Phytoplankton Algorithms and Data Assimilation: Preparing a Pre-launch Path to Exploit PACE Spectral Data

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(now retired, didn't leave a head shot)

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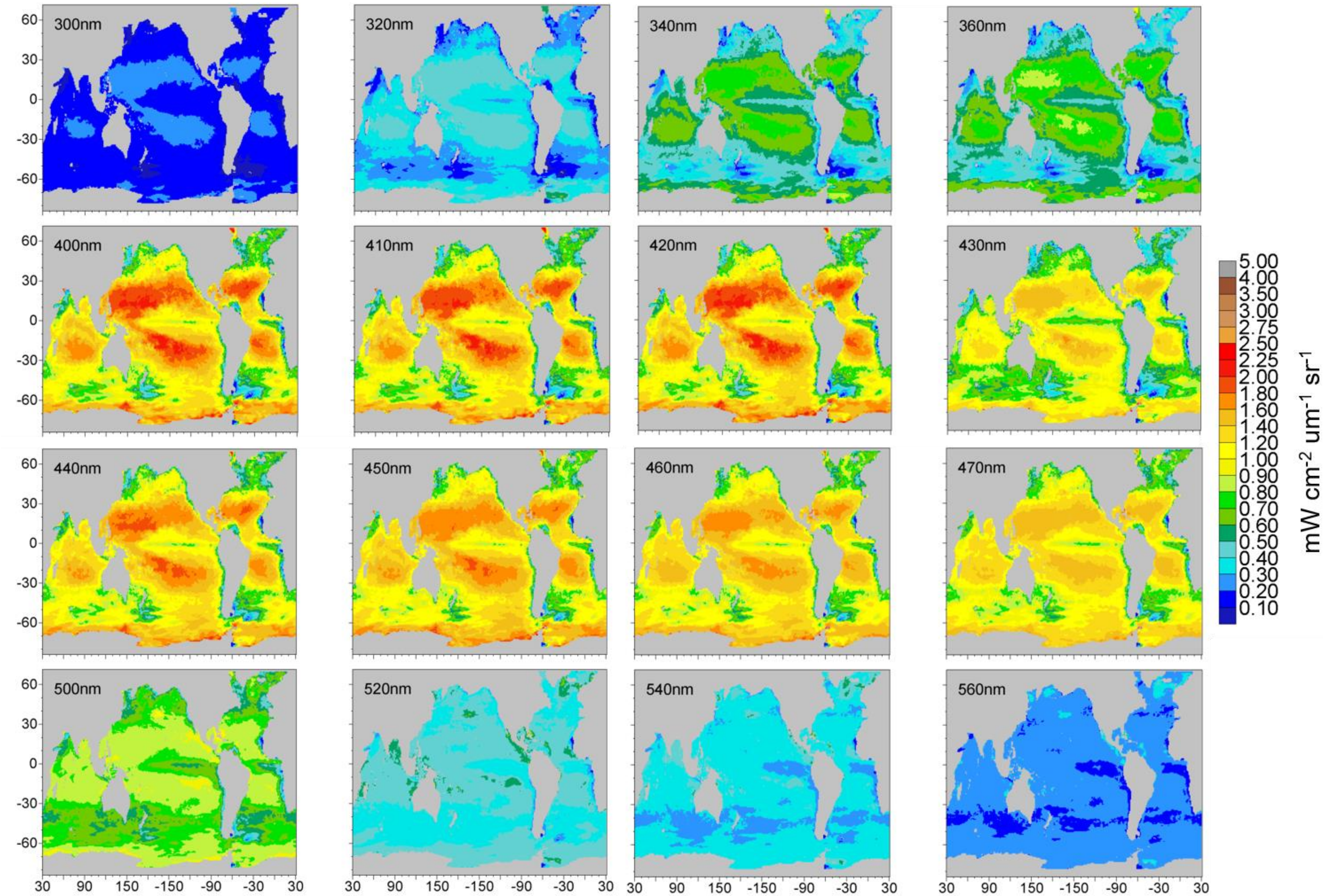
Background

- During the first PACE Science Team, we developed a hyperspectral water leaving radiance dataset

- This dataset was used in several applications. For example:
    - to test the effects that spectral and directional light have in simulations of ocean radiative transfer model (Gregg and Rousseaux 2016).
    - to develop a test granule simulation to use for algorithm development and other post-processing efforts by the PACE Project Team (GMAO and PACE Project collaboration-POC: Patricia Castellanos).

- The dataset was validated against existing multispectral ocean color satellite data



Spatial distribution of a few selected bands from the simulated global hyperspectral water leaving radiance dataset developed during the first PACE ST

Gregg W.W. and Rousseaux C.S. 2017. Simulating PACE Ocean Global Radiances. Frontiers in Marine Science , doi: 10.3389/fmars.2017.00060

PACE Science Team II

Objective:

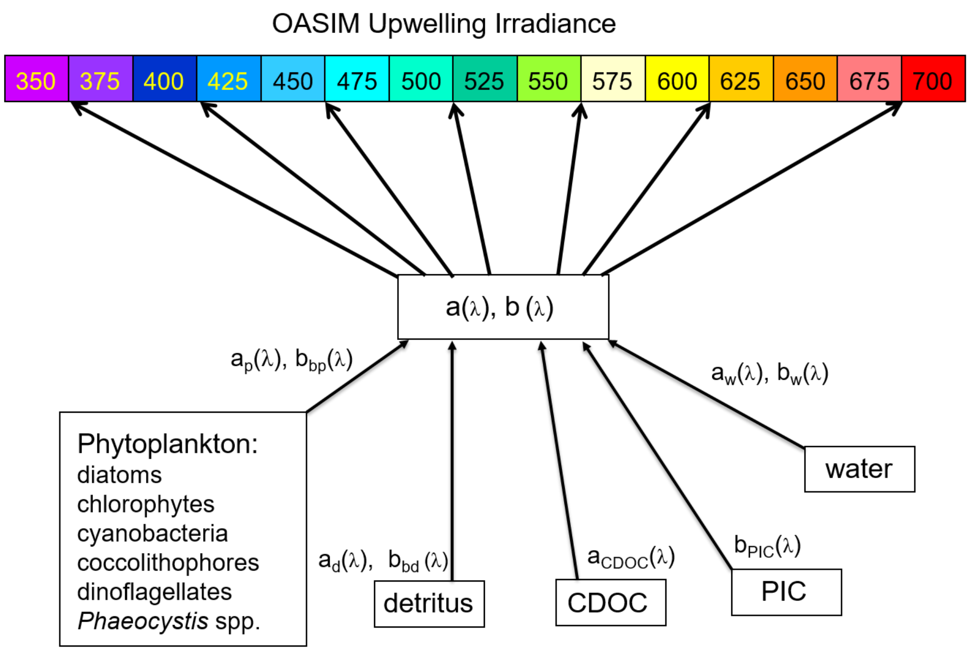
“To investigate the relationships between water leaving radiances and phytoplankton concentration and composition (SQ1*) and to develop a framework to assimilate hyperspectral water leaving radiance in a global Earth System Model (SQ2)."*

Method for SQ1:

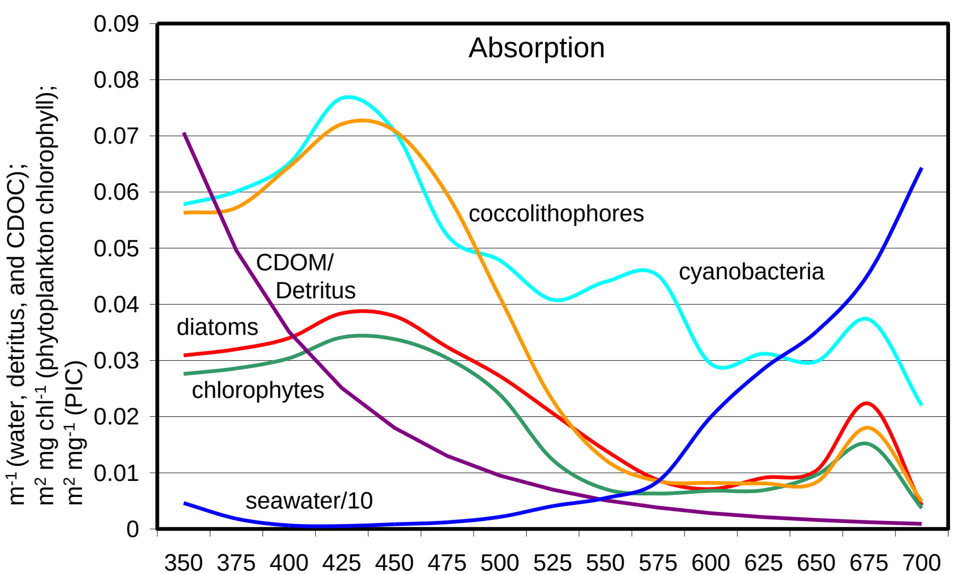
1) Use OASIM to generate water leaving radiances for individual and assemblages of phytoplankton functional groups, as well as other optically active constituents (water, detrital material, CDOM, and particulate inorganic carbon)

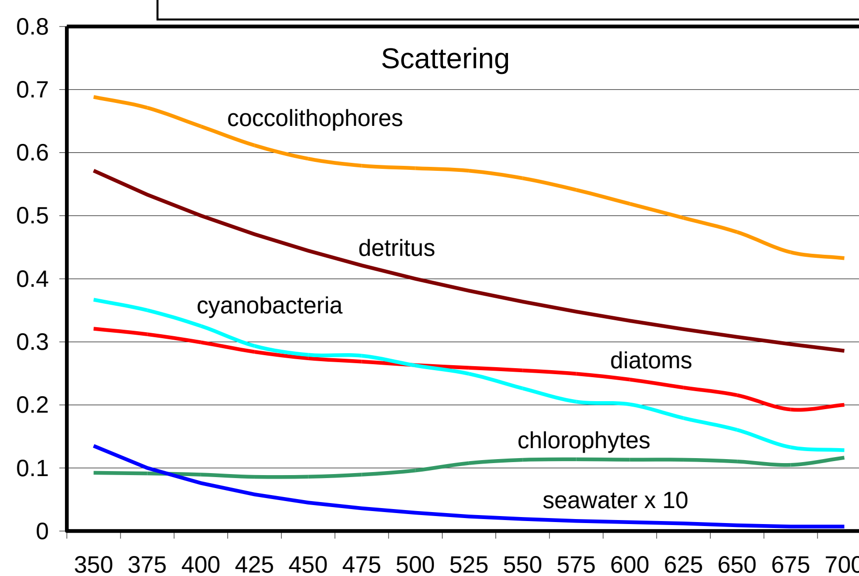
2) Test and refine algorithms developed in previous step with existing global simulated global hyperspectral water leaving radiance dataset (after calibration using existing hyperspectral instruments)

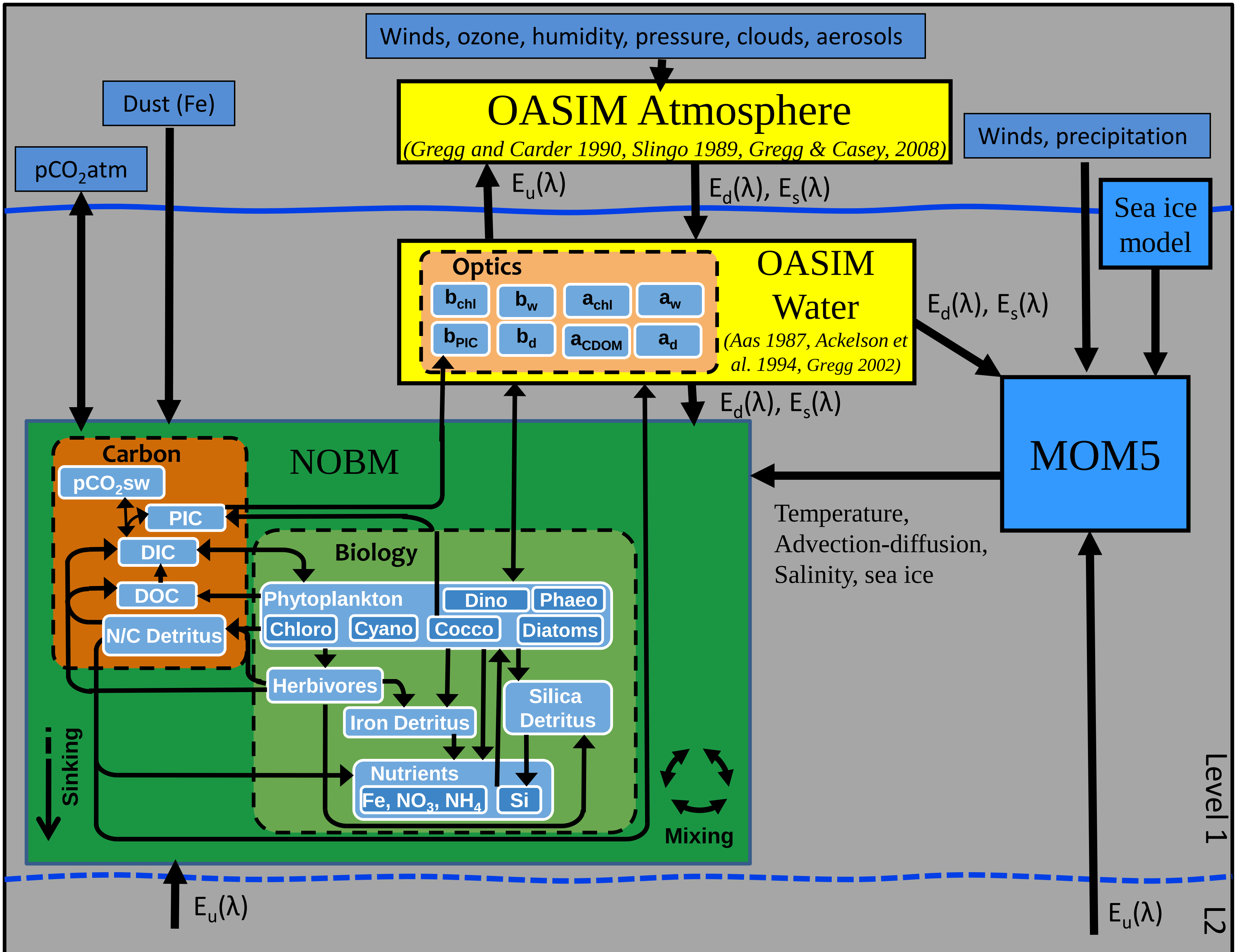
3) Use in situ data withheld from algorithm development to derive bias and uncertainty statistics



a_w, b_w	Smith and Baker 1981 (200-300 nm), (730-800 nm), Morel et al 2007 (325-475), Pope and Fry 1997 (500-720), Circio and Petty 1951 (800nm-2.5um), and Maul 1985 (2.5-4um).Lee et al
2015	(350-550) a_w only
b_b probability	0.5
a_c*, b_c* Bricaud	Morel 1987, Bricaud and Morel 1986 and et al. 1988, Ahn et al. 1992 (mass-specific coefficients)
b_b probability (2010)	Ahn et al. 1992, Morel, 1988, Whitmire et al.
a_d*, b_d*	Gallegos et al 2011 (mass-specific coefficients)
S_d=0.013	Gallegos et al 2011
b_b probability	Gallegos et al 2011
a_{cdom}*	Yacobi et al 2003; Tzortziou et al 2007 (mass-specific coefficient)
S_{aCDOM}=0.014	
b_{pic}	Gordon et al 2009
b_b probability	Balch et al 1996
ET irradiance	Thiullier et al 2003






Winds, ozone, humidity, pressure, clouds, aerosols
Dust (Fe)
pCO2atm
OASIM Atmosphere
(Gregg and Carder 1990, Slingo 1989, Gregg & Casey, 2008)
Winds, precipitation
Eu(λ)
Ed(λ), Es(λ)
Sea ice model
Optics
bchl
bw
achl
aw
bPIC
bd
aCDOM
ad
OASIM Water
(Aas 1987, Ackelson et al. 1994, Gregg 2002)
Ed(λ), Es(λ)
Ed(λ), Es(λ)
MOM5
Carbon
NOBM
pCO2sw
PIC
DIC
DOC
N/C Detritus
Biology
Phytoplankton
Dino
Phaeo
Chloro
Cyano
Cocco
Diatoms
Herbivores
Iron Detritus
Silica Detritus
Nutrients
Fe, NO3, NH4
Si
Temperature, Advection-diffusion, Salinity, sea ice
Sinking
Mixing
Level 1
Eu(λ)
Eu(λ)
L2

1) ***Use OASIM to generate water leaving radiances for individual and assemblages of phytoplankton functional groups, as well as other optically active constituents (water, detrital material, CDOM, and particulate inorganic carbon***

a) **Simulate** different concentration (or % of relative contribution) of total chlorophyll distributed among the 6 phytoplankton groups

b) **Spectral analyses** including band ratios, derivative analysis and clustering techniques (Lin et al. 2013; Torrecilla et al. 2011; Xi et al. 2017).

c) Smoothing and **derivative** parameters (filter size and band separation): compromise between the noise removal and the ability to resolve fine spectral information.

d) **HCA** will partition the datasets into clusters using a single linkage algorithm (analogous to the similarity index commonly used in algorithm development, see for example Millie et al. 2002).

e) The hyperspectral water leaving radiances generated during this phase will be converted to **look-up tables**. These tables can be used to further refine the algorithms by, for example, finding the absolute minimum differences when compared to hyperspectral water leaving radiances from natural assemblages

2) Test and refine algorithms developed in previous step with existing global simulated global hyperspectral water leaving radiance dataset (after calibration using existing hyperspectral instruments)

(1) Regrid, compare and calibrate simulated dataset with existing hyperspectral data:

- HICO (2009-2014, https://oceandata.sci.gsfc.nasa.gov/HICO/),
- PRISM (2012-2018, https://prism.jpl.nasa.gov/prism_data.html),
- AVIRIS (2006-2018, https://aviris.jpl.nasa.gov/alt_locator/)

(2) Test the ability of the algorithms to derive phytoplankton concentration and composition in a natural environment at the global scale

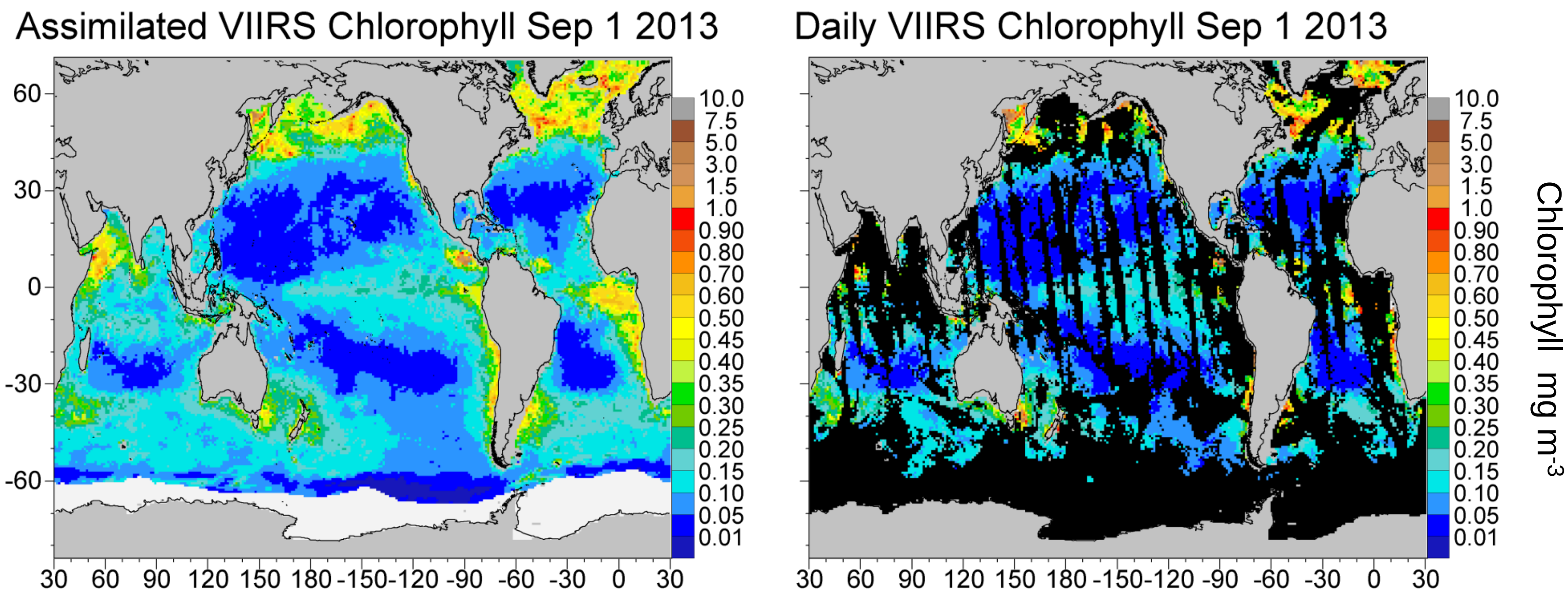
- Use for example absolute minimum differences between the look-up tables and the hyperspectral water leaving radiances from NOBM-OASIM for each locations
  - Attribute different weights to the various bands further improves the algorithms performances?
  - Do statistical approaches of different complexity (single and higher order band-ratios, multiple regression comparison between discrete values and combination of water leaving radiances, etc) decrease our bias and uncertainty?

3) *Use in situ data withheld from algorithm development to derive bias and uncertainty statistics*

- Gregg and Casey (2007): 469 observations of phytoplankton relative abundances derived from the general literature (http://gmao.gsfc.nasa.gov/research/oceanbiology/index.php)
- World of Ocean Atlas of MARine Ecosystem DATa (MAREDAT, Buitenhuis et al. 2012a, www.pangaea.de)
- The performance of the algorithms will be evaluated using parametric and non-parametric representations: correlation, relative error, root mean square error, median, semi-interquartile range.
- We will establish differences, statistical dispersion, and correlations in different regions to understand where and when our approaches succeed and where difficulties arise.

Objective:

"To investigate the relationships between water leaving radiances and phytoplankton concentration and composition (SQ1) and ***to develop a framework to assimilate hyperspectral water leaving radiance in a global Earth System Model (SQ2)."***



Ice fields are shown in white. Missing data is shown in black.

Method for SQ2:

- Use the Joint Effort for Data assimilation Initiative (JEDI), a framework that allows for the assimilation of a variety of variables within GEOS-NOBM

- Compare the model output from a run assimilating multi-spectral data products (chlorophyll, PIC and aCDOM) with the model output from a model run that assimilates hyperspectral water leaving radiances

- Produce Level-4 products of existing data product or new product if algorithm not currently available

- Can also inform the PACE Project Team on band selection, band aggregation and other information that can only be derived using an assimilation model framework where various simulations can be run at various spectral resolutions, using different bands etc

Milestone/Deliverables	Date
Use OASIM to generate water leaving radiances for individual and assemblages of phytoplankton functional types in a ‘controlled’ environment	Year 1
Develop algorithms for the phytoplankton composition using the spectra generated by OASIM alone	Year 1-2
Apply and refine the algorithms using a global simulated dataset	Year 2
Validate final phytoplankton composition and concentration algorithms using in situ dataset	Year 2-3
Develop the framework to assimilate hyperspectral water leaving radiances	Year 1-2
Assess whether the quantity and quality of data products derived from PACE can be improved by assimilating hyperspectral water leaving radiances	Year 2-3
Make the data of phytoplankton composition as well as the Level-4 hyperspectral water leaving radiance data publicly available	Year 3

- Validation plan and/or needs:

    - Data on phytoplankton composition

    - Anything to know about AVIRIS, PRISM or HICO or other hyperspectral dataset we can use to calibrate our simulated dataset

- Needs that can and cannot be met presently:

    - Looking for a postdoc on algorithm development

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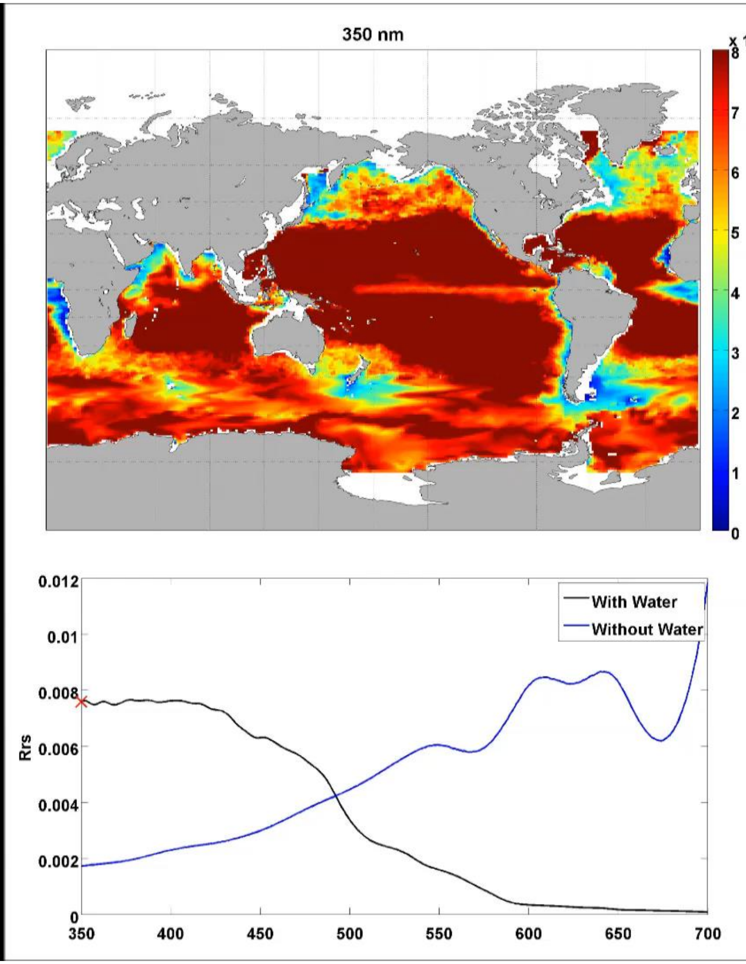
(sr^{-1})



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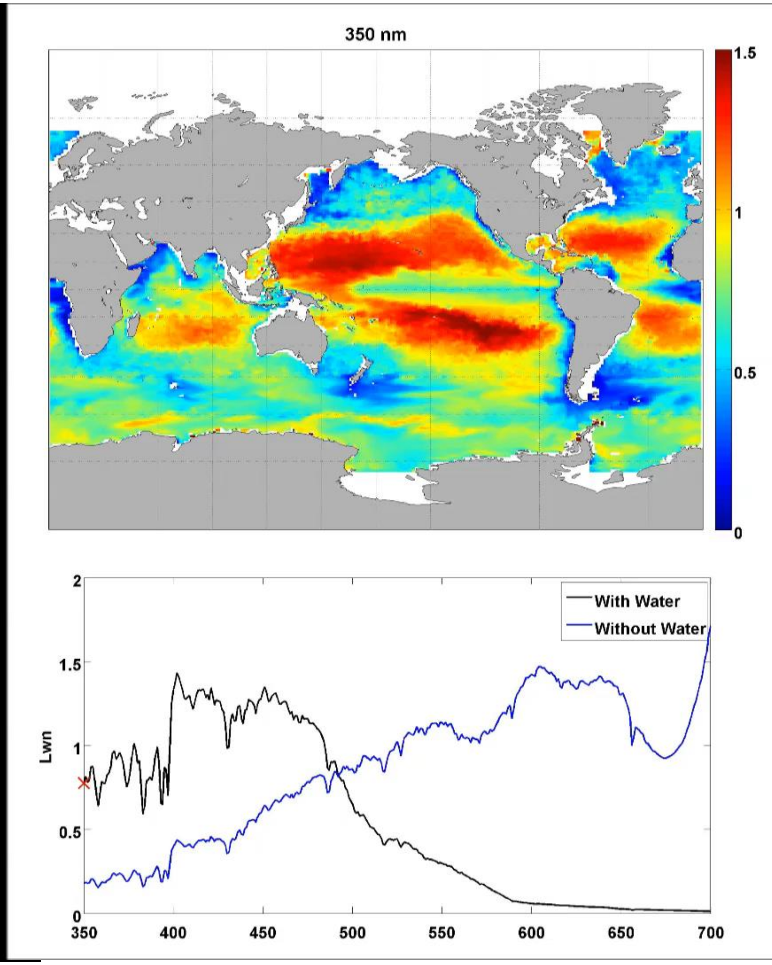
($mW\ cm^{-2}\ um^{-1}\ sr^{-1}$)



The end...

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