

Estimating normal: Synthesizing the SOCCOM array with an ocean model

2018 OCB Summer Workshop

Matt Mazloff, Ariane Verdy, ECCO, SOCCOM, et al.

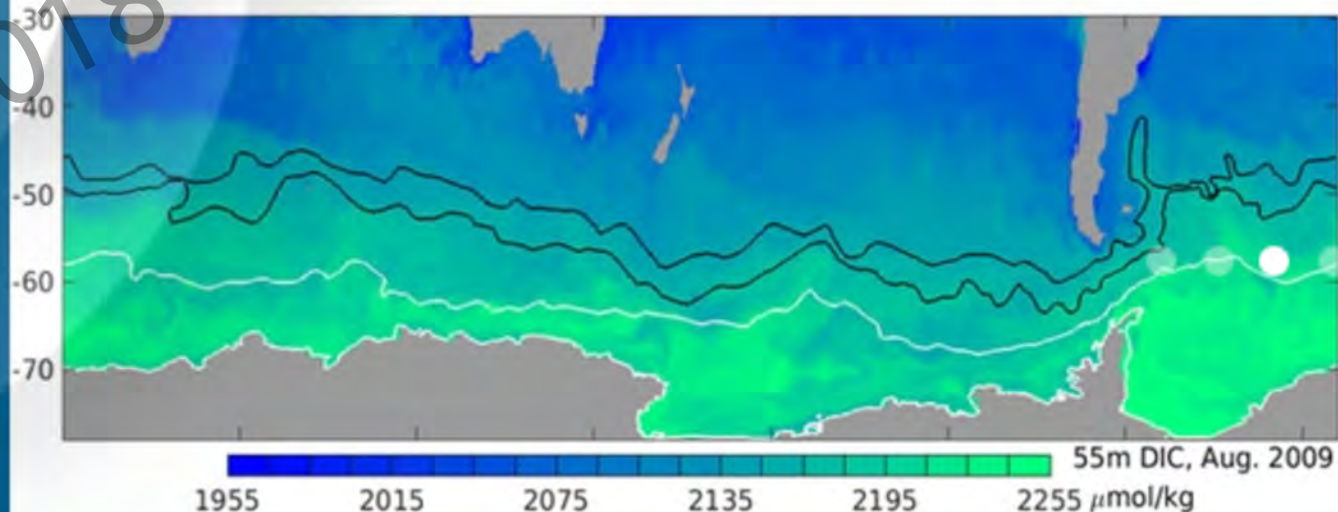


SOCCOM

Unlocking the mysteries
of the Southern Ocean

Biogeochemical SOSE
Solution Now Available

Access our 3-D estimate
of Southern Ocean
biogeochemistry

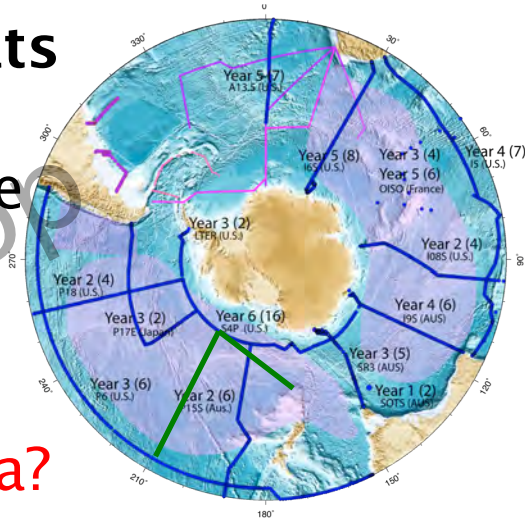


1. SOCCOM observations

(L. Talley, K. Johnson, S. Riser, E. Boss, S. Gille, A. Dickson)



200 Biogeochemical Argo floats
(10 day profiling to 2000 m)
Temperature, salinity, pressure
Oxygen, Nitrate, pH
Bio-optics



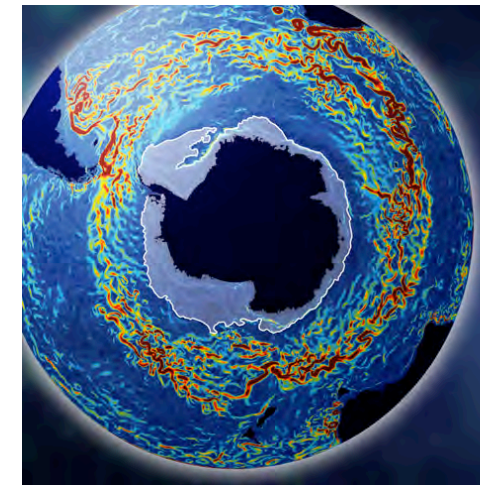
What are the value of these data?

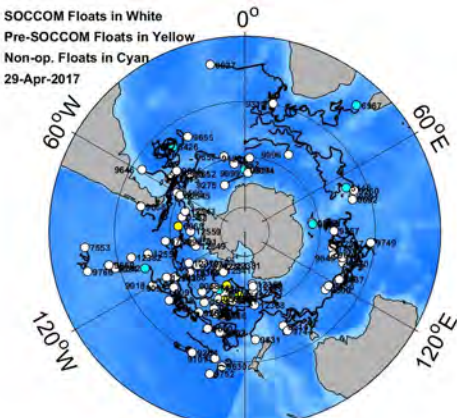
2. SOCCOM state estimation

Biogeochemical Southern Ocean State Estimate (BSOSE)

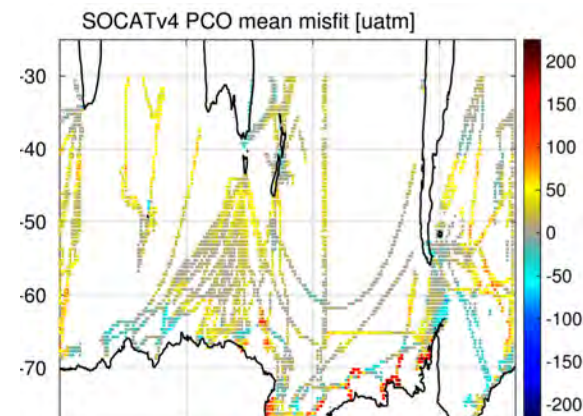
M. Mazloff, A. Verdy

What is a state estimate?





Biogeochemical constraints:



	2009	2010	2011	2012	2013	2014	2015	2016	2017
# of O ₂ profiles	2416	2142	1254	906	821	1322	1,574	1,550	2,395
# of pH profiles	0	0	0	0	0	309	564	1,126	1,624
# of NO ₃ profiles	0	0	0	116	247	463	625	1,293	2,057
Ship profiles	679	380	447	88	125	180	102	333	149
SOCAT5 pCO ₂	14,296	17,242	20,548	23,626	18,238	17,021	20,566	14,070	0



SOCOM

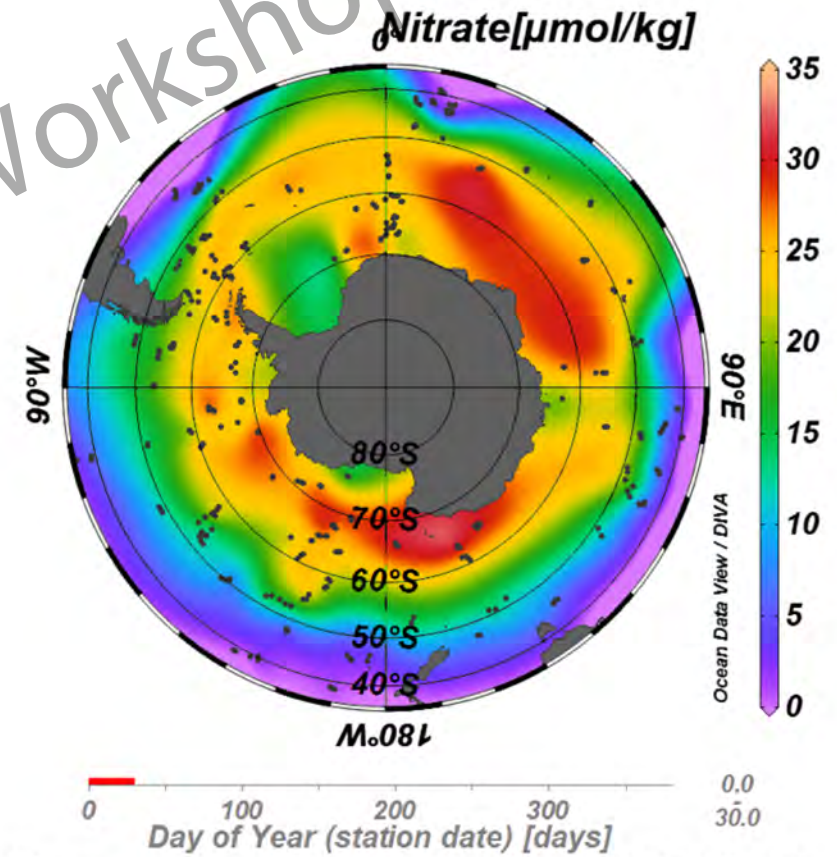
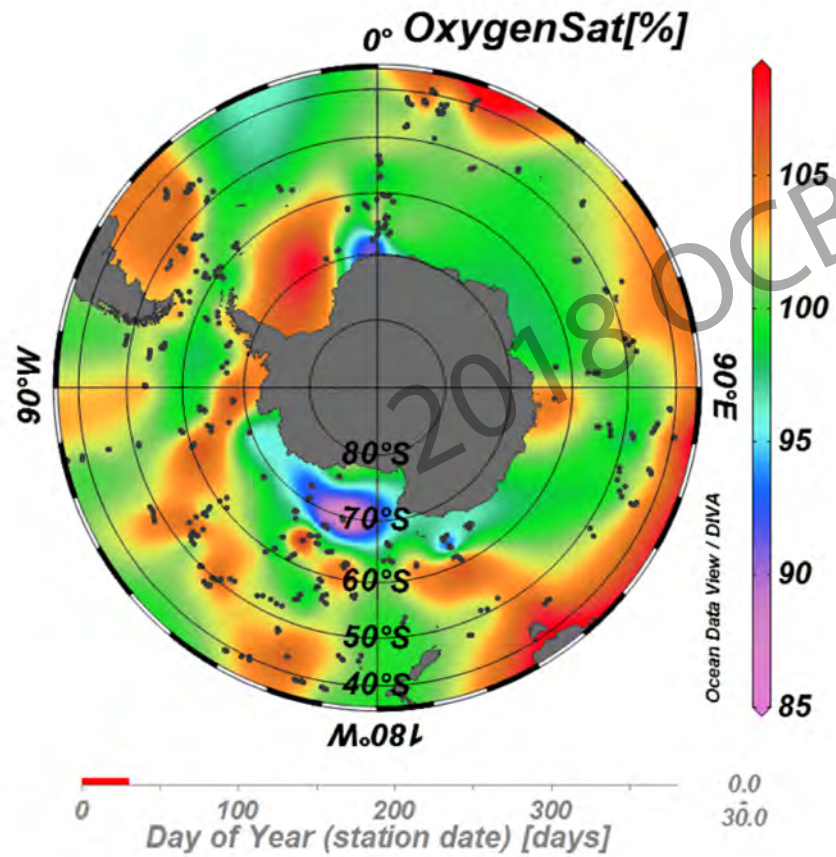
Mapping data

Non-linear statistical model
(e.g. neural network)

Numerical model
(e.g. Kalman filter or 4d-Var)

Spectrum of
complexity
and human vs
machine learning

Statistical model
(e.g. objective mapping)



Maps From Ken Johnson, MBARI

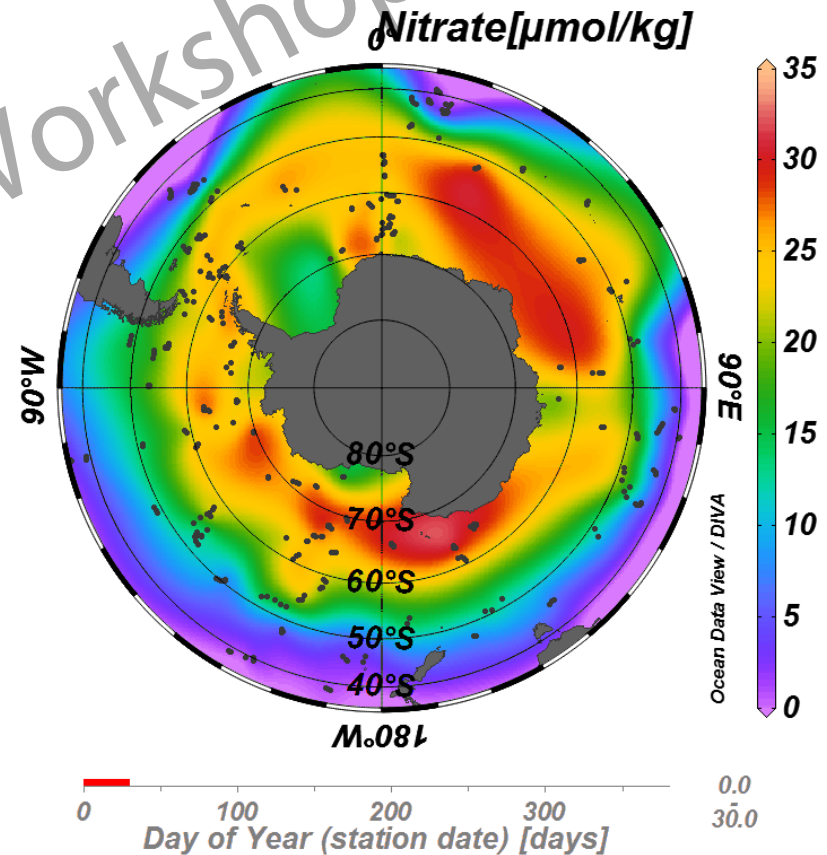
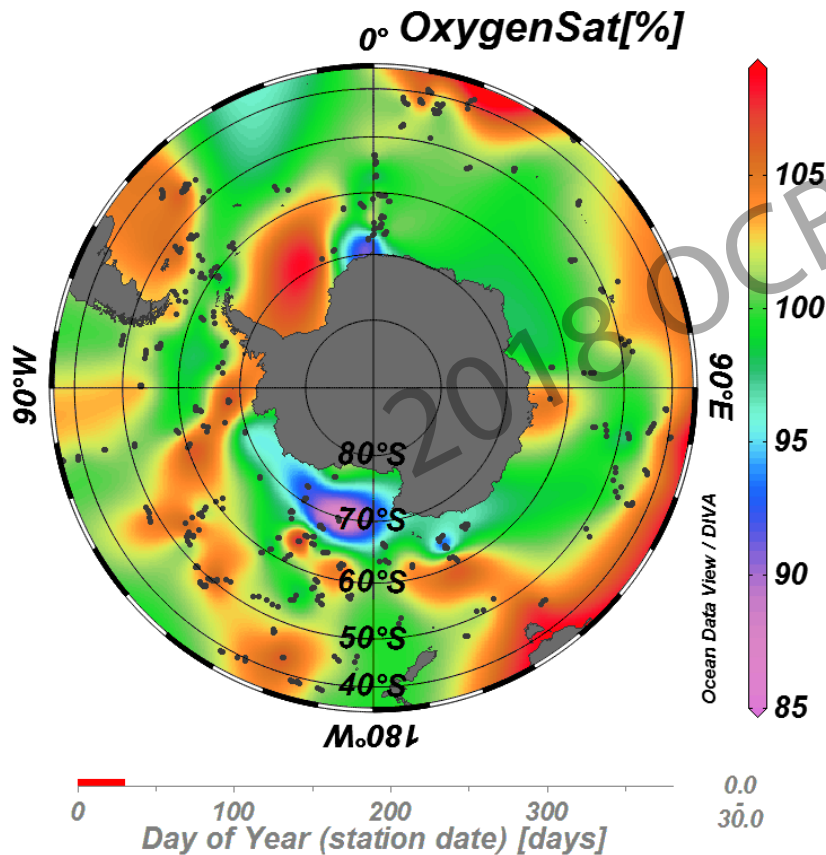
Mapping data

Non-linear statistical model (e.g. neural network)

Numerical model (e.g. Kalman filter or 4d-Var)

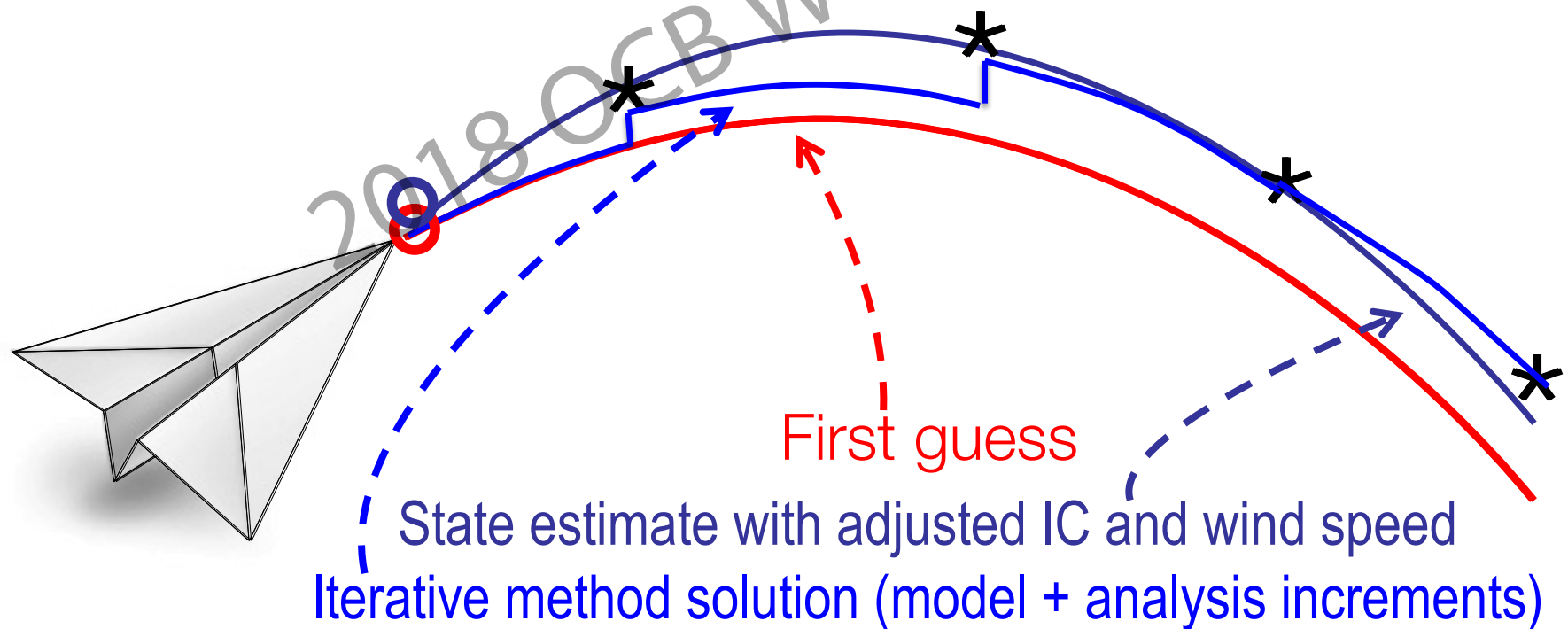
Spectrum of
complexity
and human vs
machine learning

Statistical model (e.g. objective mapping)

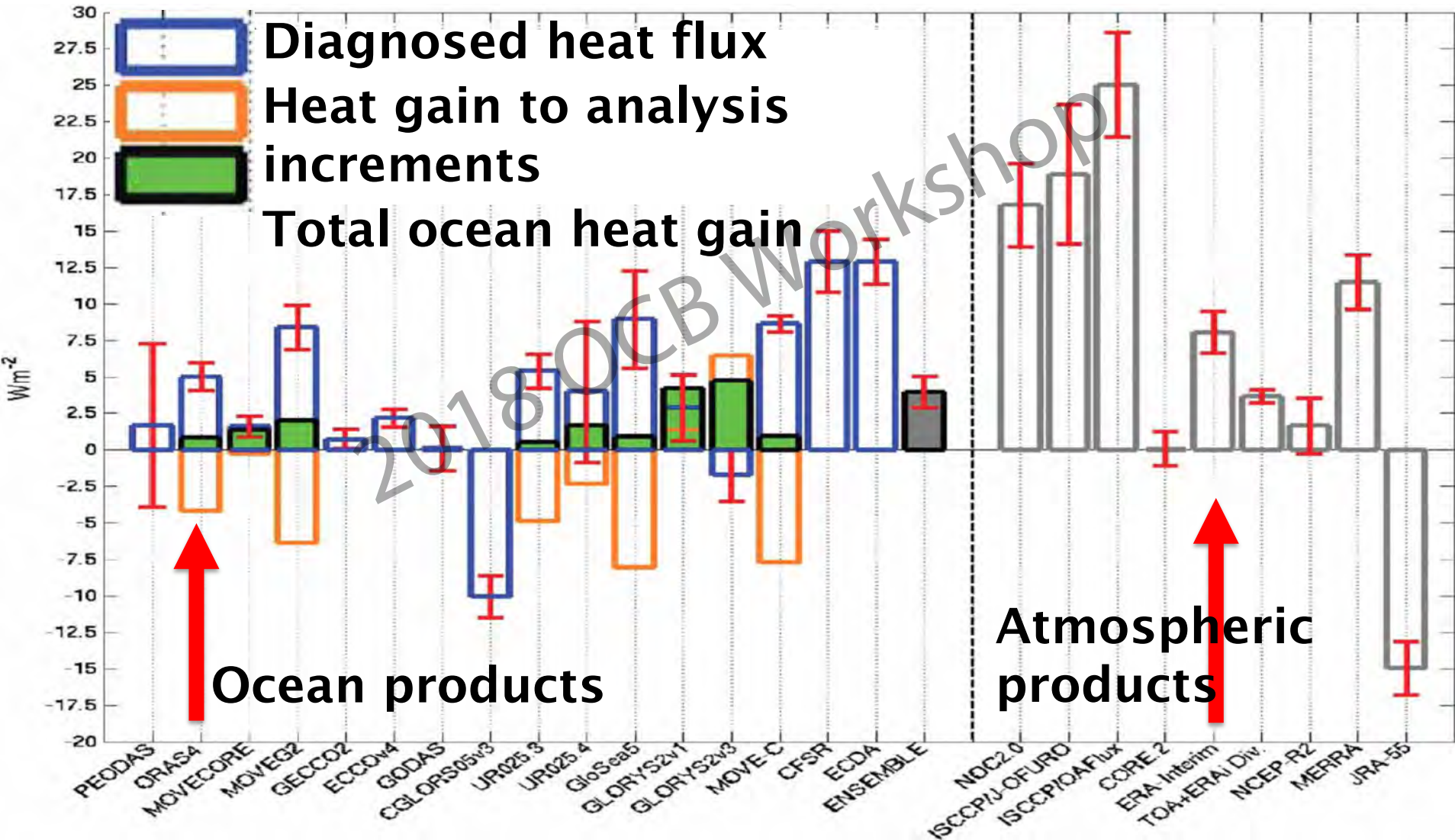


State estimation vs. Iterative methods (e.g. reanalysis)

For scientific understanding one prefers to adjusting the uncertain initial condition and “wind speed” allowing the trajectory to obey a *closed dynamical budget*. This has become known as “state estimation”.



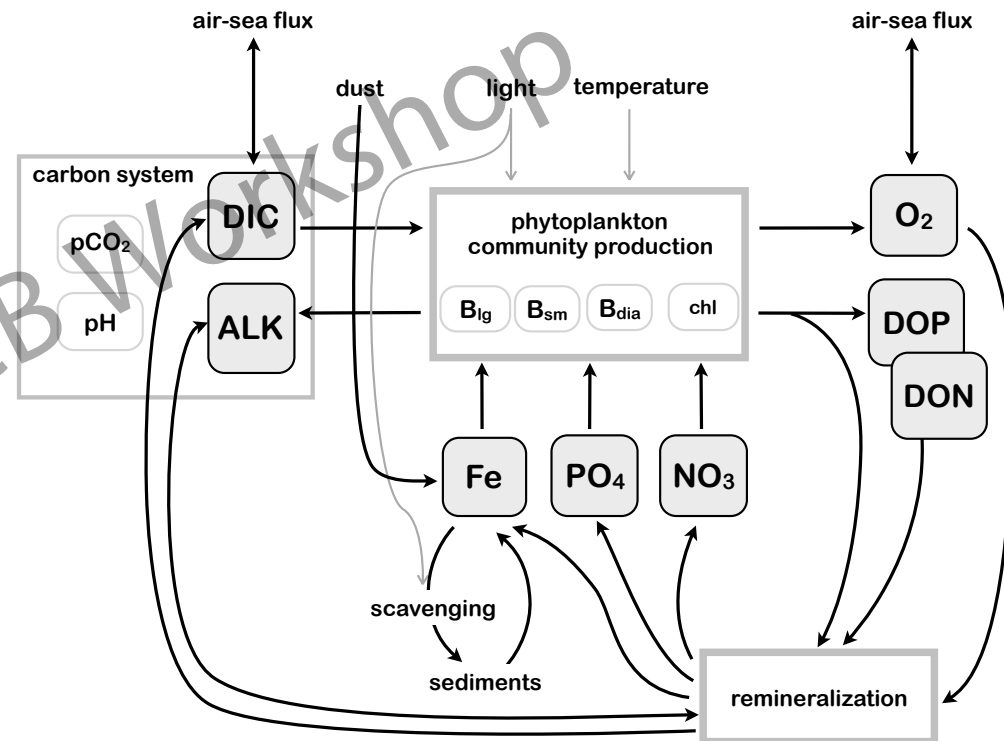
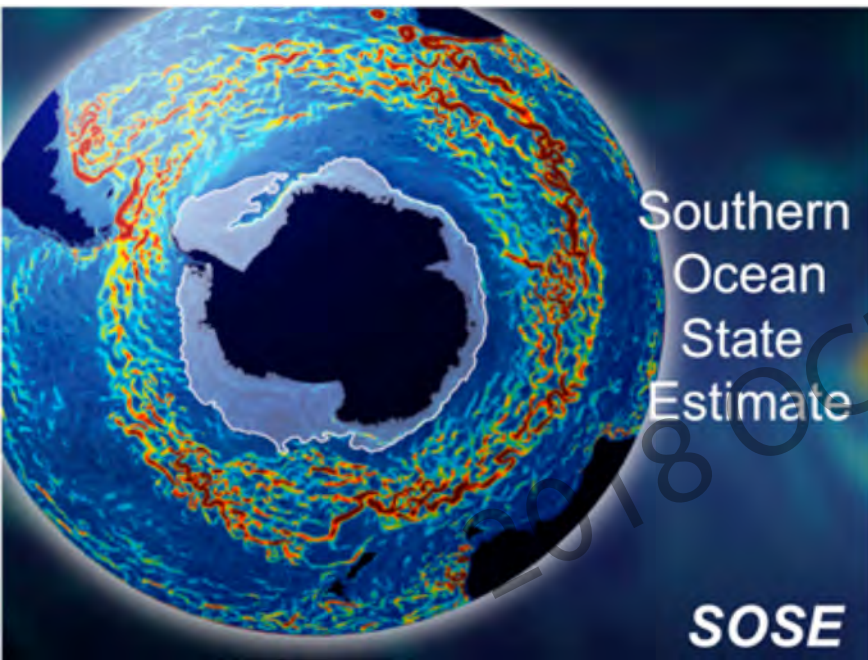
State estimation vs. Iterative methods: The Ocean Reanalyses Intercomparison Project (ORA-IP). Adapted from Balmaseda et al. 2015



The Biogeochemical Southern Ocean State Estimate (B-SOSE)

MIT general circulation model

+ BLING biogeochemistry (Galbraith et al, 2010)



observations: altimetry; sea surface temperature, sea ice concentration; profiling floats temperature, salinity, oxygen, nitrate, pH; bottle nutrients and carbon system; underway pCO_2 ; POC & CHL



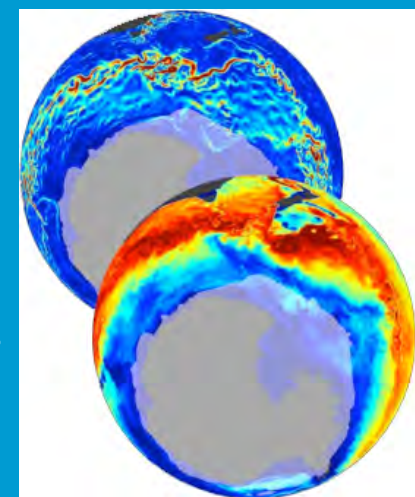
We use the adjoint method (4d-Var) to iteratively solve our weighted least-squares problem: solve for model inputs to minimize distance between model and observations.

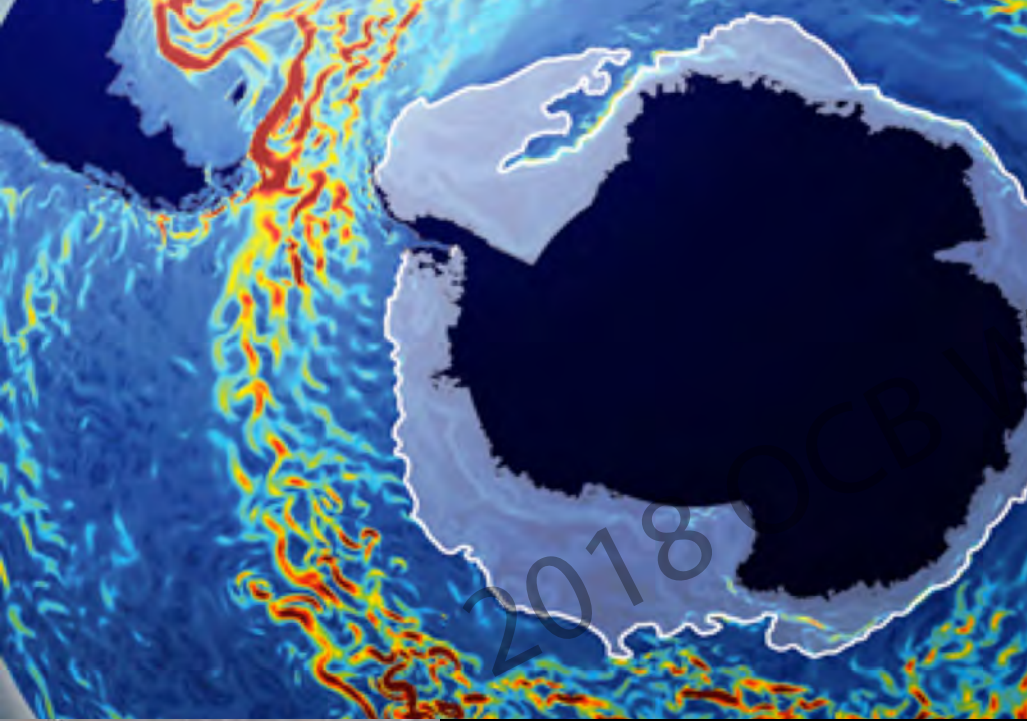
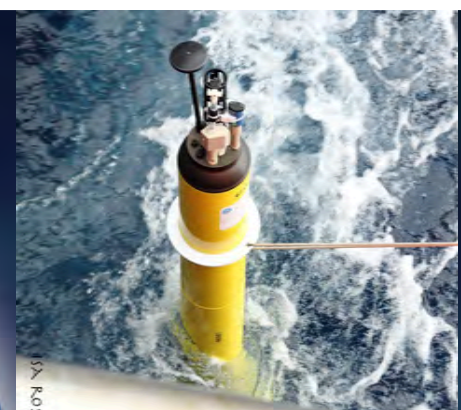
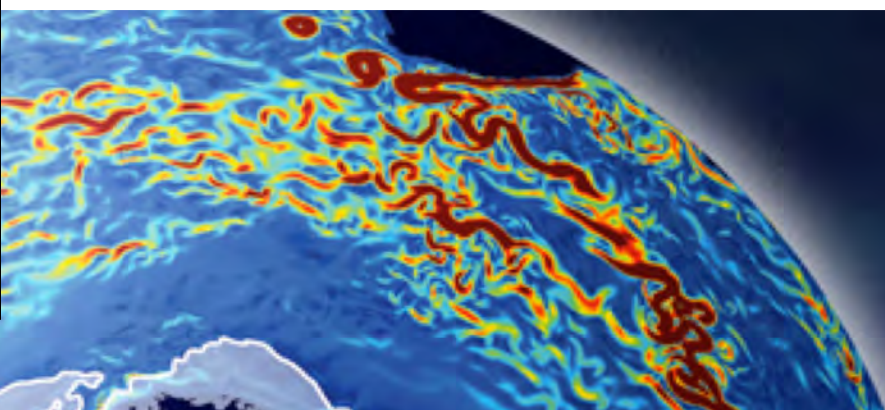
forward model with closed budgets
cost = $((obs_i - model_i) / error_i)^2$

adjust ICs and atmospheric state

produce estimate

adjoint model
sensitivity of cost to control variables





BGC-Argo is achieving substantial in situ coverage. Now appropriate to construct a state estimate synthesizing all available observations and the laws of nature represented by a general circulation model

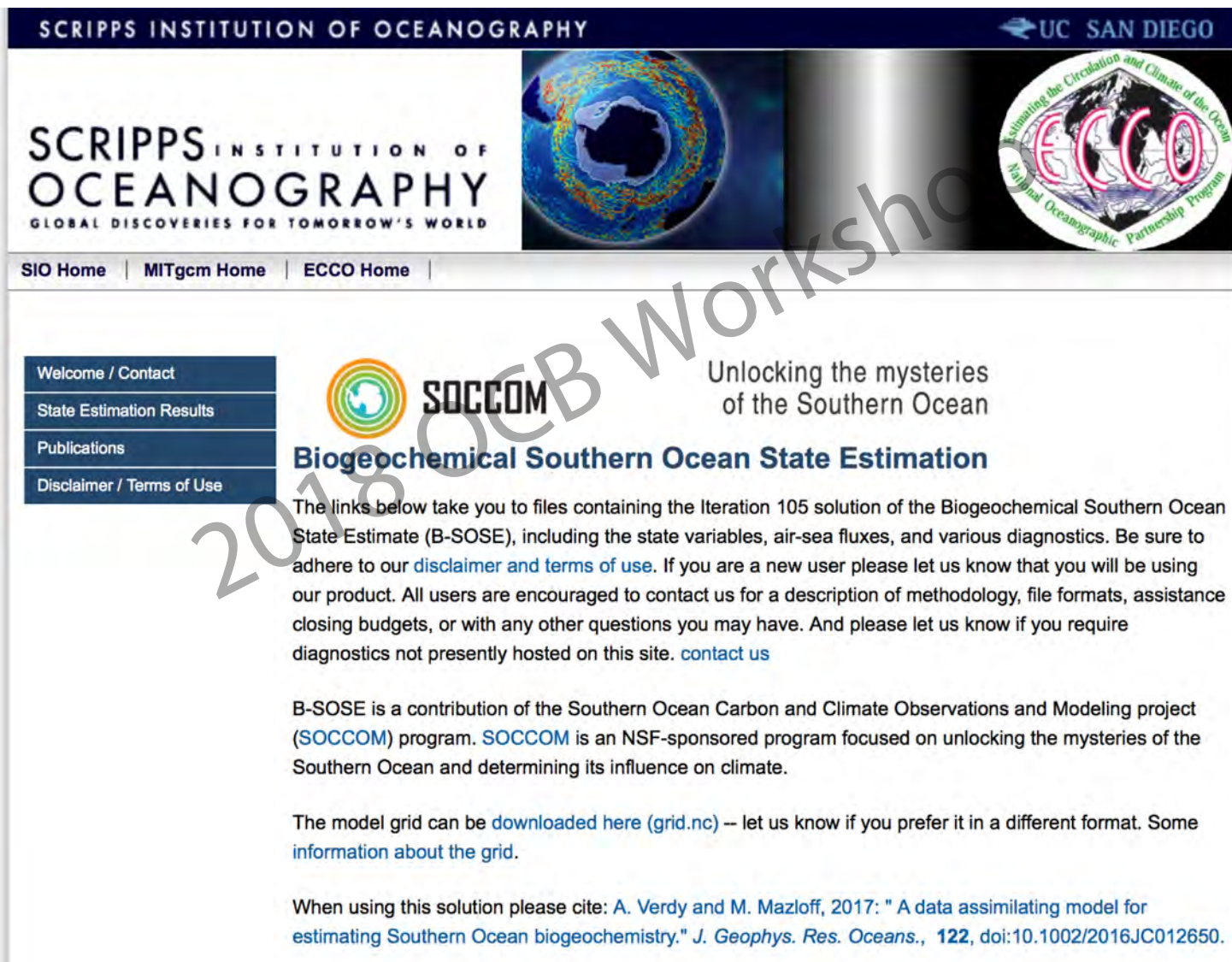
Goals

- Produce a gridded data set consistent with model physics and observations, increasing accessibility
- Provide quantitative baselines: Estimating the “normal” and a framework to understand the “normal”



2008-2012 solution publicly available: sose.ucsd.edu

Now producing a 2013 to present SOCCOM-era BSOSE



The screenshot shows the Scripps Institution of Oceanography website. At the top, there is a dark blue header with "SCRIPPS INSTITUTION OF OCEANOGRAPHY" on the left and "UC SAN DIEGO" on the right. Below the header, there are three main images: the Scripps Institution of Oceanography logo, a globe showing oceanographic data, and the ECCO logo. A navigation bar below the images contains links for "SIO Home", "MITgcm Home", and "ECCO Home".

On the left side of the page, there is a vertical menu with the following items: "Welcome / Contact", "State Estimation Results", "Publications", and "Disclaimer / Terms of Use".

The main content area features the SOCCOM logo, which consists of a stylized globe with a green and orange border. To the right of the logo is the text "SOCCOM" and "Unlocking the mysteries of the Southern Ocean". Below this is the section title "Biogeochemical Southern Ocean State Estimation".

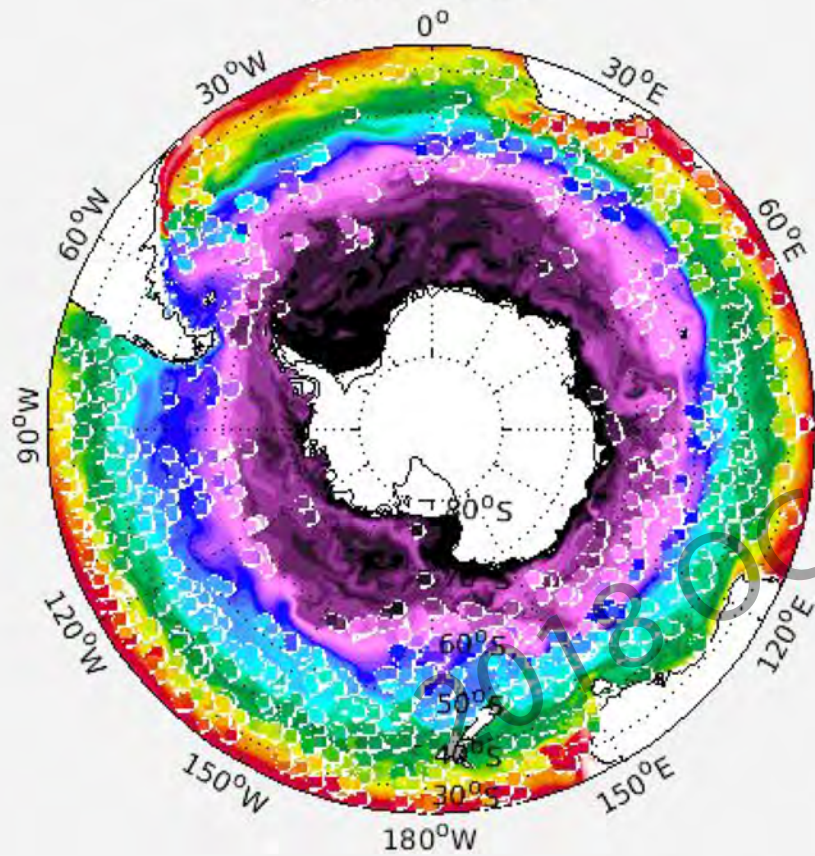
The text below the title reads: "The links below take you to files containing the Iteration 105 solution of the Biogeochemical Southern Ocean State Estimate (B-SOSE), including the state variables, air-sea fluxes, and various diagnostics. Be sure to adhere to our [disclaimer and terms of use](#). If you are a new user please let us know that you will be using our product. All users are encouraged to contact us for a description of methodology, file formats, assistance closing budgets, or with any other questions you may have. And please let us know if you require diagnostics not presently hosted on this site. [contact us](#)"

Below this is a paragraph: "B-SOSE is a contribution of the Southern Ocean Carbon and Climate Observations and Modeling project (SOCCOM) program. SOCCOM is an NSF-sponsored program focused on unlocking the mysteries of the Southern Ocean and determining its influence on climate."

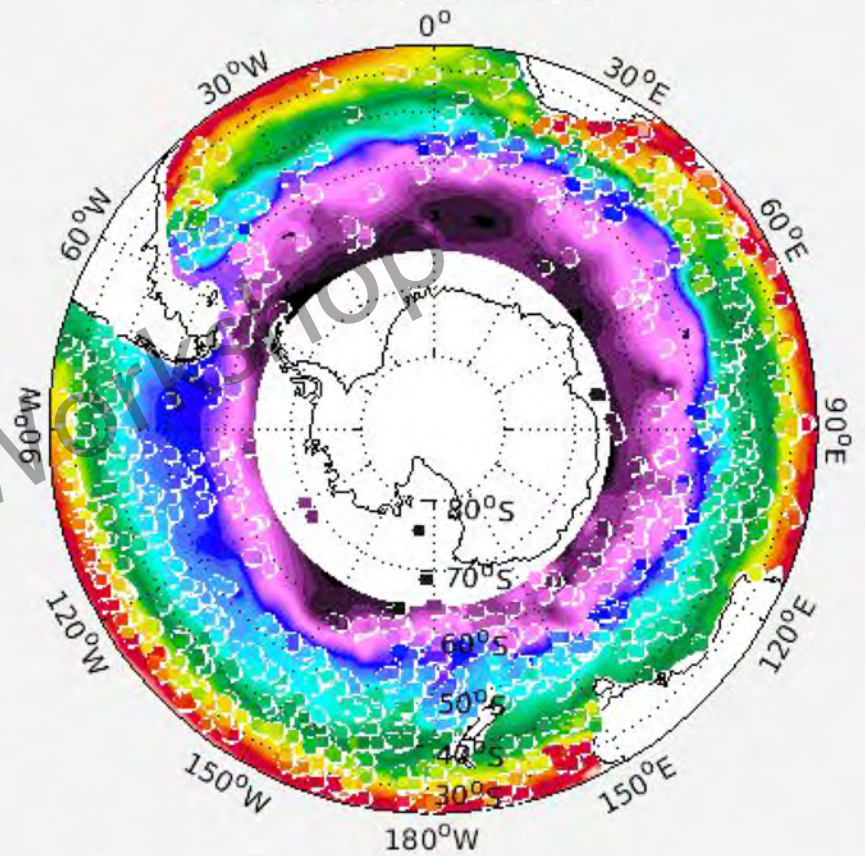
The next paragraph states: "The model grid can be [downloaded here \(grid.nc\)](#) -- let us know if you prefer it in a different format. Some [information about the grid](#)."

The final paragraph provides a citation: "When using this solution please cite: A. Verdy and M. Mazloff, 2017: " A data assimilating model for estimating Southern Ocean biogeochemistry." *J. Geophys. Res. Oceans.*, **122**, doi:10.1002/2016JC012650."

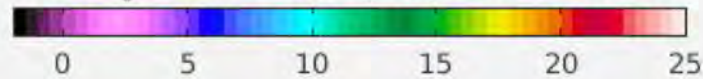
JAN 2013



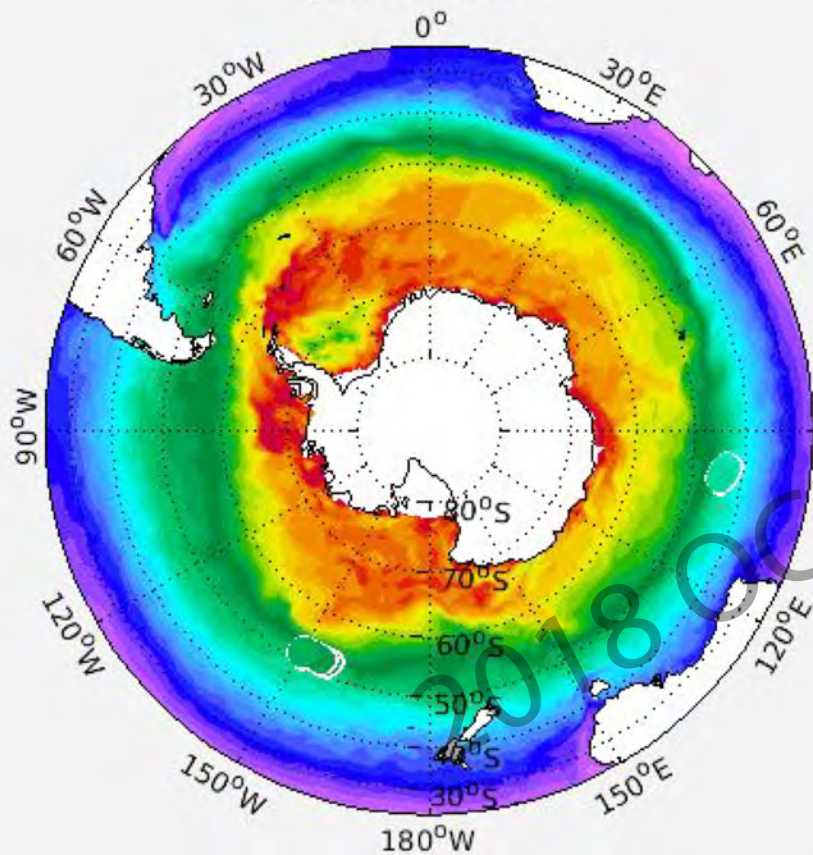
Argo (RG map)



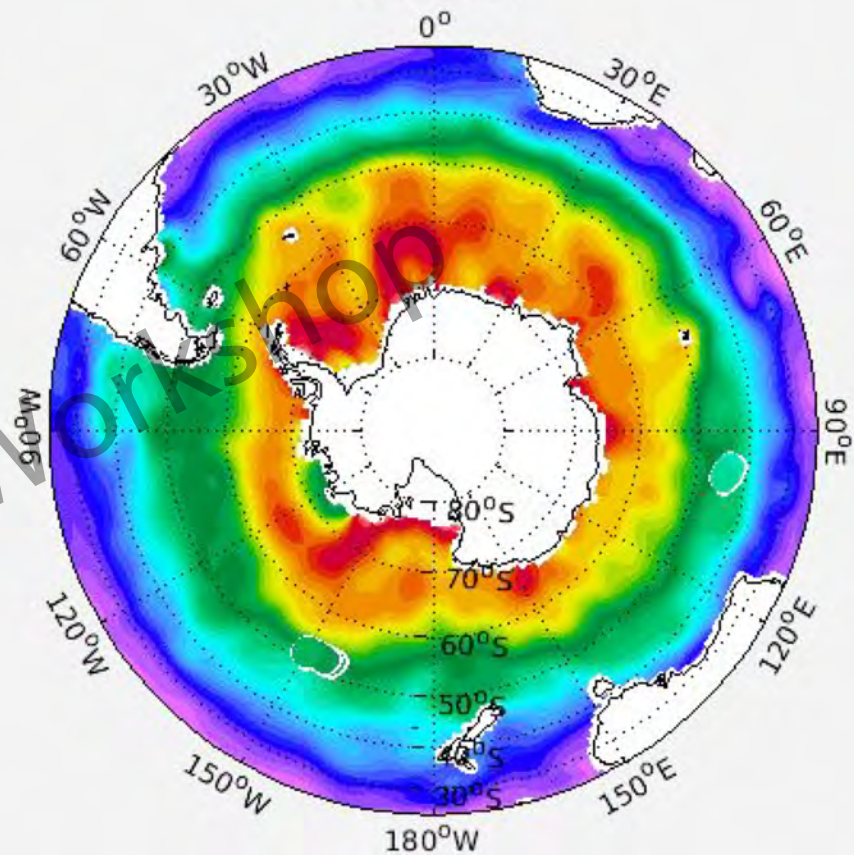
Temperature (°C) at 100 m



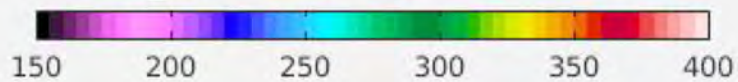
JAN 2013



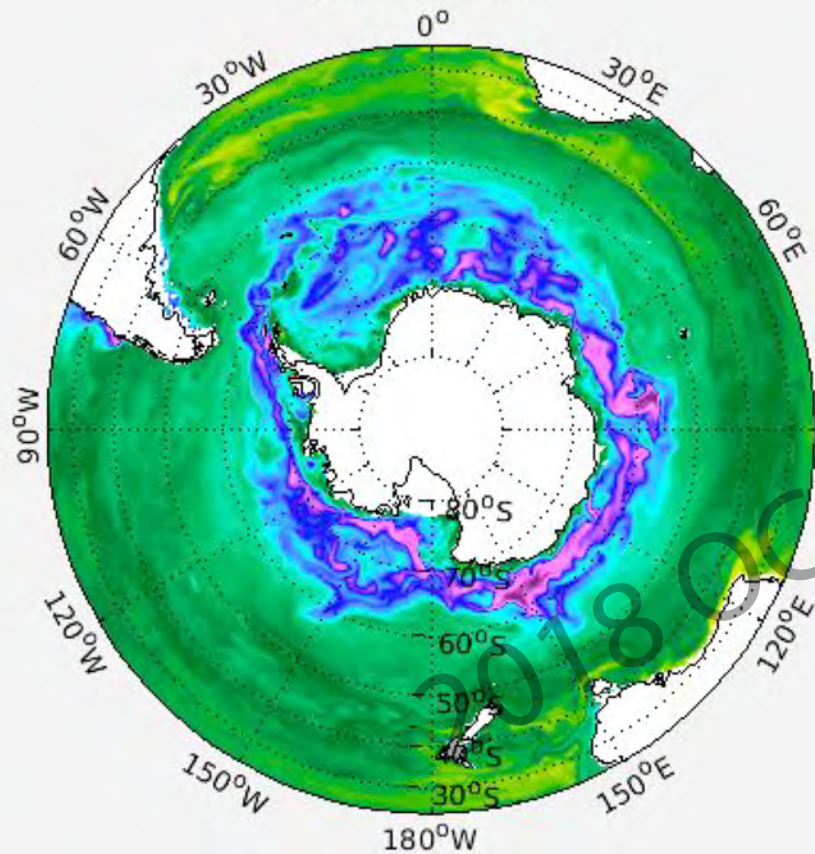
WOA 13



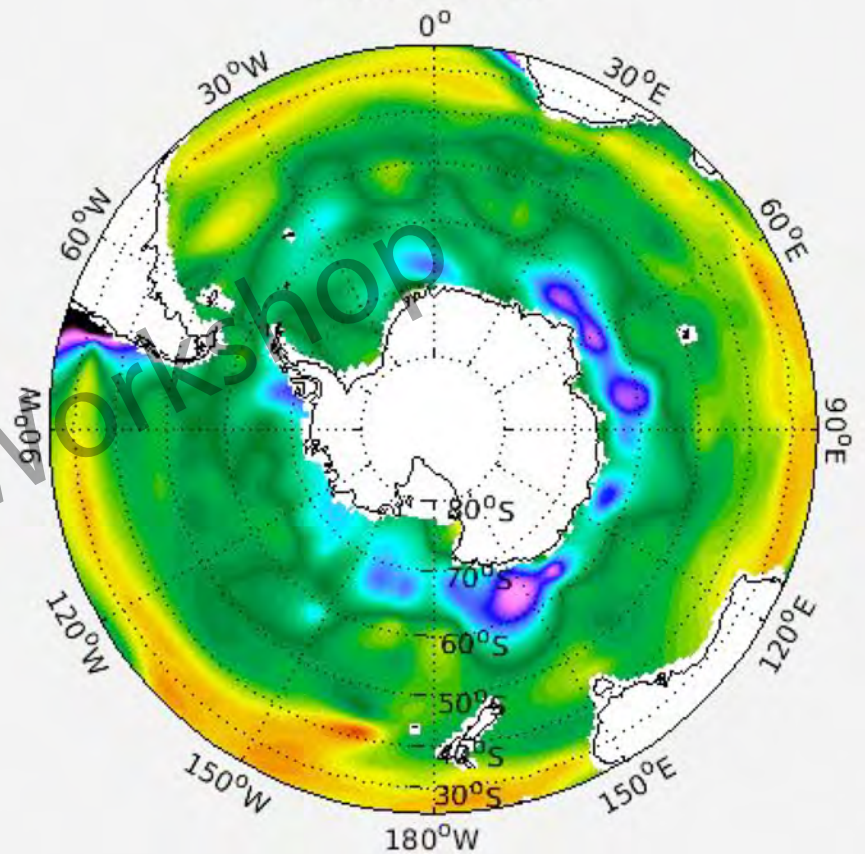
O₂ ($\mu\text{mol/kg}$) at 10 m



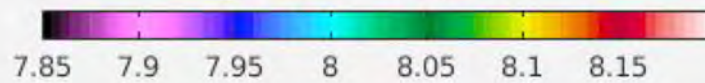
JAN 2013



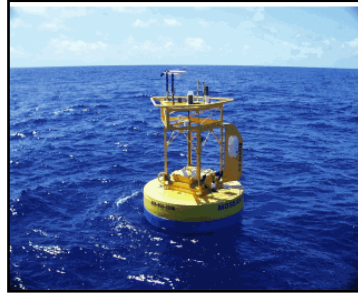
GLODAPv2



pH at 100 m



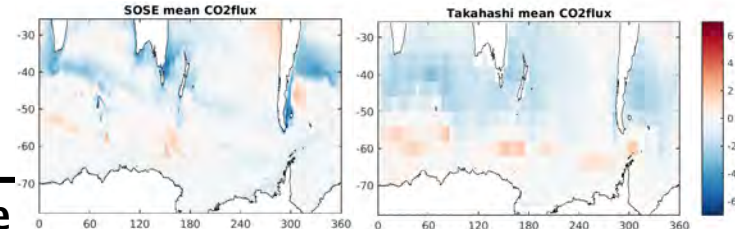
Validation against observations: holding the *model* accountable to the *data*



- **Comparisons with gridded products**
 - satellite data
 - mapped products
- **Comparisons with in situ obs.**
 - float profiles
 - shipboard measurements
- **Comparisons with estimated “quantities of interest”**
 - air-sea CO₂ flux
 - Drake Passage pCO₂
 - nutrient transport
 - across 32°S

Validation online

http://sose.ucsd.edu/bsose_valid.html



Biogeochemical state

• Comparisons with climatology:

- air-sea CO₂ flux with Takahashi climatology
- ALK, DIC, pH with GLODAPv2 climatology
- O₂, NO₃, PO₄ with WOA13 climatology

• Comparisons with mapped products:

- surface pCO₂ with SOCATv5 & Landschutzer monthly maps
- air-sea CO₂ flux with Landschutzer monthly maps
- chlorophyll with MODIS Aqua and VIIRS monthly maps

• Comparisons with in situ observations:

- pCO₂ with SOCATv5 underway
- O₂, pH, NO₃, CHL, POC with SOCCOM floats profiles
- ALK, O₂, NO₃ with GLODAPv2 profiles
- O₂ with non-SOCCOM BgcArgo profiles
- O₂ and CHL with shipboard profiles

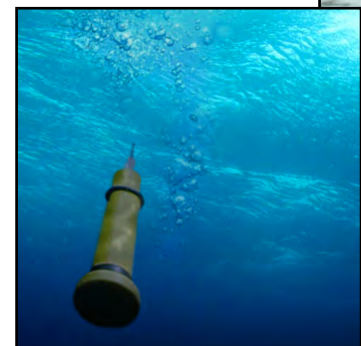
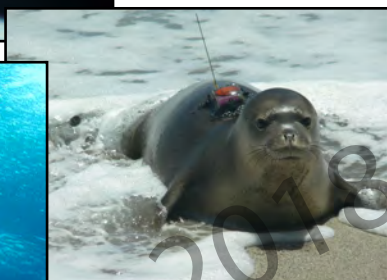
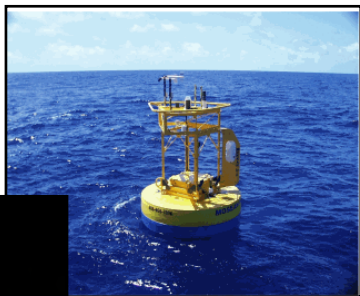
Physical state

• Comparisons with mapped products:

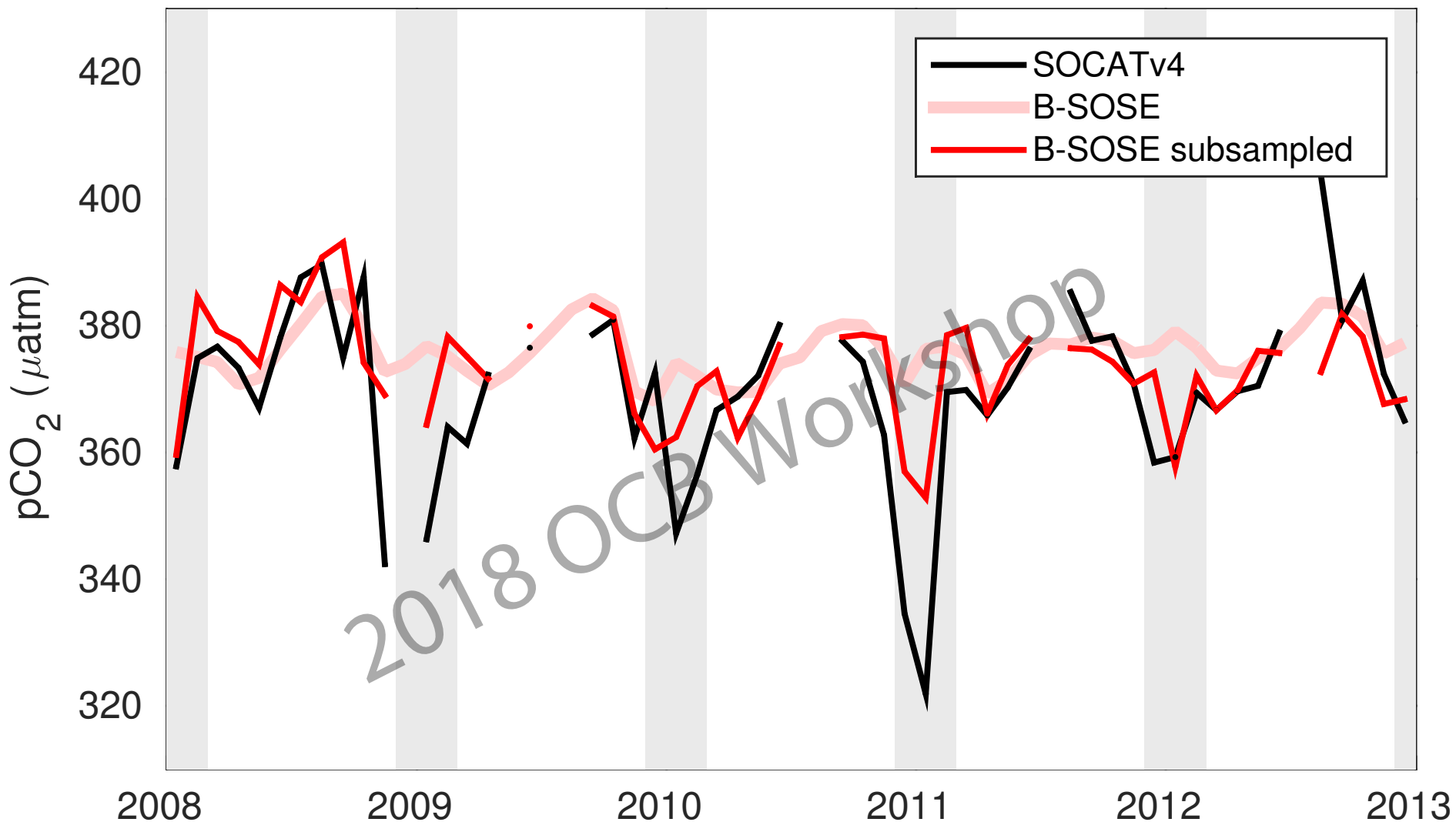
- SSH with Jason 1&2, and with AVISO maps
- SST with MW SST maps
- Ice concentration with NSIDC maps
- T, S with Argo maps

• Comparisons with in situ observations:

- T, S with Argo, MEOP, and shipboard profiles

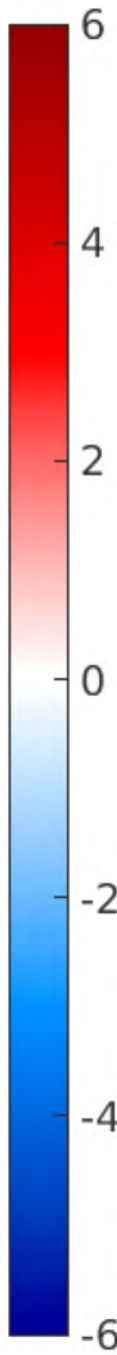
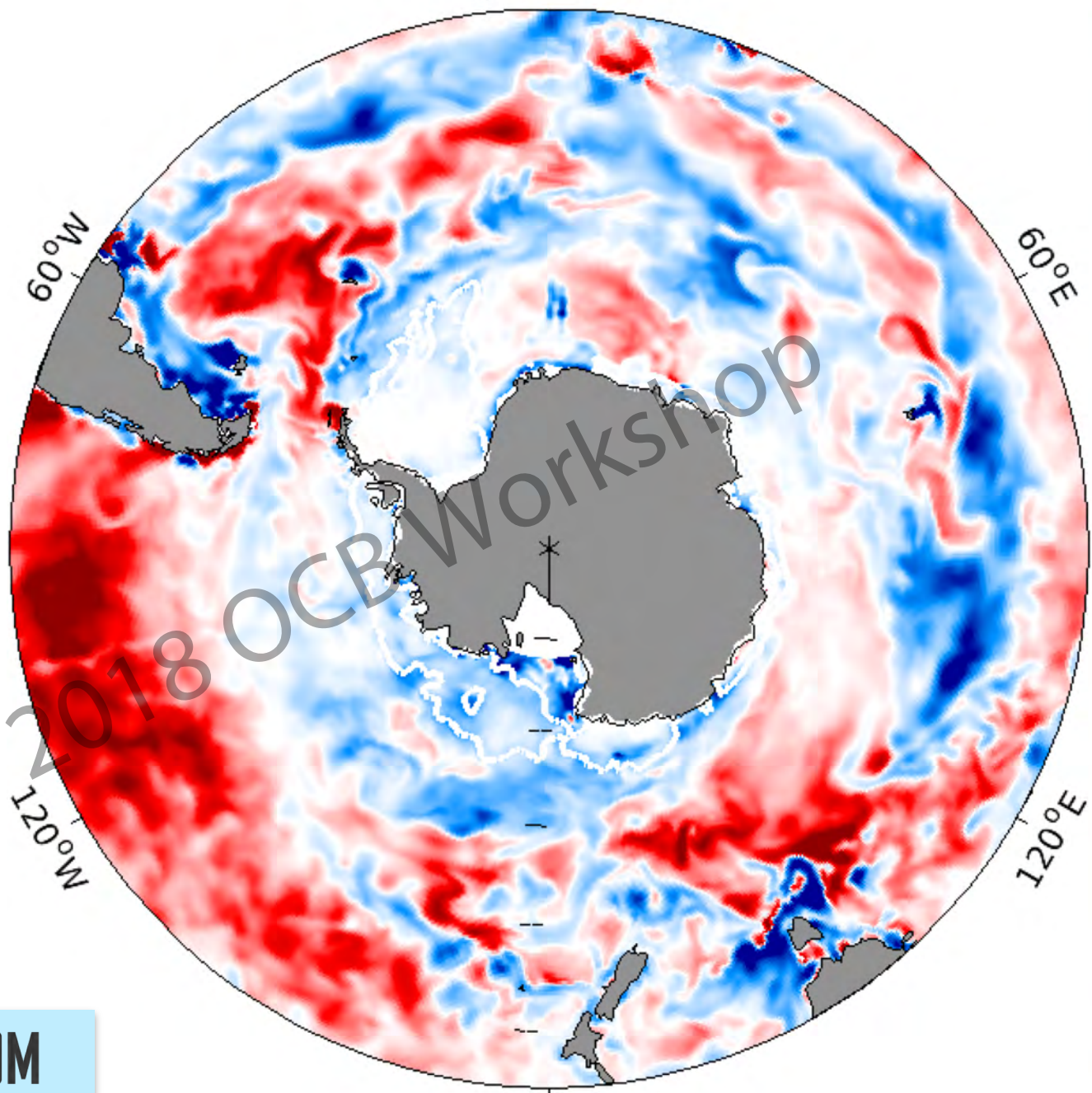


pCO₂ in Drake Passage



B-SOSE is giving a “low-pass” estimate of normal

05-Jan-2008



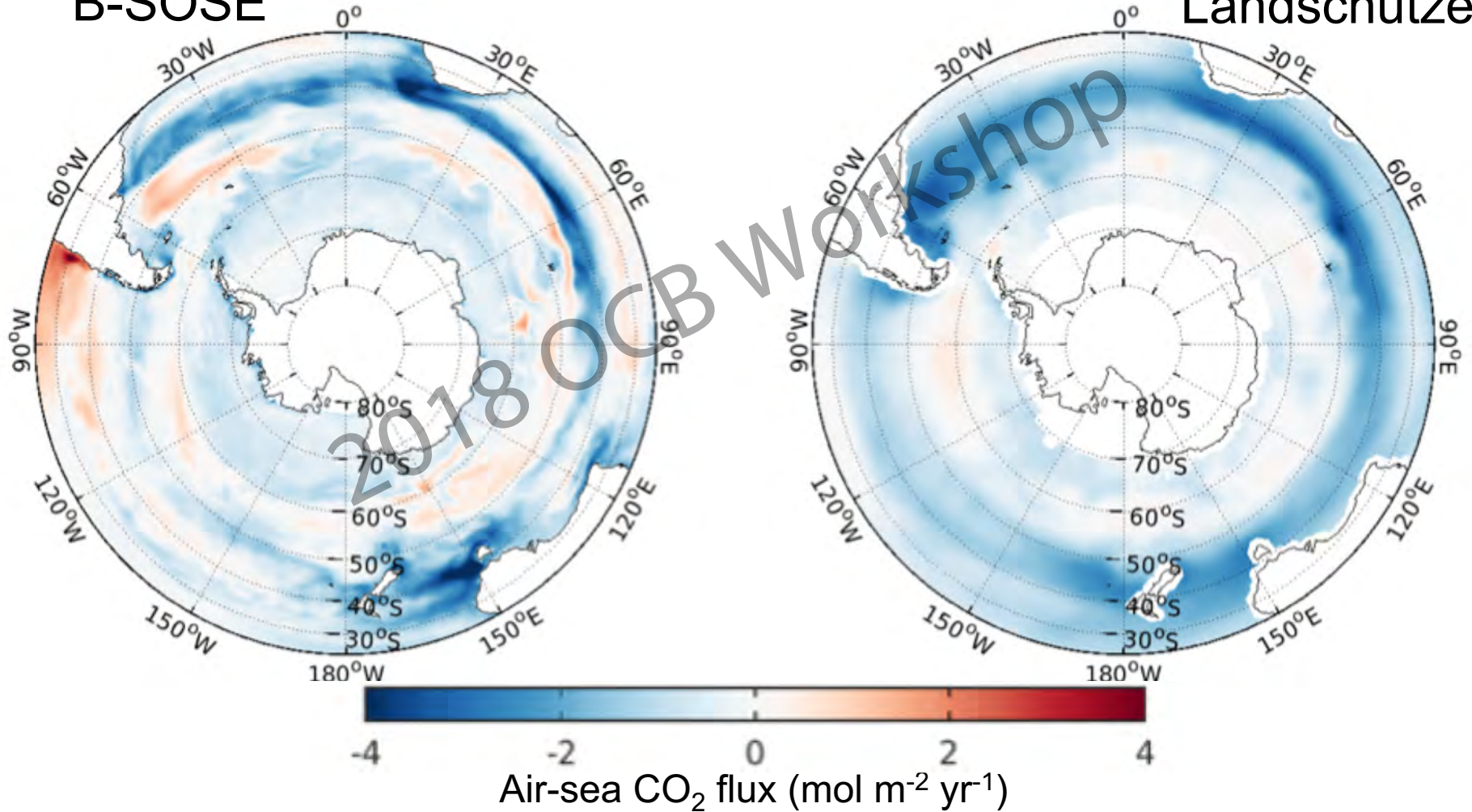
Air-sea CO₂ flux
[mol m⁻² yr⁻¹]
from B-SOSE
2008 - 2012
solution



SOCCOM

B-SOSE

Landschutzer





What's working, what not, what's next?

working:



- Multiyear BGC data assimilation via adjoint method at $1/3^\circ$.
- Closed budgets for BGC variables (DIC, ALK, O_2 , NO_3 , PO_4 , Fe).
- SOCCOM float observations as constraints.
- Establishing a BLING and B-SOSE international user base.

not working:



- CO_2 flux seasonal cycle out of phase with observations in some regions.
- In general: Biological activity weak. Surface pCO_2 high. pH low.
- Mid-lat. NCP low and Argentine Basin misfits large due to circulation
- Multigrid 4D-Var optimization at $1/6^\circ$. Some development needed.
- Some outliers still present in data constraints

next:

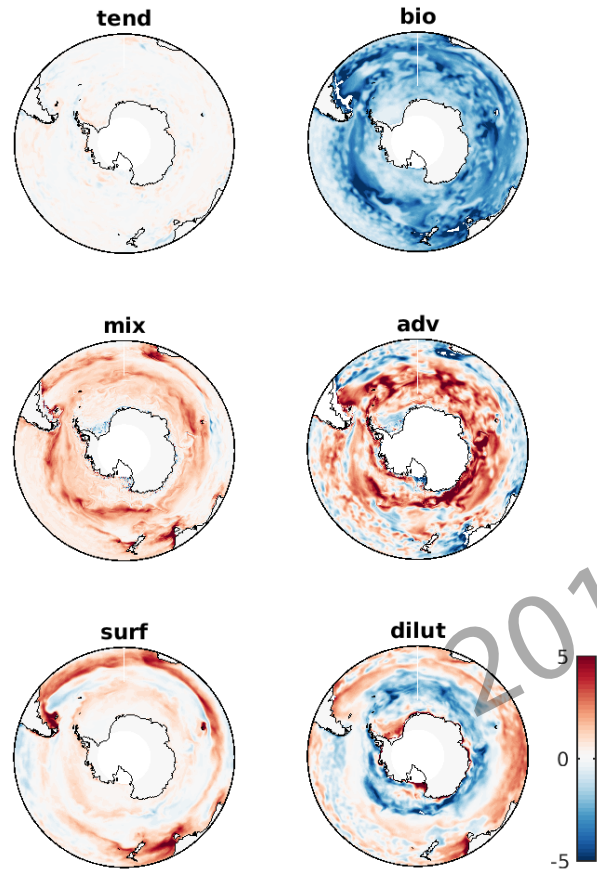


- Optical constraints and improved mixed layer fidelity for BGC.
- Removal of remaining outliers
- Reporting of misfit statistics to aid SOCCOM QC effort.
- Publication of $1/6^\circ$ B-SOSE for 2013-2017, dissemination via LAS.
- Multigrid optimization at $1/6^\circ$ for improved 2013-2018 B-SOSE.
- Extend validation to include other quantities of interest (e.g. NCP).

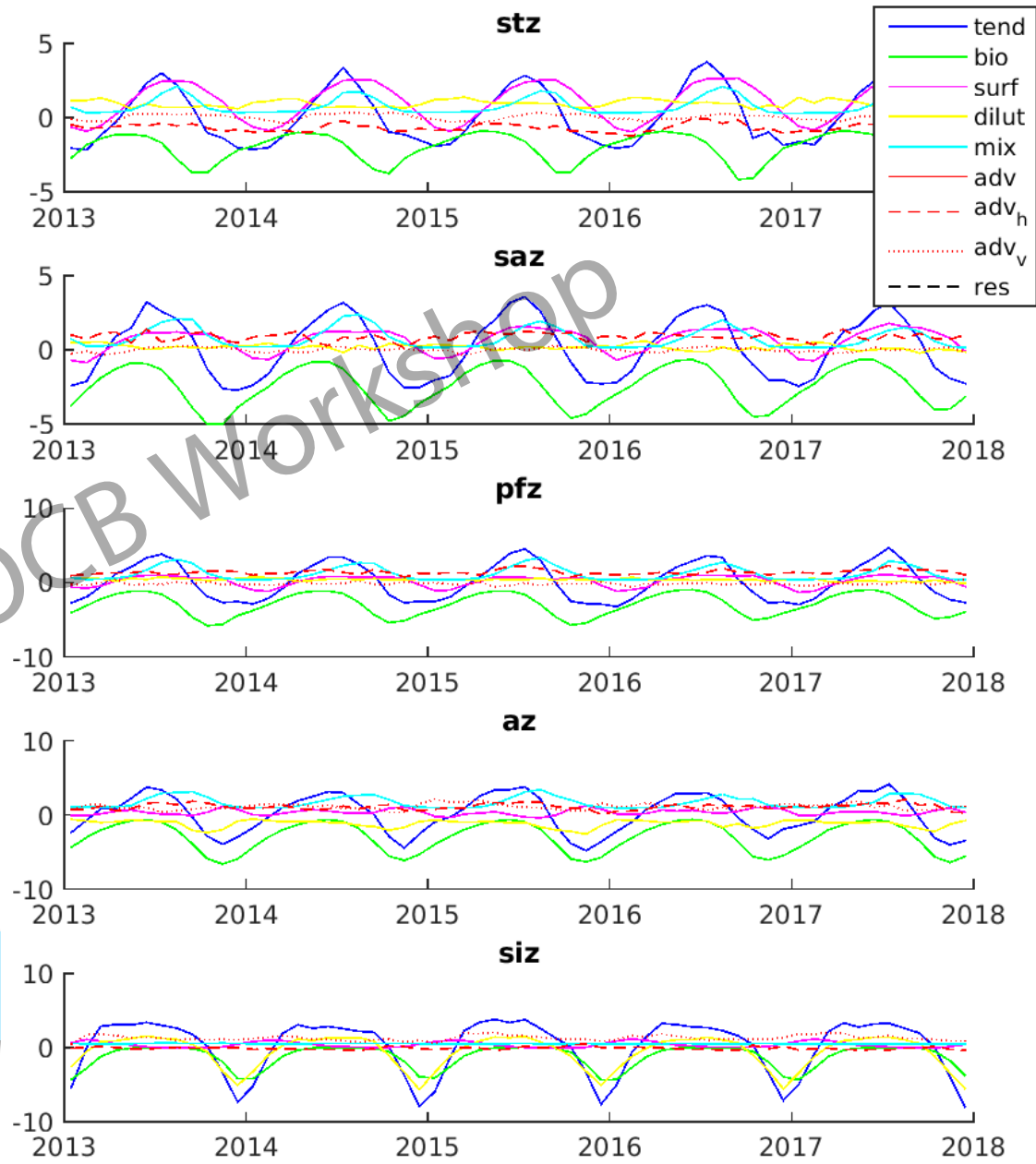
DIC budget for five regions of the Southern Ocean

<http://sose.ucsd.edu/budgets/>

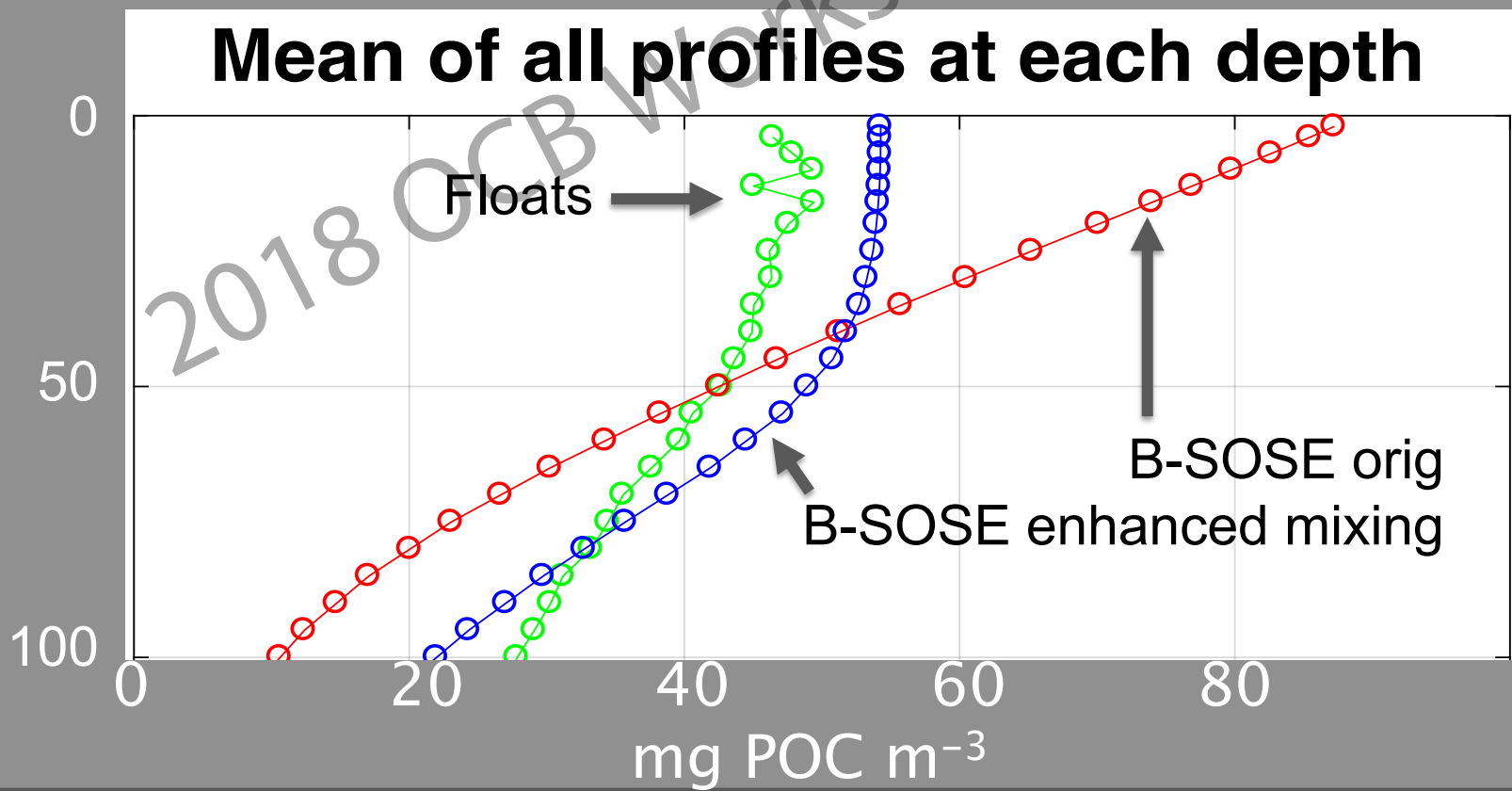
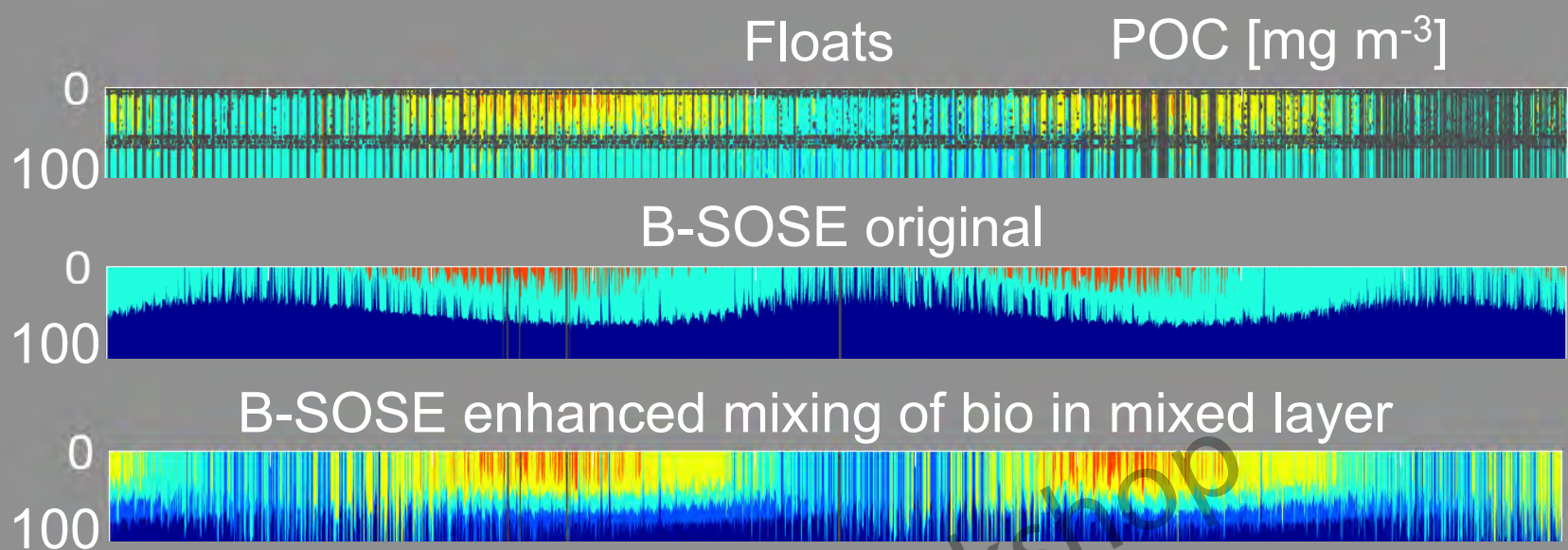
Mean



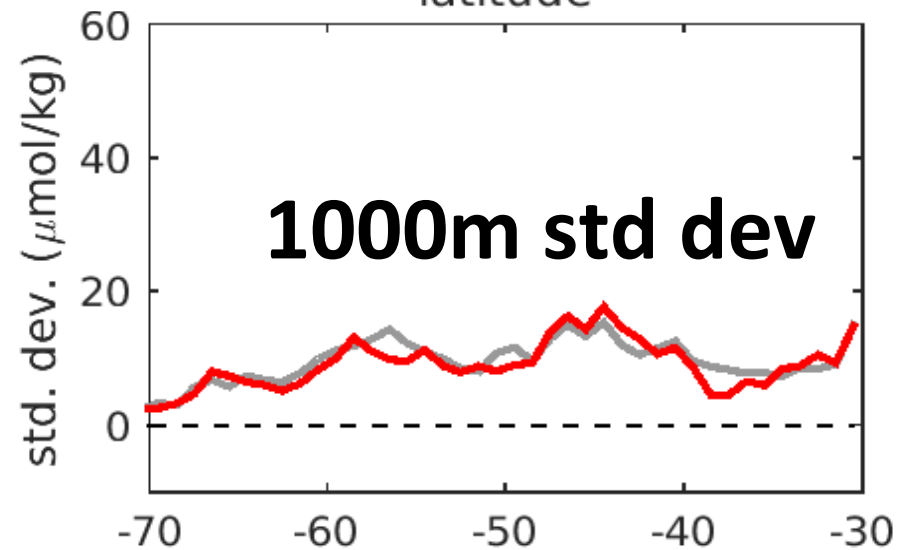
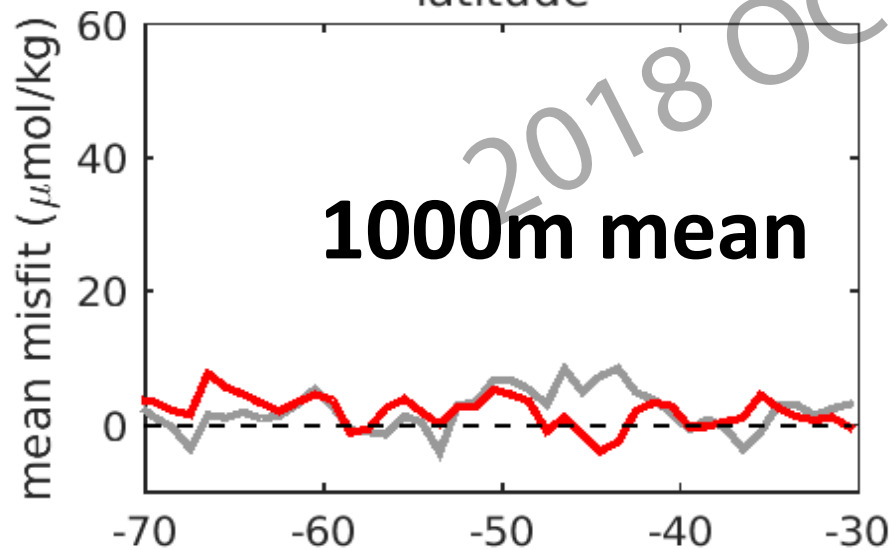
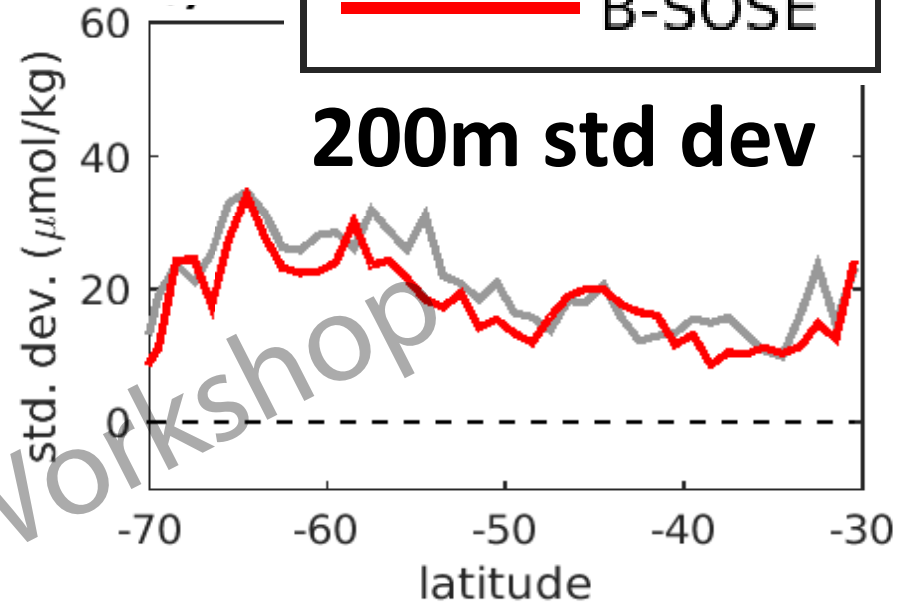
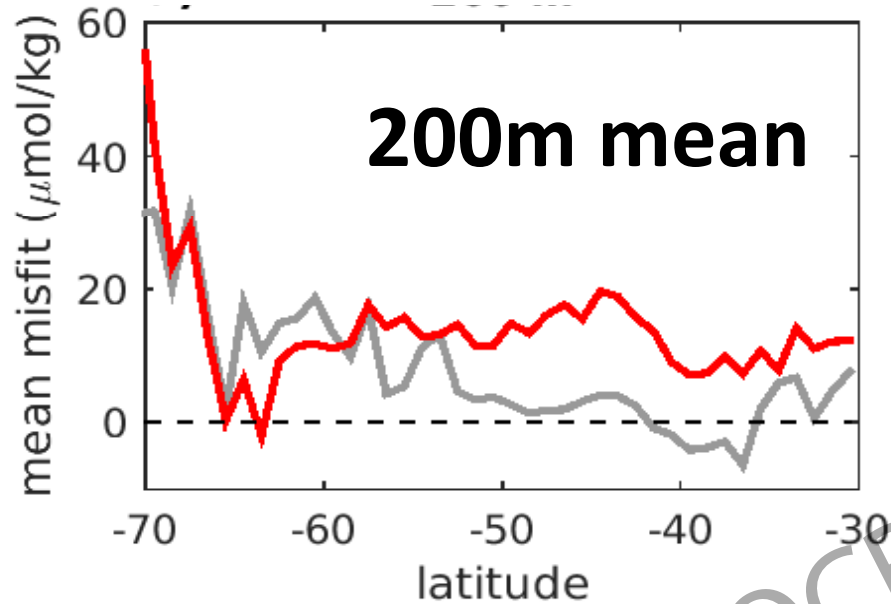
Time series



SOCCOM



2008 – 2012 B-SOSE Fit to O₂

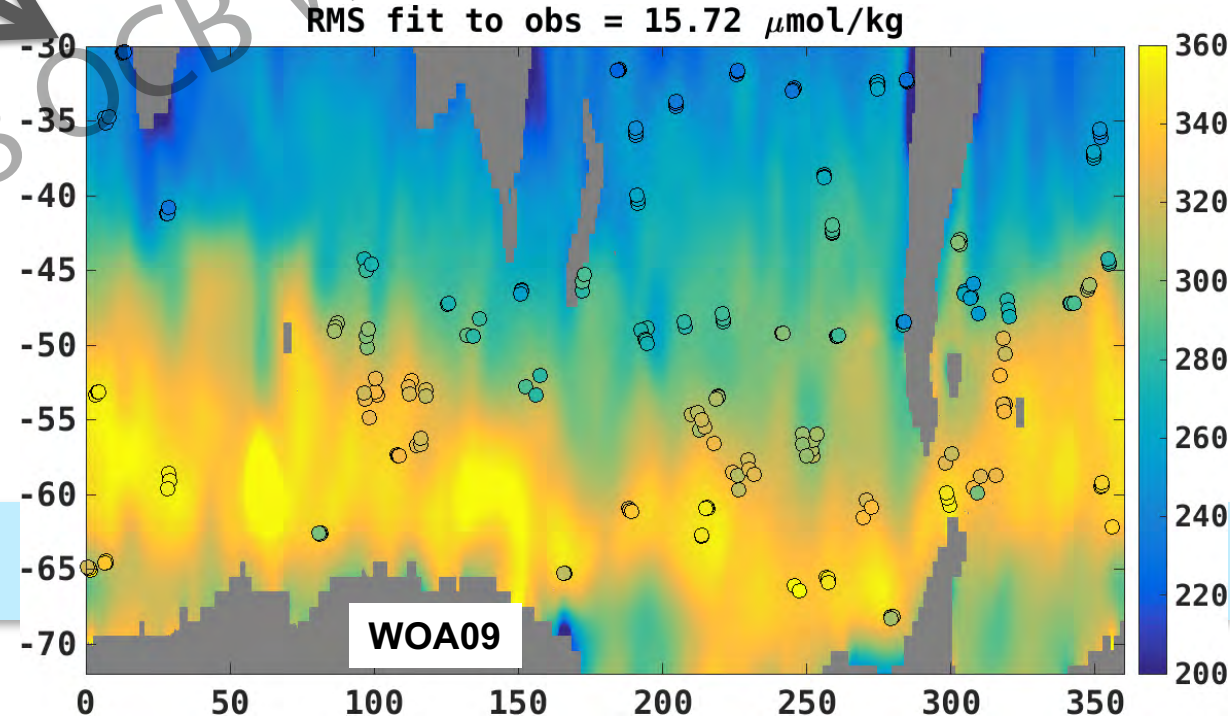
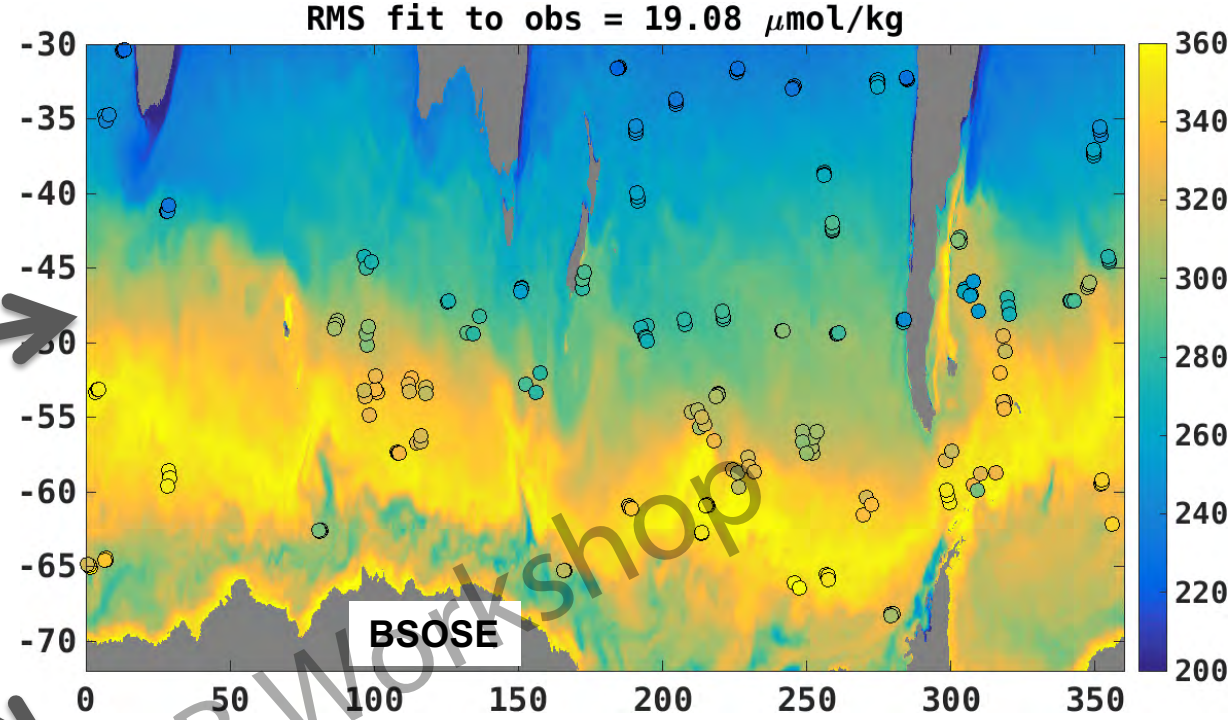


Dec. 2017 oxygen at 55 m.
BGC-Argo observations
shown with filled circles.

B-SOSE Iteration 121.
RMS fit to obs: 19.08
 $\mu\text{mol/kg}$

World Ocean Atlas 2013
climatology. RMS fit to
obs: 15.72 $\mu\text{mol/kg}$

WOA 18% more
consistent with obs.

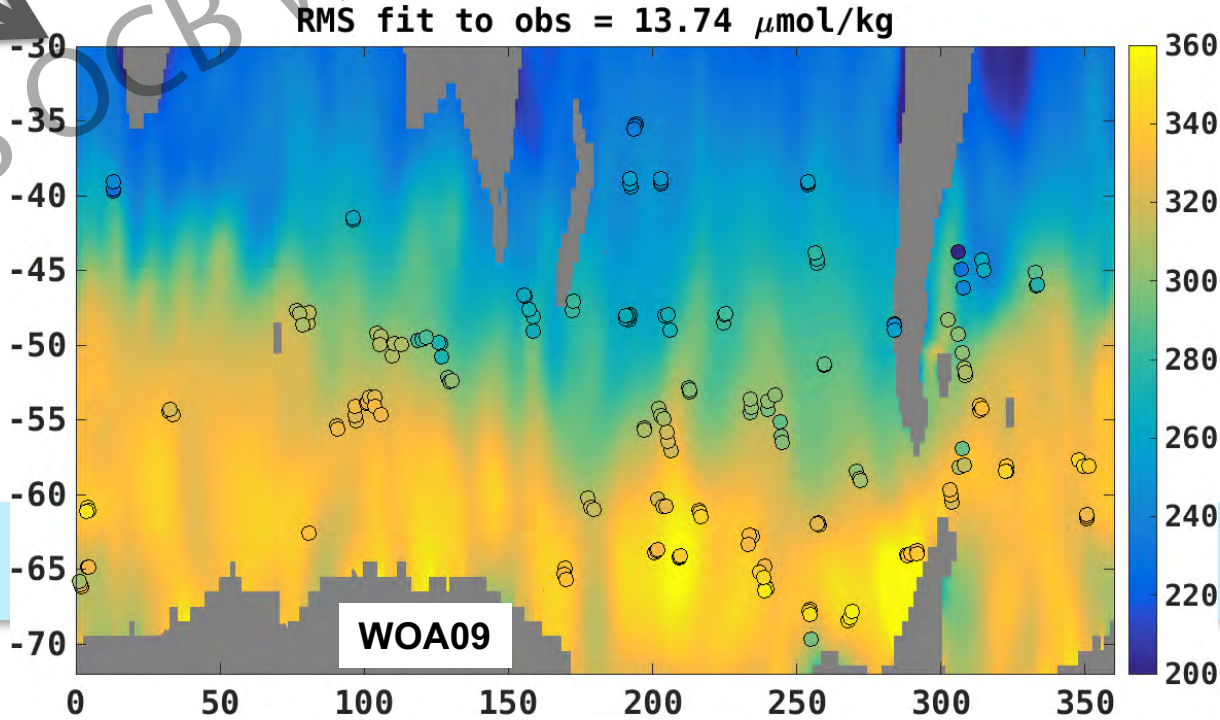
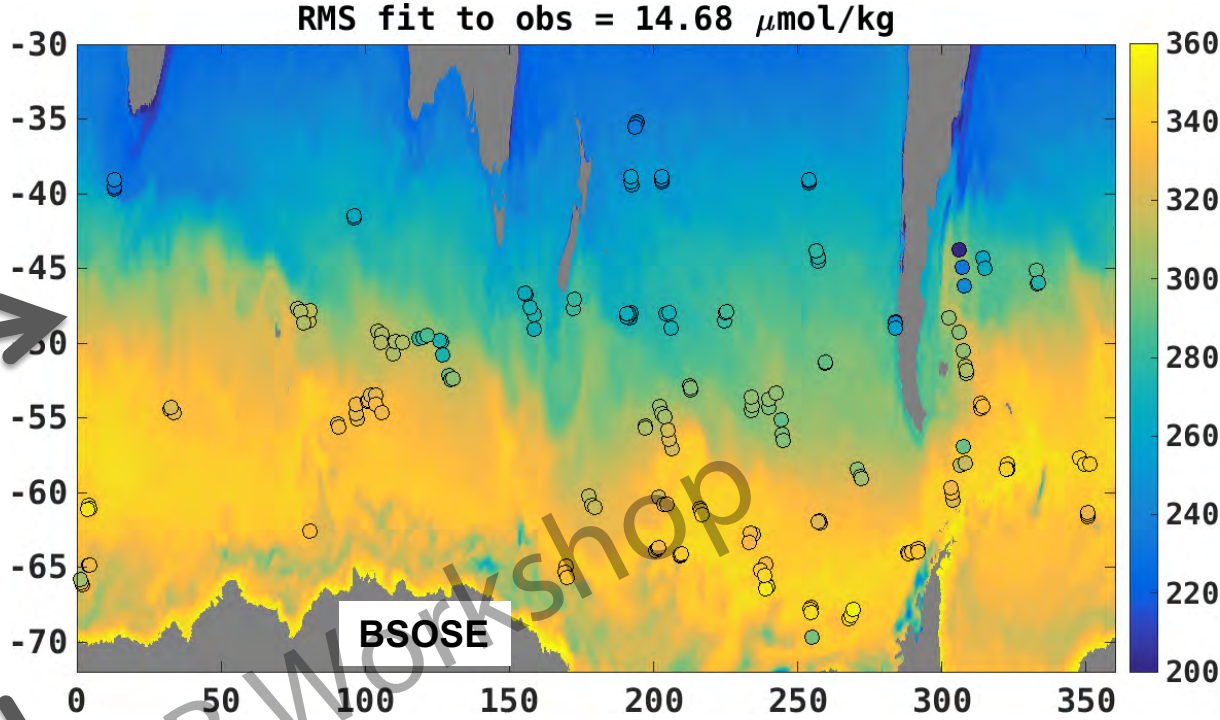


June 2017 oxygen at 55 m. BGC-Argo observations shown with filled circles.

B-SOSE Iteration 121.
RMS fit to obs: 14.68 $\mu\text{mol/kg}$

World Ocean Atlas 2013 climatology.
RMS fit to obs: 13.74 $\mu\text{mol/kg}$

WOA 6% more consistent with obs.



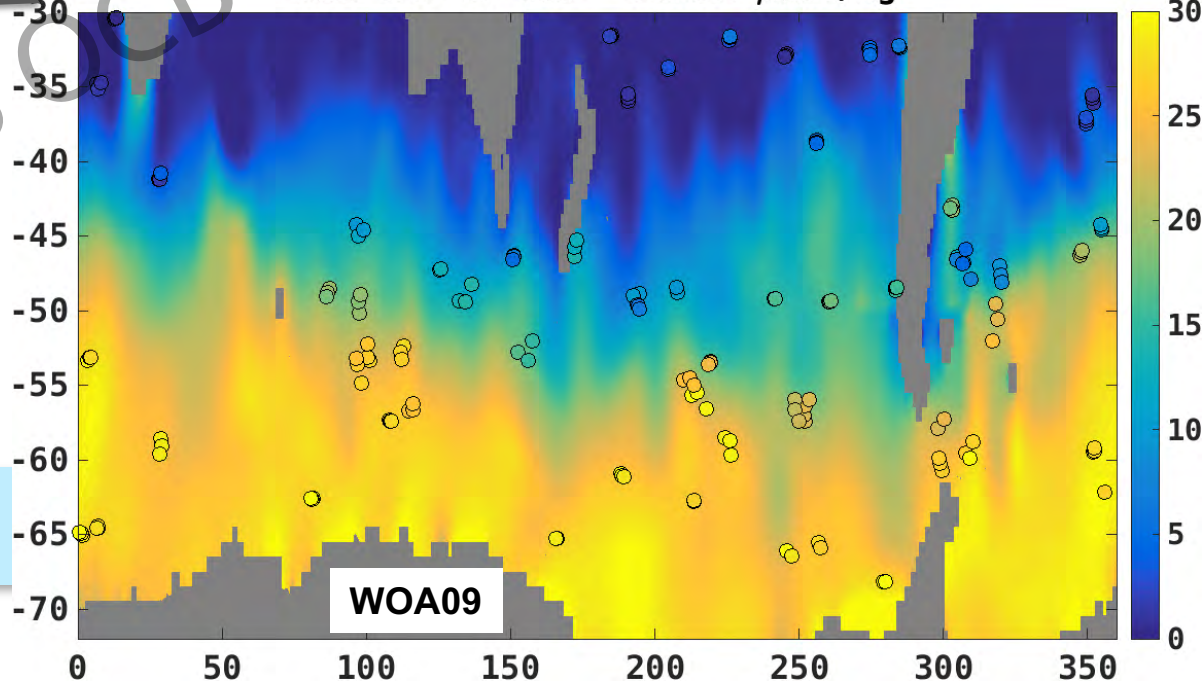
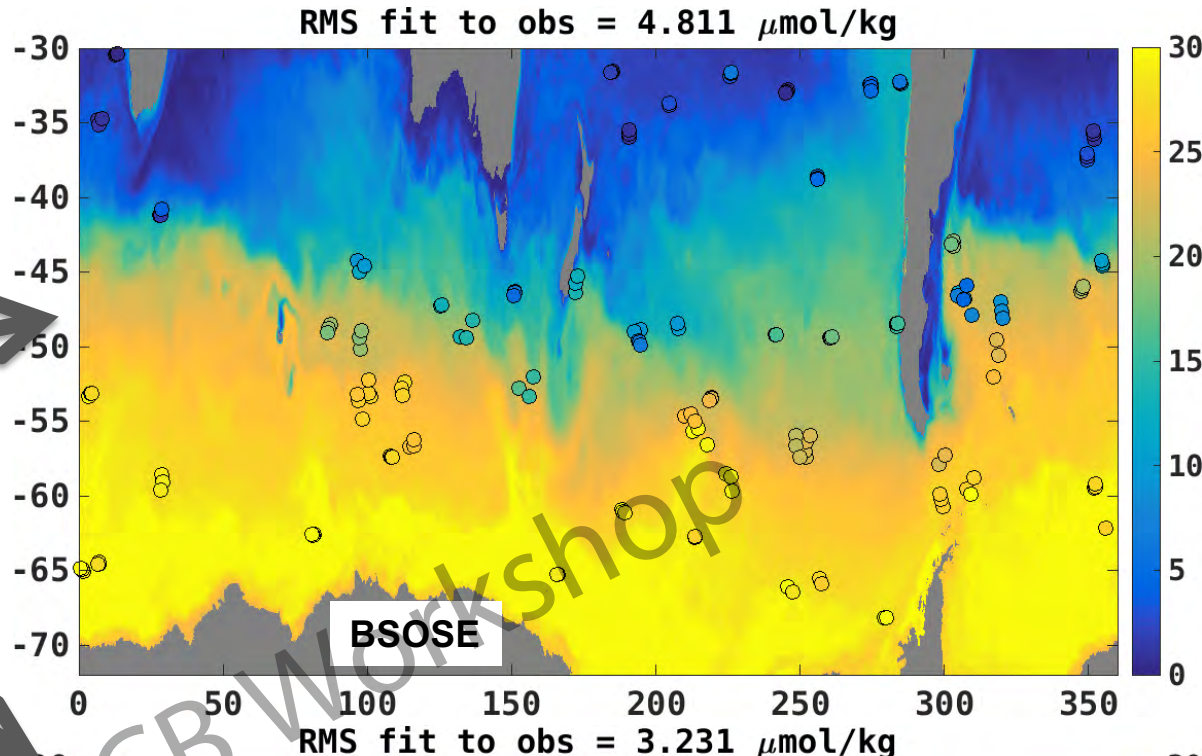
SOCCOM

Dec. 2017 nitrate at 55 m.
BGC-Argo observations
shown with filled circles.

B-SOSE Iteration 121.
RMS fit to obs: 19.08
 $\mu\text{mol/kg}$

World Ocean Atlas 2013
climatology. RMS fit to
obs: 15.72 $\mu\text{mol/kg}$

WOA 33% more
consistent with obs.

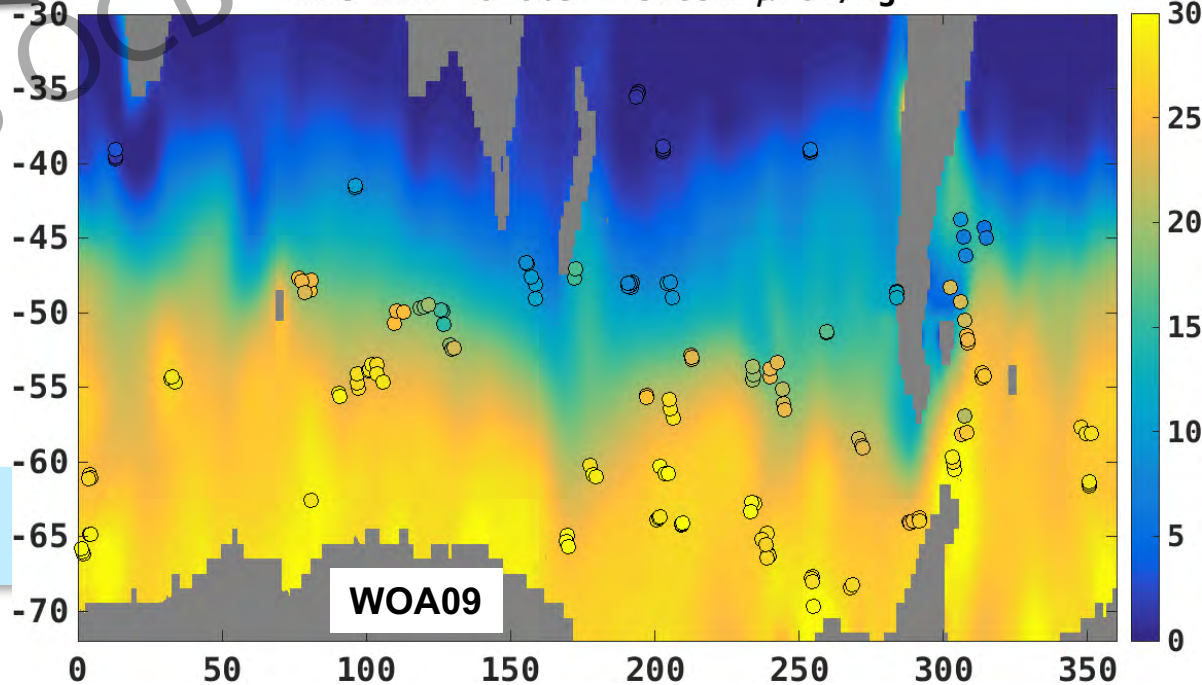
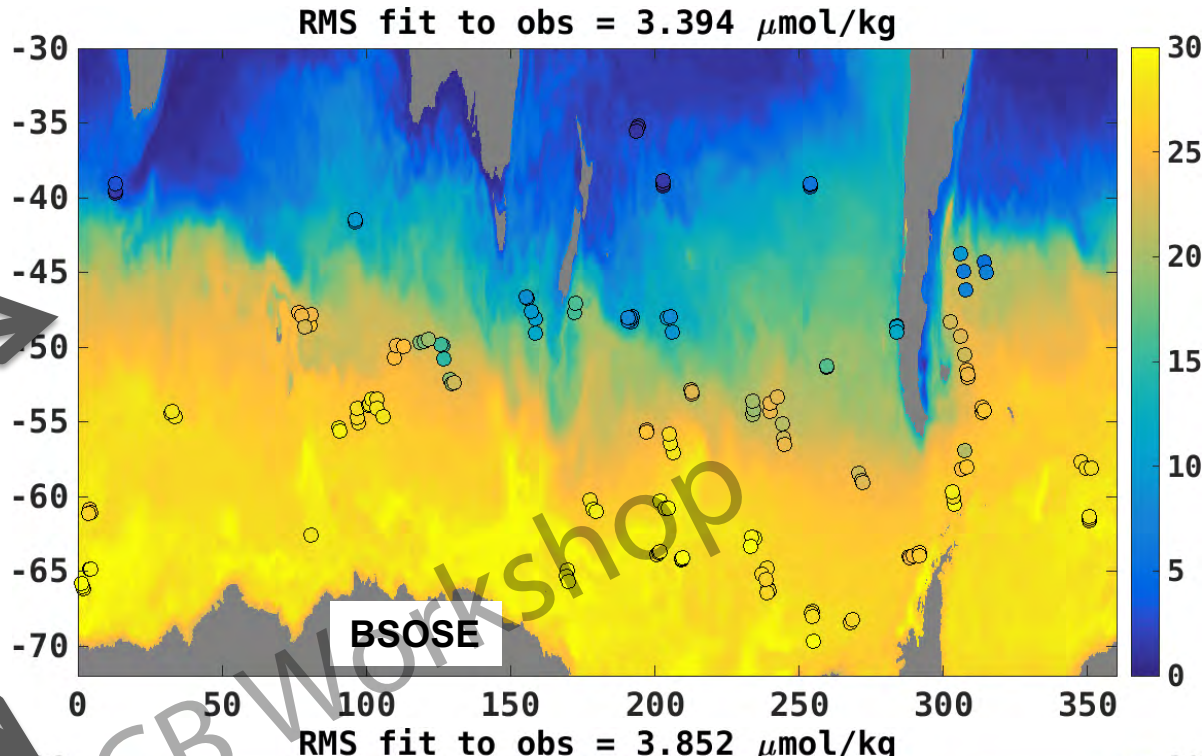


June 2017 nitrate at 55 m.
BGC-Argo observations
shown with filled circles.

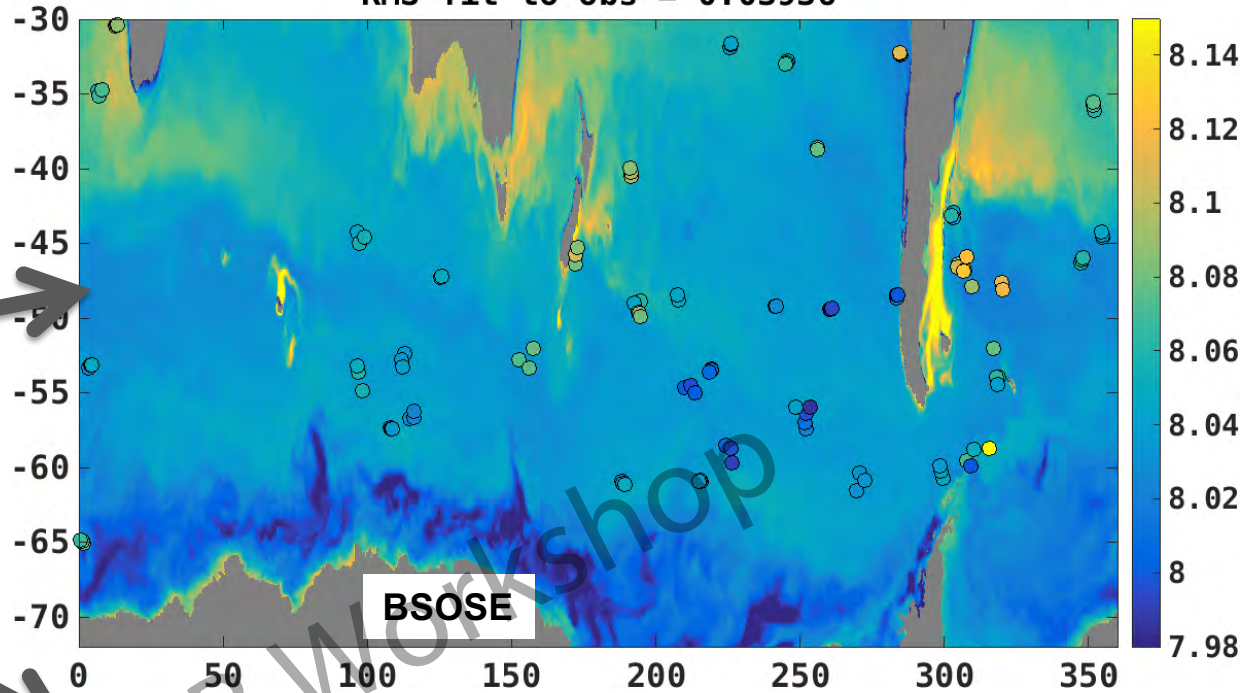
B-SOSE Iteration 121.
RMS fit to obs: 3.4
 $\mu\text{mol/kg}$

World Ocean Atlas 2013
climatology. RMS fit to
obs: 3.9 $\mu\text{mol/kg}$

B-SOSE 12% more
consistent with obs.



RMS fit to obs = 0.03936



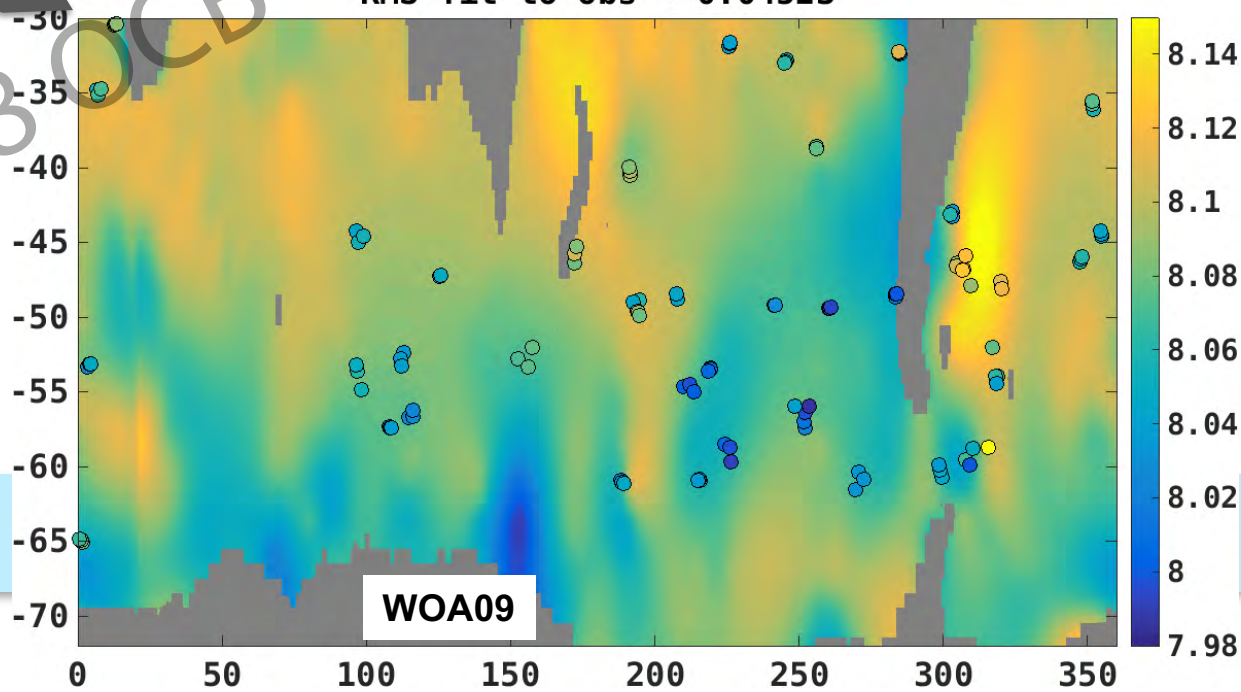
Dec. 2017 pH at 55 m.
BGC-Argo observations
shown with filled circles.

B-SOSE Iteration 121.
RMS fit to obs: 0.04

GLODAPv2 mean map.
RMS fit to obs: 0.05

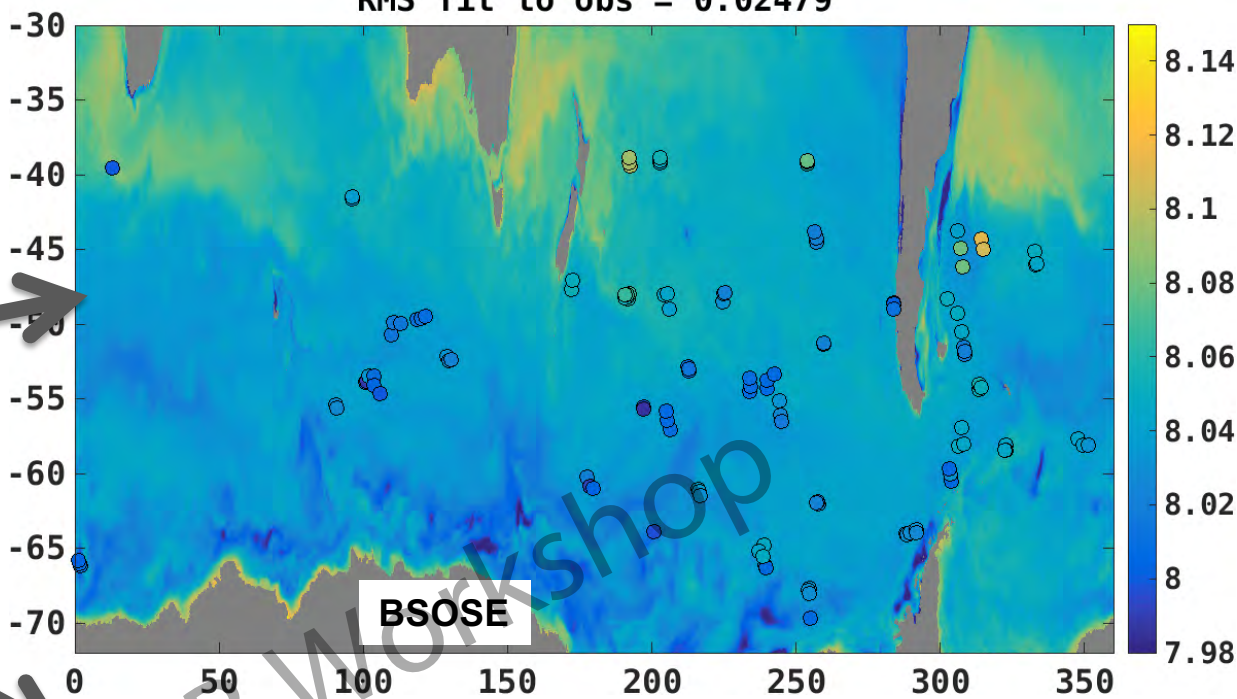
B-SOSE 13% more
consistent with obs.

RMS fit to obs = 0.04523



SOCCOM

RMS fit to obs = 0.02479

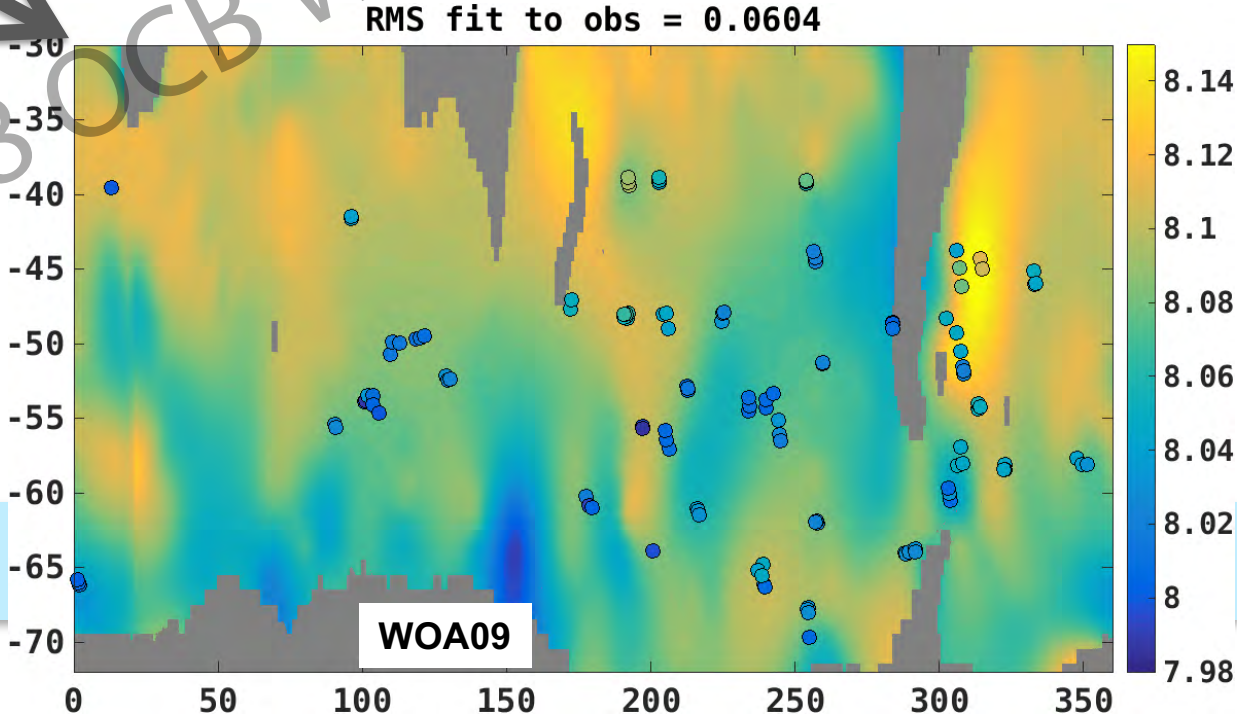


June 2017 pH at 55 m.
BGC-Argo observations
shown with filled circles.

B-SOSE Iteration 121.
RMS fit to obs: 0.02

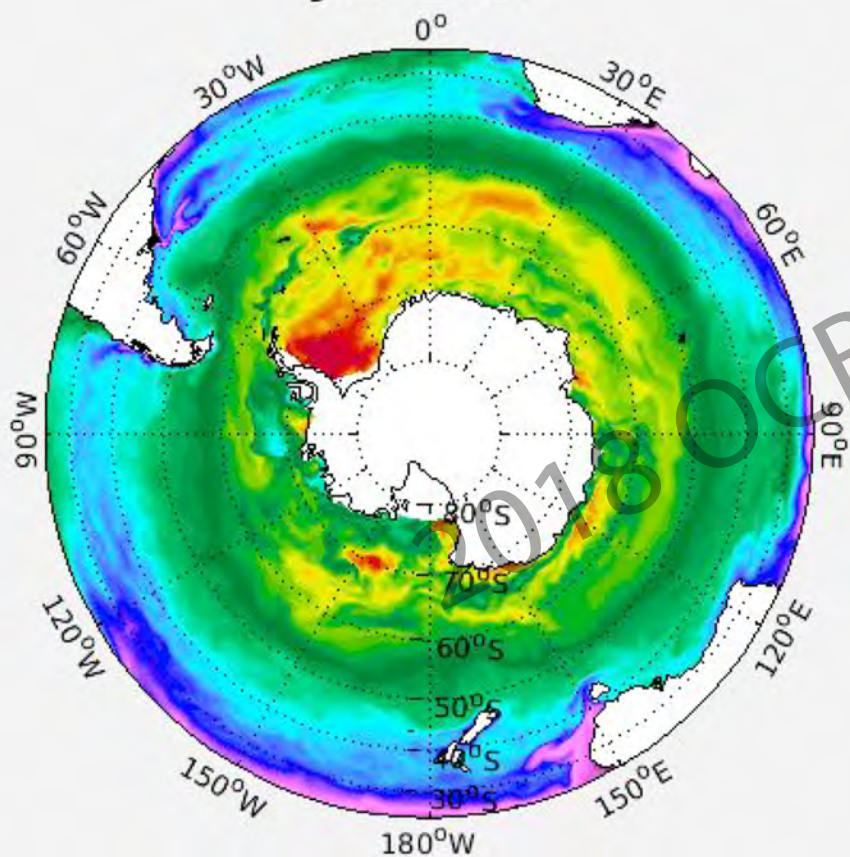
GLODAPv2 mean map.
RMS fit to obs: 0.06

B-SOSE 59% more
consistent with obs.

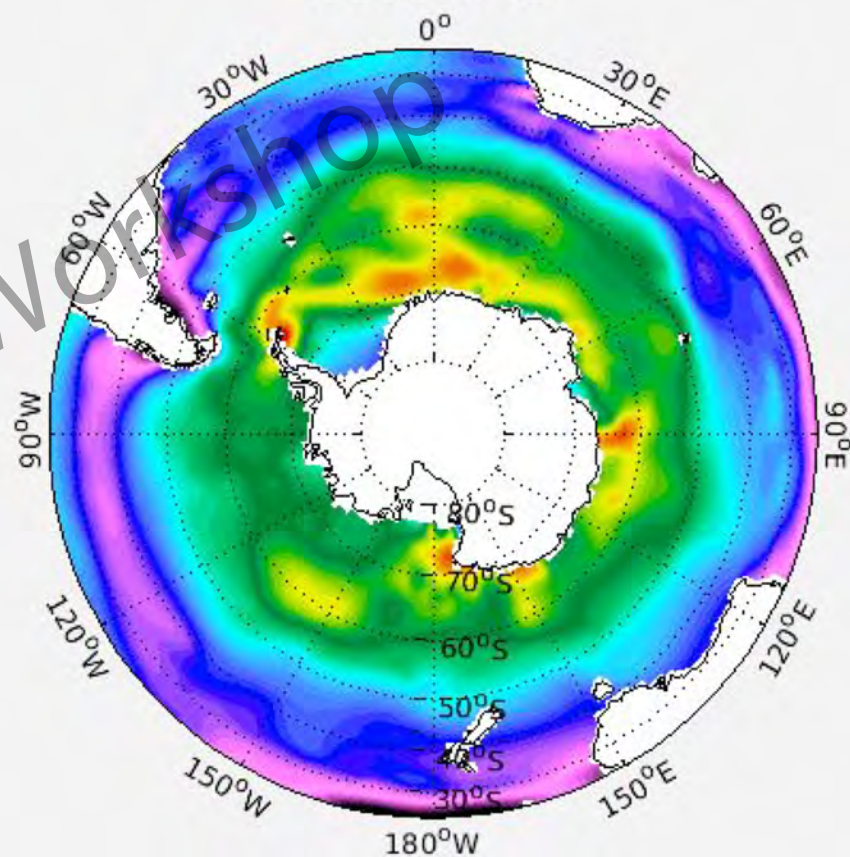




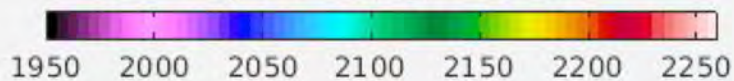
JAN 2013



GLODAPv2



DIC ($\mu\text{mol/kg}$) at 10 m



Validation

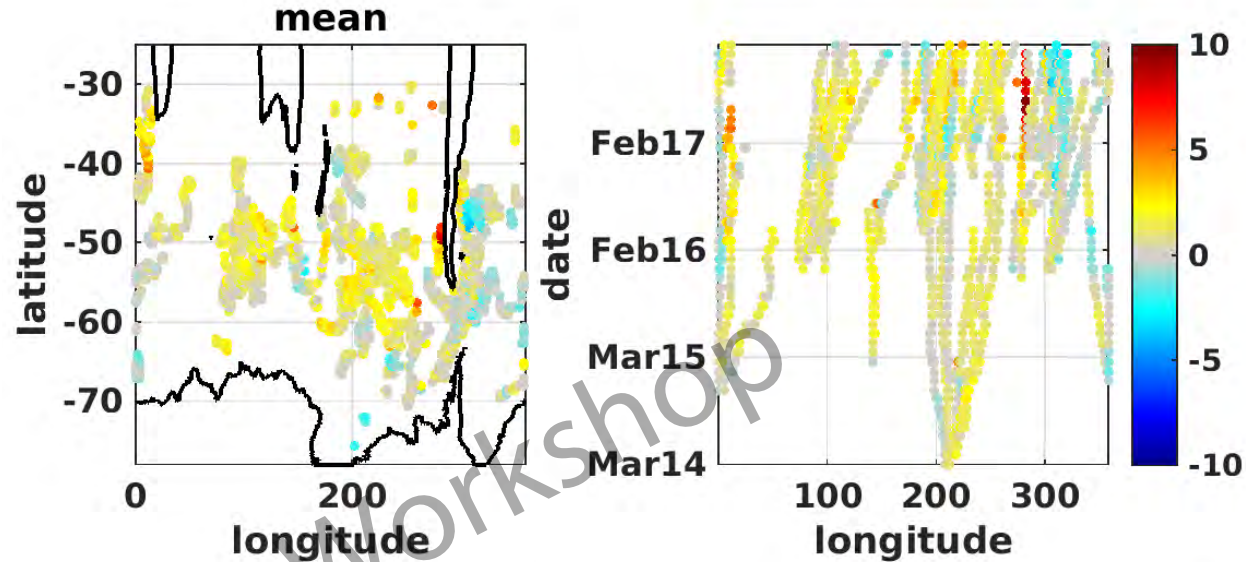
Hold the *model* accountable to the *data*

AND ALSO

Hold the *data* accountable to the *model*

Feedback to QC effort. Now posting table of largest normalized misfits.

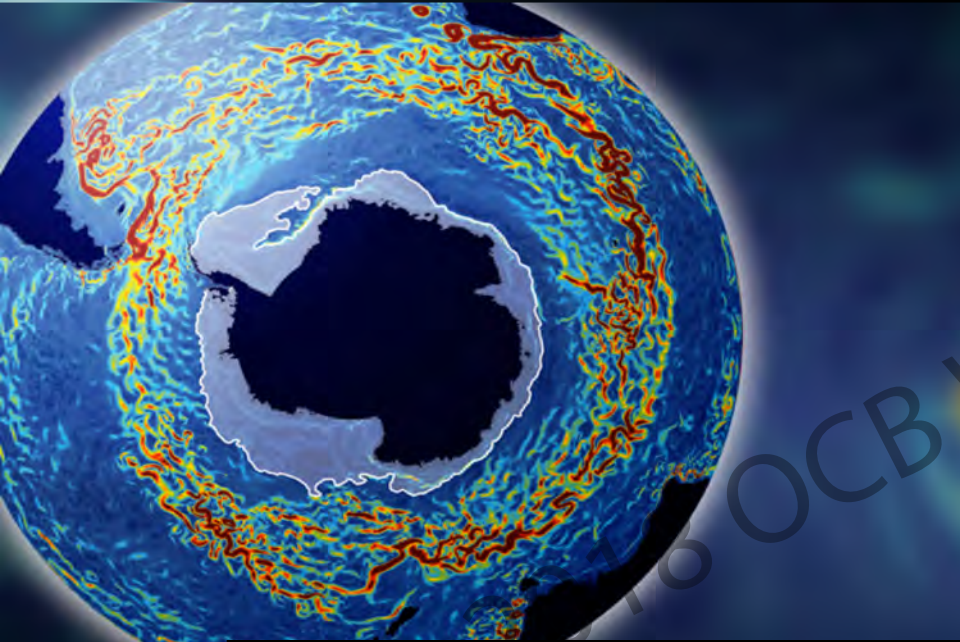
Normalized pH misfit



PH								
	Norm misfit	long	lat	depth	year	month	day	meta
1	15.1951	249.878	-48.331	375	2016	10	14	VIZ-9031LIAR//5904396-127
2	14.864	249.965	-48.424	375	2016	10	24	VIZ-9031LIAR//5904396-128
3	13.7959	249.965	-48.424	400	2016	10	24	VIZ-9031LIAR//5904396-128
4	13.6787	249.878	-48.331	400	2016	10	14	VIZ-9031LIAR//5904396-127
5	13.2064	221.665	-47.889	1700	2015	3	16	VIZ-9018LIAR//5904186-065
6	12.006	189.074	-46.714	600	2016	6	12	VIZ-9762LIAR//5904765-002
7	11.9587	189.074	-46.714	650	2016	6	12	VIZ-9762LIAR//5904765-002
8	11.8913	221.665	-47.889	1600	2015	3	16	VIZ-9018LIAR//5904186-065
9	11.7939	221.665	-47.889	1000	2015	3	16	VIZ-9018LIAR//5904186-065
10	11.754	249.878	-48.331	350	2016	10	14	VIZ-9031LIAR//5904396-127
11	11.7039	221.665	-47.889	1500	2015	3	16	VIZ-9018LIAR//5904186-065
12	11.5672	221.665	-47.889	1400	2015	3	16	VIZ-9018LIAR//5904186-065
13	-11.5256	311.423	-58.413	10	2016	11	24	VIZ-9652LIAR//5904660-032



BGC-Argo is achieving substantial in situ coverage. Now appropriate to construct a state estimate synthesizing observations and the laws of nature represented by a model



State estimate goals:

- Propagate observational information via model dynamics.
- Produce a gridded data set consistent with model physics and observations, increasing accessibility
- Provide quantitative baselines: Estimating the “normal” and a framework to understand the “normal”

sose.ucsd.edu

Input and output freely available

Code is well-document and on github

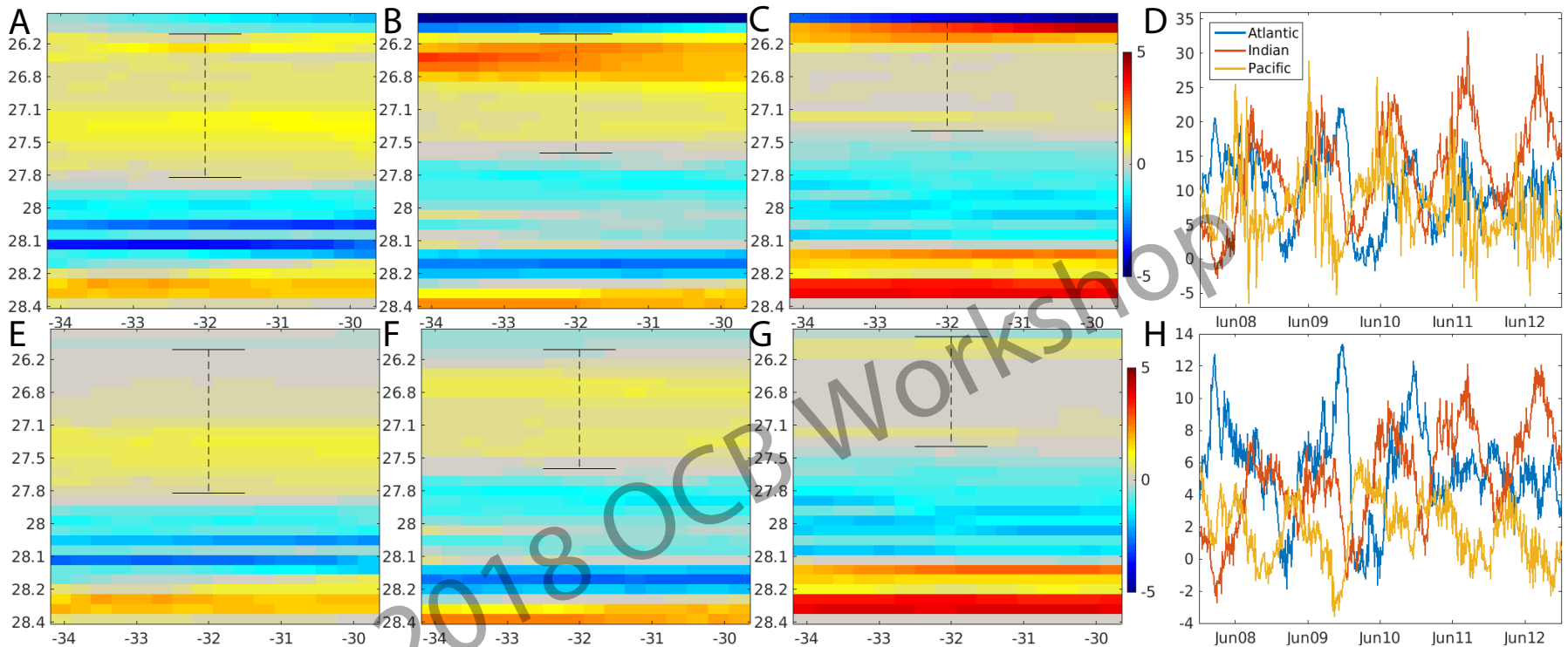
Verdy and Mazloff, 2017. JGR.



SOCCOM

2018 OCB Workshop

Nitrate transport



Volume transport in neutral density, γ , layers for the (A) Atlantic, (B) Indian, and (C) Pacific sectors of the Southern Ocean in Sv. Nitrate transport in γ -layers is shown below (E, F, G) in Tmol/yr. The transport is quantified across 32°S into the Atlantic Ocean for the layer $25.99 < \gamma < 27.76$, into the Indian Ocean for the layer $25.99 < \gamma < 27.55$, and into the Pacific for the layer $25.18 < \gamma < 27.34$ for (D) volume and (H) nitrate (layers denoted by a dashed black line).

The mean volume transport is 9.71 ± 5.07 Sv, 13.09 ± 6.77 Sv, and 7.51 ± 5.18 Sv for the Atlantic, Indian, and Pacific Oceans, where the \pm gives the standard deviation from the 3-day average time series. The nitrate volume transport for these three basins is 5.57 ± 2.94 Tmol/yr, 5.09 ± 3.06 Tmol/yr, and 1.78 ± 1.91 Tmol/yr.

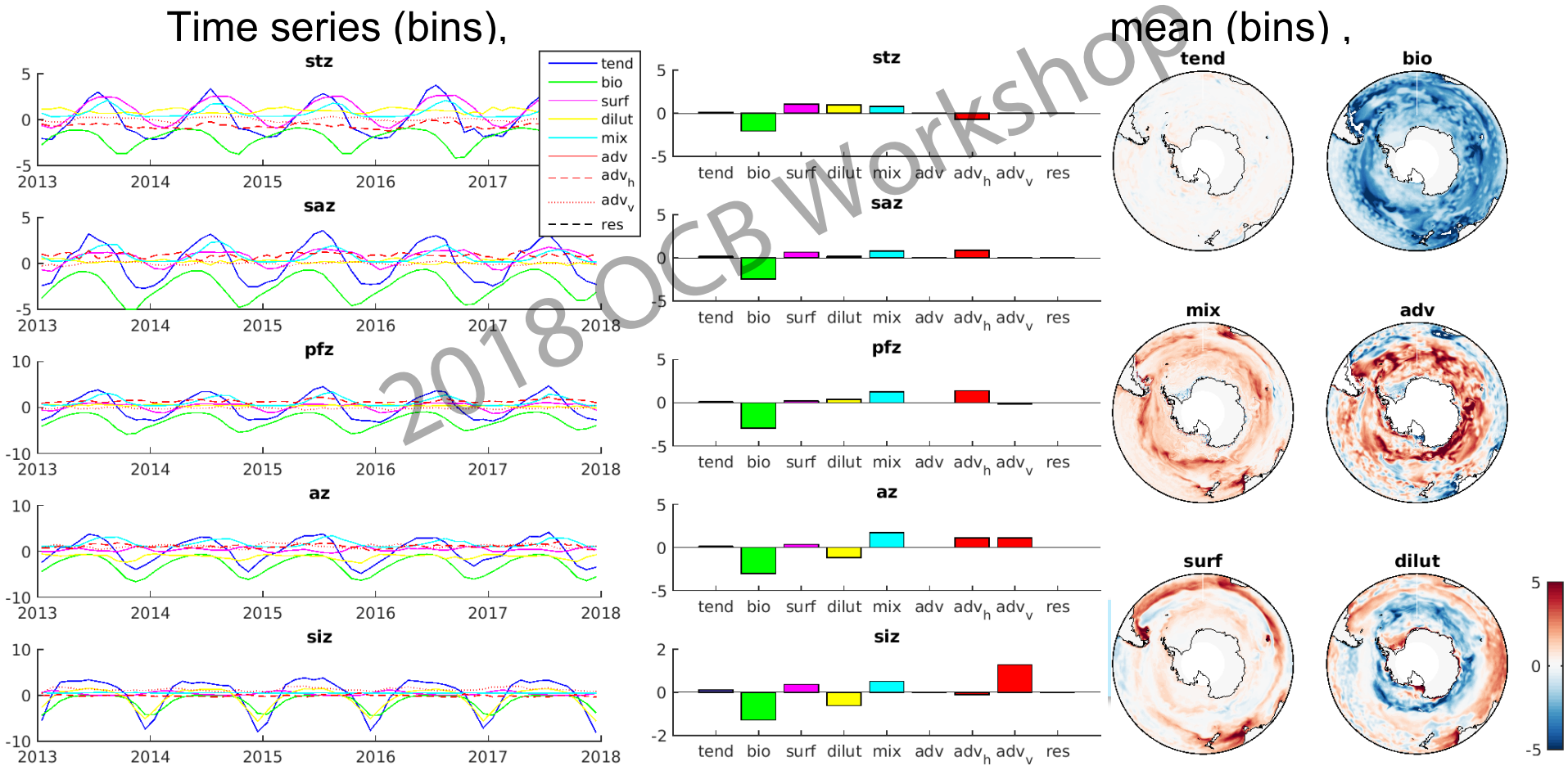
Budget diagnostic software and examples

<http://sose.ucsd.edu/budgets/>

BGC budgets being presented for BSOSE iteration 105 (2008-2012)

In development. Currently has: DIC, O₂, NO₃, and FE for top 150m and top 650m

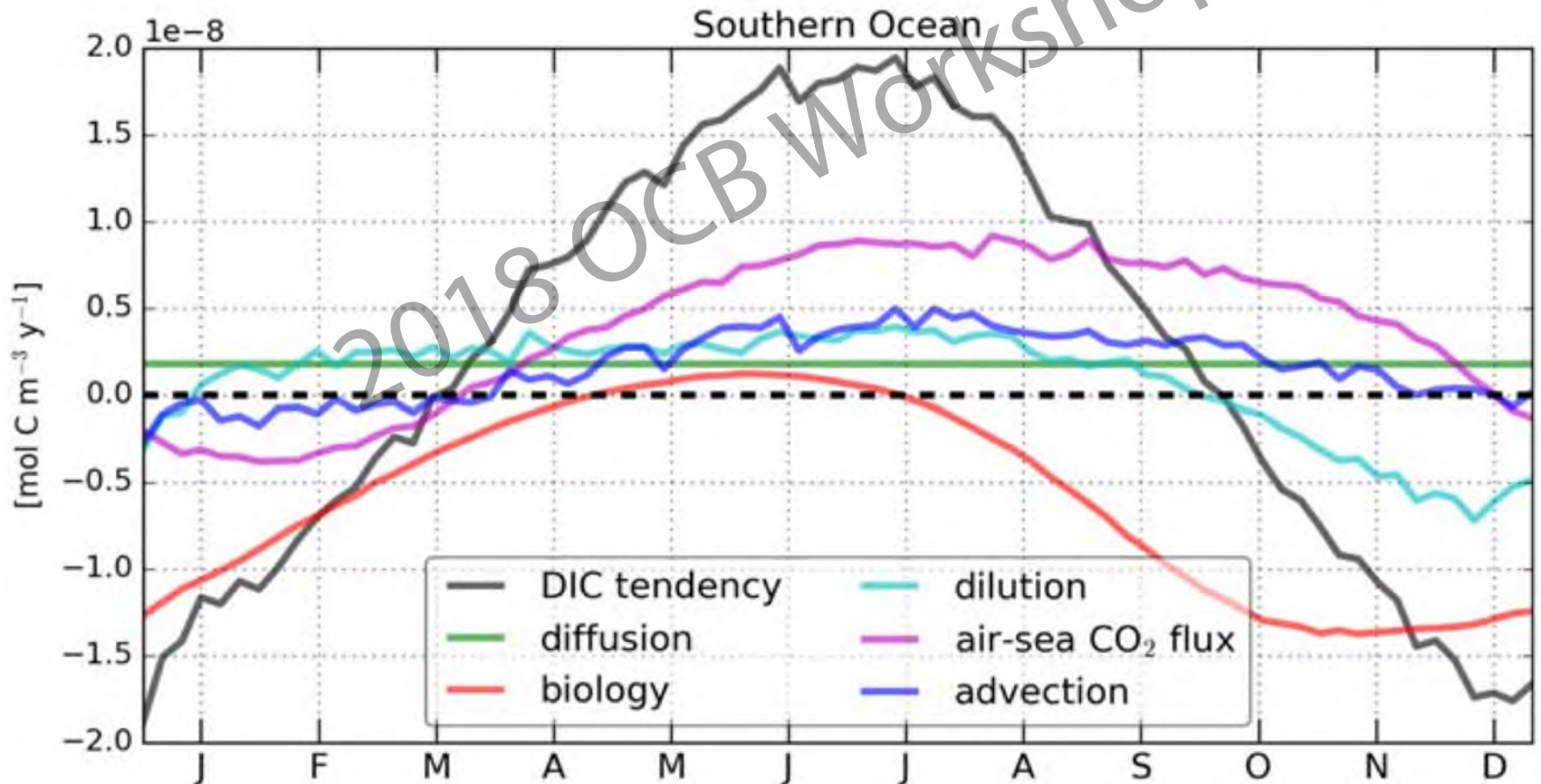
For five regions of the Southern Ocean we present:



The Southern Ocean DIC budget analyzed in a state estimate revealing the impact of components at various time and space scales. **Rosso et al., 2017**

Seasonal cycle averaged 26.6°-78°S =>

$$\text{adv} + \text{dif} + \text{bio}, \text{air-sea}, \text{dilution} = d\text{DIC}/dt$$





Extensive work on observing system design and mapping methods using the B-SOSE model, machine learning techniques, float data, and satellite data

- ❖ Correlation scales of heat and carbon content and their fluxes as first guess at observational density requirements. **Mazloff et al., 2018**

Mazloff et al., 2018

- ❖ Assessment of importance of sampling strategy and T,S covariance for NO₃ reconstruction. **Liang et al., 2018**

Liang et al., 2018

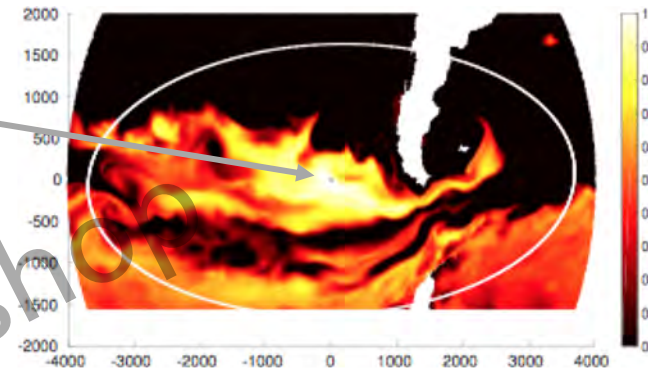
- ❖ Assessment of importance of covariance and sampling strategy for mapping O₂ at 100 m via “Random Forest” machine learning technique. **Giglio et al., 2018**

Giglio et al., 2018

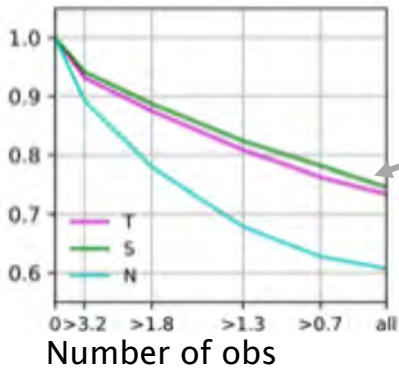
- ❖ Methodology developed to estimate where a float will be in 100 days based on 1/12° model. Validate estimate with actual trajectories. **Wang et al., 2018**

Wang et al., 2018

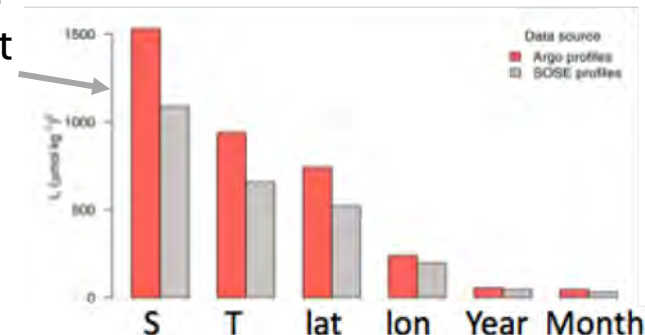
Correlation to OOI location



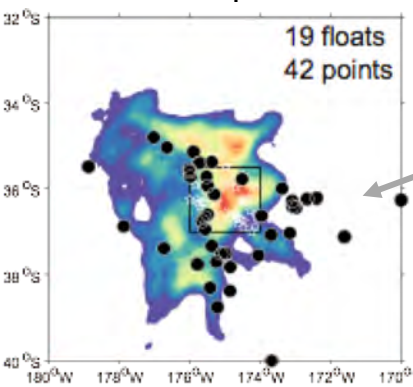
Error



Importance of variable



PDF of final position



Changing biogeochemical budgets and the role of the ocean in climate and supporting marine resources

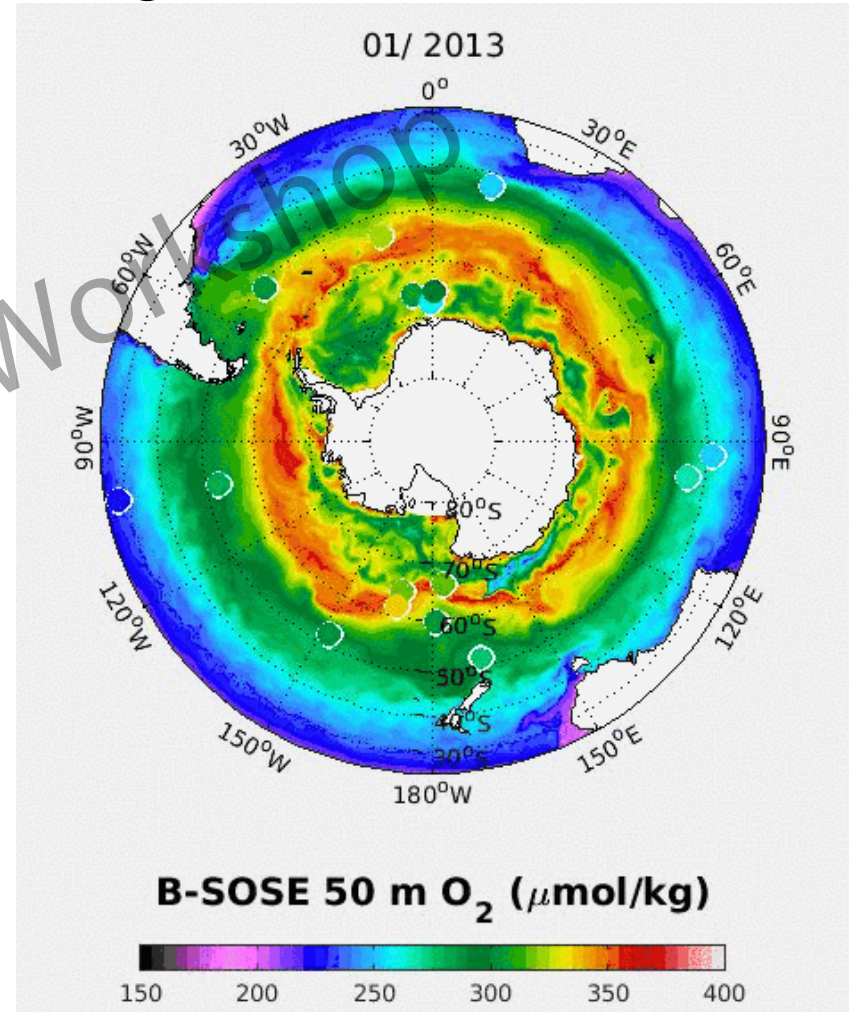
For B-SOSE results and validation:

<http://sose.ucsd.edu/>

Don't hesitate to request diagnostics or assistance with analysis!

References:

- Verdy and Mazloff, 2017. A data assimilating model for estimating Southern Ocean biogeochemistry. *JGR*.
- Rosso, Mazloff, Verdy, and Talley, 2017. Space and time variability of the Southern Ocean carbon budget. *JGR*.
- Mazloff, Cornuelle, Gille, and Verdy, 2018. Correlation Lengths for Estimating the Large-Scale Carbon and Heat Content of the Southern Ocean. *JGR*.



O₂ at 50m. Floats superimposed on B-SOSE