MERIS	Globcolour merged (GSM)
N intersections	722	722	743	743
Mean Error carbontracker-insitu (μatm)	3.07	3.58	3.02	3.53
Mean Error inferred-insitu (μatm)	0.12	-0.49	-0.04	-0.66
Mean Absolute Error carbontracker-insitu (μatm)	21.67	21.20	21.52	20.88
Mean Absolute Error inferred-insitu (μatm)	18.08	16.36	17.91	15.54
Mean Relative Error carbontracker-insitu	0.059	0.058	0.059	0.055
Mean Relative Error inferred-insitu	0.049	0.044	0.048	0.041

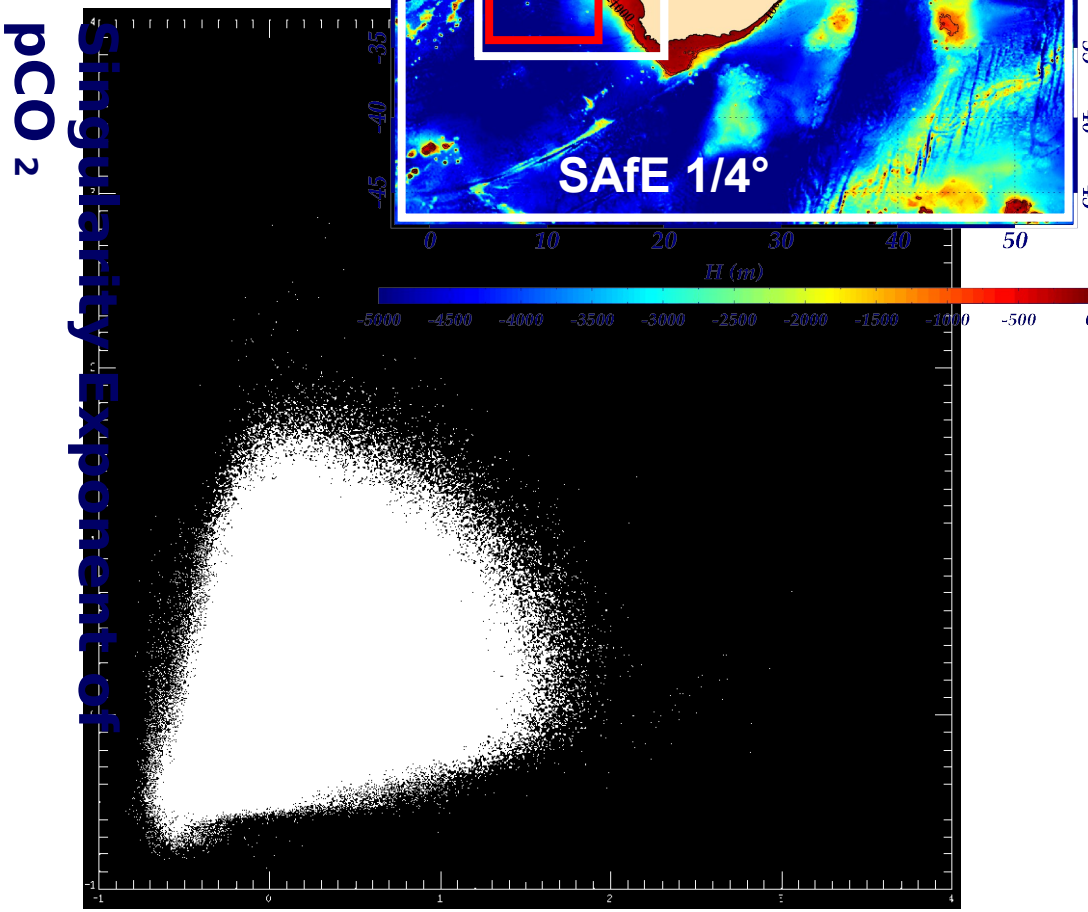
Values for merged inferred pCO2 are closer to insitu measurement than MERIS inferred pCO2. GSM as a better candidate

Properties diagrams of SE: pCO_2 vs SST and pCO_2 vs Chl-a



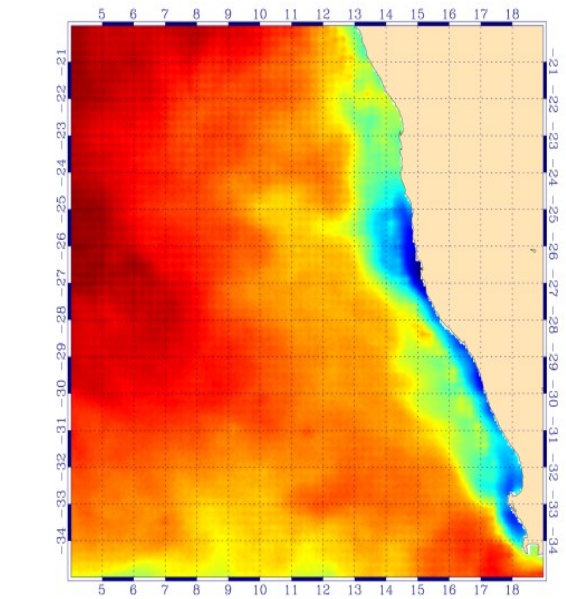
Singularity Exponent of SST

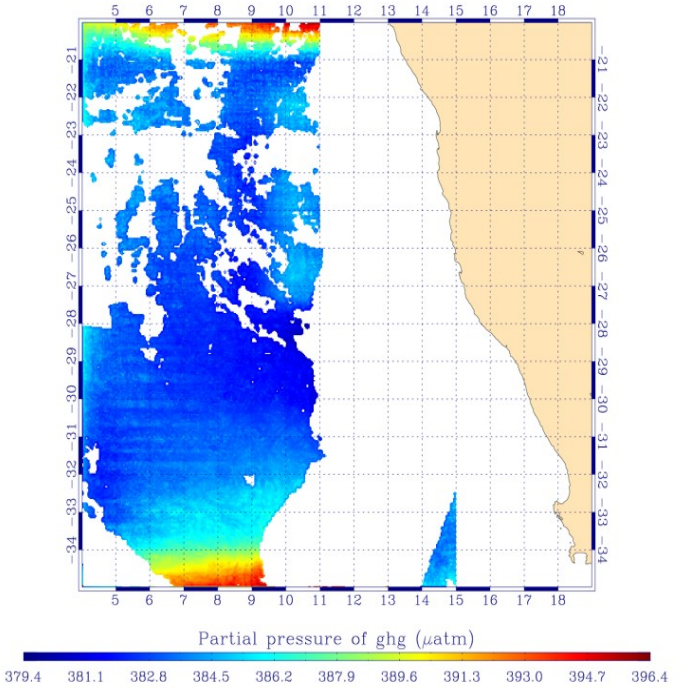
10 years of IPSL present : 1990-2000 with downscaled winds over the Benguela upwelling (Machu et al.,2014)

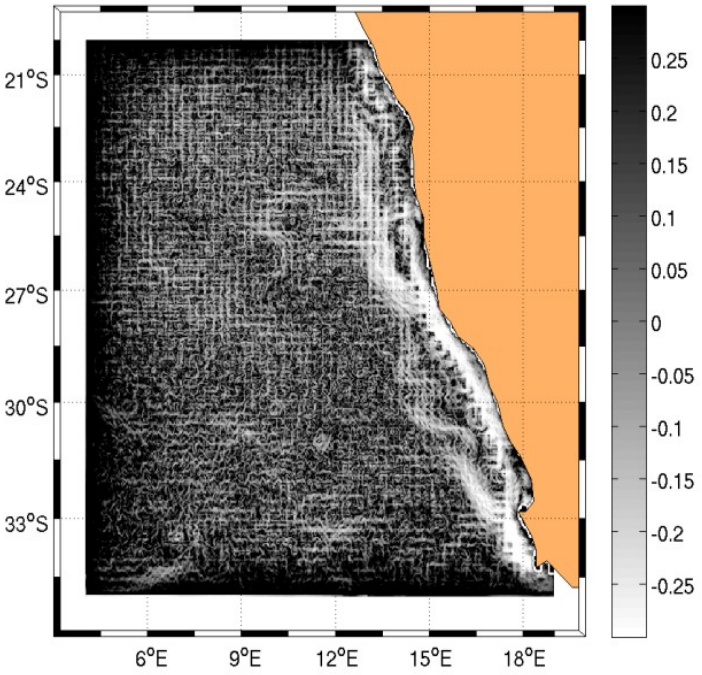


Singularity Exponent of Chl-a

Effect of merged OSTIA SST in the infererence of superresolution pCO2







OSTIA SST introduce regular and periodic horizontal lines in the background.

Singularity exponents show clearly this grid pattern.
Singularity exponents as a powerfull tool to detect spurious patterns in data sets.