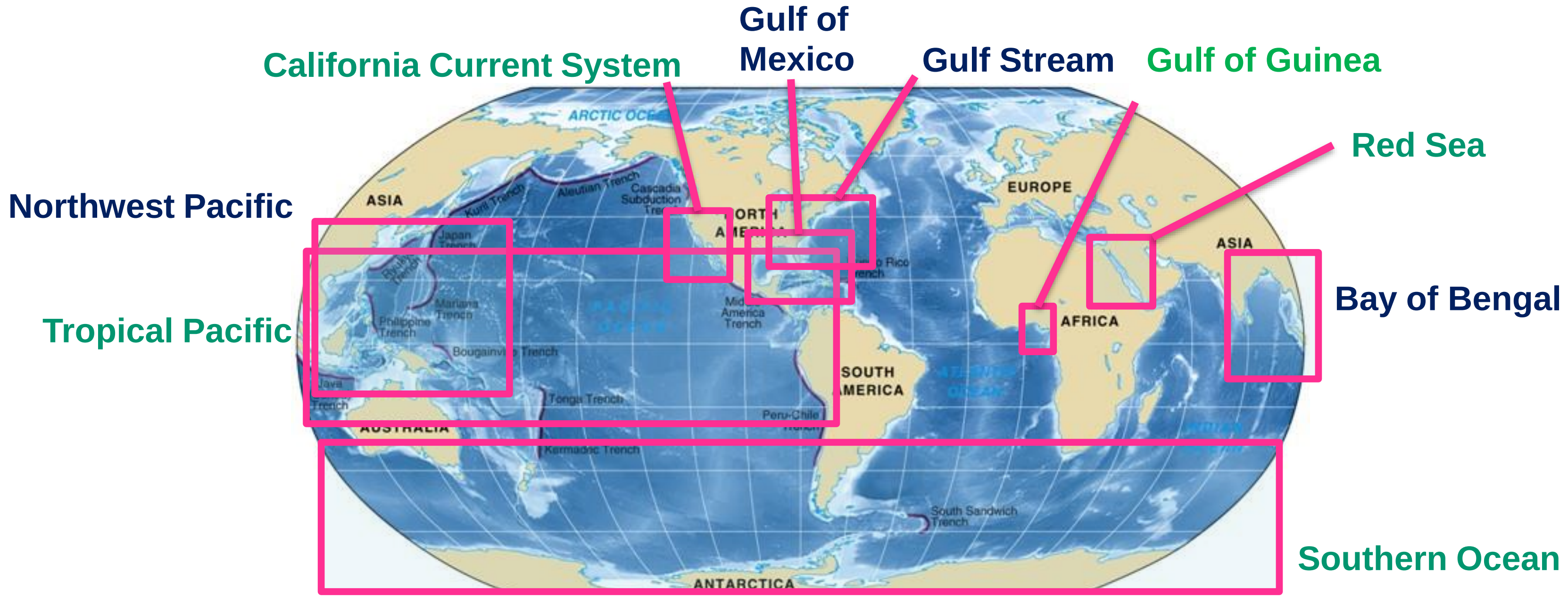
Regional state estimation activities at Scripps Institution of Oceanography

Matt Mazloff, Ariane Verdy, Ganesh Gopalakrishnan, Bruce Cornuelle



A synthesis of Verdy and Mazloff et al 2017 study, "A data assimilating model for estimating Southern Ocean biogeochemistry"

ECCO Summer School

May 27, 2025

B-SOSE

Biogeochemical Southern Ocean State Estimate

Ariane Verdy

Matt Mazloff

SCRIPPS INSTITUTION OF OCEANOGRAPHY

UC San Diego

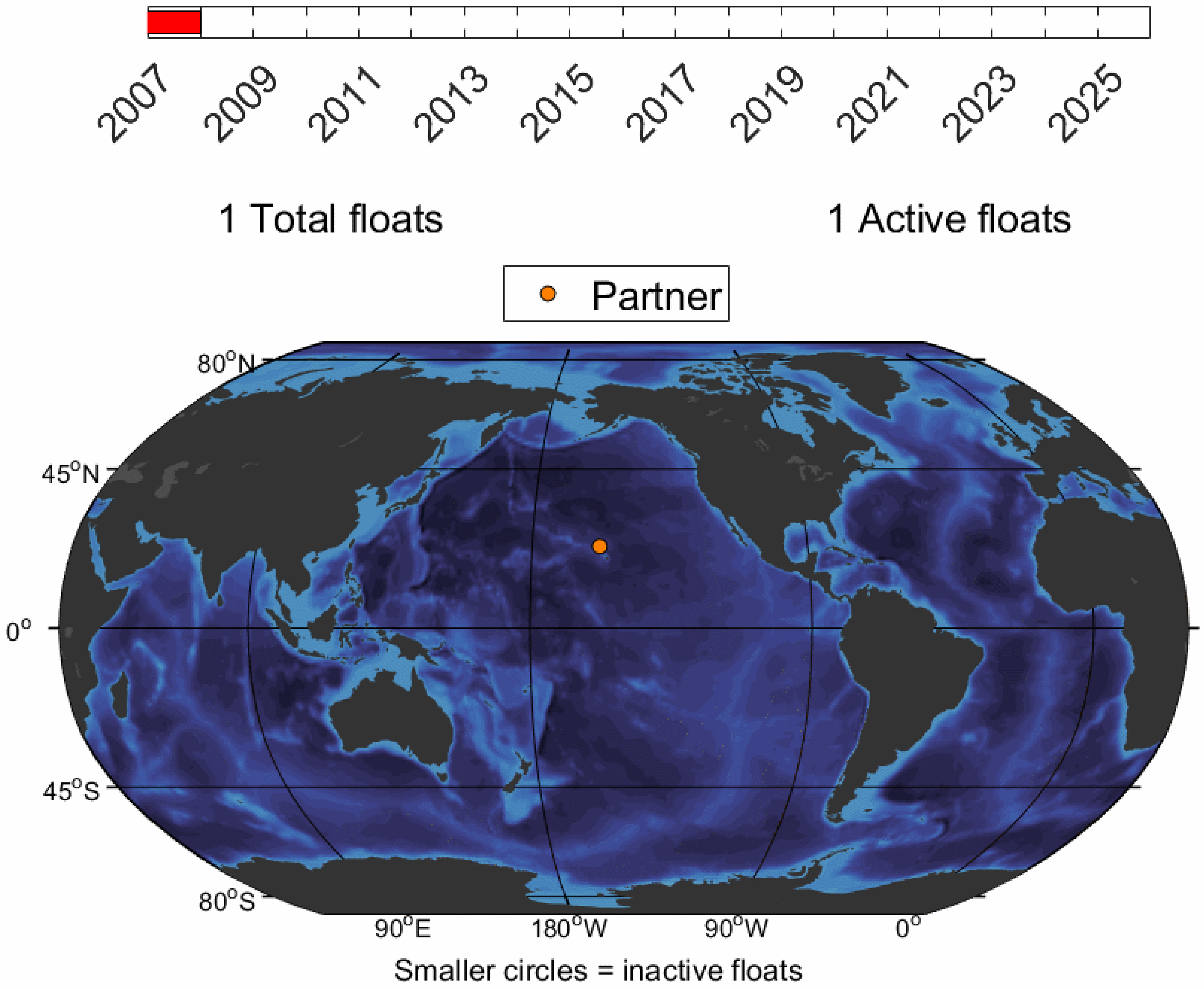
With help from ECCO consortium, Lynne Talley, Sharon Escher, Bruce Cornuelle, Joellen Russell, Jorge Sarmiento, John Dunne, Eric Galbraith, and many others

SOCCOM

Unlocking the mysteries of the Southern Ocean

Southern Ocean Climate and Carbon Observations and Modeling

- Thirteen year NSF-funded project (2015 - 2027) to transform our understanding of the Southern Ocean, a major sink of carbon and heat
- Headquartered at Princeton/UCSD; involves over 85 participants at 14 partner institutions
- Goals:
  - Deploy over 320 Argo floats with BGC sensors
  - High-resolution modeling and state estimation
  - Outreach



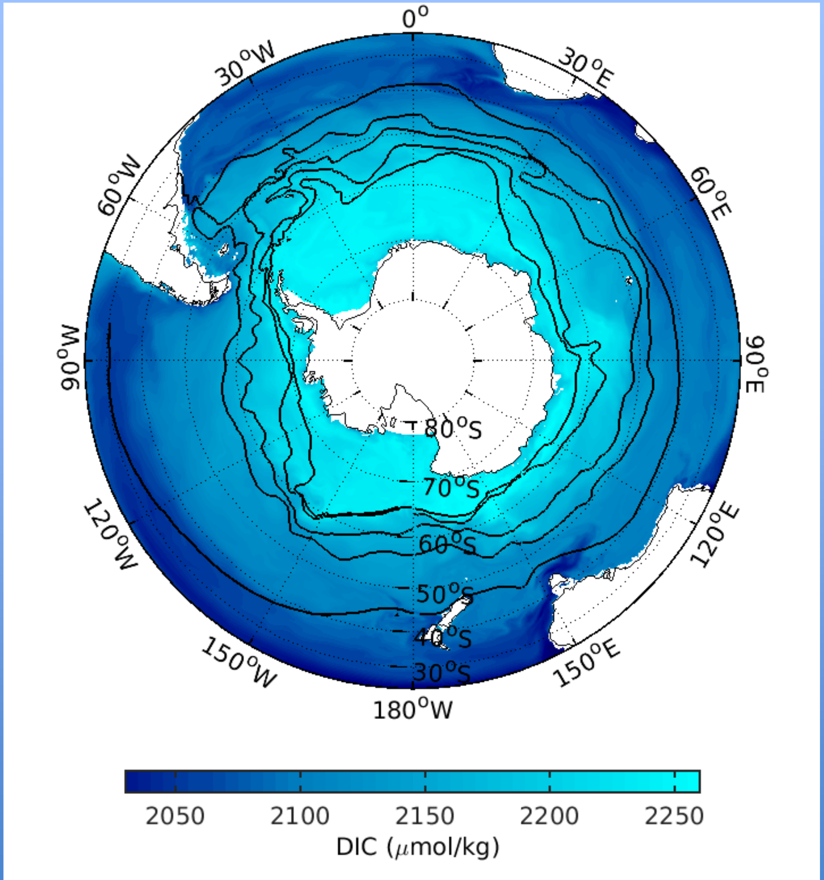
2007
2009
2011
2013
2015
2017
2019
2021
2023
2025
1 Total floats
1 Active floats
Partner
80°N
45°N
0°
45°S
80°S
90°E
180°W
90°W
0°
Smaller circles = inactive floats

What is a BGC-Argo float?

Mature sensor suite

- biooptical sensors: chlorophyll fluorescence, backscatter, light intensity.
- chemical species: dissolved oxygen, nitrate, and pH.

Ken Johnson, MBARI



Snapshot of the simulated dissolved inorganic carbon (DIC) concentration at 100 m on February 1, 2009. Black contours show the mean position of Antarctic Circumpolar Current fronts (Orsi 1995).

summary:

use **model + observations** to estimate carbon system over the past ~10 years

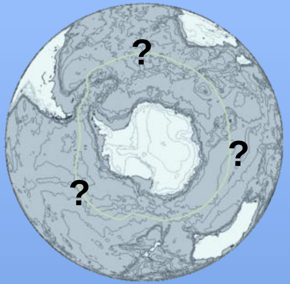
multi-year estimate = a continuous model run, which has **closed budgets** for mass / heat / salt / BGC tracers (DIC, O_2, NO_3, …)

the output is available online (**sose.ucsd.edu**) for analysis and comparisons with models

4D-Var, “adjoint” method

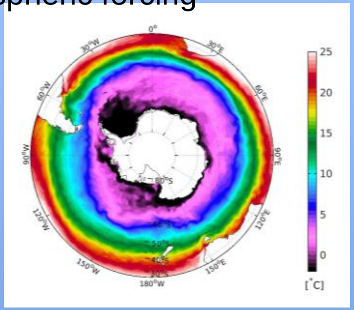
1. State estimation

models are used to hindcast the ocean state (T, S, V, SSH)



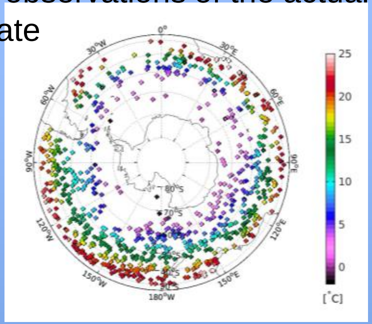
e.g. Southern Ocean 2013-2017

using inputs: initial conditions & atmospheric forcing



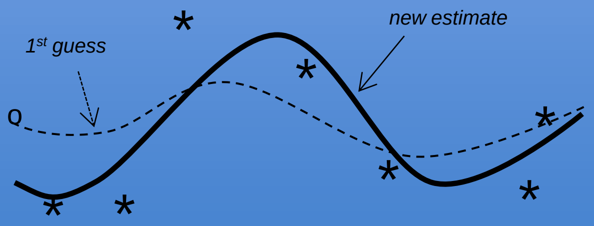
e.g. T & S from Argo maps, winds & air temp, etc. from ECMWF

adjust those inputs to bring the model closer to observations of the actual ocean state



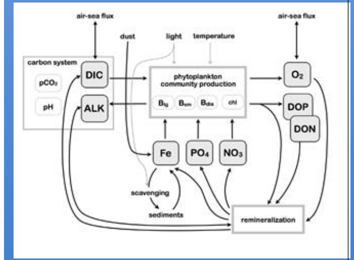
e.g. from Argo profiles, satellites, …

minimize the “cost function” :

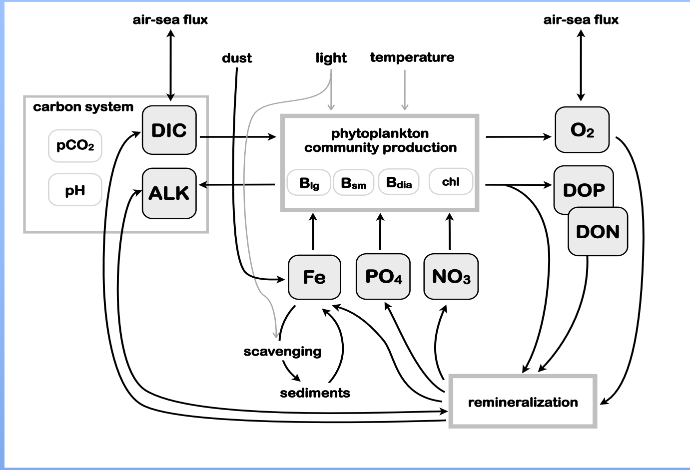


Σ (weighted model-observations misfit)^2
+ Σ (weighted adjustment to inputs)^2

B-SOSE: biogeochemical + physical state optimized together



ecco-group.org



The science:

The model is our hypothesis of how the world works.

We made assumptions for computational efficiency.

If we understand the ocean, those assumptions will give us the answers we expect.

If we don’t understand, we must go back and make a new hypothesis – a new model

Can we simulate the observed ocean pCO2?

Once we have a good model (i.e. the forward problem), we can better use observations (i.e. the inverse problem)

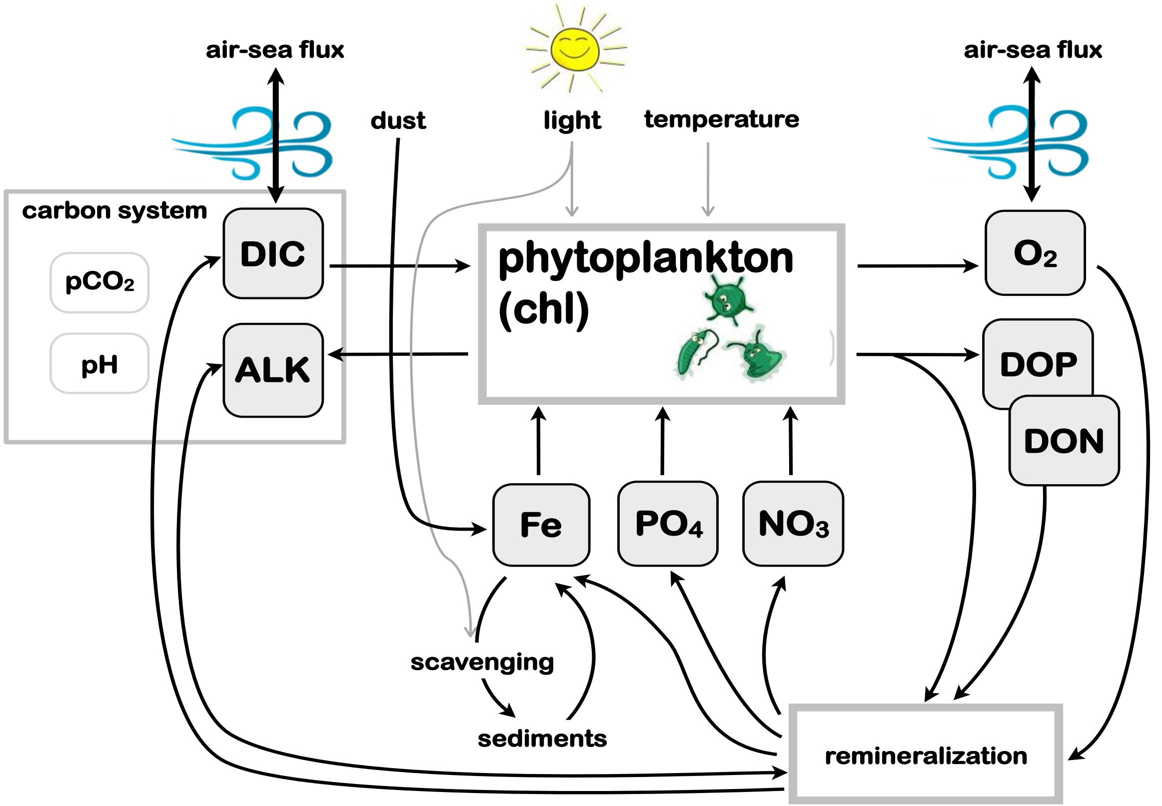
Penny, et al., Observational Needs for Improving Ocean and Coupled Reanalysis, S2S Prediction, and Decadal Prediction, Front. Mar. Sci., 2019

- Data assimilation is essentially an automation of the scientific method.
- A hypothesis is made and encoded in a numerical model.
- This model is then used to make predictions that can be tested against new observations.
- Prediction accuracy is then examined and provided as feedback to modify the model and methods, and the process repeats.

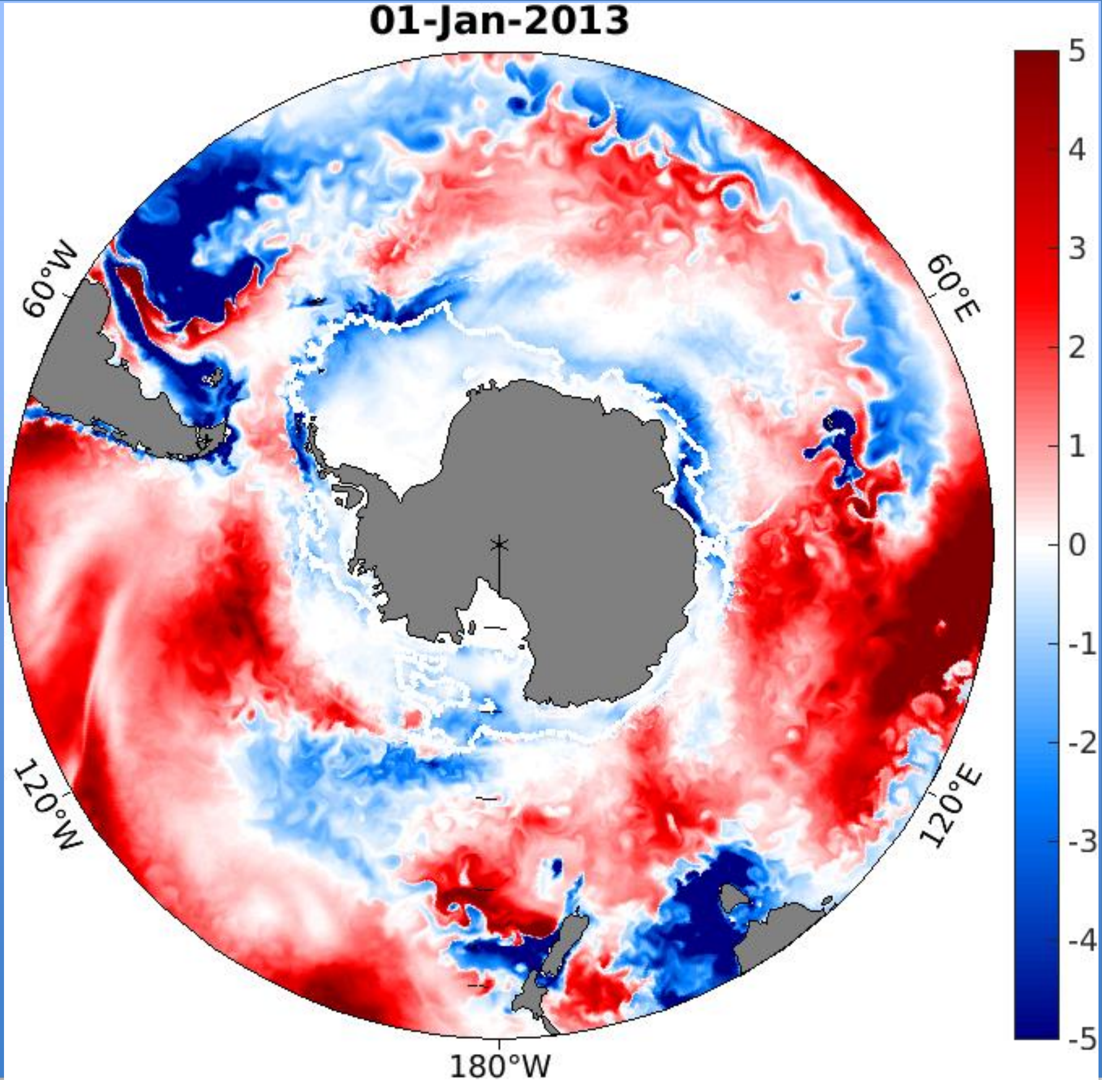
Slide from Bruce Cornuelle

2. BGC MODEL

Model: N-BLING, evolved from BLING



All prognostic and diagnostic variables are estimated; can be compared / constrained to observations

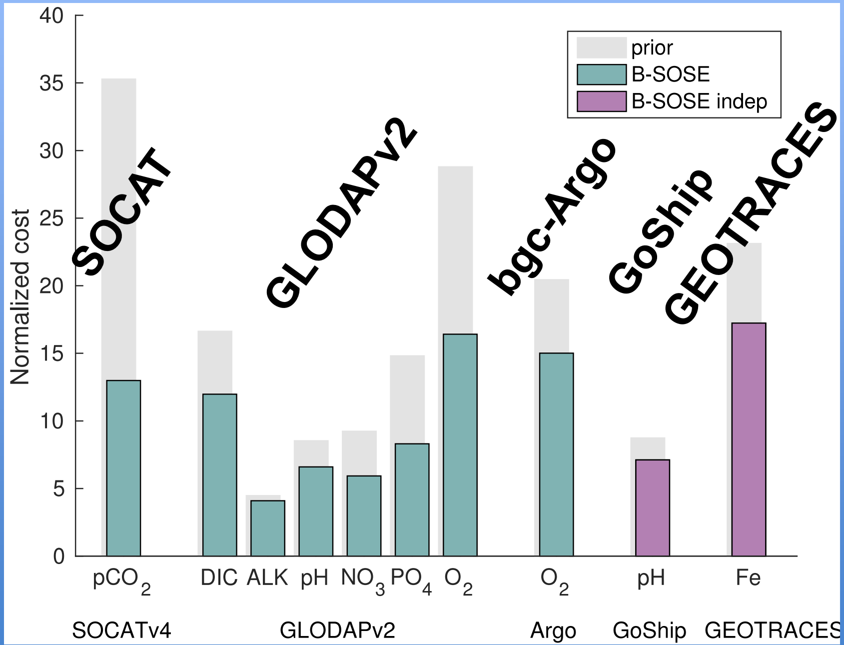


Air-sea CO_2 flux [mol m^{-2} yr^{-1}]
B-SOSE Iteration 122 solution

3. PRODUCT

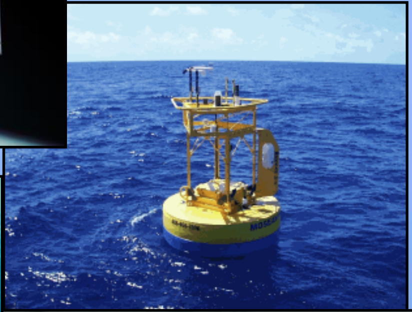
2008-2012, 1/3 degree

Verdy and Mazloff (2017), A data assimilating model for estimating Southern Ocean biogeochemistry, JGR-Oceans



2013-2021⁺ in production

(with SOCCOM BGC-Argo float constraints)


validation

* = assimilated

Comparisons with gridded products

* ocean color (chl, POC)
* altimetry
* microwave SST
* sea ice
Argo monthly mapped product
GLODAPv2, WOA13, SOCAT climatologies
Landschützer monthly mapped product

Comparisons with in situ observations

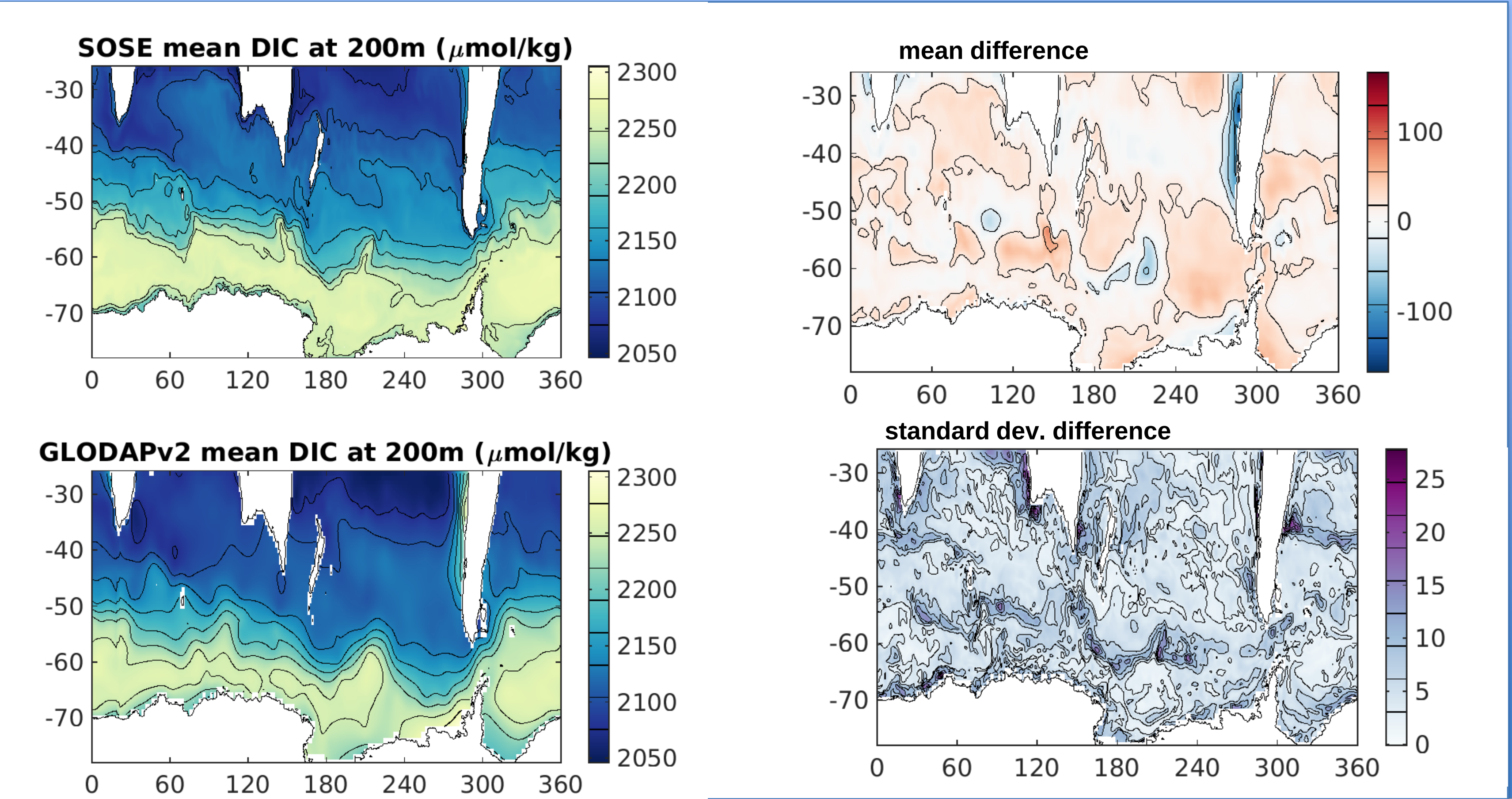
* Argo profiles (T,S)
* calibrated bgc-Argo (O_2)
* SOCCOM floats
* SOCAT (pCO_2)
* GLODAPv2 (carbon, nutrients)
* CTD (T, S, O_2, chl)
* XBT, MEOP, PIES
GEOTRACES

Comparisons with estimated “quantities of interest”

air-sea CO_2 flux
Drake Passage pCO_2
nutrient transport across 32°S

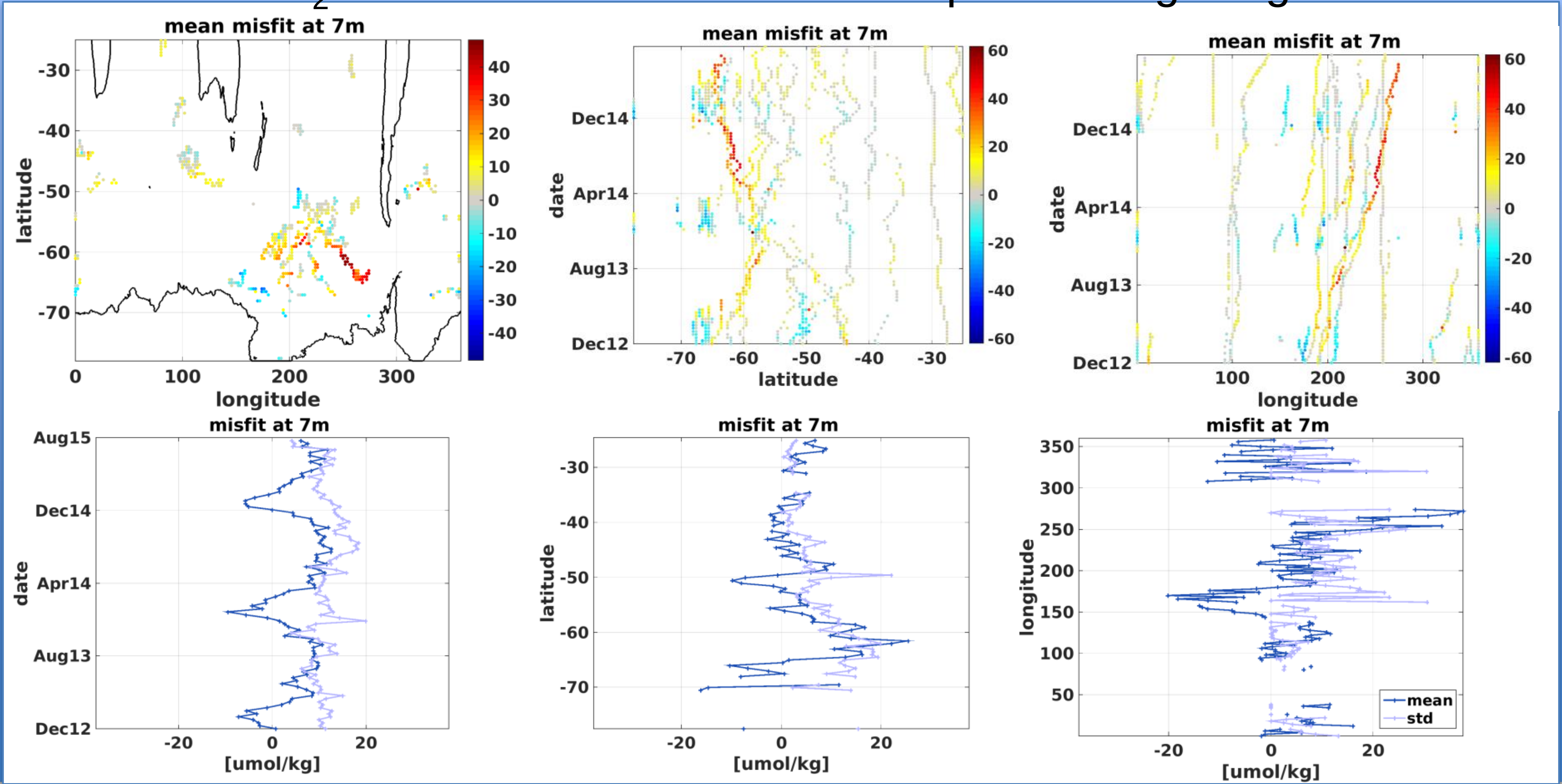
Comparisons with gridded products

200 m DIC in B-SOSE 2013-2017 is compared to GLODAPv2



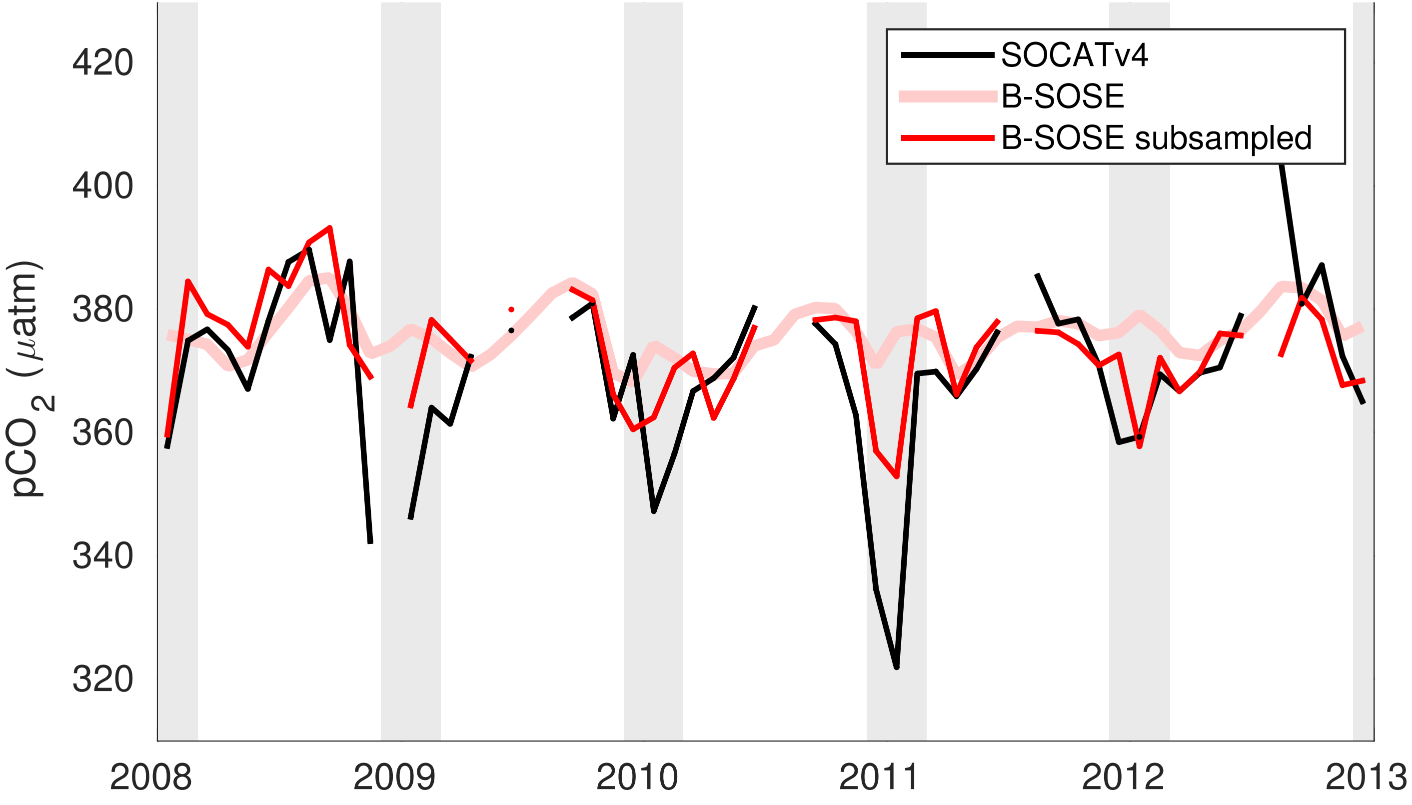
Comparisons with in situ observations

7 m O_2 in B-SOSE 2013-2017 is compared to bgc-Argo



Comparisons with "quantities of interest"

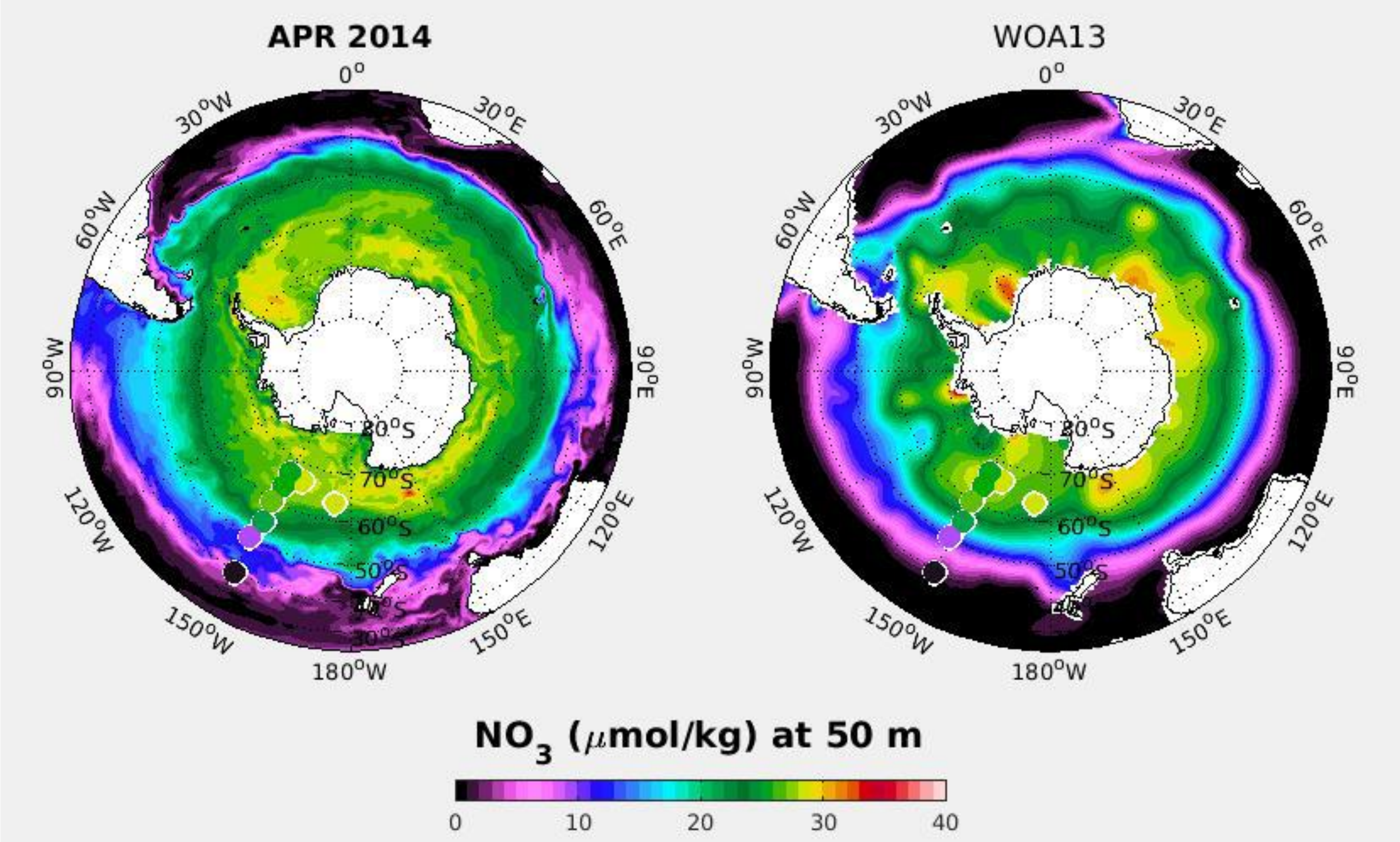
pCO_2 in B-SOSE 2008-2012 is compared to Drake Passage time series



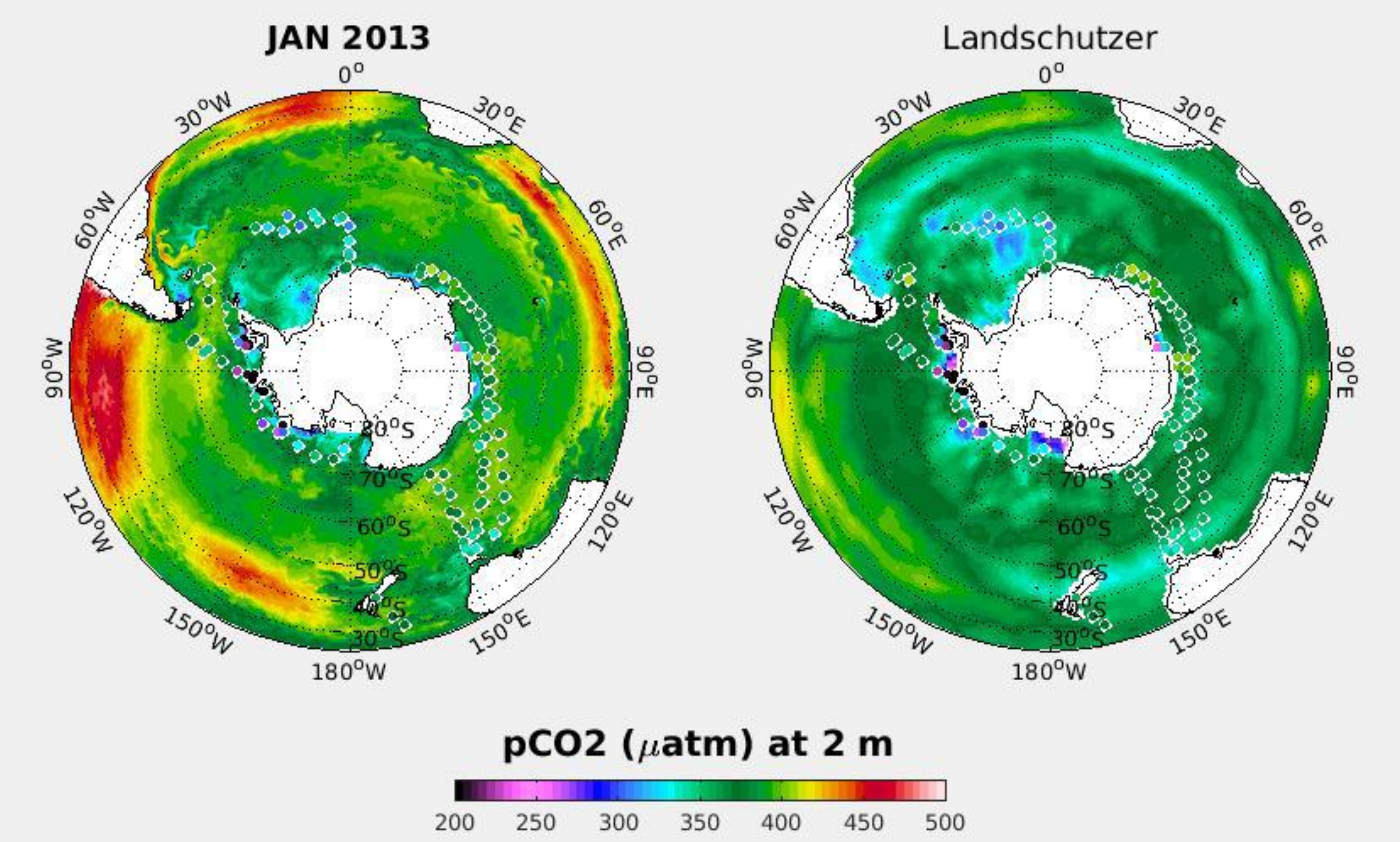
Monthly-averaged pCO_2 in Drake Passage (75°W to 55°W, south of 50°S) from SOCATv4 observations (black) [Bakker et al., 2016; Munro et al., 2015a, 2015b], and from B-SOSE (area average in pink; subsampled at the location of observations in red). Summer months are shaded gray.

B-SOSE & climatology

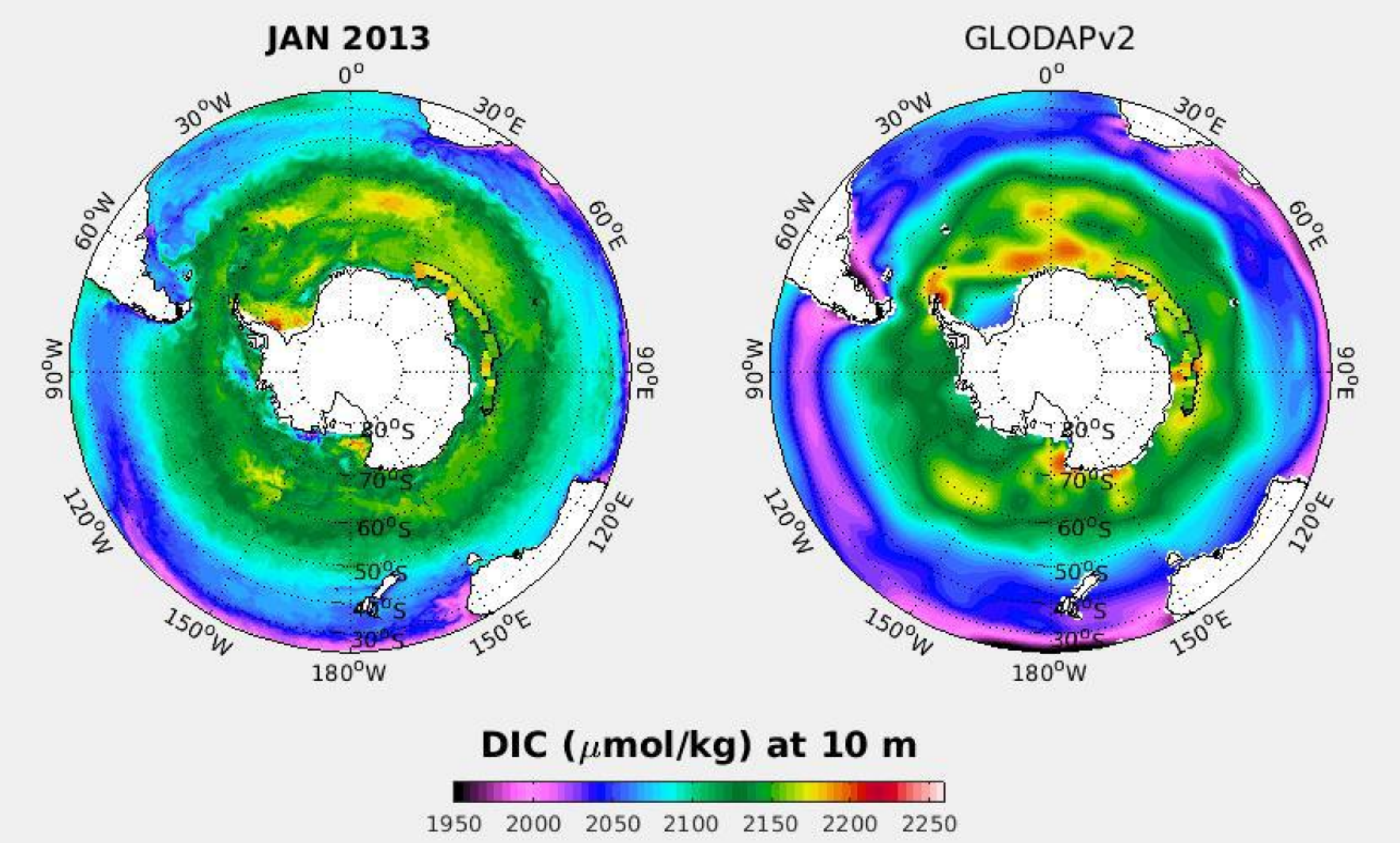
with SOCCOM float observations



B-SOSE vs Landschutzer CNN

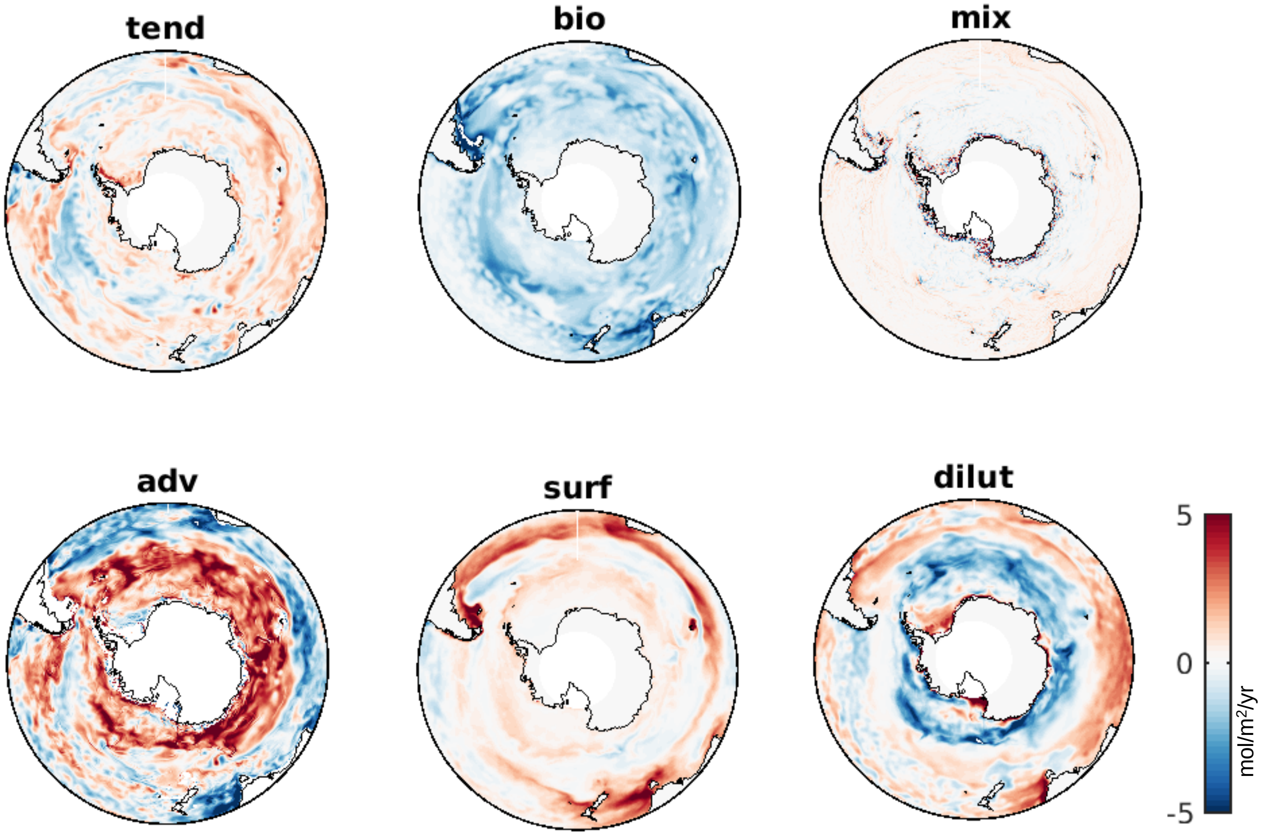


B-SOSE vs climatology

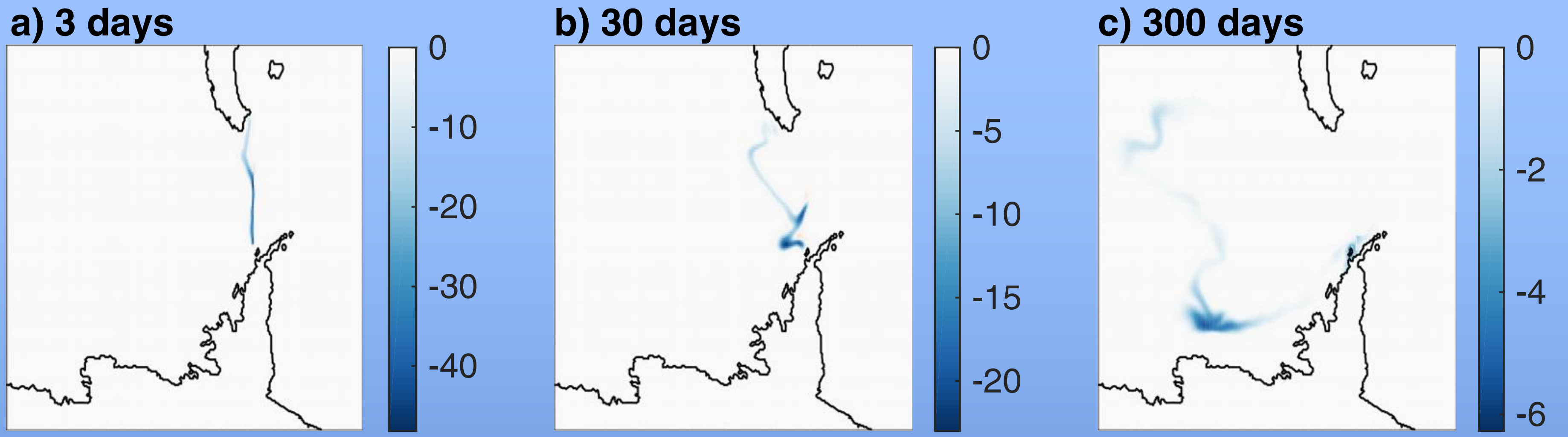


Budgets

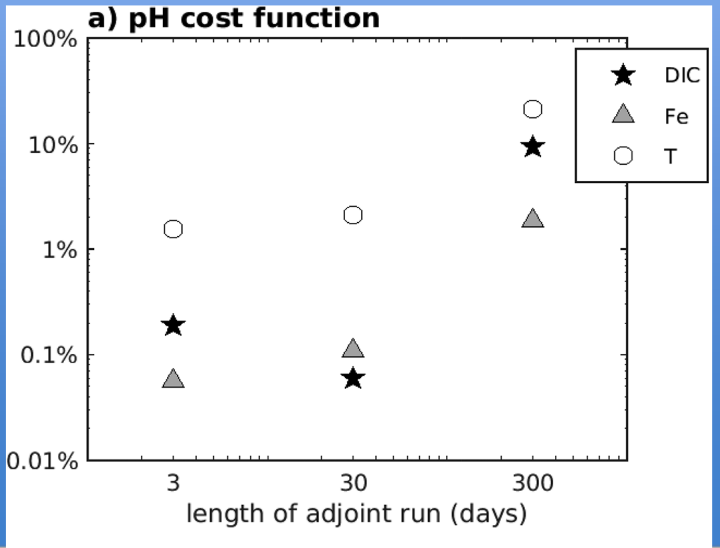
DIC in the top 650 m, 2008-2012



Rosso et al. (2017), Space and time variability of the Southern Ocean carbon budget. JGR-Oceans.



Depth-integrated sensitivity of the pH cost function to DIC after 3, 30, and 300 days of adjoint integration. Units are (micromol C/ kg)$^{-1}$ /m.

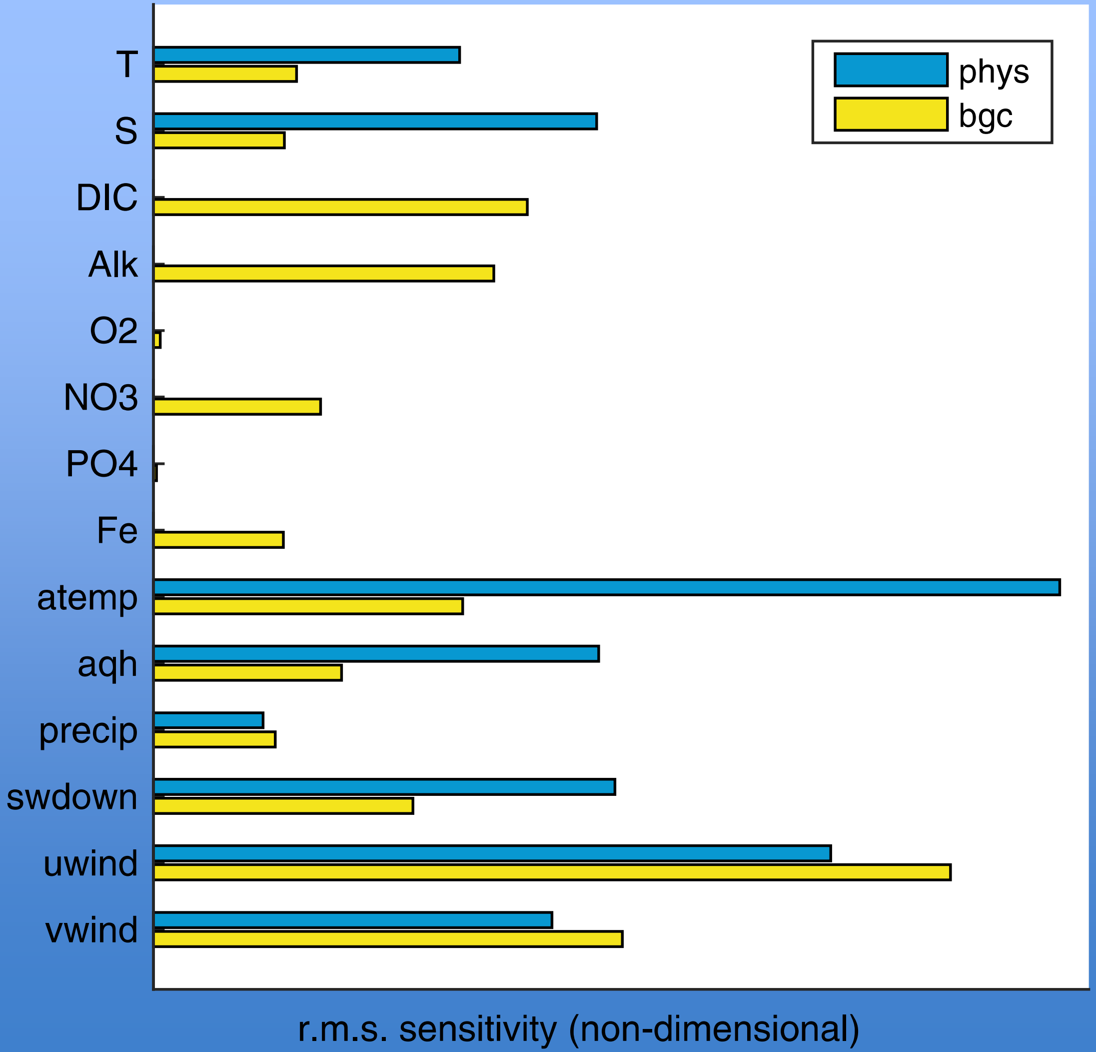


Error in adjoint sensitivities relative to the true sensitivities from finite difference perturbation experiments.

Sensitivity to the B-SOSE controls for the physical constraints (blue) and biogeochemical constraints (yellow) during 2008 in the prior run.

Sensitivities are normalized by the uncertainty on each control and the root mean square (r.m.s.) is plotted.

Controls are: initial conditions for potential temperature, salinity, and six biogeochemical tracers (DIC, alkalinity, oxygen, nitrate, phosphate, and iron) as well as timevarying atmospheric state (surface air temperature, surface air humidity, precipitation, shortwave downwelling radiation, zonal wind speed, and meridional wind speed).

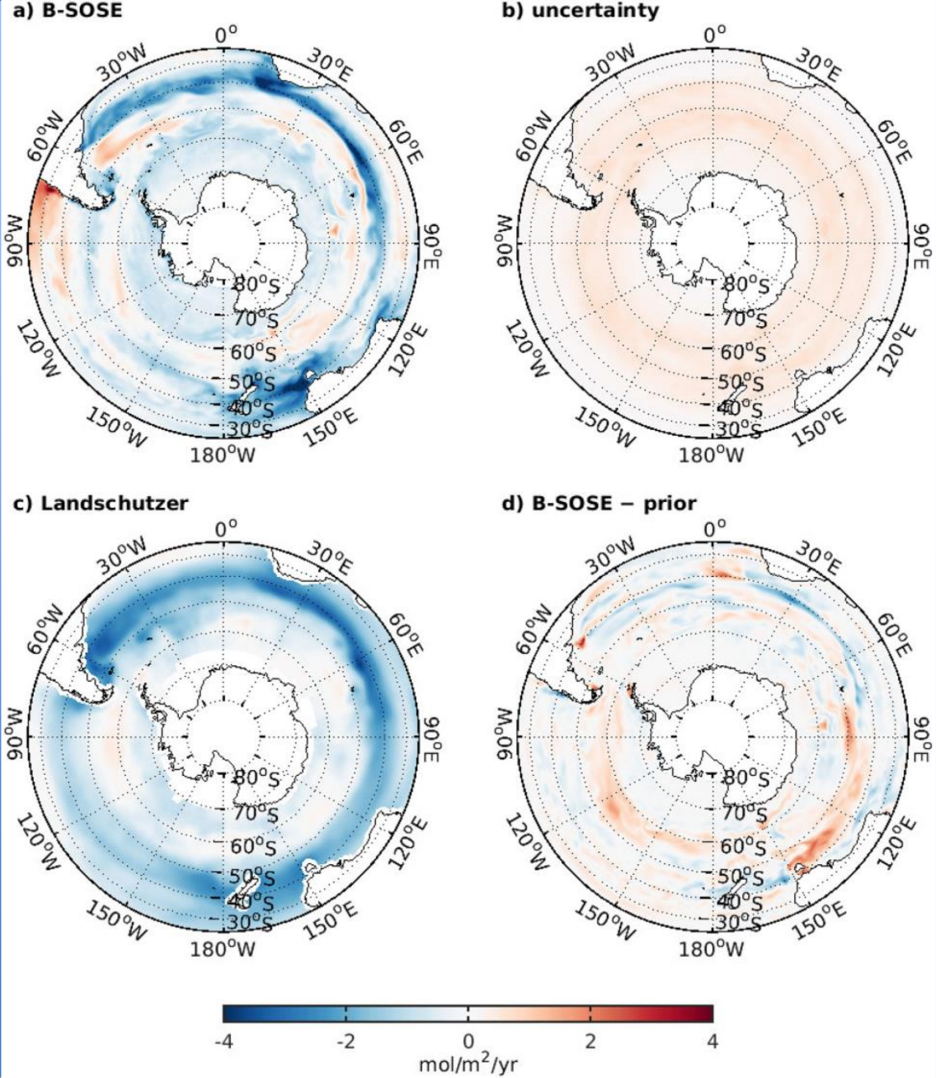


Mean air-sea flux of CO2 for 2008–2011

(a) BSOSE

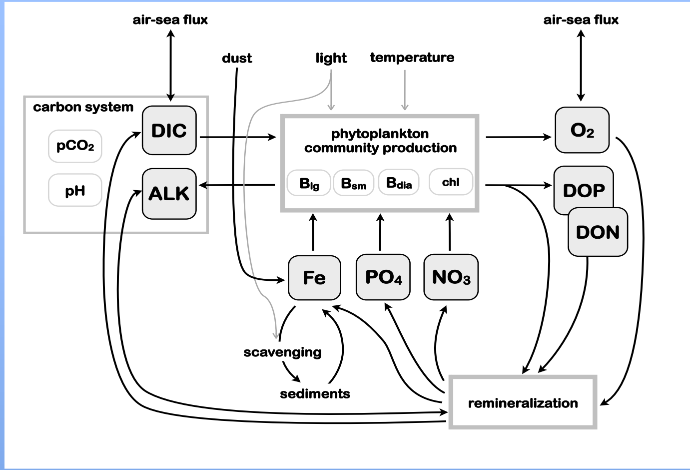
(c) Landschutzer et al. [2015].

Positive fluxes are into the atmosphere



(b) Uncertainty of the B-SOSE air-sea CO2 flux estimated from an ensemble sensitivity experiment. The maximum uncertainty value is estimated to be 1.00 $mol/m^2/yr$.

(d) Difference in air-sea CO2 flux between the state estimate and the “prior,” forward model run. The magnitude of the correction resulting from data assimilation exceeds the uncertainty estimate in > 70% of domain.



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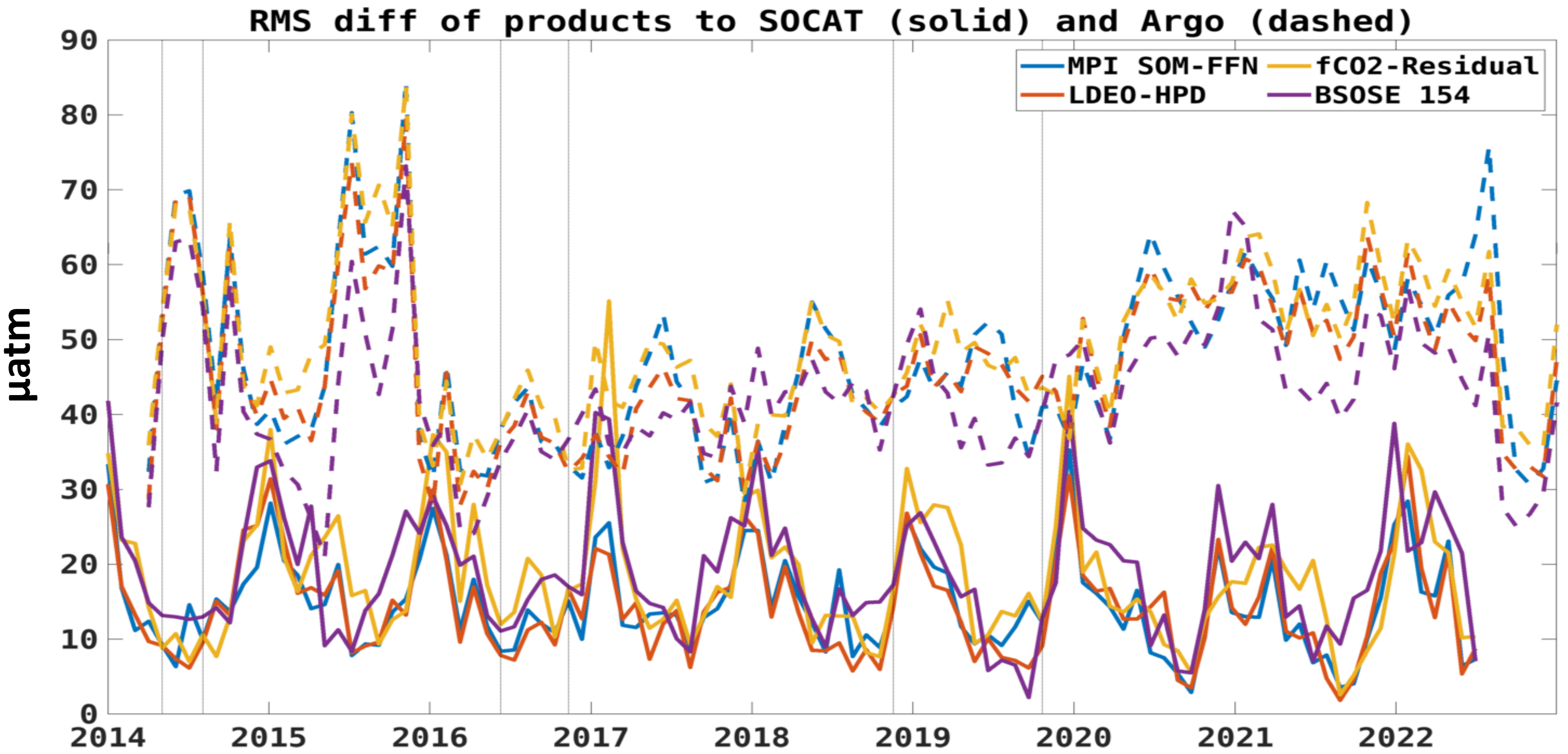
Surface ocean pCO2 comparisons to data

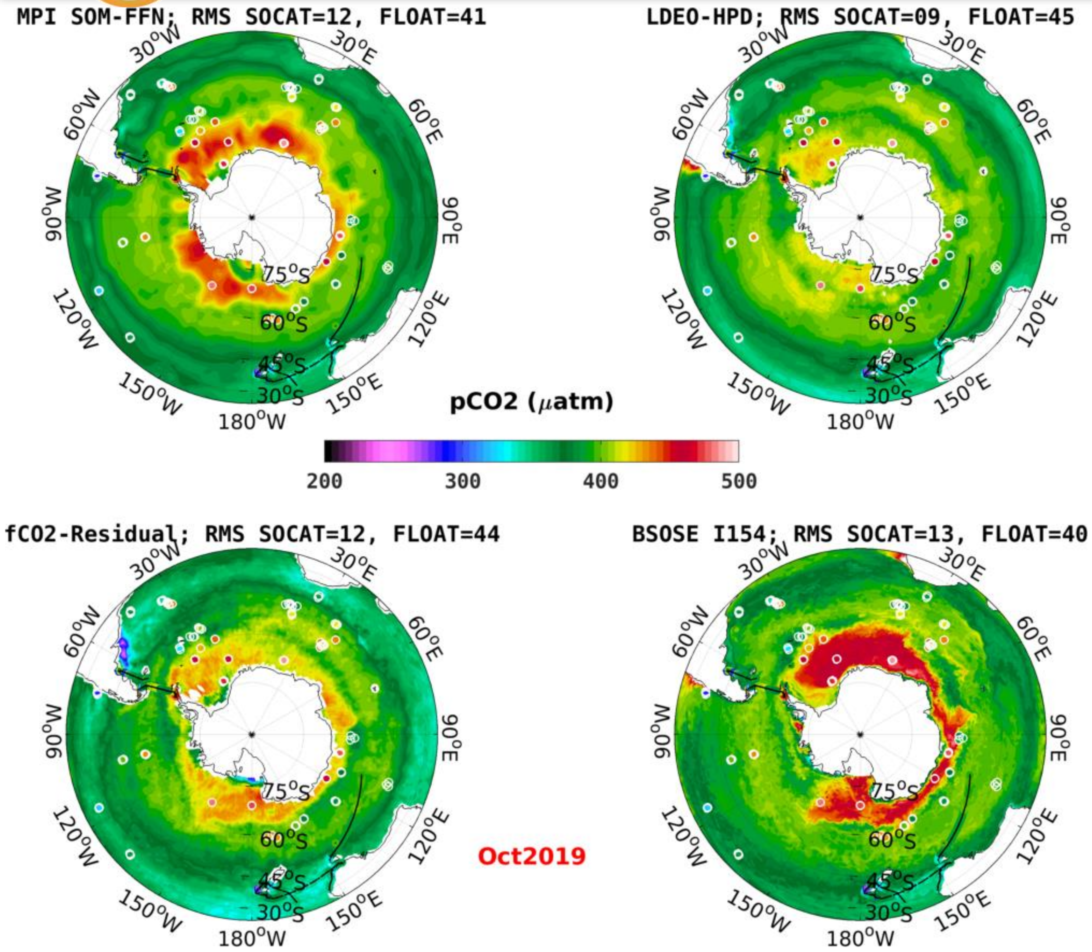
root-mean-square (RMS) differences between the products and the data in μatm

Product	SOCAT fCO2	Float canyon pCO2
MPI SOM-FFN pCO2	17.9	48.2
LDEO-HPD fCO2	17.7	46.8
fCO2-Residual fCO2	23.5	49.6
B-SOSE I154 pCO2	23.4	43.5

Surface ocean pCO2 comparisons to data



Surface ocean pCO2 comparisons to data

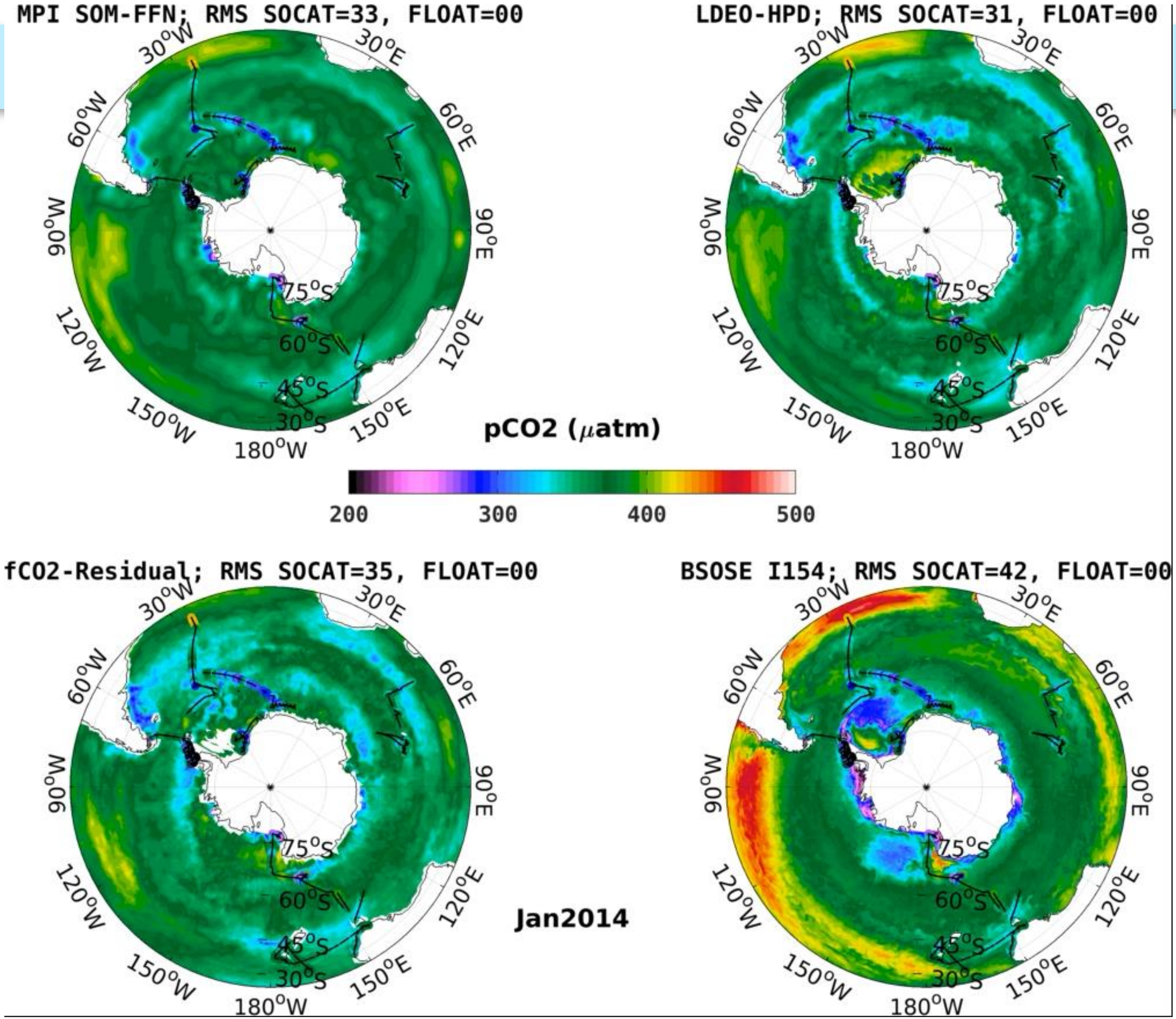


SOCCOM

Surface ocean pCO2 comparisons to data

More data (informed from OSSEs) will improve consistency and reduce

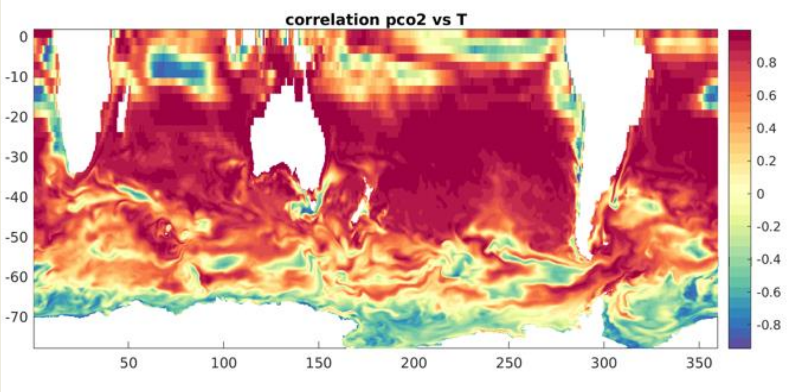
uncertainty



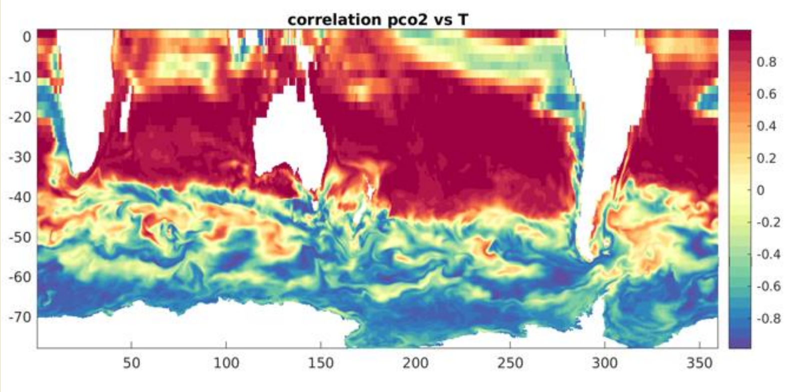
pCO2 optimization (in progress by Angela Kuhn)

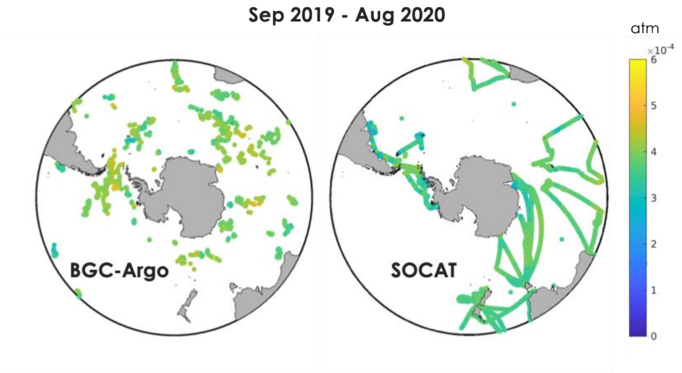
Corrects seasonal phasing and spatial biogeochemical dynamics

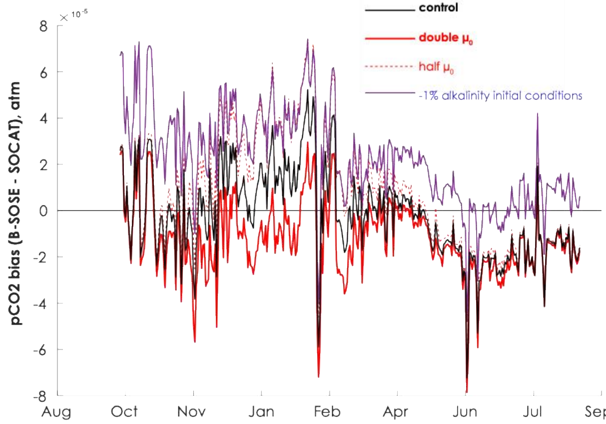
Control run:



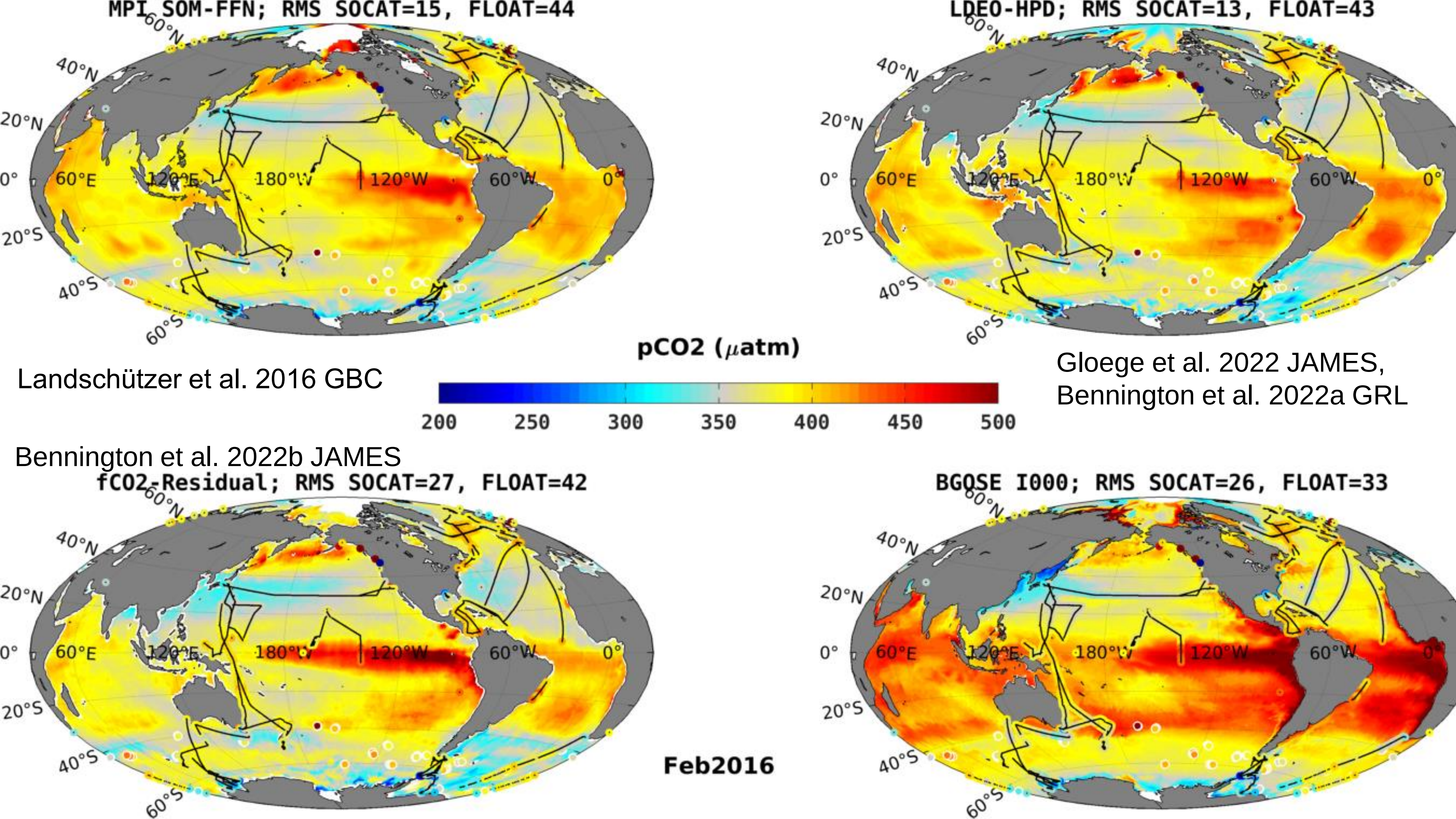
Optimized run:



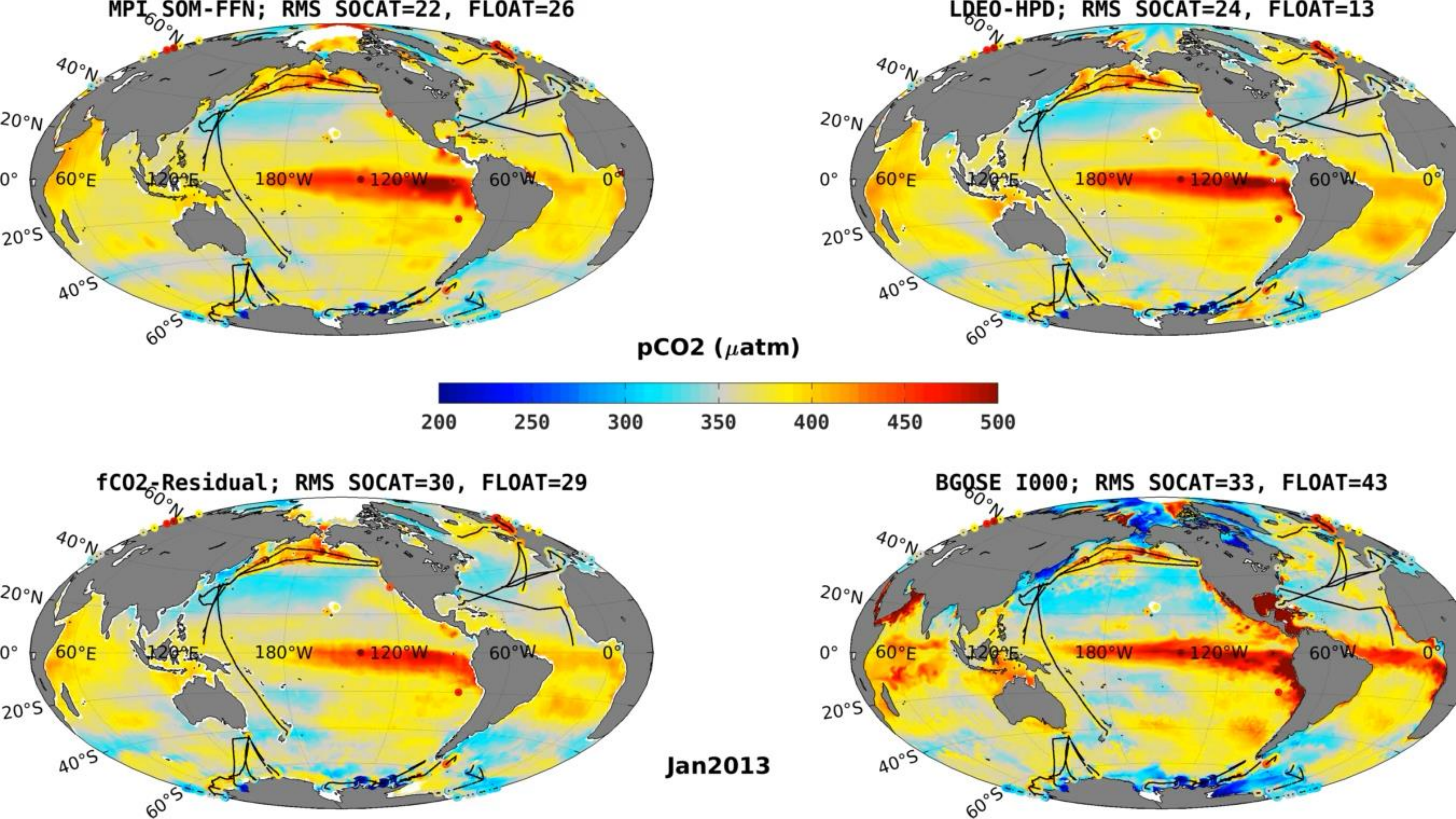


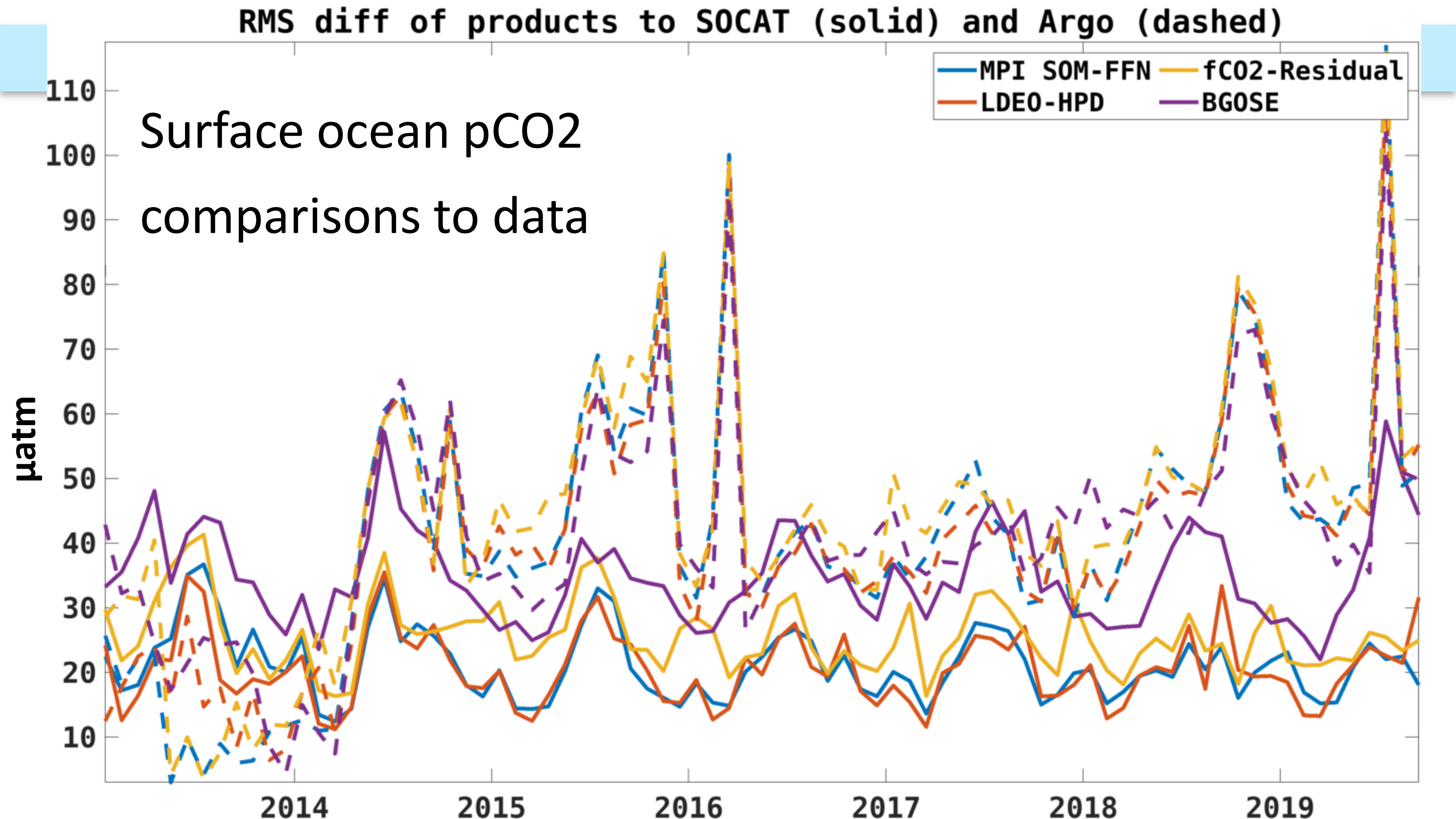


Temporal and spatial **surface pCO_2** patterns will be optimized using both **BGC-Argo** and **SOCAT** observations.

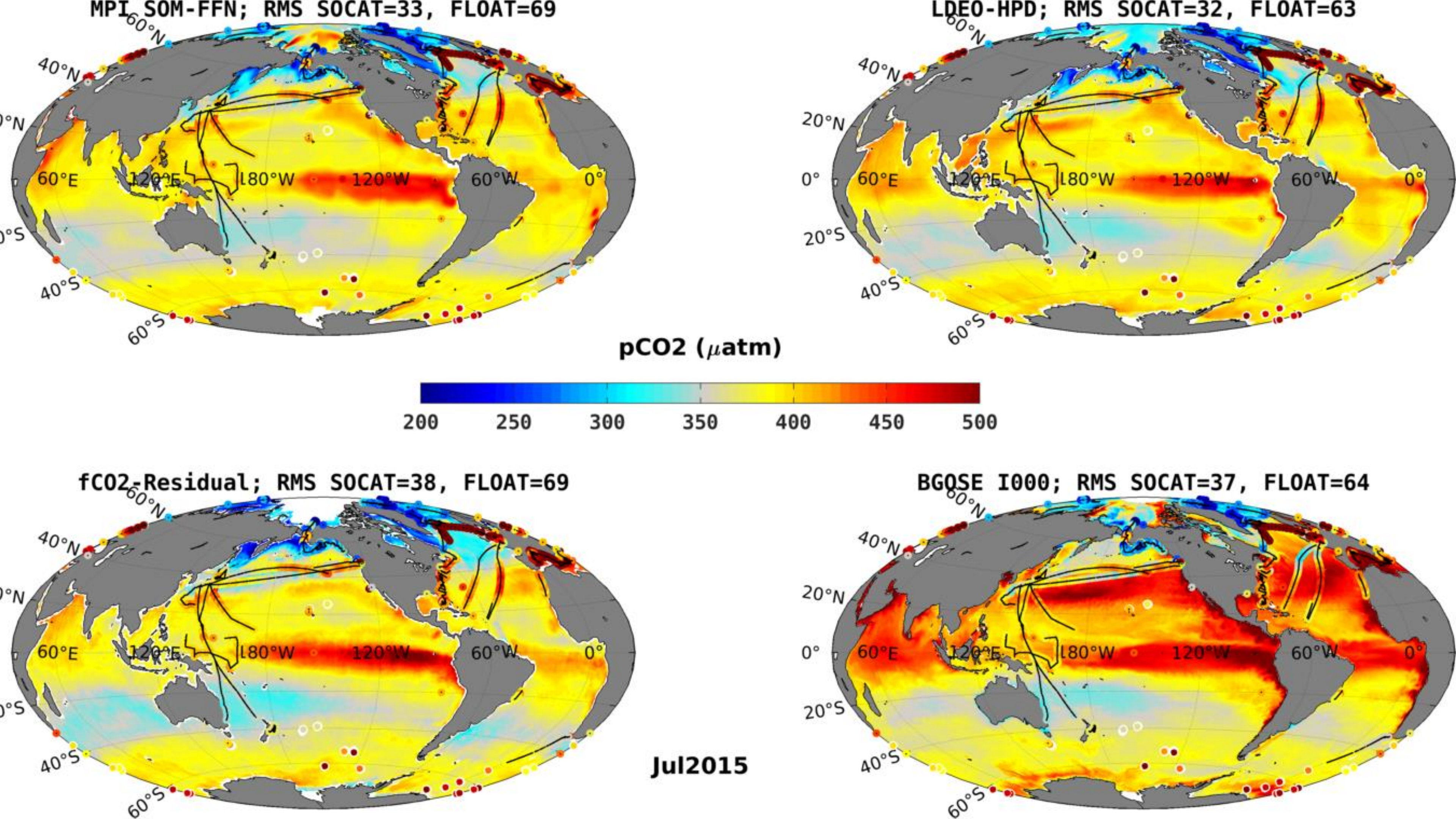


MPI SOM-FFN; RMS SOCAT=15, FLOAT=44
LDEO-HPD; RMS SOCAT=13, FLOAT=43
pCO2 (μatm)
200
250
300
350
400
450
500
Landschützer et al. 2016 GBC
Gloege et al. 2022 JAMES,
Bennington et al. 2022a GRL
Bennington et al. 2022b JAMES
fCO2-Residual; RMS SOCAT=27, FLOAT=42
BGOSE I000; RMS SOCAT=26, FLOAT=33
Feb2016
60°N
40°N
20°N
0°
20°S
40°S
60°S
60°E
120°E
180°W
120°W
60°W


MPI SOM-FFN; RMS SOCAT=22, FLOAT=26
LDEO-HPD; RMS SOCAT=24, FLOAT=13
pCO2 (μatm)
200 250 300 350 400 450 500
fCO2-Residual; RMS SOCAT=30, FLOAT=29
BGOSE I000; RMS SOCAT=33, FLOAT=43
Jan2013
60°N 40°N 20°N 0° 20°S 40°S 60°S
60°E 120°E 180°W 120°W 60°W 0°

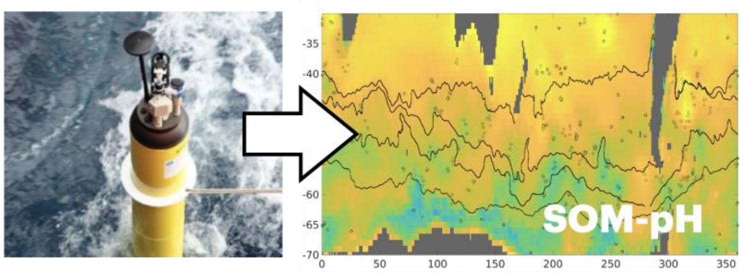


RMS diff of products to SOCAT (solid) and Argo (dashed)
MPI SOM-FFN
fCO2-Residual
LDEO-HPD
BGOSE
Surface ocean pCO2
comparisons to data
µatm
110
100
90
80
70
60
50
40
30
20
10
2014
2015
2016
2017
2018
2019

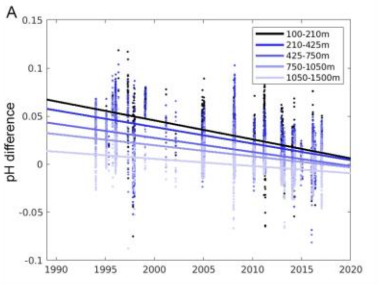


MPI SOM-FFN; RMS SOCAT=33, FLOAT=69
LDEO-HPD; RMS SOCAT=32, FLOAT=63
pCO2 (μatm)
200 250 300 350 400 450 500
fCO2-Residual; RMS SOCAT=38, FLOAT=69
BGOSE I000; RMS SOCAT=37, FLOAT=64
Jul2015
60°N
40°N
20°N
0°
20°S
40°S
60°S
60°E
120°E
180°W
120°W
60°W

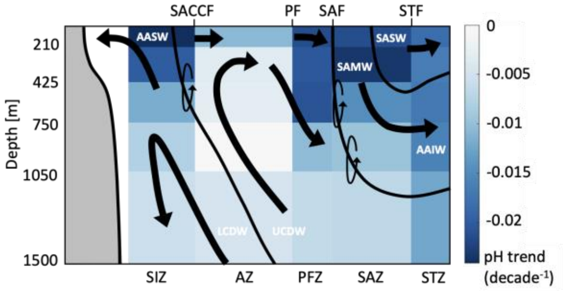
BGC-Southern Ocean State Estimate (B-SOSE)



1) we make a **bias-corrected pH climatology** [available at http://sose.ucsd.edu/] by removing the objectively mapped misfits between B-SOSE and bcg-Argo float data



2) we compare that pH climatology to ship data to **detect trends** (**up to -0.02 per decade**) in 5 frontal zones and 5 depths

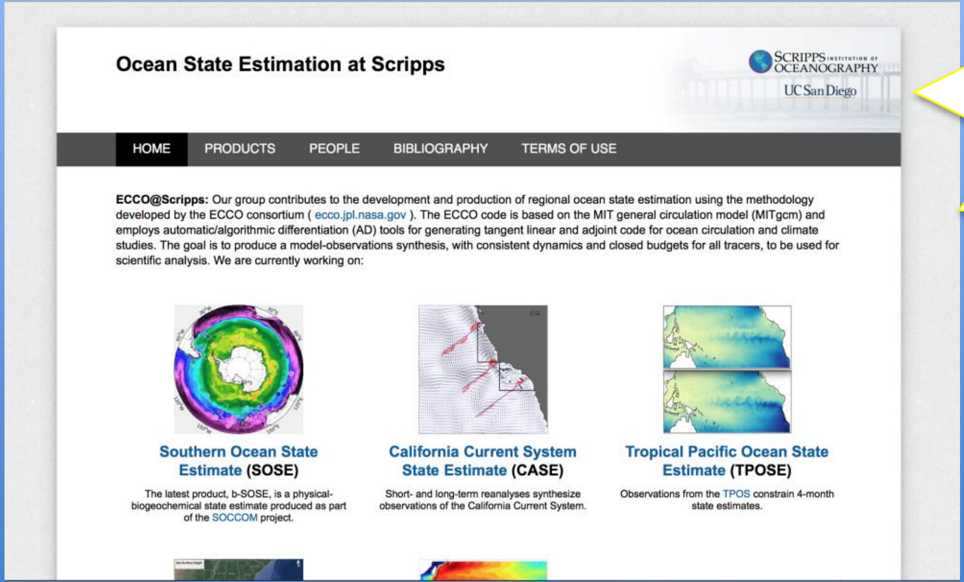


3) we can explain the trends in the context of the meridional **overturning circulation**

Mazloff et al. (2023). **Southern Ocean Acidification Revealed by Biogeochemical-Argo floats**. JGR-Oceans

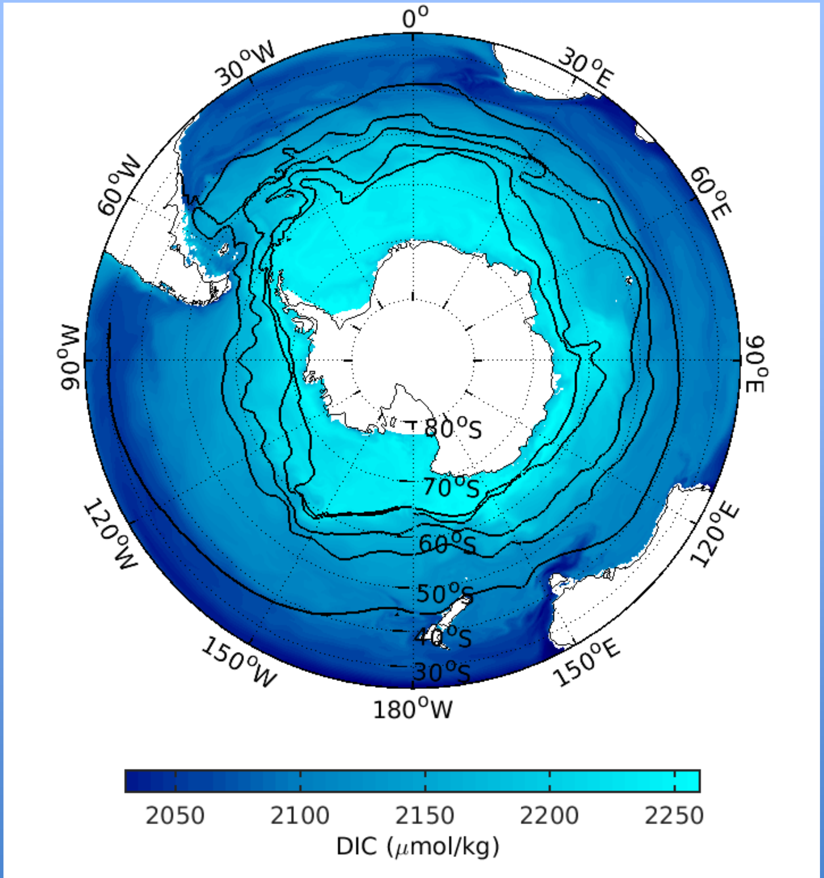
Getting the products

B-SOSE output: sose.ucsd.edu
+ validation
+ documentation



- netCDF
- CF compliant
- **available for model comparisons!**

MITgcm BLING model and adjoint: github.com/MITgcm/MITgcm



Snapshot of the simulated dissolved inorganic carbon (DIC) concentration at 100 m on February 1, 2009. Black contours show the mean position of Antarctic Circumpolar Current fronts (Orsi 1995).

summary:

use **model + observations** to estimate carbon system over the past ~10 years

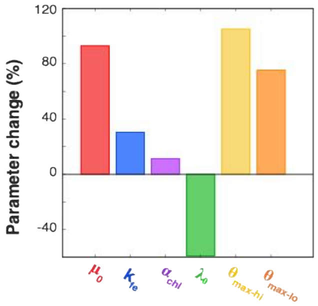
multi-year estimate = a continuous model run, which has **closed budgets** for mass / heat / salt / BGC tracers (DIC, O_2, NO_3, …)

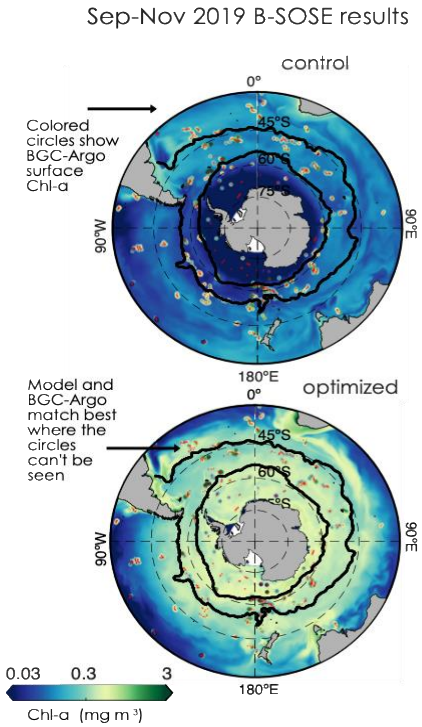
the output is available online (**sose.ucsd.edu**) for analysis and comparisons with models

- Extra slides related to projects

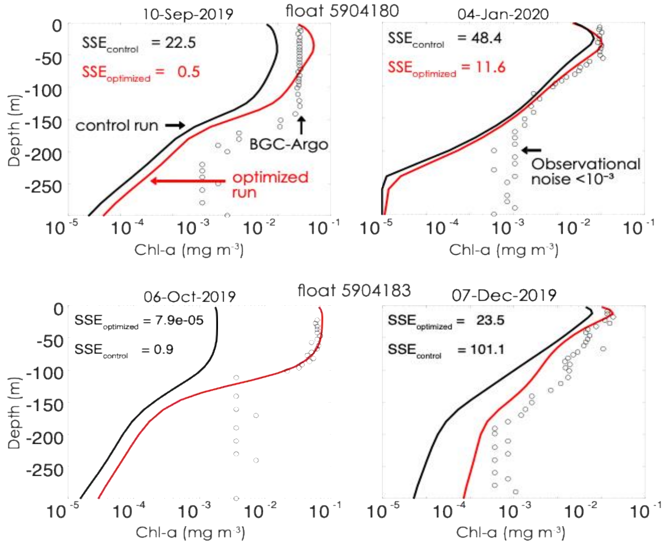
Angela Kuhn, et al. 2025. Sensitivity of chlorophyll vertical structure to model parameters in the Biogeochemical Southern Ocean State Estimate (B-SOSE). *JGR: Biogeosciences*. https://doi.org/10.1029/2024JG008300

Parameters changes ranged between -60% to +110% of original values.

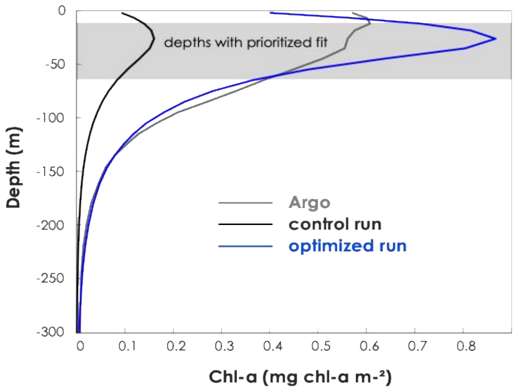




Significant **improvements** were obtained in the match to seasonal **spatial patterns** and individual BGC-Argo **chlorophyll profiles.**



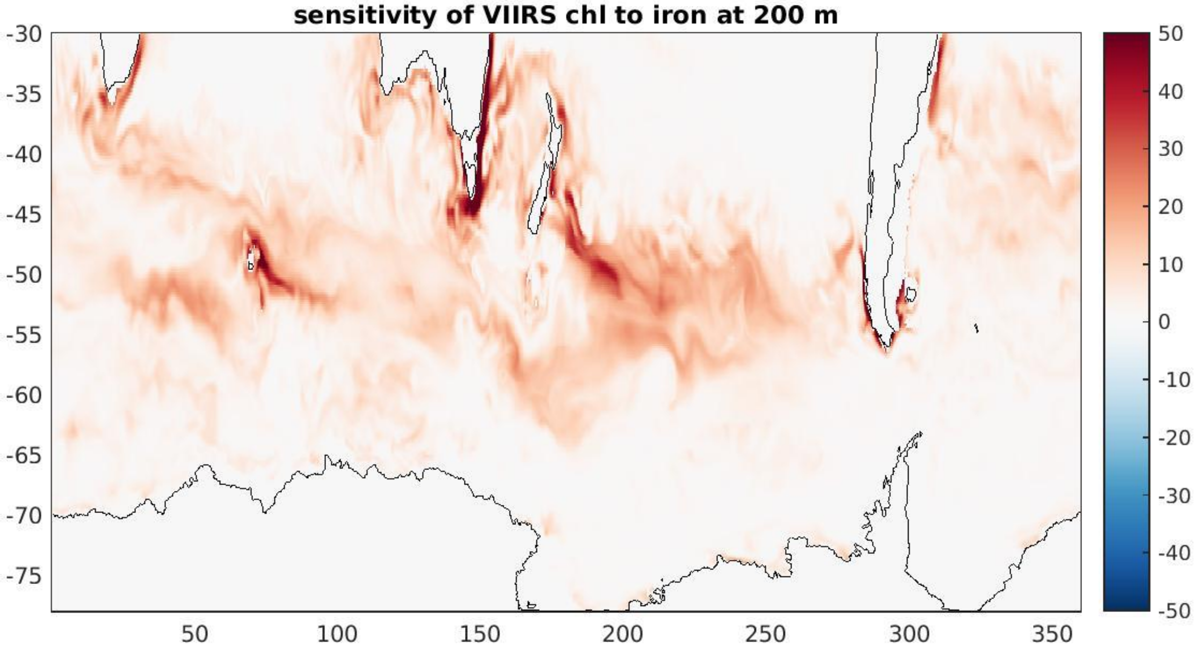
The **optimized parameters reduced misfits** (BGC-Argo vs B-SOSE) of the average chlorophyll profiles by **~60% of RMSD.**



Turbulence, **species succession**, and **susceptibility to grazing** are **key parameterizations** for development of subsurface chlorophyll maxima in the Southern Ocean.

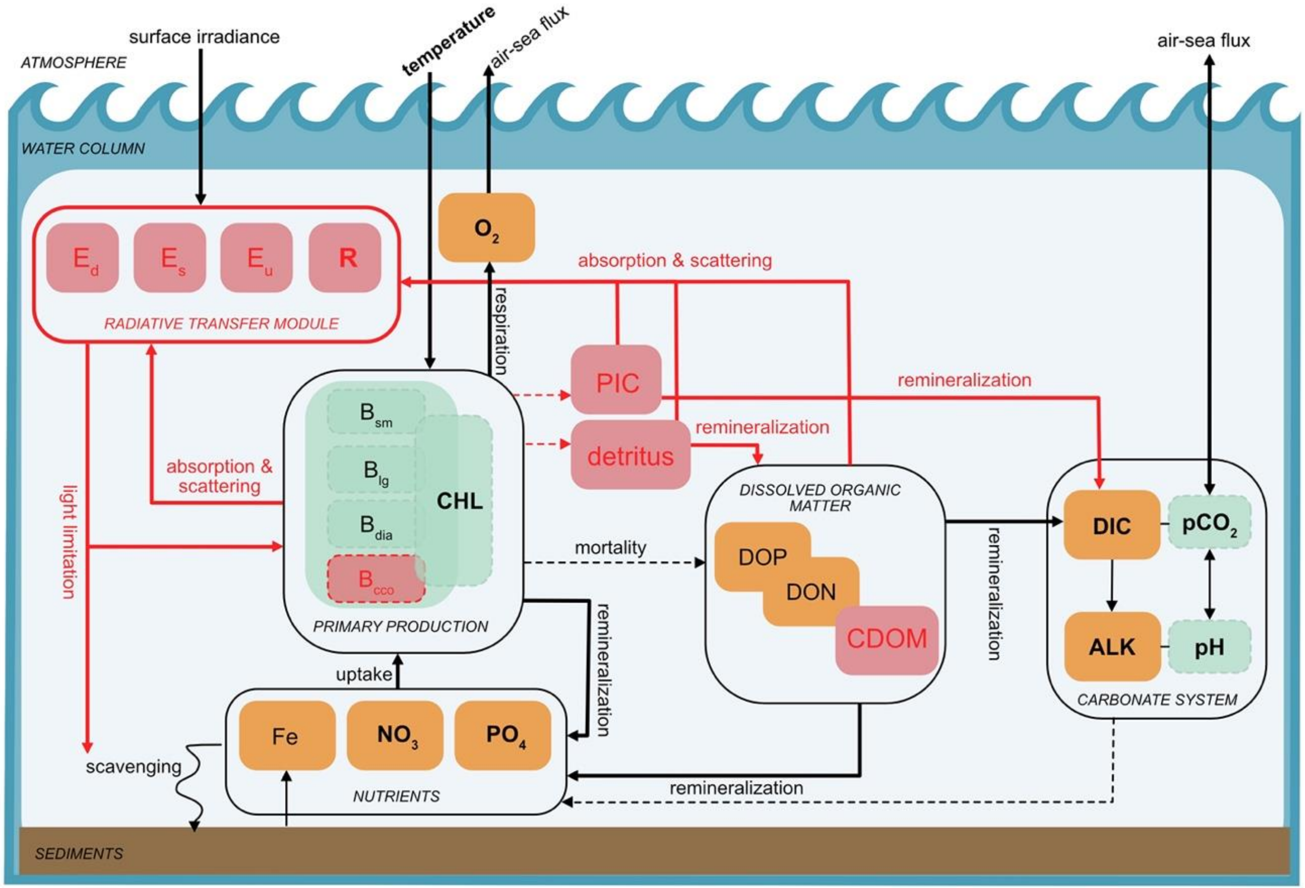
Assimilating ocean color observations

cost function = surface chlorophyll from VIIRS satellite, 2013



red = where adding iron would reduce the misfit with observations

Model: N-BLING, evolved from BLING



Proposed code additions to code to enable radiative transfer module

(Proposed by Angela Kuhn)