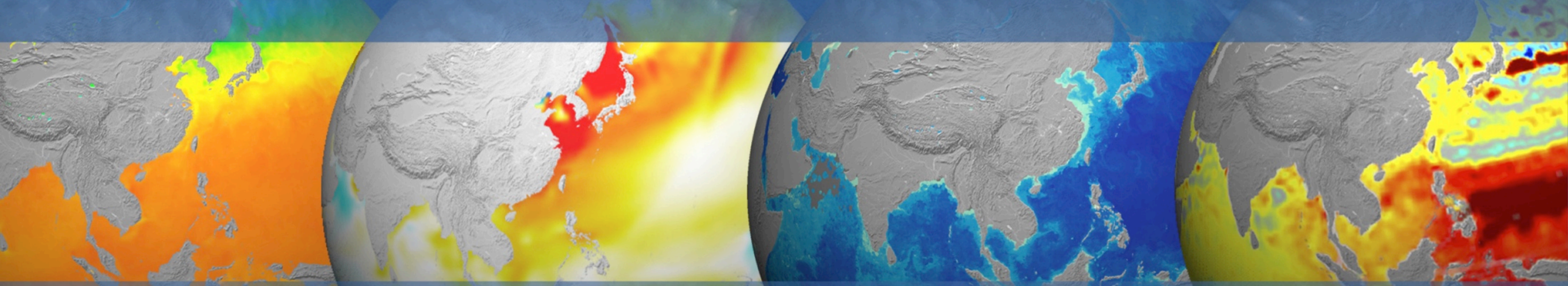
ESA–MOST China Dragon 4 Cooperation

→ ADVANCED TRAINING COURSE IN OCEAN AND COASTAL REMOTE SENSING



12 to 17 November 2018 | Shenzhen University | P.R. China

Estimating Ocean Acidification from space

Roberto Sabia – Telespazio/Vega UK for European Space Agency (ESA)

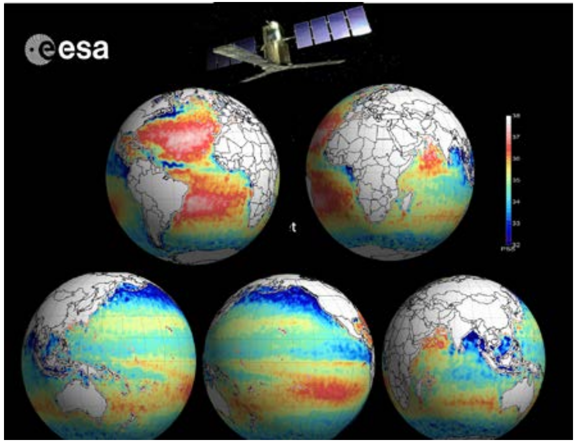
Hosted by

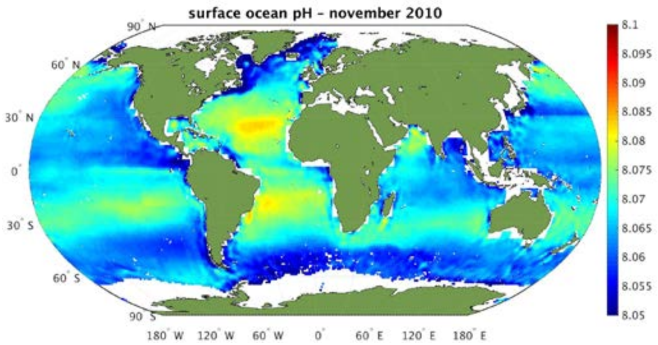
Course lectures/practical – R. Sabia

Mon 12 Nov, 16.00 – SSS from SMOS

Mon 12 Nov,, 17.00 – SSS using SNAP
Pi-MEP and SMOS data (Practical)

Fri 16 Nov, 14.00 – Ocean Acidification
from space

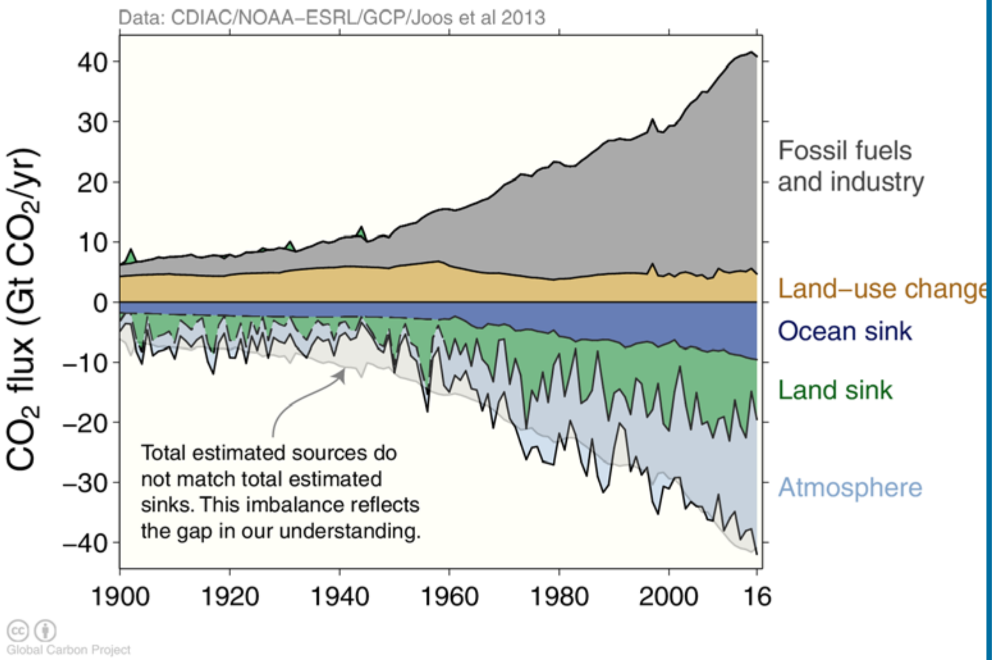




Outline

- Background: the Ocean Acidification context
- Motivation / Objectives: the remote sensing perspective
- The ESA Pathfinders-OA project
    - Total Alkalinity derivation and performance
    - Dissolved Inorganic Carbon derivation and performance
- Additional OA-relevant studies (ocean pH, Omega-aragonite etc.)
- ESA OceanSODA objectives / workplan – new project
- Remarks and perspectives

Anthropogenic emissions and CO2 sources/sinks



Budget Imbalance: 6% (0.6 GtC/yr)
(the difference between estimated sources & sinks)

9.4 GtC/yr (88%)

1.3 GtC/yr (12%)

Sources

4.7 GtC /yr (46%)

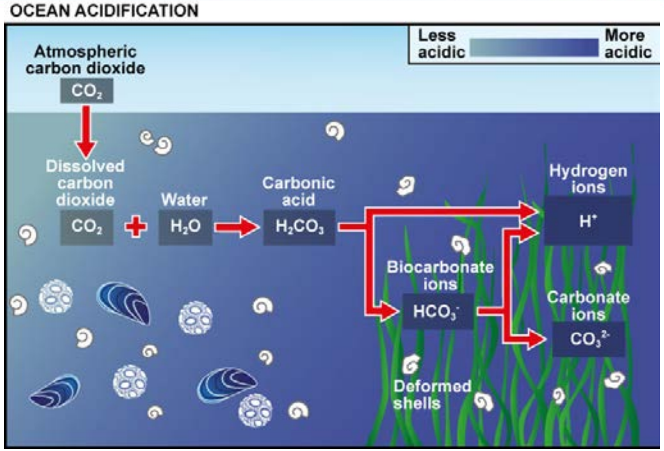
3 GtC /yr (30%)

2.4 GtC /yr (24%)

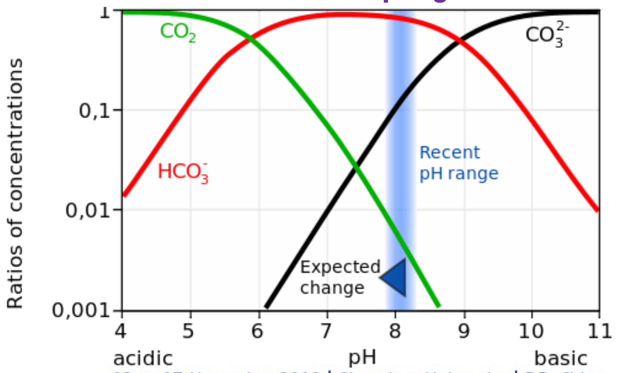
Sinks

The Ocean Acidification problem (i)

- The surface ocean currently absorbs approximately one third of the excess atmospheric carbon dioxide (CO2), mitigating the impact of global warming.
- This anthropogenic CO2 absorption by seawater determines, however, a reduction of both ocean pH and the concentration of carbonate ion and causes wholesale shifts in seawater carbonate chemistry.
- This can also lead to a decrease in calcium carbonate saturation state Ω, with potential implications for marine animals, especially calcifying organisms and the overall trophic chain
- Average global surface ocean pH has already fallen from a pre-industrial value of 8.2 to 8.1, corresponding to an increase in acidity of about 30%. Values of 7.8–7.9 are expected by 2100, representing a doubling of acidity.
- The overall process is referred to as Ocean Acidification (OA), with profound impacts at scientific and socio-economic level.



Credits: UK OA programme



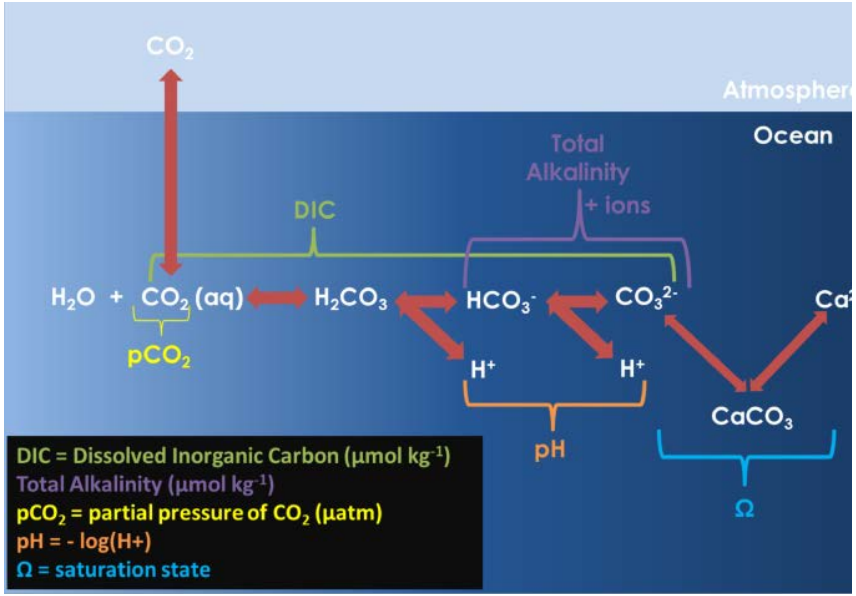
Bjerrum plot

The Ocean Acidification problem (ii)

Areas that could be particularly vulnerable to OA include:

- **upwelling regions (C02-rich waters)**
- **the oceans near the poles (cold water)**
- **coastal regions (freshwater discharge)**

Additional potential complexity: acidic inputs from rivers, intense bio respiration, atm. deposition



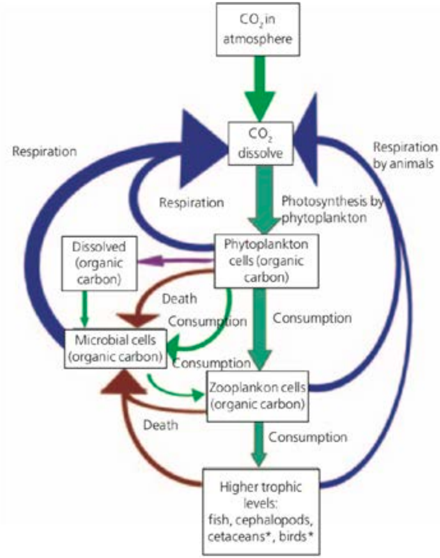
OA potential implications:

- **Biodiversity loss**
- **Coral reefs ecosystems health**
- **Coastal protection from storms**
- **Fisheries**
- **Food provision**
- **Economy**

The Ocean Acidification problem (iii)

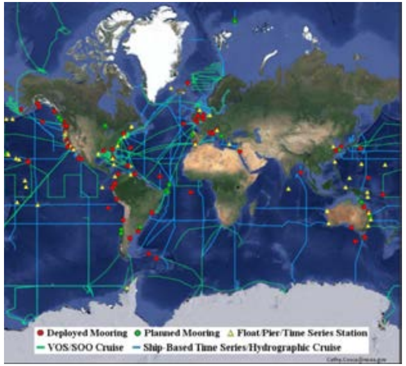
(Potential) Detrimental effects on marine biota (variable among species/taxa) and environment:

- **Biomineralization potential prevention**
- **Potential dissolution of shells**
- **Functional stress and respiration metabolism**
- **Growth/photosynthetic rates alteration**
- **Reproduction rates alteration**
- **Energy balances alteration**
- **Nutrients uptake, nitrogen fixation and primary production alteration**
- **Biogeochemical cycles alteration**
- **Speciation shifts (beyond carbonate system – e.g., B, P, Si, N, Fe etc.)**
- **Sound absorption**
- **Light scattering**



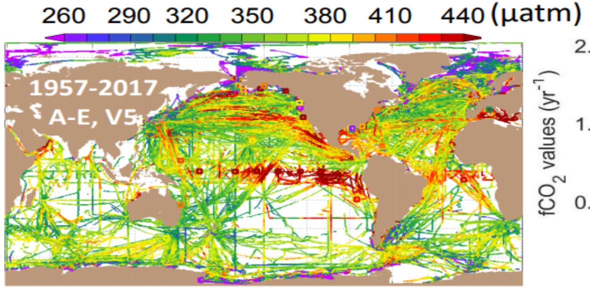
The OA changing scenario occurs in concomitance with other anthropogenic stresses (global warming, pollution, overfishing, coral reef bleaching).

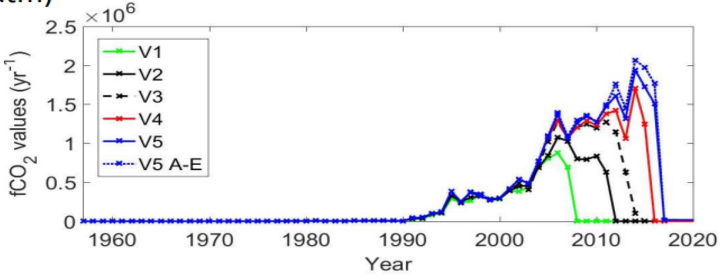
- International efforts are devoted to develop a coordinated strategy for monitoring OA, with an eager need for global and frequent observations of OA-relevant parameters;
- In 2012, OA researchers formed the Global OA Observing Network (GOA-ON) to bring together datasets and resources. Yet, datasets acquired are mostly relevant to in-situ measurements, laboratory-controlled experiments and models run.



Surface Ocean CO_2 Atlas at 10!

SOCAT - SURFACE OCEAN CO_2 ATLAS -
www.socat.info





Global synthesis and gridded products of surface ocean fCO_2
(fugacity of CO_2) in uniform format with quality control;
No gap filling; Annual public releases;
V5: 21.5 million fCO_2 values from 1957-2017, accuracy < 5 µatm (flags A-D);
Plus calibrated sensor data (< 10 µatm, flag E);
Online viewers, downloadable (text, NetCDF), ODV;
Documented in ESSD articles;
Fair Data Use Statement;
Community activity with >100 contributors worldwide.

(**Pfeil et al., 2013; Sabine et al., 2013; Bakker et al., 2014, 2016, all in ESSD**)

OA remote sensing (i)

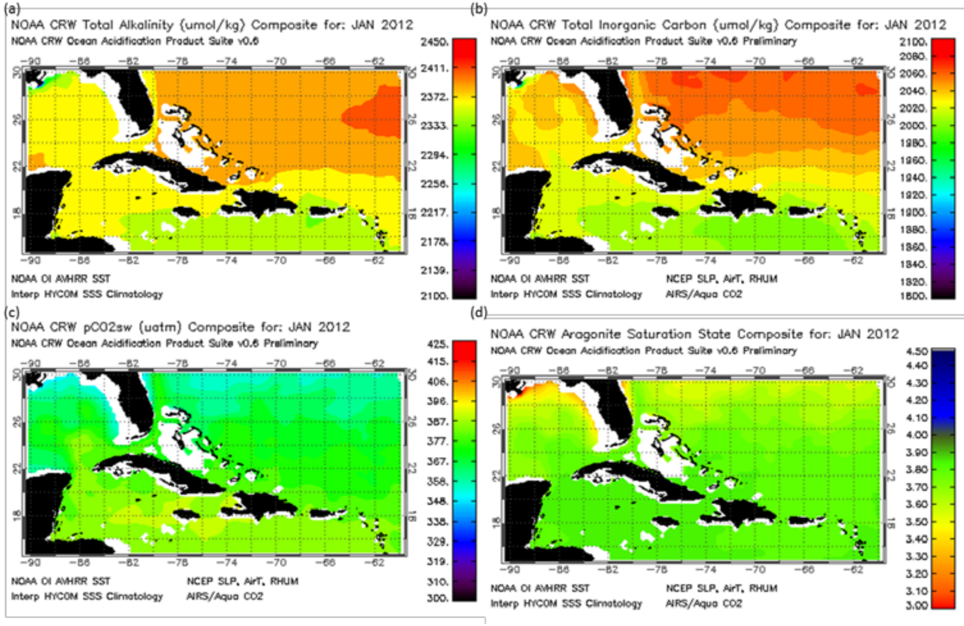
- Remote sensing technology can be integrated by providing synoptic and frequent OA-related observations, complementing in-situ carbonate chemistry measurements at different spatial / temporal scales.
- Benefits of EO:
    - Upper ocean inorganic carbon cycle spatial and temporal dynamics (especially on seasonal time-scales)
    - Focus on extremes and episodic events not captured by in-situ measurements or regional hotspots
    - Poorly-sampled open ocean provinces
    - Supporting research tied to OA
- Passive microwave measurements are key for studying and monitoring marine carbon.

OA remote sensing (ii)

- Preliminary products developed so far are mainly regional or derived with a limited variety of satellite datasets.
- The overall objective is to quantitatively and routinely infer marine carbonate system variables by means of EO:

  1) developing new algorithms and data processing strategies to overcome the relative immaturity of OA satellite products currently available, and

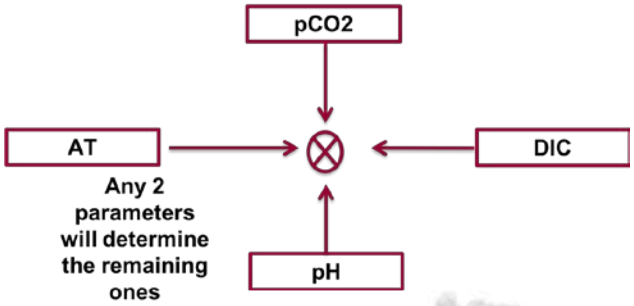
  2) producing a global, temporally evolving, suite of OA-relevant satellite-derived products.



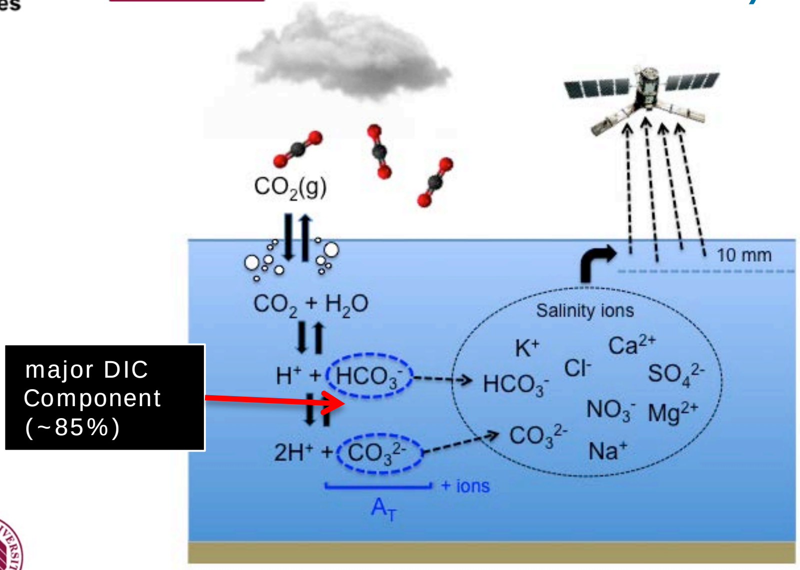
Several regional algorithms exist using combinations of EO and model data to retrieve OA parameters (e.g. NOAA OAPS)

Carbonate system parameters

- **Total Alkalinity (TA) -> buffering capacity of a water body. Measure of the ability of a solution to neutralize acids and thus to resist to changes in pH;**
- **pCO2 -> Partial pressure of CO_2 in surface seawater**
- **Dissolved Inorganic Carbon (DIC or C_T) –> sum of aqueous CO_2 gas, carbonic acid, bicarbonate and carbonate ions**
- **pH -> ($-\log_{10}[H^+]$)**
- **Omega -> $[CO_3^{2-}]\,[Ca^{2+}]/K_{sp}$ – usually referred as Ω-ar, since aragonite is approximately 50% more soluble than calcite**
- **First order effect: shift in the ratio DIC:TA**
  - **Increase ratio -> higher CO2, lower pH and lower omega**
  - **Decrease ratio -> lower CO2, higher pH and higher omega**



Off-the-shelf numerical routines for inorganic carbon speciation computation (e.g, CO2SYS and SeaCarb)



TA variability attributed for 80% to SSS

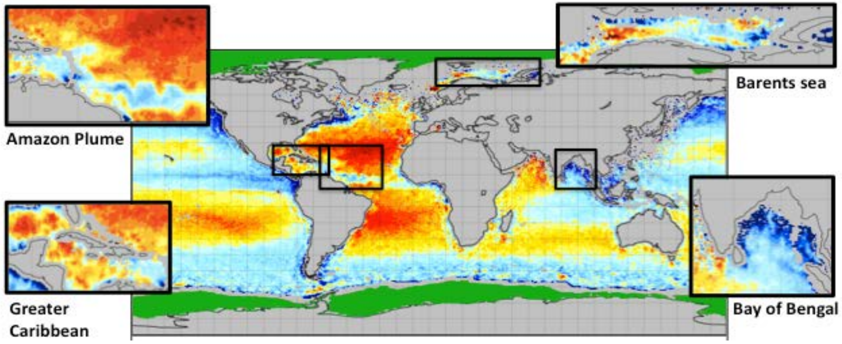
Atmosphere-ocean gas fluxes – ESA OceanFlux

ESA STSE Pathfinders-OA – objectives/set-up

Pathfinders-OA was an ESA STSE project to exploit EO in the context of Ocean Acidification whose objectives were:

- Collect relevant datasets (in situ, EO and model) and create a large database **of EO / in-situ matchups**
- Assess existing relations and develop **novel algorithms** to retrieve OA parameters from space for several case studies
- **Validate** EO-derived products with available in-situ data and climatologies
- Generate **open source software tools**

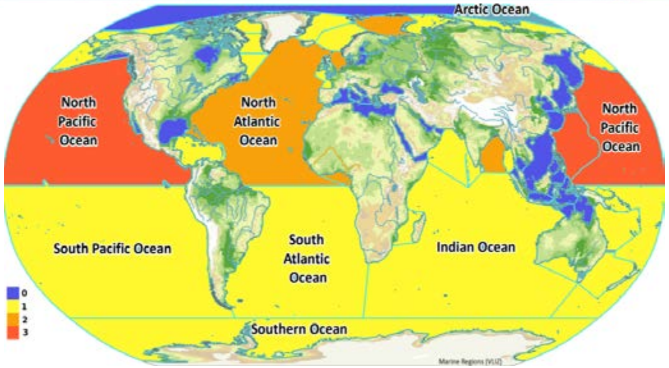
stse support to science element



SOURCE	DATE RANGE	LOCATION	PARAMETERS	N
CORA (inc. Argo, Pirata +)	2003-2014	Global	SST, SSS	1,000,000+
GLODAP	1972-1999	Global	AT,DIC,NO_{3-},SST,SSS	10,000+
CARINA	1977-2006	Arctic, Atlantic, Southern Ocean	AT,DIC,pH,SST,SSS	1500+
LDEO	1980-2013	Global	pCO_2,SST,SSS	6,000,000+
SOCAT	1991-2011	Global	pCO_2,SST,SSS	6,000,000+
OWS Mike	2001-2006	Arctic	AT,DIC,SST,SSS	1000+
Helen Findlay	2012-2014	Arctic	AT,DIC,SST,SSS	100+
Joe Salisbury	2013	Bay of Bengal	pCO_2,SST,SSS	130+
Punyasloke Bhadury	2014	Bay of Bengal	AT,pH,SST,SSS	100+

www.pathfinders-oceanacidification.org

ESA STSE Pathfinders-OA – parameterisations



Existing algorithms are most frequent in the north Pacific, north Atlantic, Bay of Bengal and Barents Sea

Existing parameterizations	
pCO2	SST, Chl-a, SSS, MLD
TA	SSS, SST, nitrate
DIC	SST, Chl-a, SSS
pH	SST, Chl-a, O2, nitrate

Parameters function of salinity
TA
K_{sp}
Gas solubility (ɑ)
Stoichiometric dissociation const.
Carbonate system speciation

ESA STSE Pathfinders-OA – TA and DIC methods

Global, Amazon Plume, Bay of Bengal and GC regions:

Two TA algorithms:

- **Lee et al 2006 (Lee06) uses SSS and SST;**
- **Takahashi & Sutherland 2013 (Taka13) uses SSS and NO_3^-.**

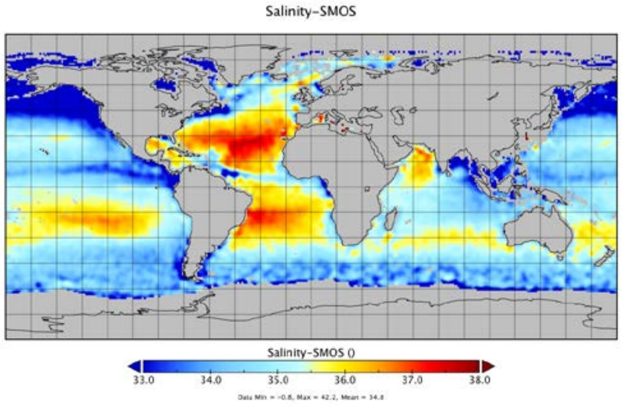
One DIC algorithm:

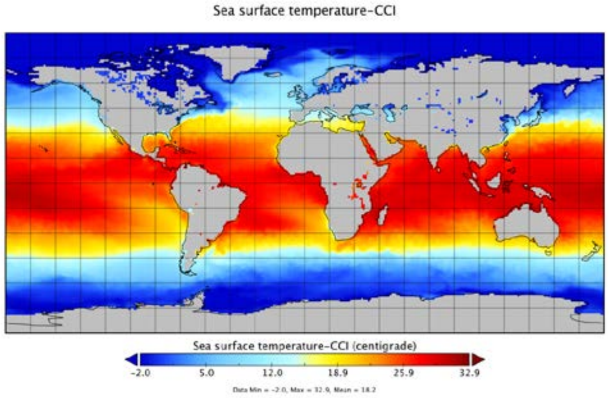
- **Lee et al 2000 (Lee00) uses SSS, SST and NO_{3-}**

Evaluated using CARINA, GLODAP *in situ* data of >10,000 pts

Potential inputs:

- ***In situ* re-analysis data: Coriolis Ocean database for re-analysis (CORA) SST and SSS**
- **Climatology: LDEO SST and SSS, World Ocean Atlas (WOA) NO_{3-}**
- **Satellite data: SMOS SSS, Aquarius SSS, ESA CCI SST**
- **Model data: HADGEM2-ES TA (used directly) or NO_{3-} (used in Taka13 or Lee00)**





Sample input datasets: SMOS SSS in psu (top), CCI SST in ° C (bottom)

1. Convert all data (*in situ*, climatology, model, satellite) binned to daily and monthly 1º x 1º, and to 50km polar stereographic in the Arctic.

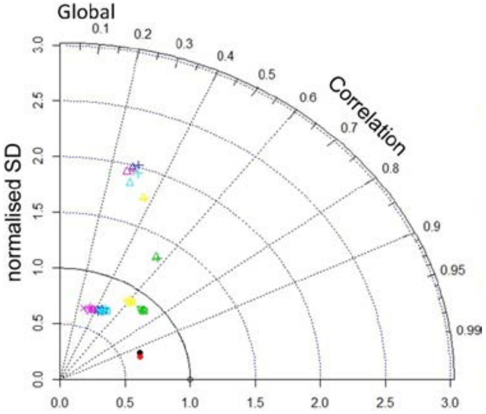
1. Identify locations and times where we have *in situ* carbonate parameters to compare with estimates generated from empirical algorithms.

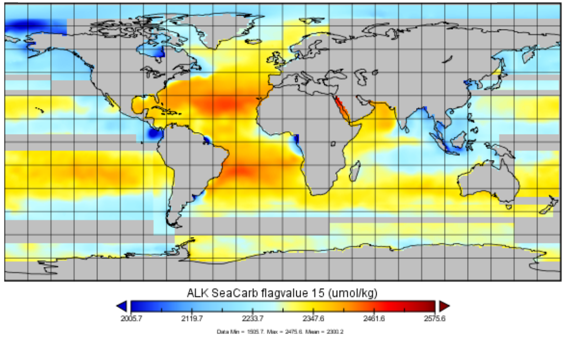
2. Create a ranked list of the performance of each C_T, A_T, pH and pCO_2 algorithm with each different set of data inputs.

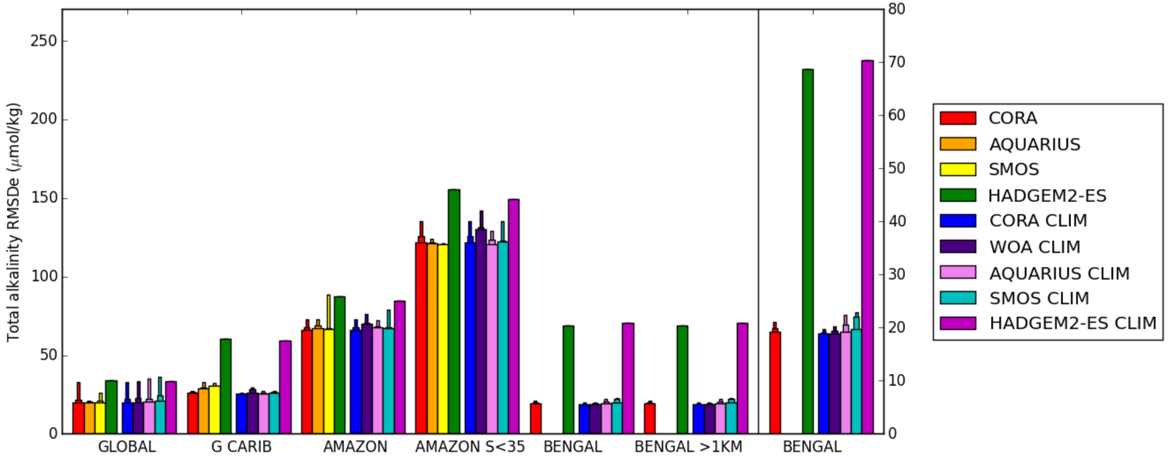
   a. Calculate all statistics for all possible comparisons for each model (optimal characterisation of each model, e.g. accuracy assessment).

   b. Calculate all statistics for only common data points for each model (allows models to be ranked based on choice of input data).

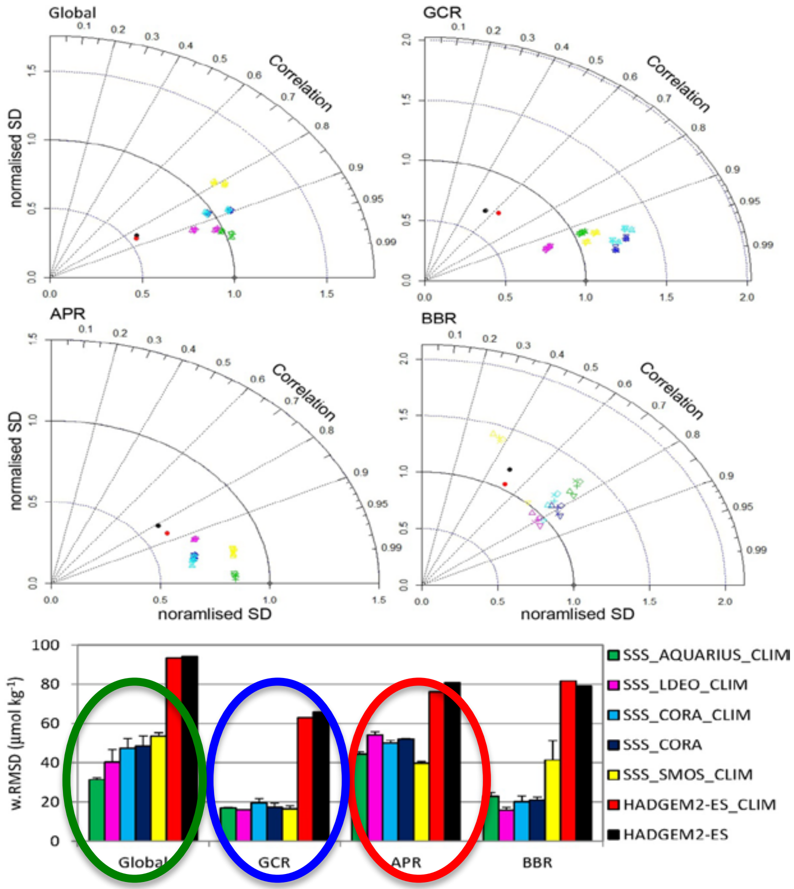
ESA STSE Pathfinders-OA – TA round-robin







- **Possible to exploit the salinity-alkalinity relationship using satellite data.**
- **Satellite SSS (SMOS and Aquarius) outperform or equal other approaches for TA**
- **Estimated total uncertainty of state of the art TA and CT measurements are ~0.5% (or ~10 µmol kg-1) - From space we have 20 µmol kg-1 for global case!**



Aquarius driven models outperform all others for Global region.

RMSD is lowest for Greater Caribbean Region (GCR).

SMOS and Aquarius driven models have comparable performance to in situ data driven models for GCR.

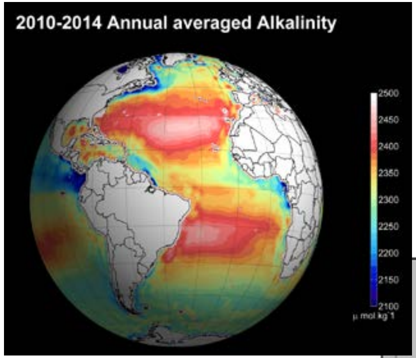
SMOS and Aquarius driven models out perform in situ data driven models in Amazon Plume Region (APR)

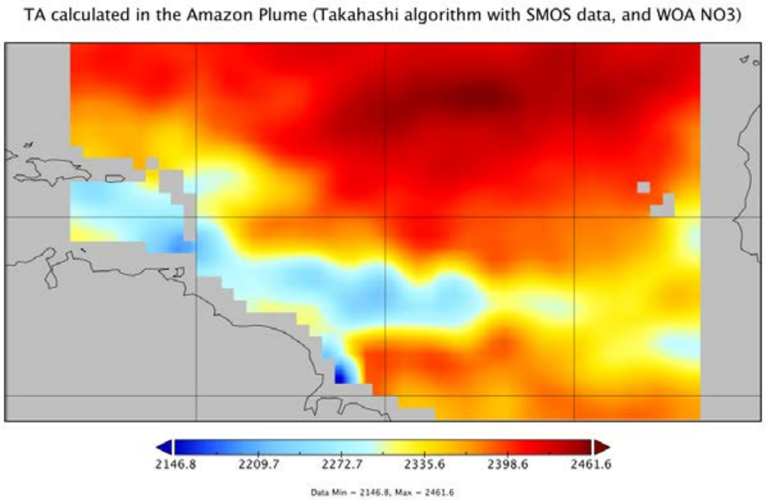
ESA STSE Pathfinders-OA – round-robin concl.

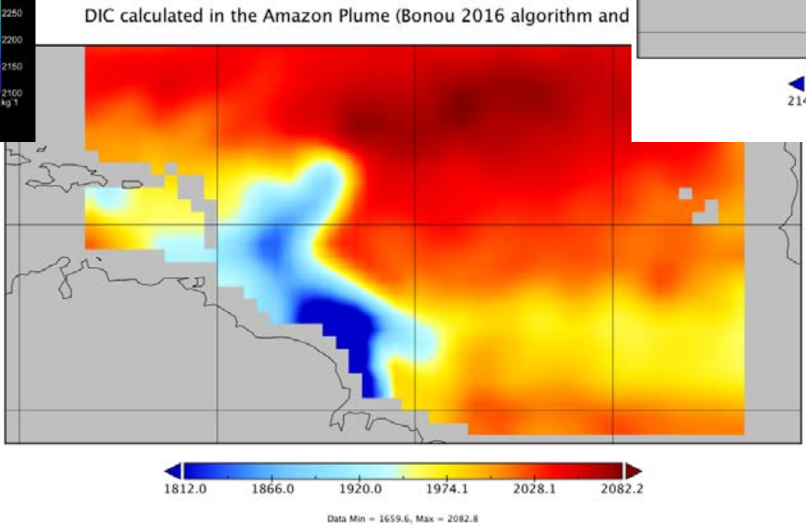
1. Possible to exploit the salinity-alkalinity relationship using satellite data.
2. Satellite SSS (Aquarius is slightly better than SMOS) equal or outperforms other approaches globally for both TA and DIC.
3. Satellite SSS (SMOS and Aquarius are comparable) outperforms other approaches in the Amazon Plume for both TA and DIC.
4. Regional results are more variable: satellite SSS performance is comparable to others in the Greater Caribbean, but worse for TA in the Barents Sea.
5. More in situ data are needed in the Arctic regions to parameterise and test the algorithms.
6. HadGEM2-ES performs well in the Barents Sea.

ESA STSE Pathfinders-OA – project outcomes

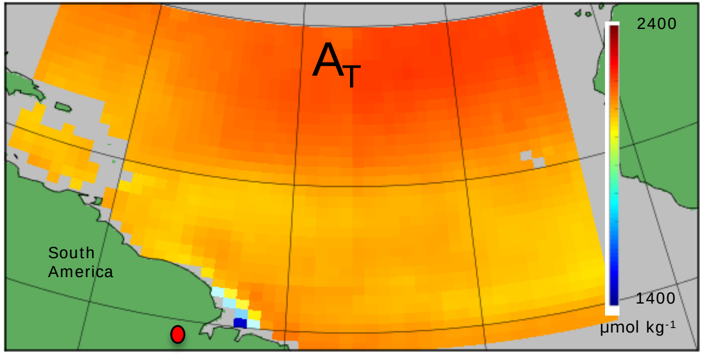
Total Alkalinity (buffering capacity of a water body to neutralize acids) averaged over 2010-2014 (credits: ESA Pathfinder-OA project)

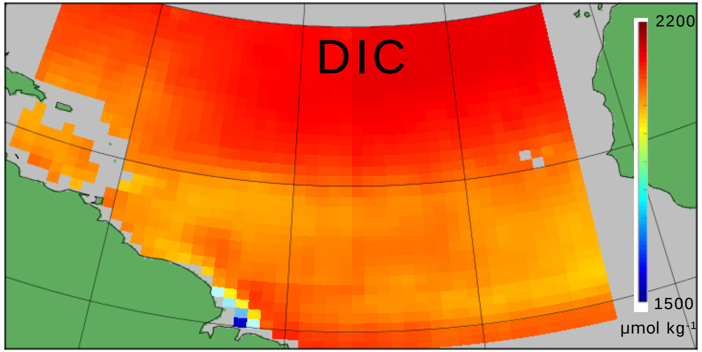






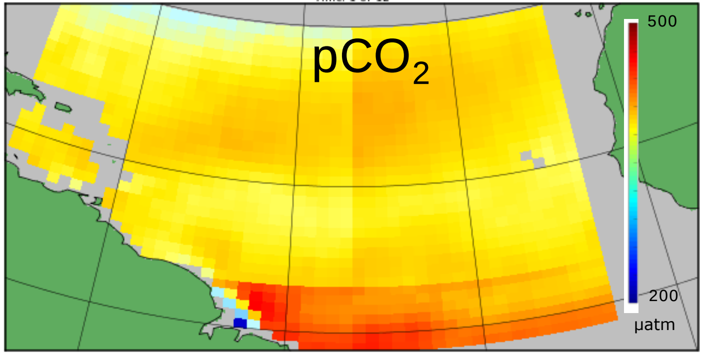
Sample Total alkalinity (top), and Dissolved Inorganic Carbon (left) in the Amazon plume

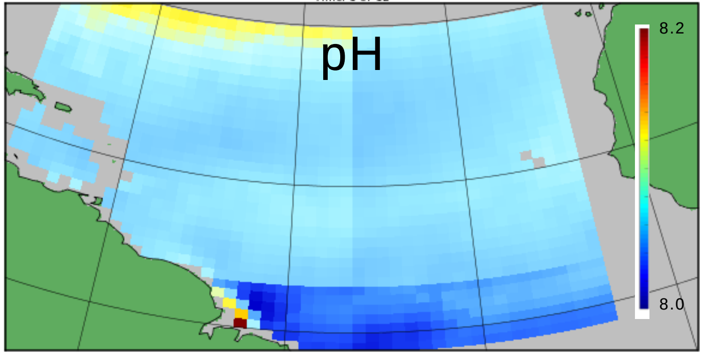




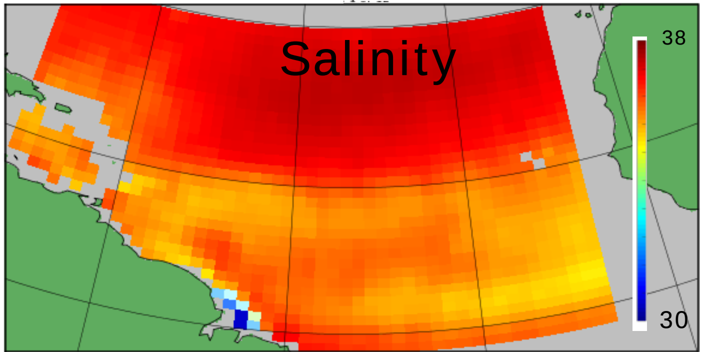
Time: 1 of 12

Time: 1 of 12





Derived Marine carbonates parameters time series



ESA STSE Pathfinders-OA – outreach

University of Exeter

PML | Plymouth Marine Laboratory

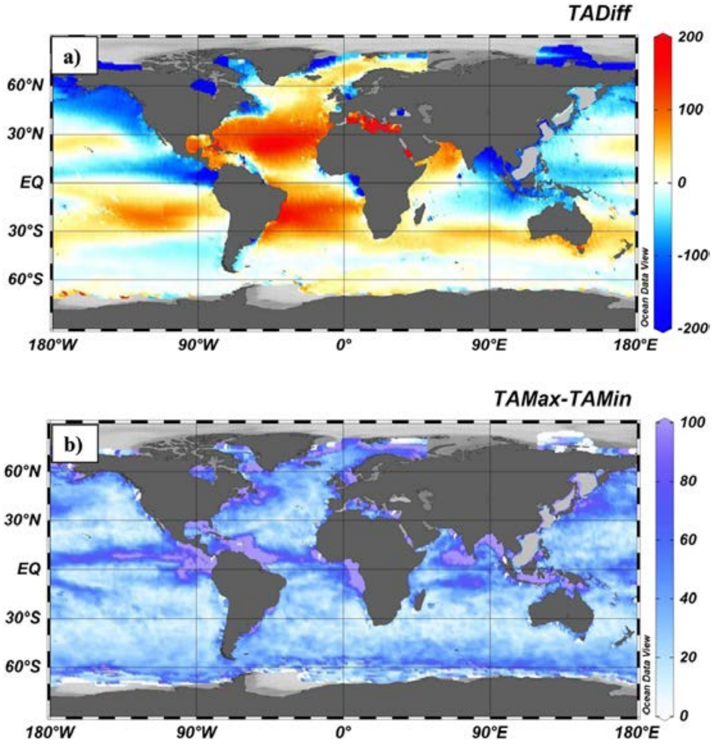
Ifremer

TELESPAZIO VEGA
UNITED KINGDOM
A Finmeccanica / Thales Company

esa

stse
support to science element

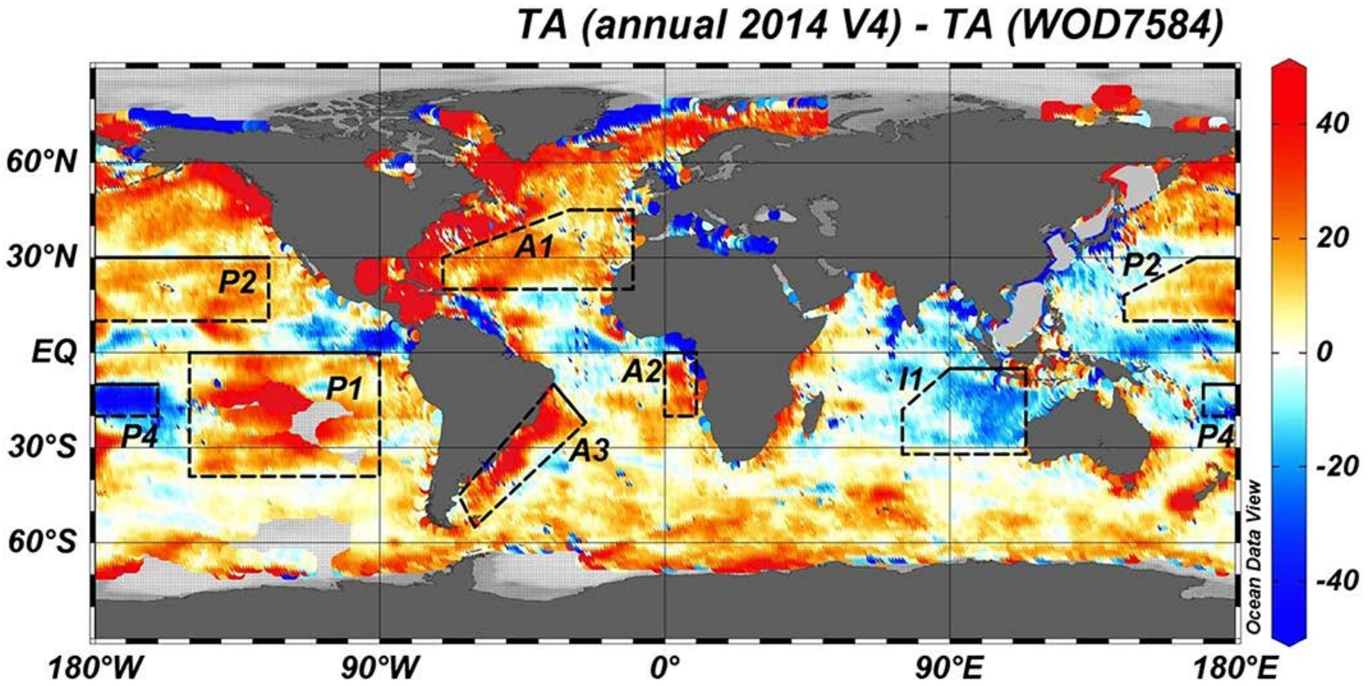
Alkalinity from space: Global variability of total alkalinity, and amplitude of the seasonal cycle. (Aquarius, 2014)



From Fine et al, 2017: Geophysical Research Letters
Volume 44, Issue 1, pages 261-267, 5 JAN 2017 DOI: 10.1002/2016GL071712
http://onlinelibrary.wiley.com/doi/10.1002/2016GL071712/full#grl55372-fig-0002

Additional studies – Aquarius TA

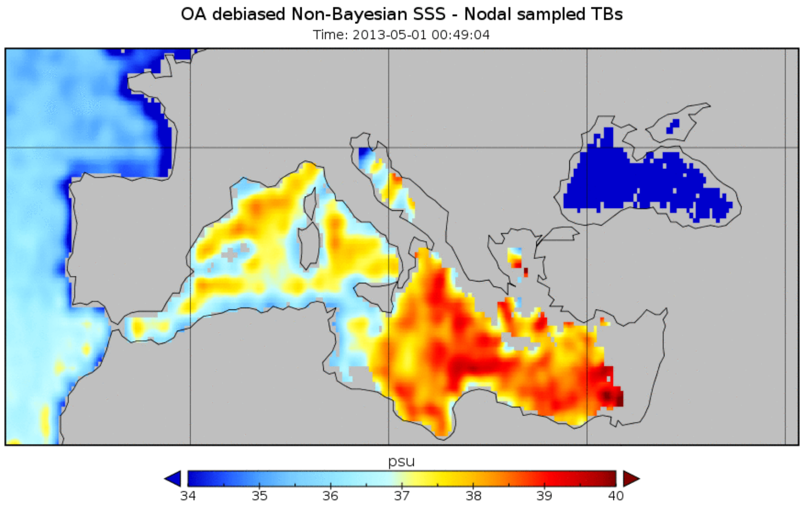
Changes in ocean total alkalinity over recent decades: from Aquarius satellite data (2014) compared to Conkright et al climatology (1975-2014)



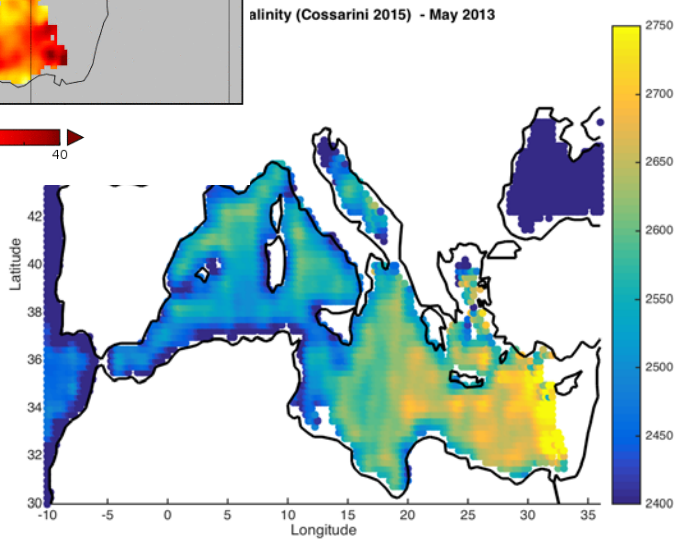
Additional studies – SMOS Med TA

TA in the Med significantly higher than in the open ocean. West-east increasing gradient. In the surface layers, TA has a remarkable seasonal cycle.

In the Med, different regions present different TA/SSS relationships -> positively correlated in the open sea areas of the Med; negatively in regions of fw influence. Not possible to study this basin relying on global parameterizations.



Novel preliminary approach (Nodal sampling) to tackle RFIs and extend coverage to the east and in regional seas

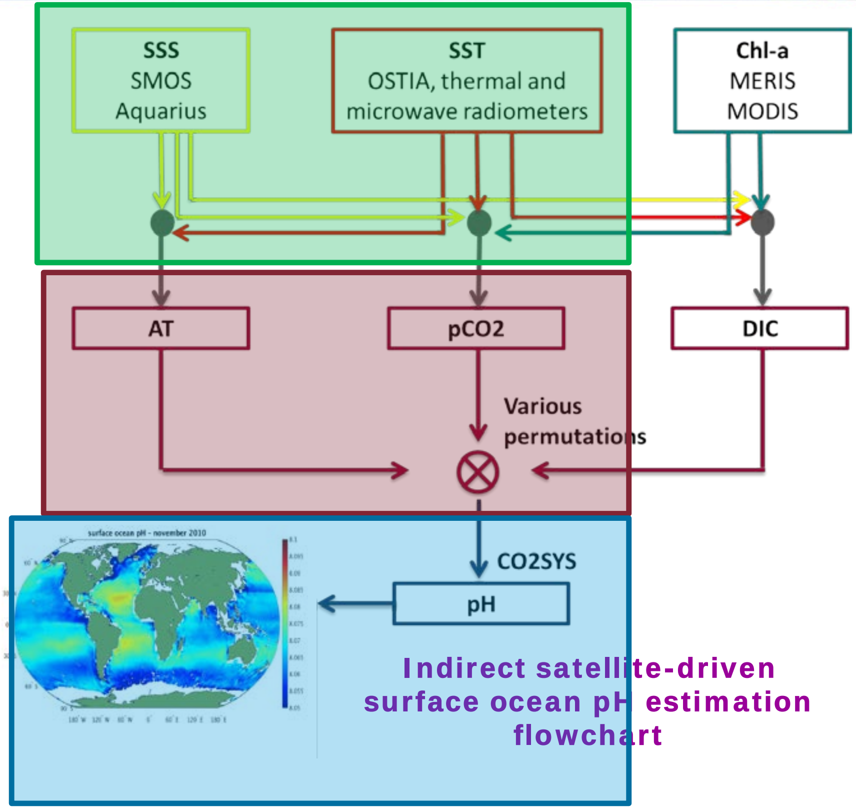


Derived Alk for a sample month with Cossarini 2015 algorithm.

Sabia et al. 2018

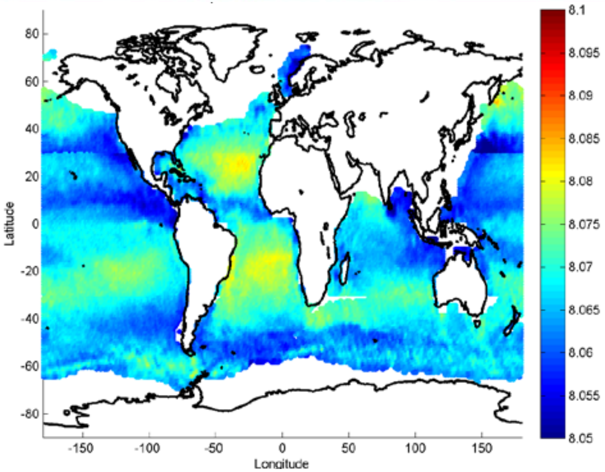
Additional studies – pH and Ω-ar (i)

- Satellite datasets (SSS, SST) forcing
  - SMOS L3 SSS OI, ascending passes (courtesy SMOS-BEC, Barcelona)
  - OSTIA GLO-SST-L4-NRT-OBS-SST-MON-V2 at ¼ deg- distributed by MyOcean
- Stress on satellite SSS, assessing its impact in the OA-related variables estimation and monitoring
- Uncertainties coming from the remote sensing data accuracies, from the quality of the algorithms and the adequacy of the carbonate system pairing choice
- pCO2 2010-normalized updated climatology, ESA OceanFlux-GHG project (courtesy J. Shutler and ESA Pathfinders-OA project)
- [Lee et al., 2006] AT and [Takahashi and Sutherland, 2013] formulation; Different (5 or 24) parameterizations for the various ocean basins
- CO2SYS software package v1.1 2011
- Total pH scale, surface pressure

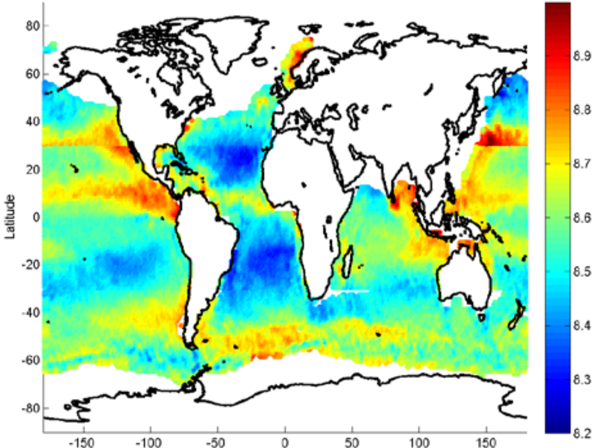


Indirect satellite-driven surface ocean pH estimation flowchart

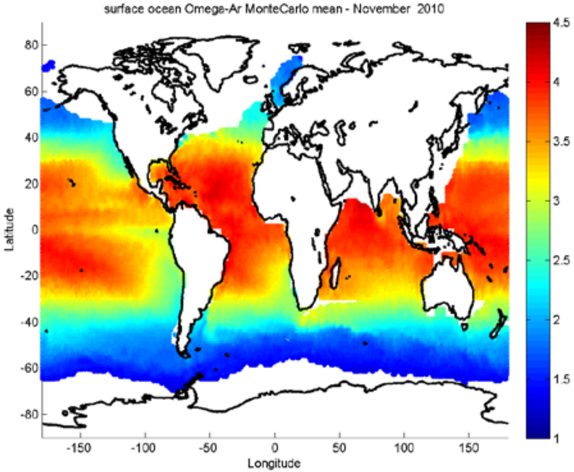
Additional studies – pH and Ω-ar (ii)



Sample Surface ocean pH



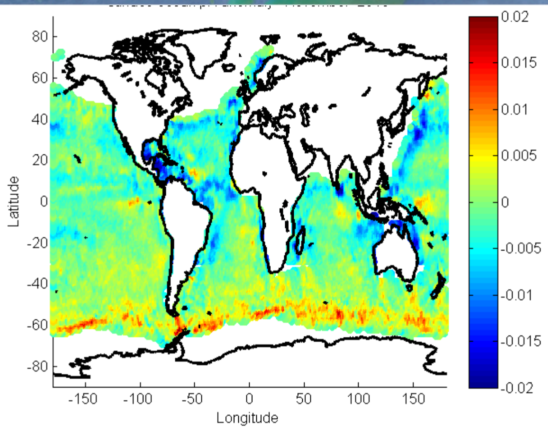
Sample Surface [H+] concentration

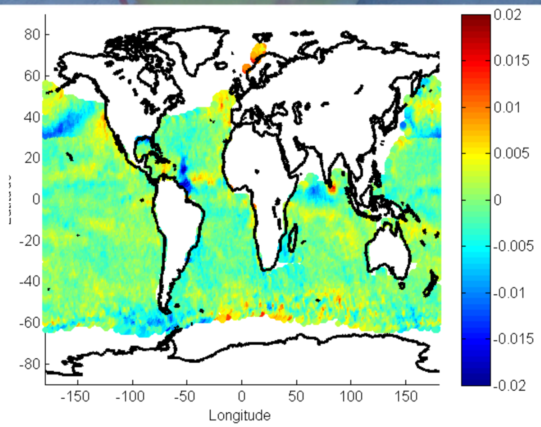


Sample Surface Omega-Aragonite

([Ca++][CO3--]/Ksp)

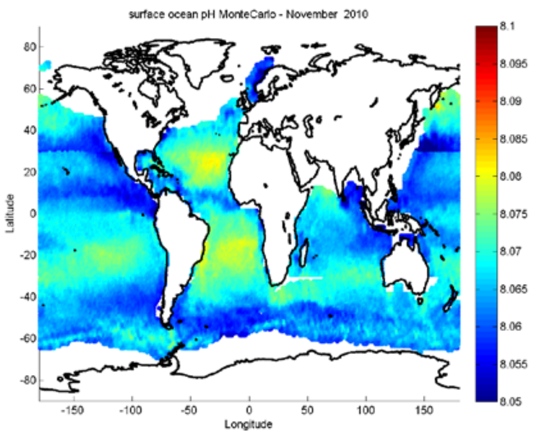
Additional studies – pH and Ω-ar (iii)

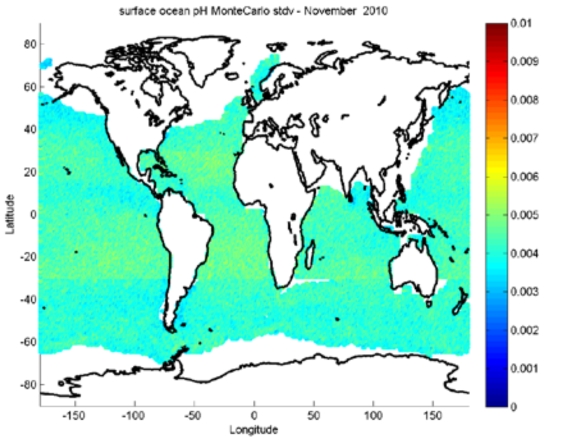




Anomaly wrt WOA climatology and Seasonal Variability

Anomaly vs variability	Mean	StDev
pH anomaly	-0.0009	0.0040
pH variability	0.0006	0.0028





SSS(1,n) = SSS + rand(n) * sigma(SSS)
SST(1,n) = SST + rand(n) * sigma(SST)

Mean pH and Stdv

(100 Montecarlo)

- **Misfit computation (satellite-clima)**
- **L3 ensemble statistics**
- **Propagation into pH computation**

Error prop.	Ensemble mean	Ensemble StDev
pH	8.0665	0.0039 [0.0066]

ESA OceanSODA - objectives

- Deepen acquaintance with the **state of the art** of the OA research
- Generate a **match-up database** (in-situ / EO / models) to perform algorithms development, validation activities and scientific analyses
- Assess spatio-temporal **natural variability** of the carbonate system parameters and satellite data **sensitivity** to them
- Quantify satellite data **uncertainties with their propagation** into related carbonate system parameters
- Explore and develop **novel algorithms** and methods to advance the synergistic exploitation of the satellite data to produce carbonate system parameters estimates
- **Validate** the developed products against a reliable and representative ensemble of in-situ data
- Produce a public **Experimental datasets** of long-term products at global and regional scales
- Explore the potential impact of the products on science, applications and society through dedicated **Impact studies**
- Produce a **scientific roadmap** to indicate research avenues to pursue and assess the degree of operationalization of the derived products
- Promote the results of the activity through a dedicated **workshop**, communication material and dialogue with the relevant communities.

ESA OceanSODA - focus

Focus on pH, AT, Ω_A (but all analysis will include C_T and pCO_2).

Create the matchup database (radial sampling of data, calculating missing parameters using SeaCarb).

Algorithm retraining for global and 6 regionals.

Develop the pH litmus test.

Develop neural network type approaches.

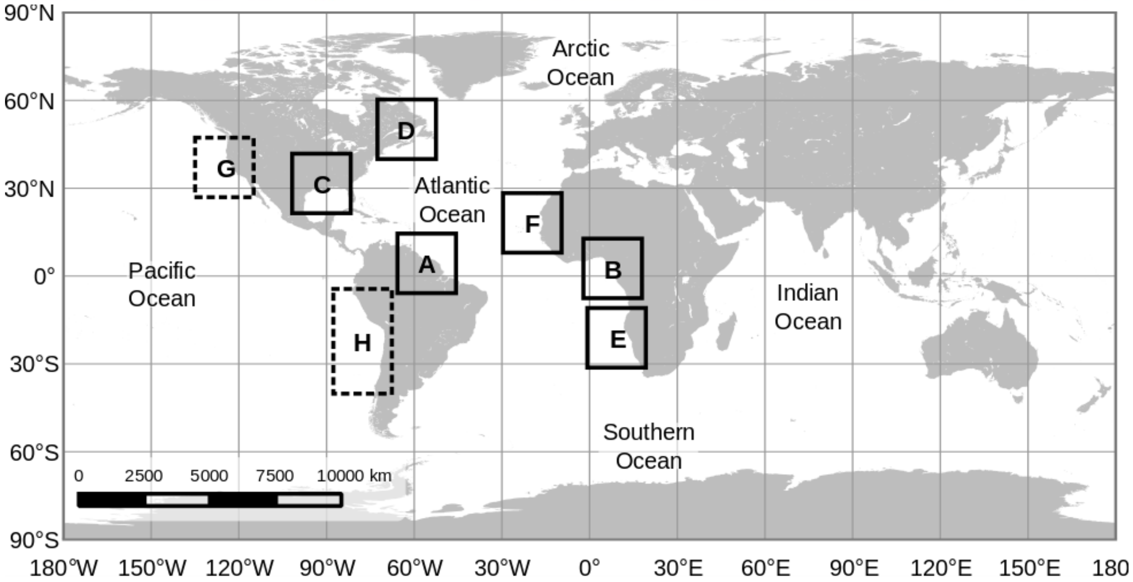
Inter-comparison to characterise total uncertainty in each approach.

Three dedicated science and impact studies (large river flows, upwelling and extreme OA and compound events).

Co-created impact studies with WWF and NOAA.

Stakeholder workshop and community paper.

ESA OceanSODA – study regions



Study regions (**global and six geographic regions**, and two further alternative regions) within *OceanSODA* will include areas of river plumes (large freshwater discharge) in the Amazon and Orinoco (A), Congo (B), Mississippi (C), St Lawrence estuary and outflow (D), and vulnerable eastern boundary upwelling systems, in the Benguela (E) and Canary (Mauritanian, F) upwelling systems. Possible alternative upwelling systems (to replace E or F) are the Californian (G) or the Humboldt (H)

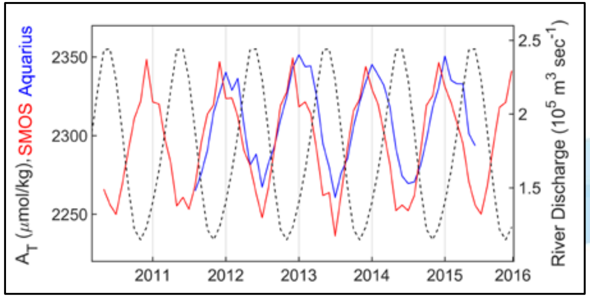
ESA OceanSODA – intercomparison strategy

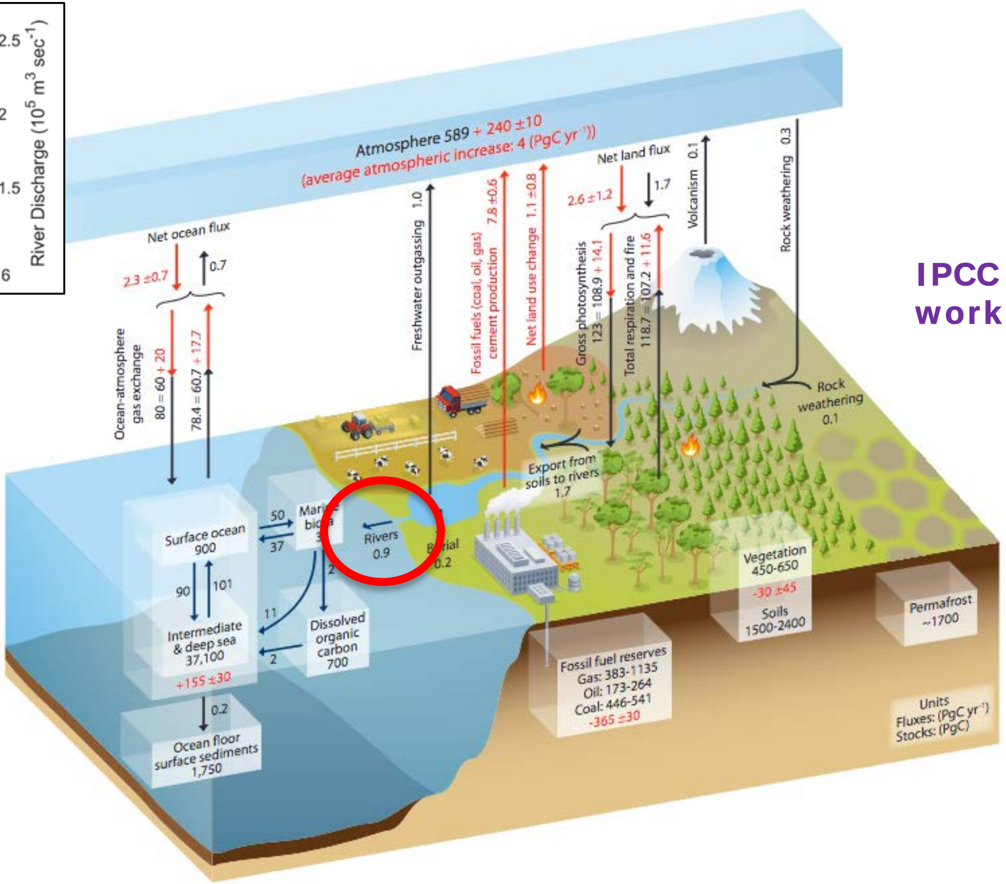
Sources of carbonate estimates (i.e. data to be inter-compared)

- **Results from published algorithms.**
- **Results from retrained algorithms.**
- **Results from neural network approaches.**
- **CMIP6 model outputs.**
- **Region model outputs (if appropriate).**

- **Main validation dataset: GLODAPv2.**
- **Round-robin inter-comparison and validation of all outputs in global plus 6 regions of interest.**
- **Use performance metrics developed within Pathfinders-OA.**
- **All uncertainties will be propagated through the analysis.**

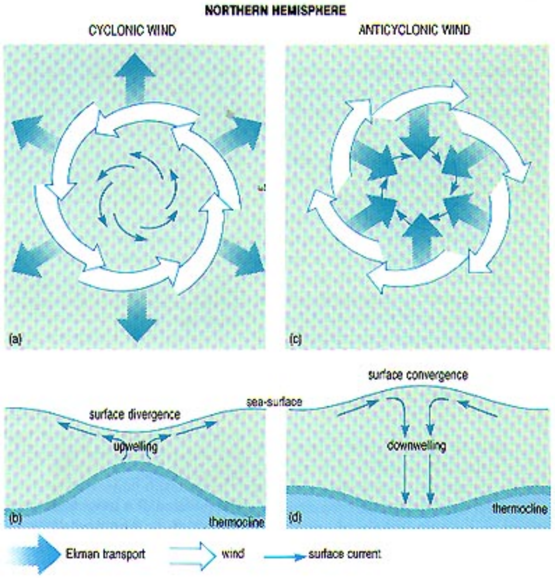
ESA OceanSODA – scientific/impact study #1: large riverine inputs/MPAs

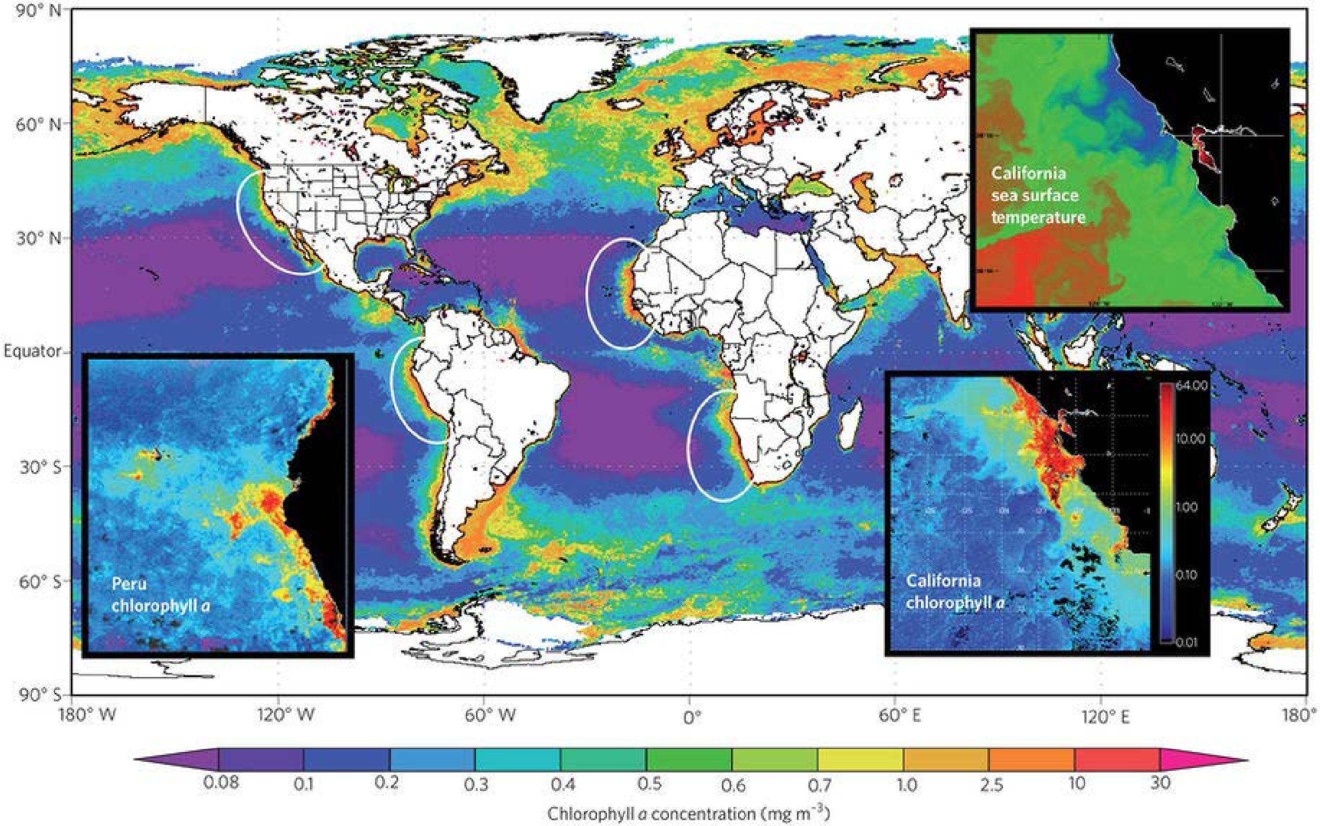




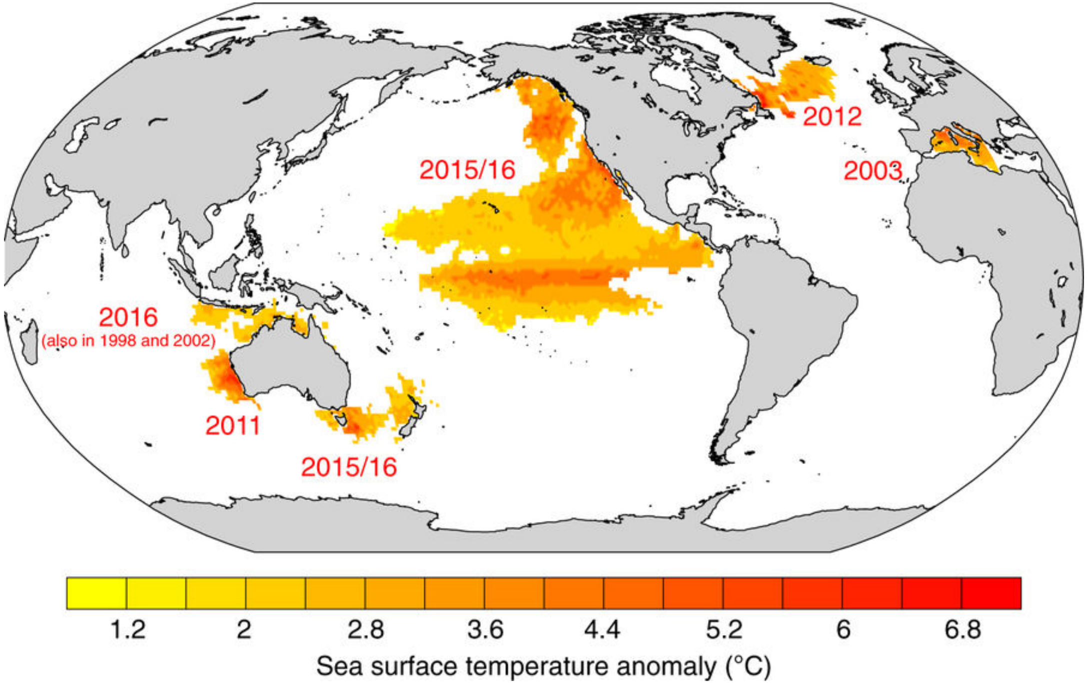
IPCC 5th Assessment, working group I (2014)

ESA OceanSODA – scientific/impact study #2: upwelling/fisheries





ESA OceanSODA – scientific/impact study #3: extreme OA-compound events/coral reef health



Recent marine heat wave (from the literature), from Frolicher and Laufkotter, 2018

Summary, Remarks and Perspectives

- Identified a methodological framework to exploit satellite EO assets in the OA context (distinct focus on satellite SSS); Satellite-based TA, DIC, Ω-ar and surface ocean pH inference. Extend temporal domain and geographical analysis including remaining carbonate system parameters, performing different permutations.
- Pathfinders-OA TA and DIC round-robin exercise showing striking global performances with satellite inputs
- Additional studies on TA, pH and Omega dynamical features and sensitivities and satellite datasets error propagation

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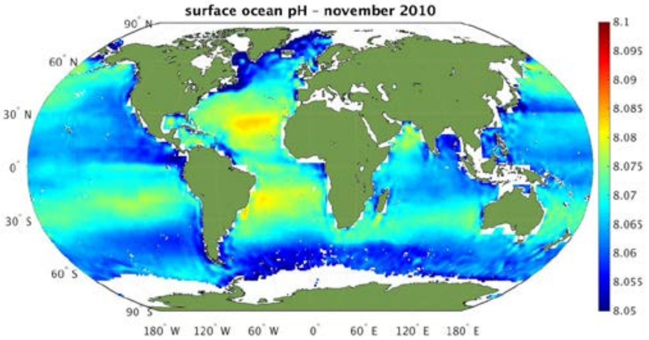
- Foster the advancement of the embryonic phase of OA-related remote sensing, inferring novel value-added satellite products -> OceanSODA project
- Unify fragmented remote sensing efforts in terms of resolution and variety of datasets used, capitalizing on the recent addition of satellite SSS
- Fine-tune algorithms to derive a surface ocean pH atlas, baseline to assess OA severity
- Mid-term objective: quasi-operational surface ocean OA-related variables derivation at different time scales
- Outreach: bridging the gap between the satellite and in-situ communities, benefiting from their cross-fertilization and feedback

Thank you

谢·谢！

Contact:
roberto.sabia@esa.int



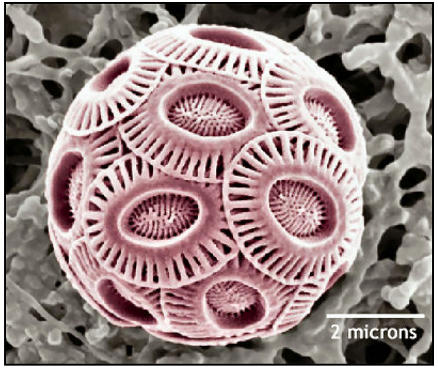
Environmental Science & Technology
Feature
pubs.acs.org/est

Salinity from Space Unlocks Satellite-Based Assessment of Ocean Acidification

Peter E. Land,[*,†] Jamie D. Shutler,[‡] Helen S. Findlay,[†] Fanny Girard-Ardhuin,[§] Roberto Sabia,[‖] Nicolas Reul,[§] Jean-Francois Piolle,[§] Bertrand Chapron,[§] Yves Quilfen,[§] Joseph Salisbury,[⊥] Douglas Vandemark,[⊥] Richard Bellerby,[#] and Punyasloke Bhadury[∇]

stse support to science element

http://www.esa.int/Our_Activities/Observing_the_Earth/SMOS/SMOS_on_acid



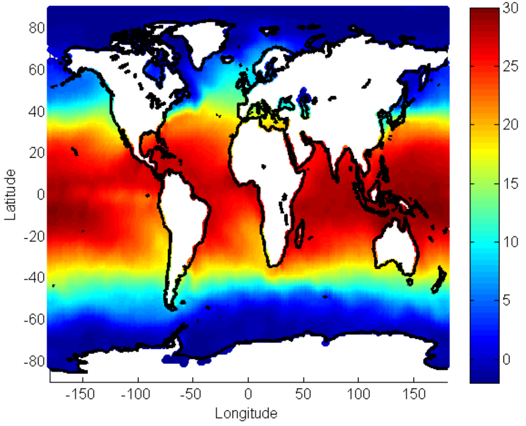
- Chemical subspecies that are biologically relevant:
  - CO2,
  - [H+] ->
  - [CO32-] -> omega

Biological processes affecting OA can be diagnosed by virtue of their covariance with ocean colour.

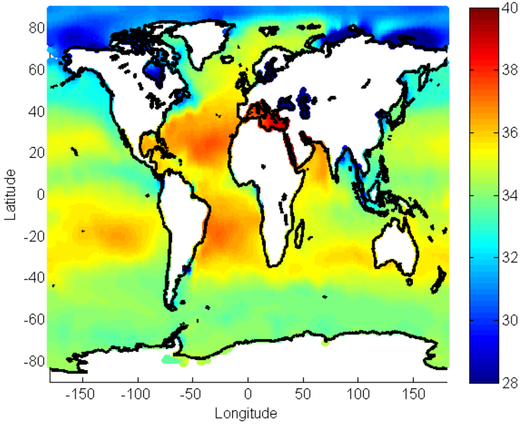
TA – ops defined as the sum of weak bases (carbonate, bicarbonate, boron, etc.) which can combine with free protons. Evap concentrates compounds thus increasing TA; opposite for Precip.

Back-up slides

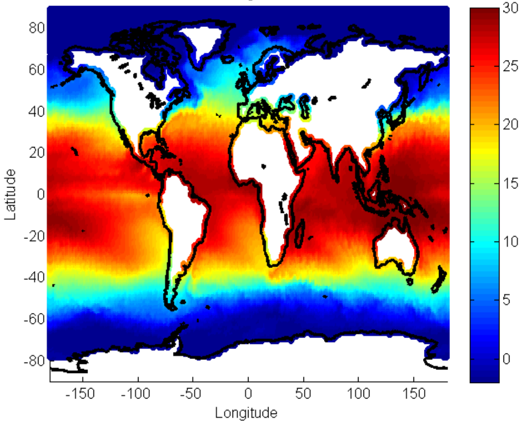
WOA2009 SST - December



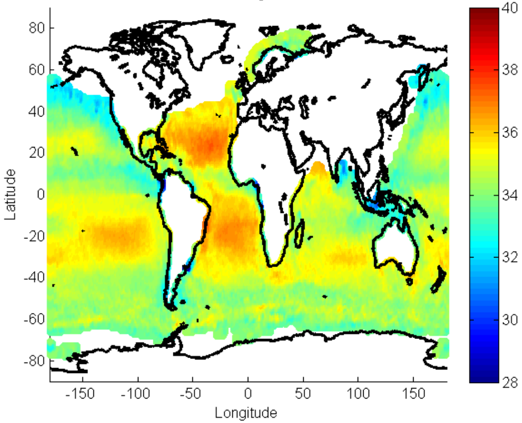
WOA2009 SSS - December



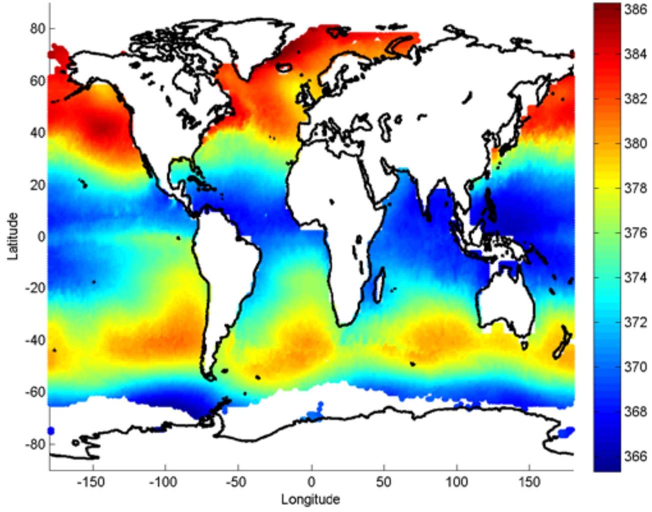
OSTIA SST L4 1 deg - December 2010



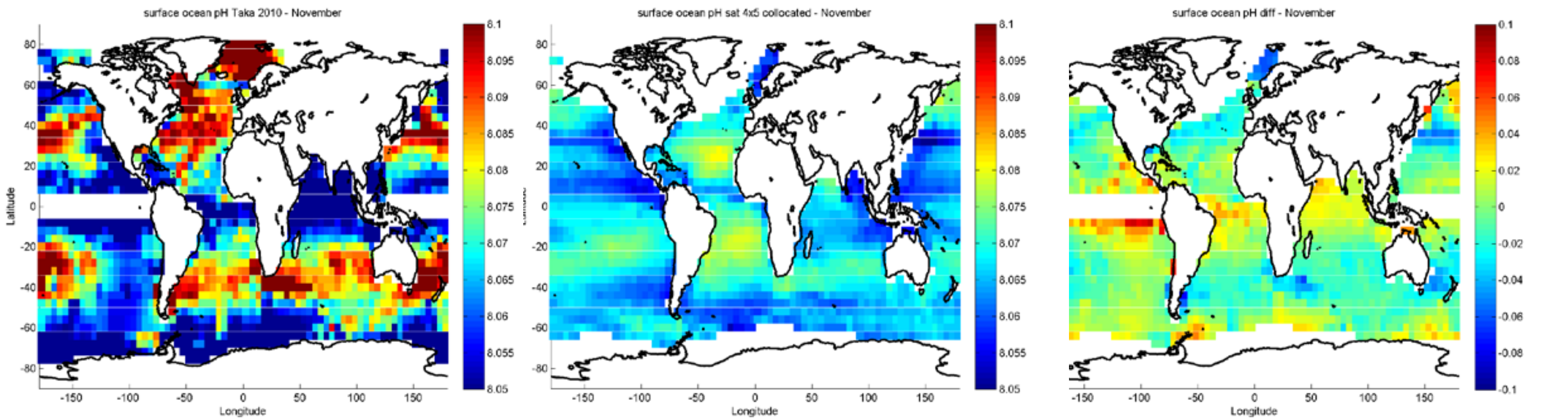
SMOS L3 OI SSS 1 deg - November 2010



seawater pCO2 - November 2010



pH climatology consistency check



Takahashi 2014 climatological surface pH, Monthly maps 4x5 deg grid

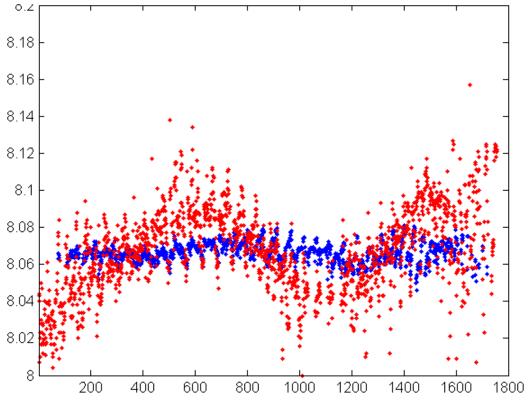
- **Computed from AT and pCO2**
- **AT derived with Takahashi 2013 fitting (24 parameterizations with NO3) – P-Alk**
- **Forcing WOA climatology SSS and SST**
- **Carbon chemistry model: Luecker 2000**

(left to right) Takahashi 2014 climatological surface pH,

Satellite- based surface pH,

Difference surface pH map and plot

	Misfit mean	Misfit StDev
pH_diff	-0.002	0.021



T_A summary

For global T_A, Lee06 has the best results (N~4000): Aquarius SSS RMSD=45 µmol kg^{-1}, SMOS 52, HadGEM2 60, CORA 69, WOA 73

For Greater Caribbean T_A (N~60) Taka13 performs best: CORA SSS RMSD=15, SMOS 19, WOA 21, Aquarius (Lee06) 22, HadGEM2 70

For Amazon plume T_A, (N~400) Taka13 performs best: SMOS SSS RMSD=42, Aquarius 47, CORA (Lee06) 54, WOA (Lee06) 57, HadGEM2 78

For Bay of Bengal T_A (N~20), Lee06 performs slightly better: CORA SSS RMSD=17, WOA 22, Aquarius 33, SMOS 36, HadGEM2 219

DIC summary

For global DIC studies, Aquarius SSS has the best results with RMSD=30 μmol kg^{-1}, LDEO 33, CORA 41, SMOS 45, HadGEM2 52

For Greater Caribbean DIC, SMOS and CORA SSS perform best with RMSD=15, LDEO 16, Aquarius 17, HadGEM2 65

For Amazon plume DIC, SMOS SSS performs best with RMSD=38, Aquarius 40, CORA 44, LDEO 49, HadGEM2 71

For Bay of Bengal DIC, LDEO and CORA perform best with RMSD=15, SMOS 20, Aquarius 22, HadGEM2 79

For Barents Sea DIC, LDEO SSS performs best with RMSD=36, Aquarius 48, HadGEM2 63, SMOS 126, no CORA data