Detecting Change in the Global Ocean Biosphere using SeaWiFS Satellite Ocean Color Observations

Part 2: Confronting Bio-Optical Complexity

David Siegel

Earth Research Institute, UC Santa Barbara

david.siegel@ucsb.edu

Much help from Chuck McClain, Mike Behrenfeld, Stéphane Maritorena, Norm Nelson, Bryan Franz, David Antoine, Jim Yoder and many others…

eLecture 1

- Review satellite ocean color basics
- Highlight important findings from SeaWiFS

  Interpret climate-relevant trends in chlorophyll

eLecture 2

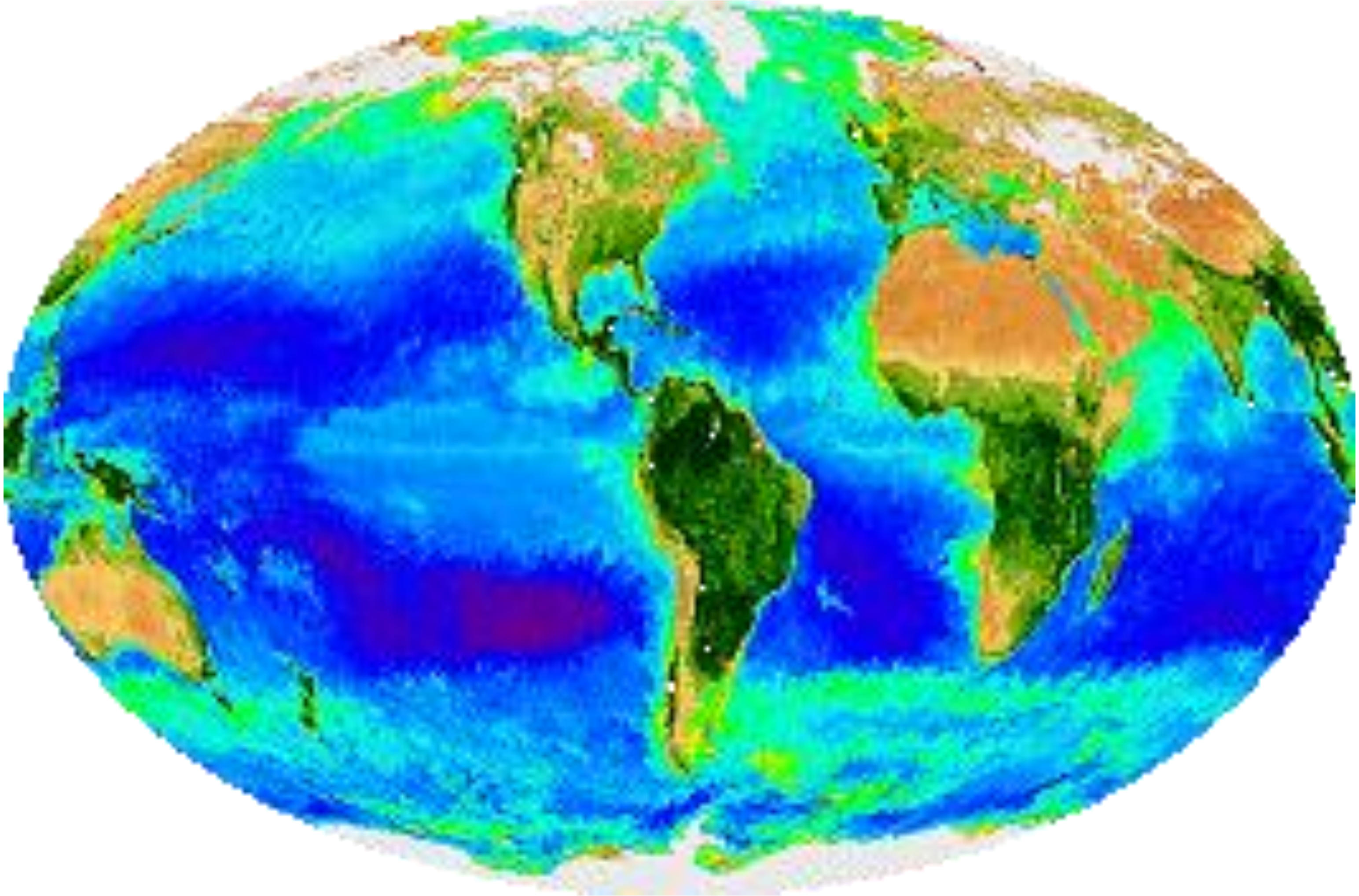
- Introduce open ocean bio-optical complexity

  Retrieve relevant inherent optical properties (IOPs)

  Confront the trends with changes in IOPs

- Introduce steps forward (NASA's PACE mission…)

Global Chlorophyll



http://oceancolor.gsfc.nasa.gov/SeaWiFS/HTML/SeaWiFS.BiosphereAnimation.html

Chlorophyll is Great…

We can [finally] see the ocean biosphere!

- Assess local to global scale variations
- Trends of change on decade time scales

Chlorophyll is easily measured in the field

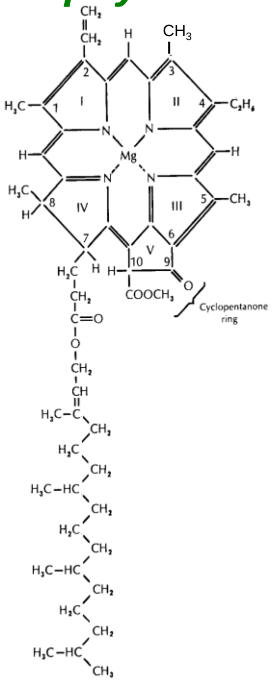
- Lots of data for building & validating algorithms

We can also assess net primary production

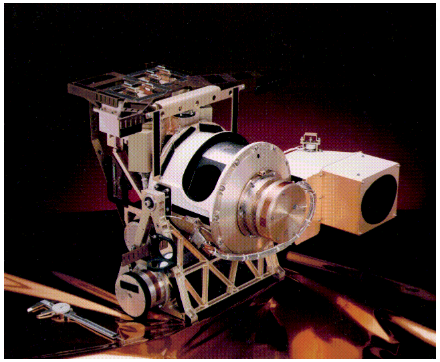
- Model NPP as f(Chl & light) - other ways too…

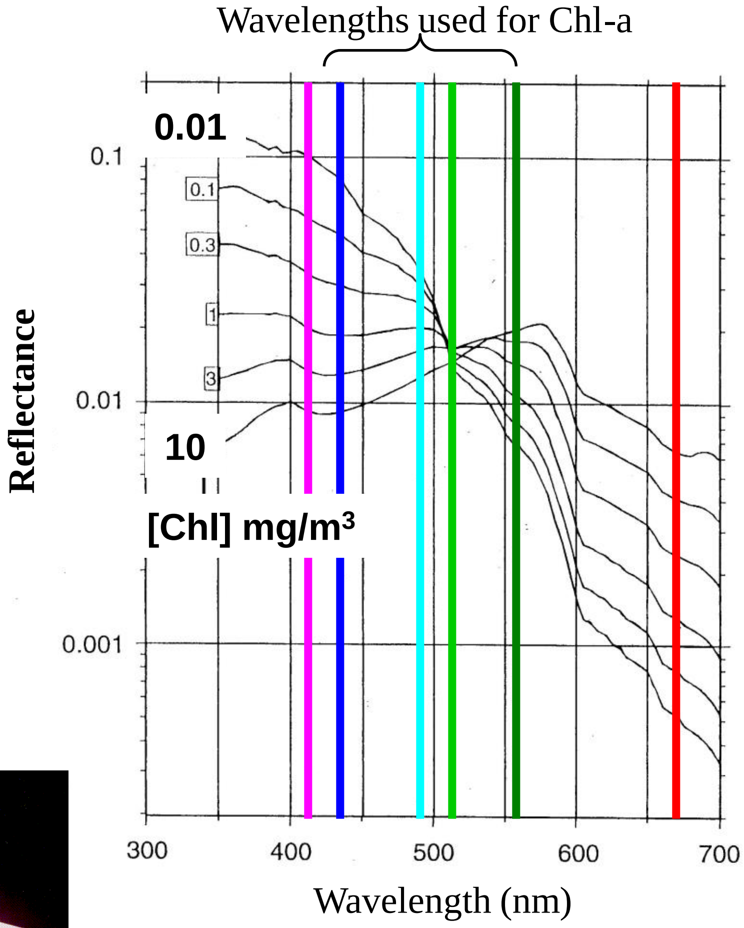
Operational Chl-a Algorithms

Chlorophyll-a



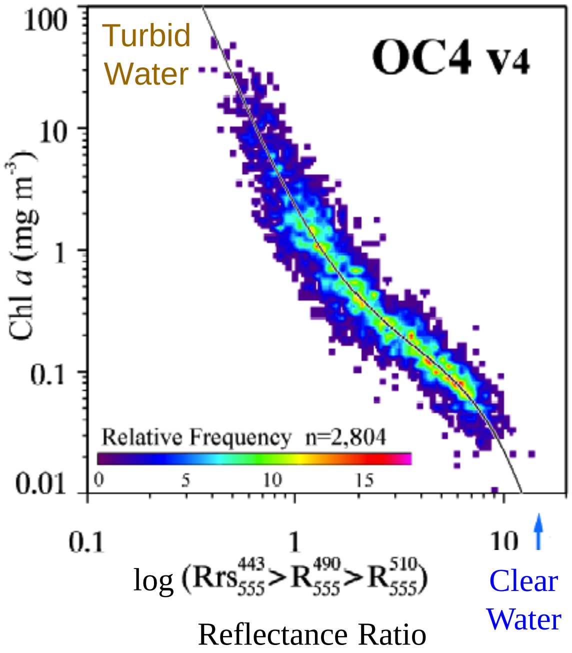
SeaWiFS





Marine Spectral Reflectance vs. Chlorophyll-a

Chlorophyll Algorithm: Empirical "Band-Ratio" Regression



But, chlorophyll is …

Not Often What We Want

Phytoplankton biomass is biogeochemically relevant, not chlorophyll

To get biomass we need to know Chl/C

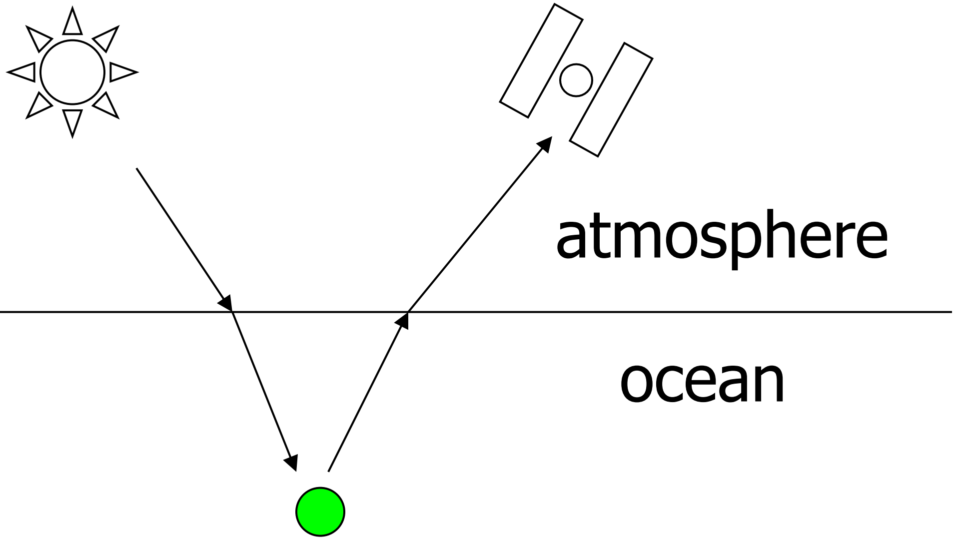
But Chl/C = f(light, nutrients, species, etc.)

Nor is it The Whole Story

There’s more in the ocean that affects ocean color than just chlorophyll

What is Ocean Color?

- Light backscattered from the ocean but is not absorbed



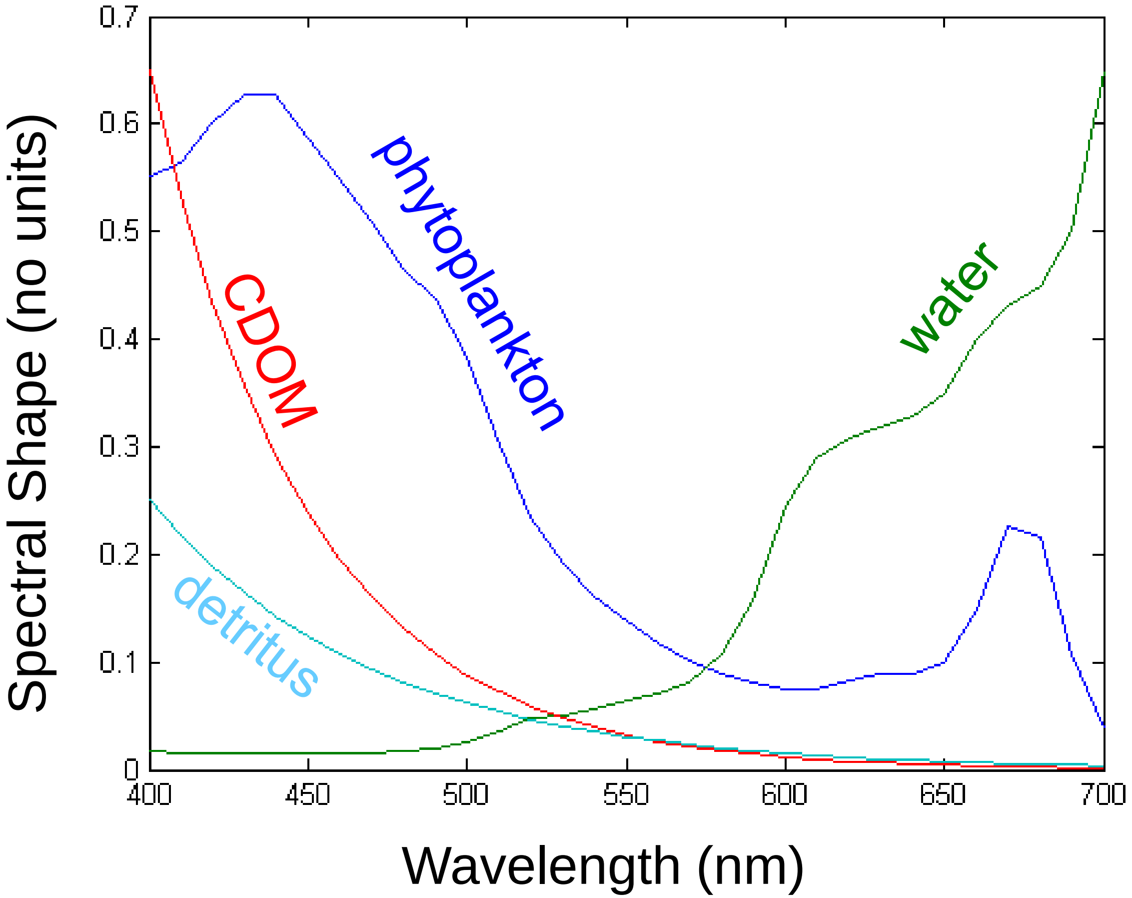
- Reflectance = f(backscattering/absorption)

$$\boxed{R_{rs}(\lambda) = f(b_b(\lambda) / a(\lambda))}$$

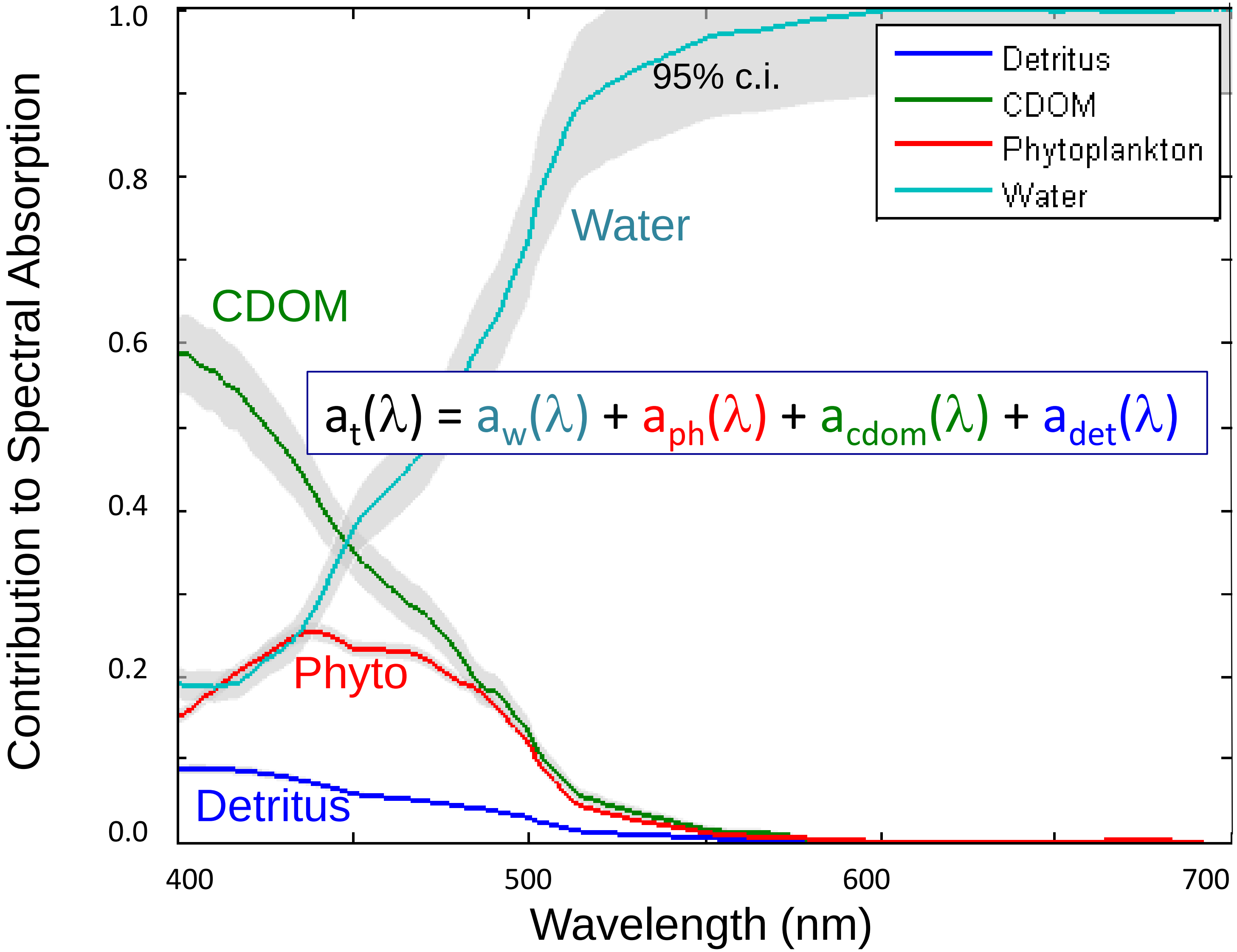
Absorption of Light in Seawater

Total abs = water + phyto + CDOM + detritus

$$a(\lambda) \quad = a_w(\lambda) + a_{ph}(\lambda) + a_g(\lambda) + a_{det}(\lambda)$$



Spectral Absorption Components



$$a_t(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{cdom}(\lambda) + a_{det}(\lambda)$$

Siegel et al. RSE [2013]

Backscattering of Seawater

Total b_b = water + particle = $b_{bw}(\lambda)$ + $b_{bp}(\lambda)$

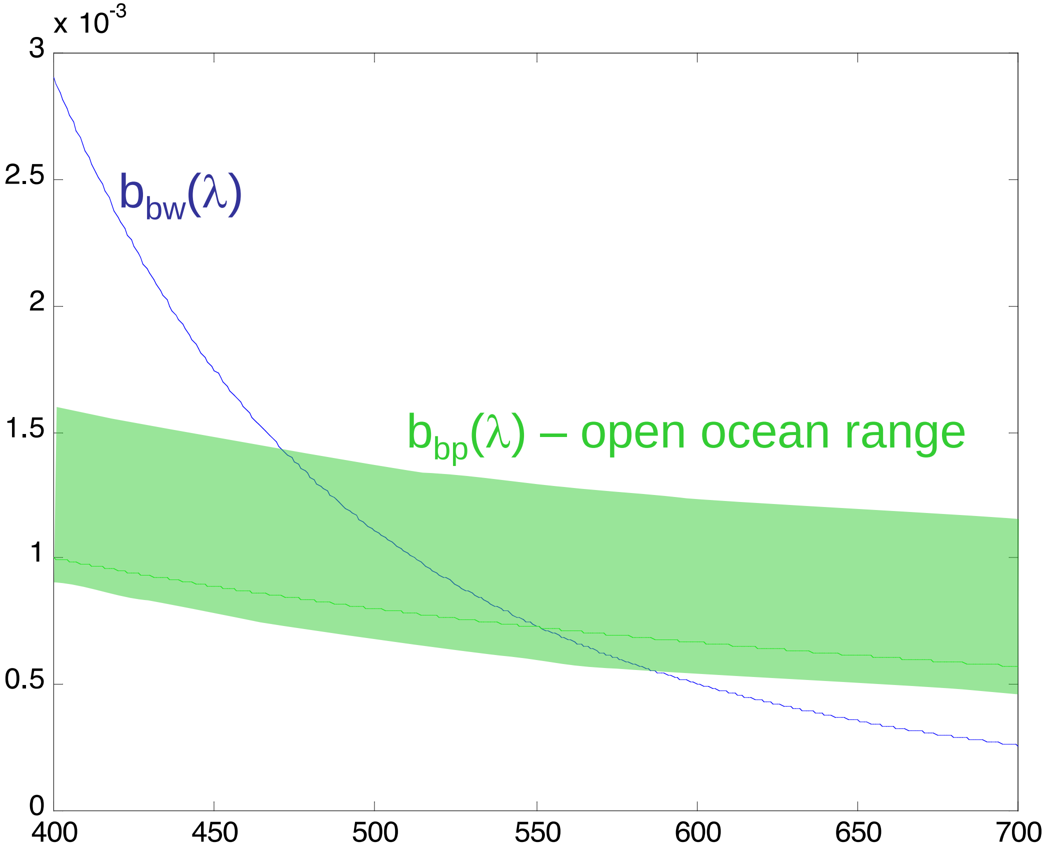
Backscattering is very small

Open ocean & most coastal waters…

- water dominates $\lambda < 450$ nm
- particles $\lambda > 550$ nm
- theoretically - small particles
- but b_{bp} variability is too large

Coastal waters under terrestrial influences…

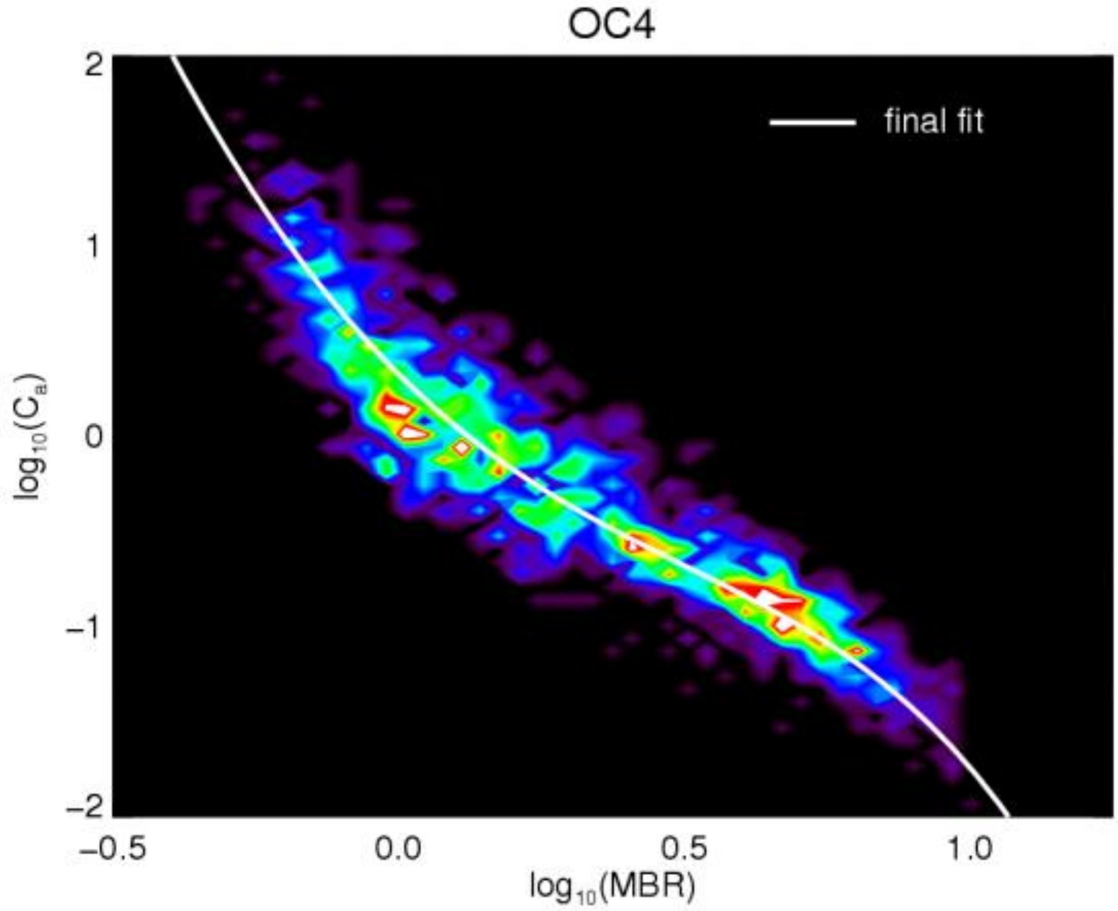
- deviations can occur



SeaWiFS Chlorophyll Algorithm

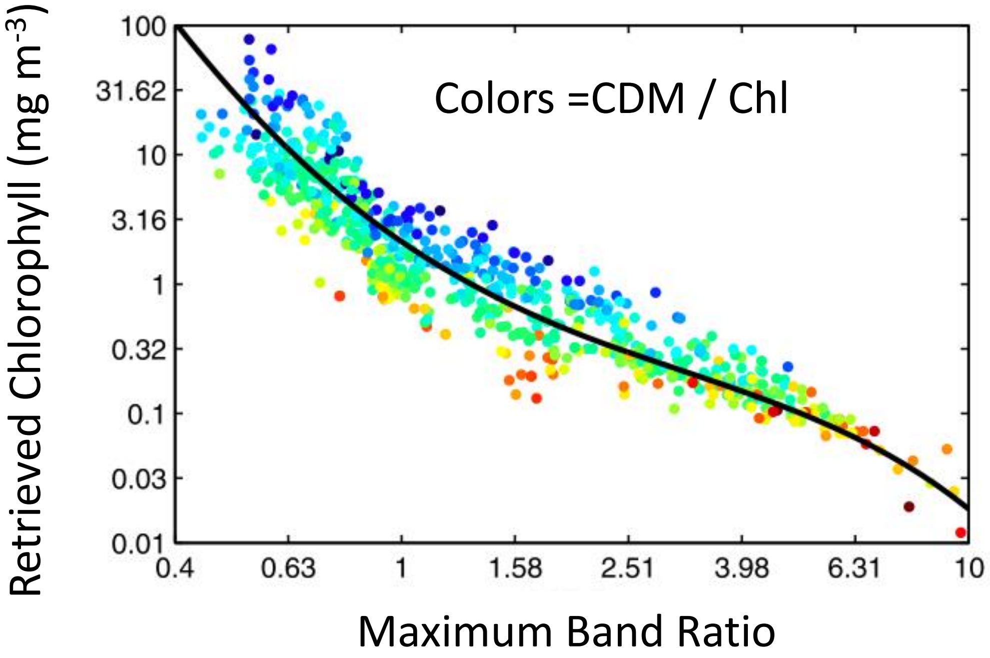
OC4v6 algorithm

- Empirical
- Maximum Band Ratio of $R_{rs}(\lambda)$'s (443/555, 489/555 & 510/555)



From GSFC reprocessing page following O'Reilly et al. [1998] JGR

Do Empirical Algorithms Work?



Szeto et al. [2011] JGR

Analysis of NOMAD data

- CDM = $a_{cdom}(443) + a_{det}(443)$ (dissolved & detrital absorption)
- Large biases in Chl retrievals due to CDM (mostly CDOM)
- CDM effects need to be removed to observe phytoplankton processes

Semi-Analytical Models

- Enables independent retrieval of several IOPs
  - Utilizes all available spectral information
  - Typically three IOPs are retrieved using SeaWiFS
  - Separates phytoplankton from other IOPs
- Combines theory & observations
  - Theory enables model to be useful over a wide range of conditions
  - Observations are used to adjust model constants

What IOPs Can Be Retrieved?

- Ocean color is like your computer monitor
  - Basically, you get 3 colors (like RGB, HSL, etc.)
- Typically you get the Open Ocean Color Trio
  - Chlorophyll, CDM & particle backscattering
  - Chl & CDOM (with water) set the color balance and BBP sets the brightness level
  - Maybe more - size, community structure, etc.

What the trio tells us…

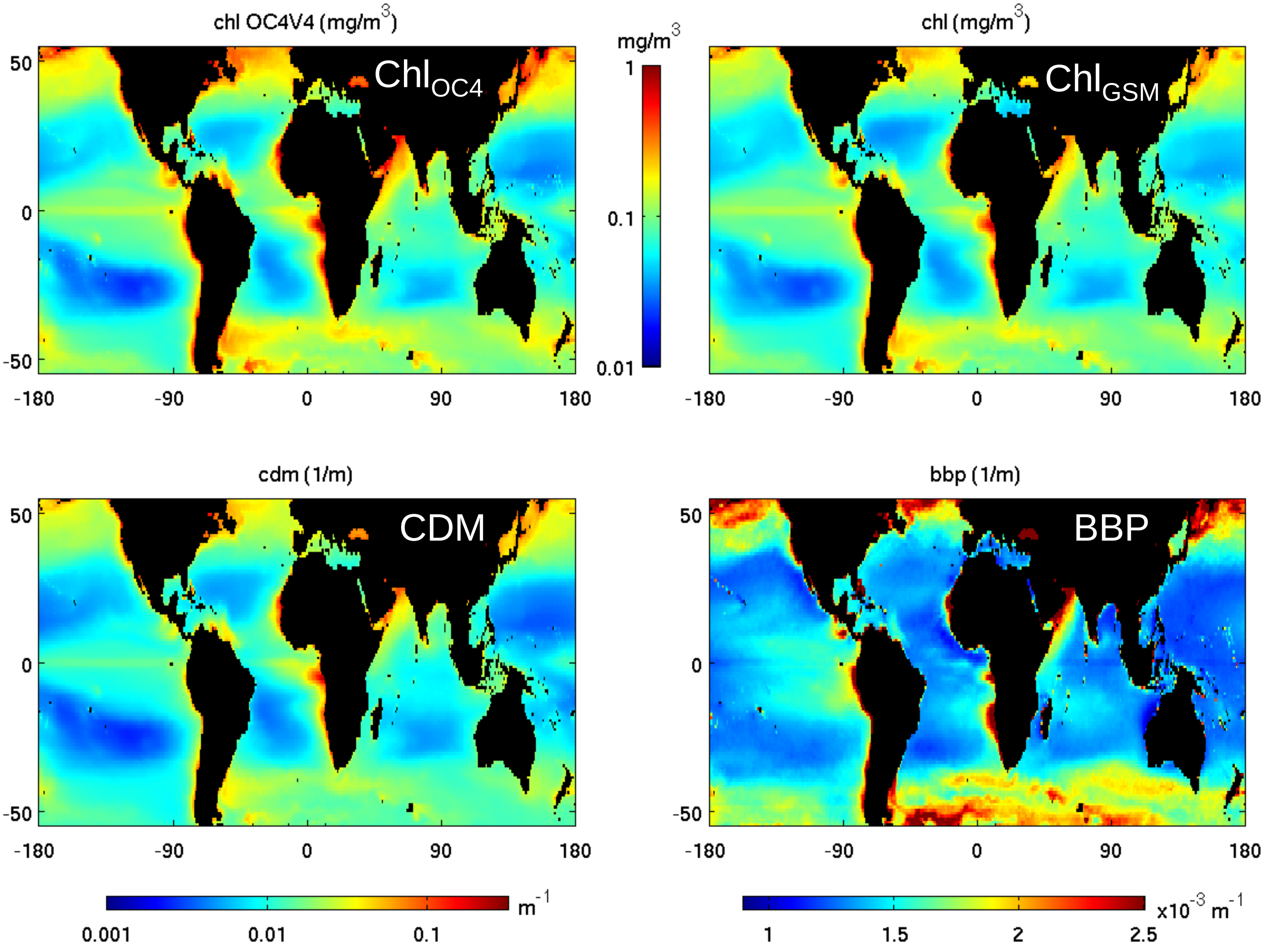
Property	**What's Sensed**	**Regulating Process**	**Forcing Mechanism**
BBP particulate backscatter	Particle biomass Suspended sediment	Primary production Terrestrial inputs	Nutrient input/upwelling Land/ocean interactions Dust deposition??
Chl chlorophyll concentration	Chlorophyll biomass	Primary production Physiological changes of phytoplankton C:Chl	Nutrient input/upwelling Growth irradiance & nutrient stress
CDM colored detrital materials	CDOM Detrital particulates	Heterotrophic production Photobleaching Terrestrial inputs	Upwelling/entrainment UV light dosage Land/ocean interactions

Siegel et al. (2005) JGR

GSM Semi-Analytic Model

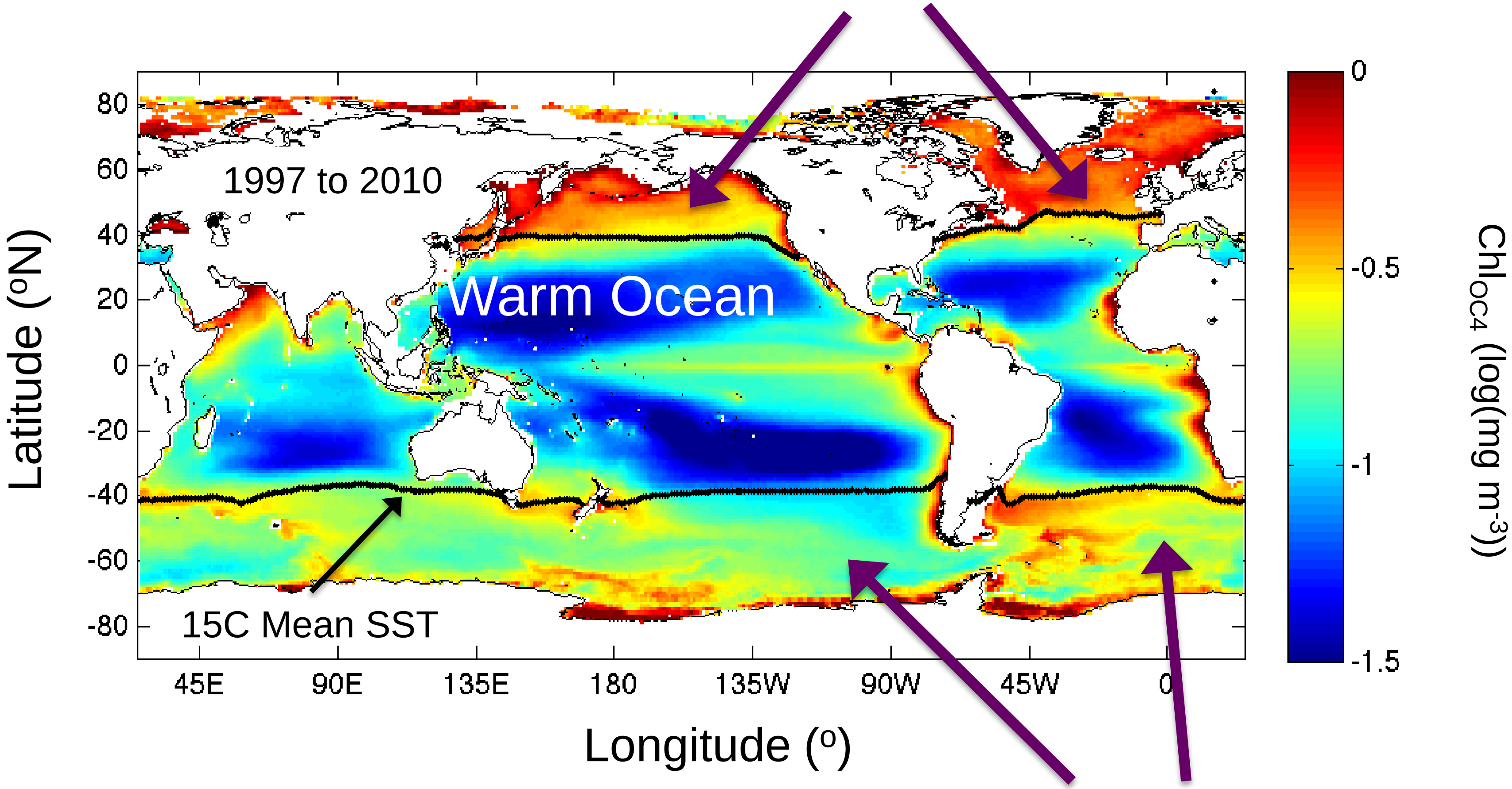
- Retrieves three relevant properties (CDM, BBP, Chl)
  - CDM = $a_{cdom}(443)+a_{det}(443)$ & BBP = $b_{bp}(443)$
- Assumptions…
  - Relationship between $R_{rs}(\lambda)$ & IOP's is known
  - Component spectral shapes are constant
  - Water properties are known
- Model coefficients fit w/ field obs (Maritorena et al. AO, 2002)
- Global validation statistics for Chl_{GSM} with SeaWiFS are nearly as good as for Chl_{OC4} (Siegel et al. RSE, 2013)
- Similar models are available (QAA, GIOP, etc.)

The Ocean Color Trio



Revisiting Empirical Algorithm Results

Cool NH Ocean



1997 to 2010

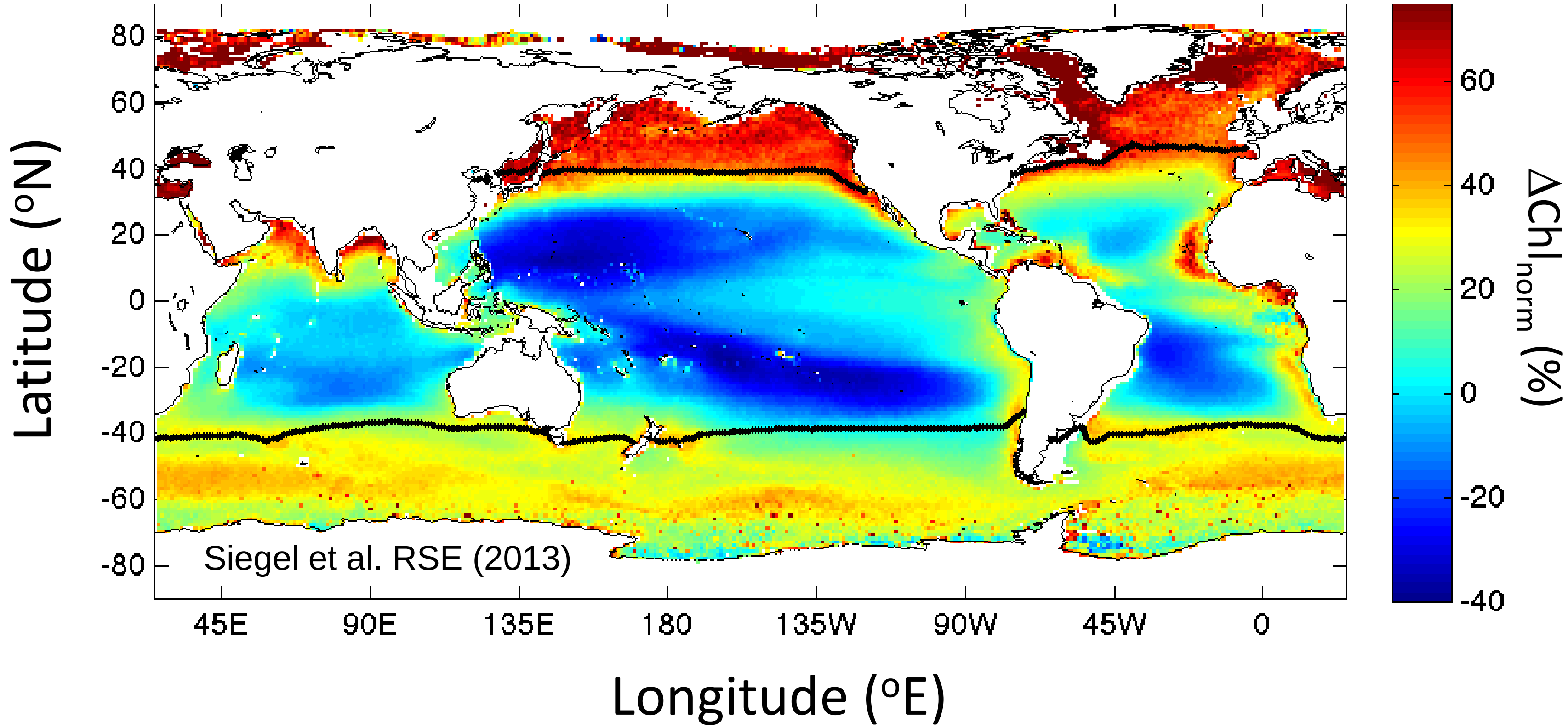
Warm Ocean

15C Mean SST

Cool SH Ocean

Siegel et al. RSE (2013)

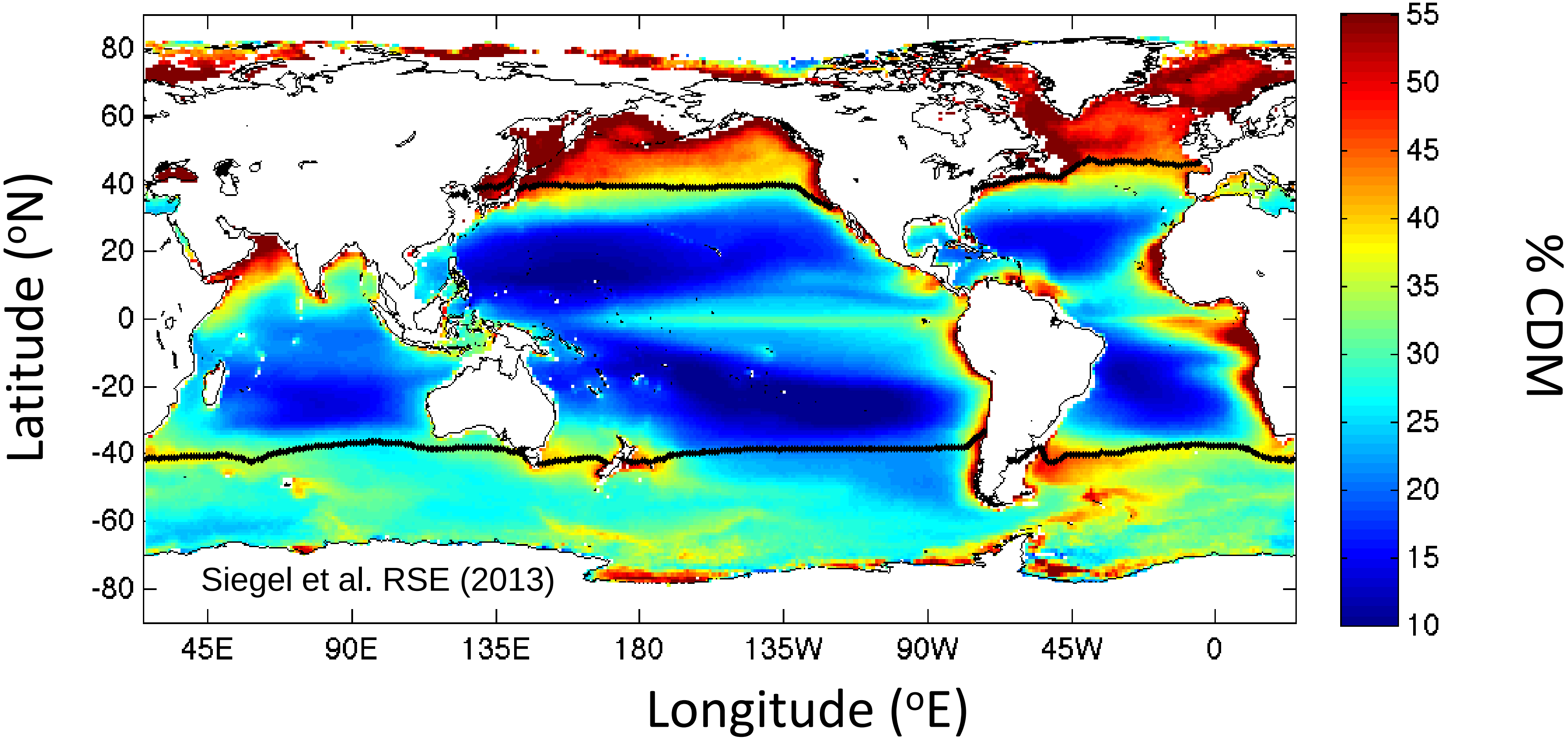
Differences Between OC4 & GSM Chl



Siegel et al. RSE (2013)

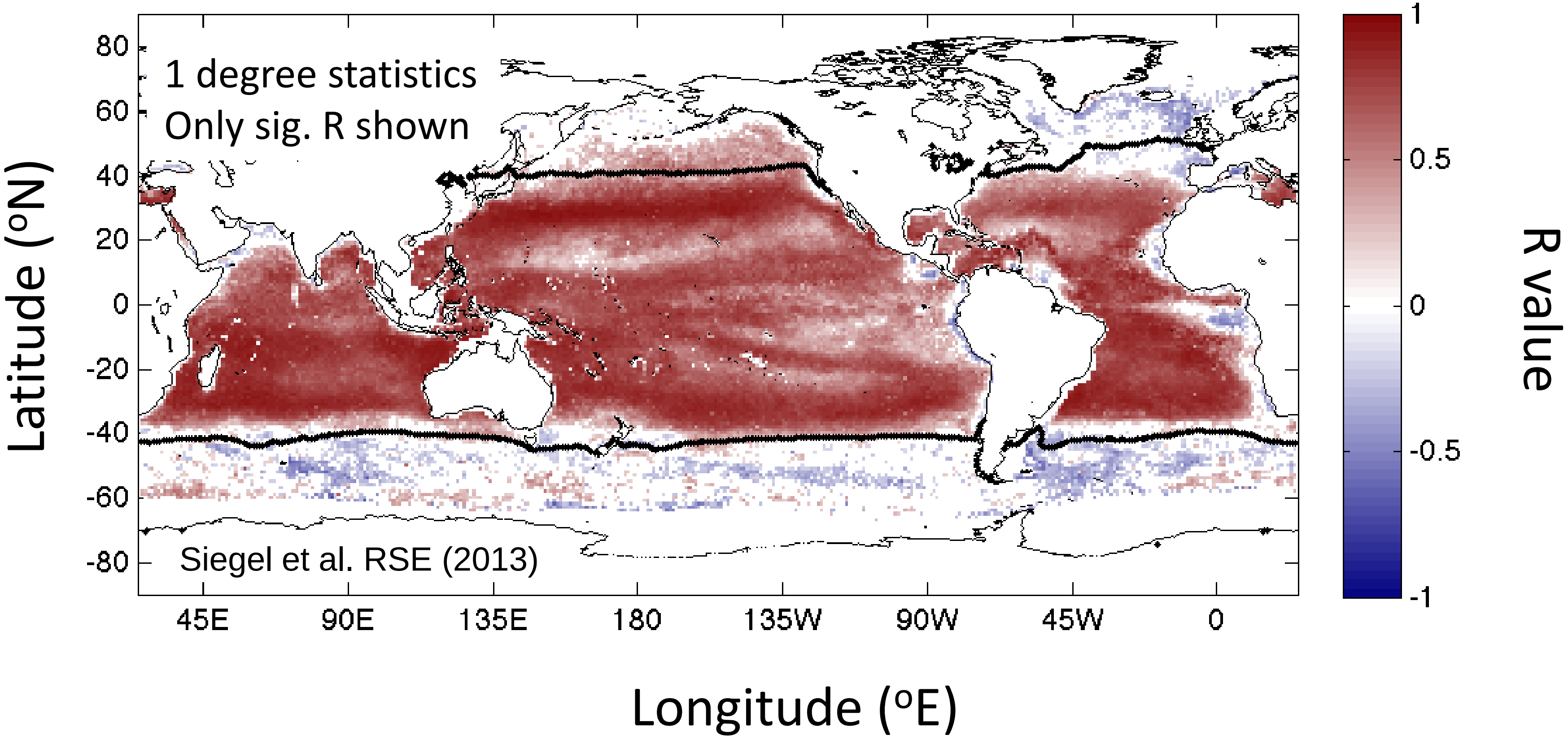
- $\Delta \text{Chl}_{\text{norm}} = 100 * (\text{Chl}_{\text{OC4}} - \text{Chl}_{\text{GSM}})/\text{Chl}_{\text{GSM}}$
- $\text{Chl}_{\text{OC4}} > \text{Chl}_{\text{GSM}}$ by ~60% in high NH, by rivers, etc.
- Chl_{OC4} ~20% lower in subtropical gyres
- Chl_{OC4} ~30% higher in the Southern Ocean

Mean Contribution of CDM



- %CDM = $a_{cdm}(443) / (a_{cdm}(443)+a_{ph}(443))$
- High in subpolar NH oceans & low in subtropical oceans
- Mean patterns for %CDM & ΔChl_{norm} are well correlated (R=0.66)

Correlations of $\Delta\mathrm{Chl}_{norm}$ & %CDM

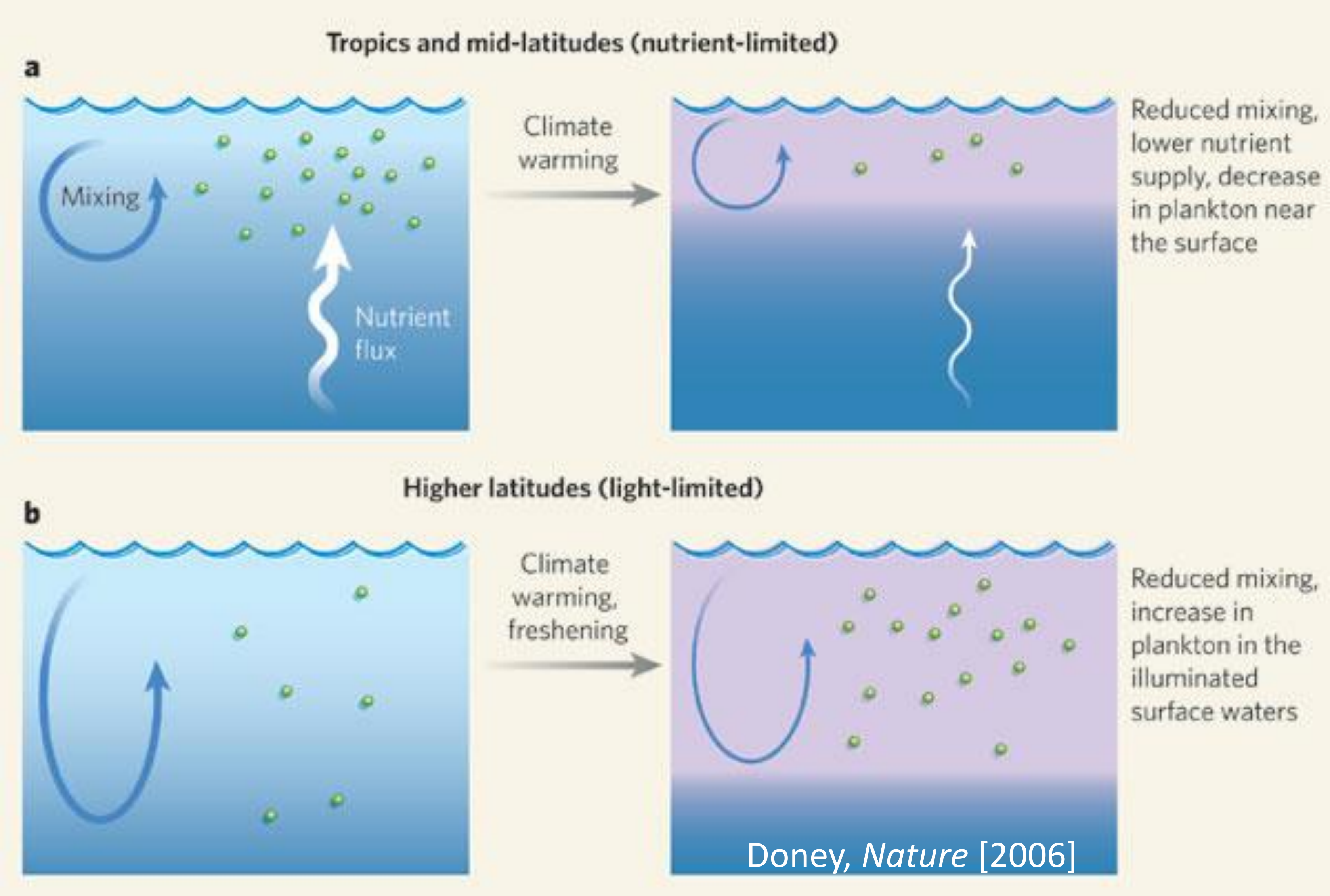

1 degree statistics
Only sig. R shown
Siegel et al. RSE (2013)

- Positive correlation between $\Delta\mathrm{Chl}_{norm}$ & %CDM in warm ocean
- Correlations are mixed for regions where mean SST < 15C

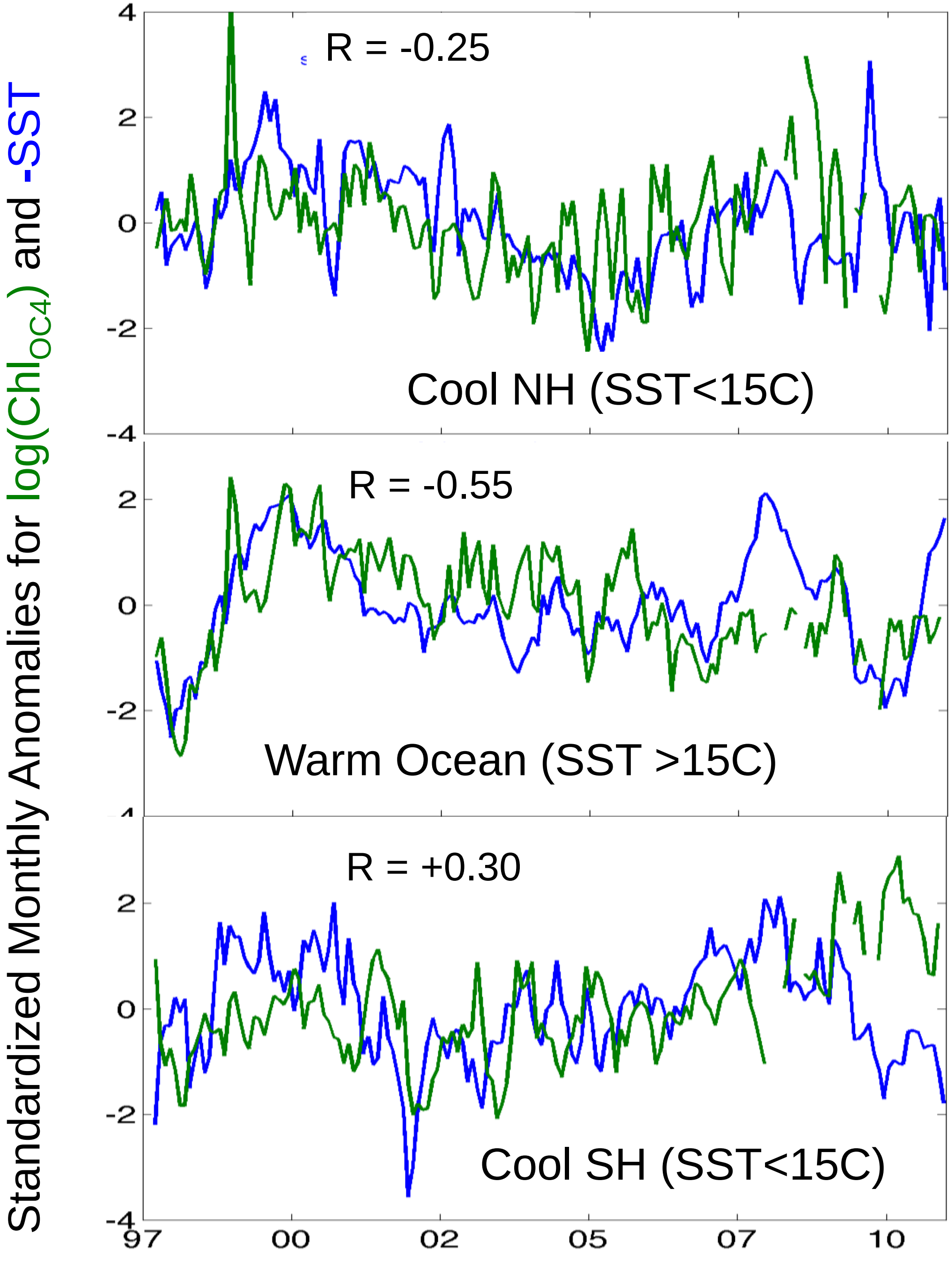
Empirical Algorithms & CDM

- Mean patterns in $\Delta \mathrm{Chl}_{\mathrm{norm}}$ & %CDM are well related especially for warm & NH cool oceans
- Changes in time of $\Delta \mathrm{Chl}_{\mathrm{norm}}$ & %CDM are well correlated for the warm ocean but not outside
- Both point to large influences of CDM on empirical (band-ratio) ocean color algorithms
- What do the CDM-corrected chlorophyll concentrations look like?

Phytoplankton in a Changing Climate



Doney, *Nature* [2006]



Siegel et al. RSE (2013)

Increasing Chl$_{OC4}$
Decreasing SST

Decreasing Chl$_{OC4}$
Increasing SST

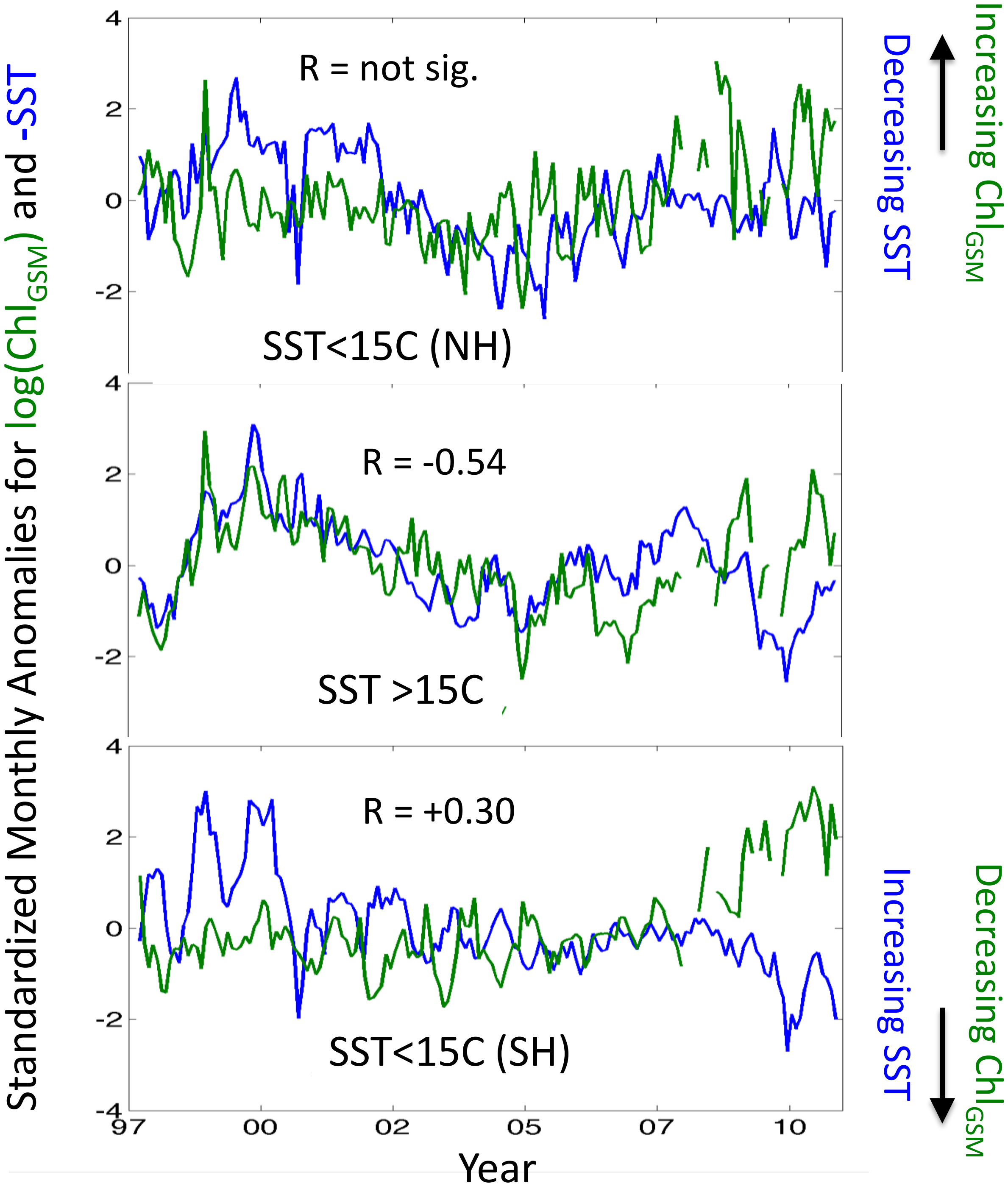
Trends by Basin

Not Significant
+0.035 °C/y

-0.18 %/y
+0.015 °C/y

+0.83 %/y
+0.029 °C/y

What do semi-analytical models say?



Trends by Region

+0.79 %/y

+0.035 ^{o}C/y

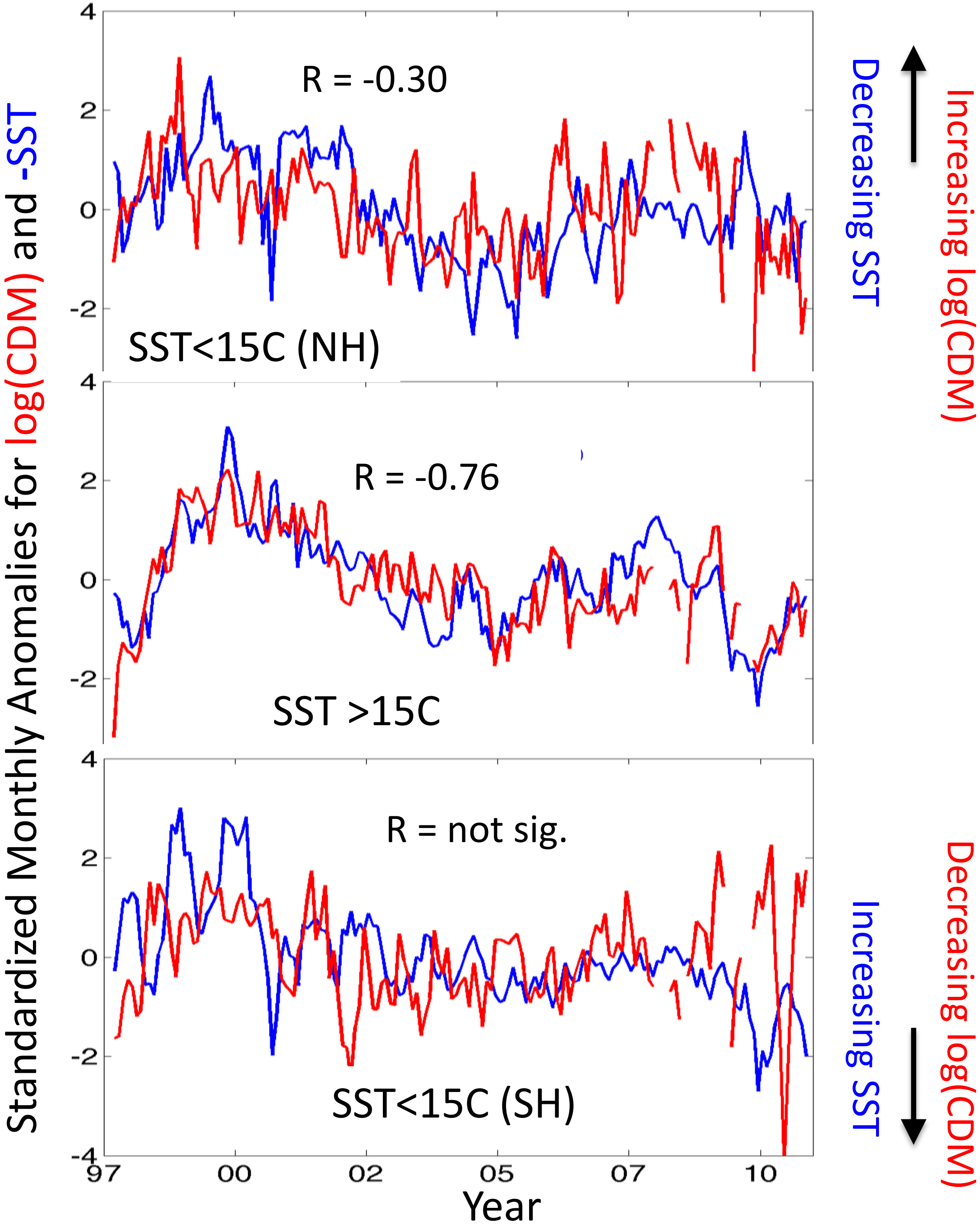
not significant

+0.015 ^{o}C/y

+1.03 %/y

+0.029 ^{o}C/y

But Chl$_{OC4}$ shows decreases in warm ocean?



Trends by Region

-0.56 %/y
+0.035 ^{o}C/y

-0.31 %/y
+0.015 ^{o}C/y

not sig
+0.029 ^{o}C/y

CDM explains $\mathrm{Chl}_{\mathrm{OC4}}$ decreases in warm ocean!!

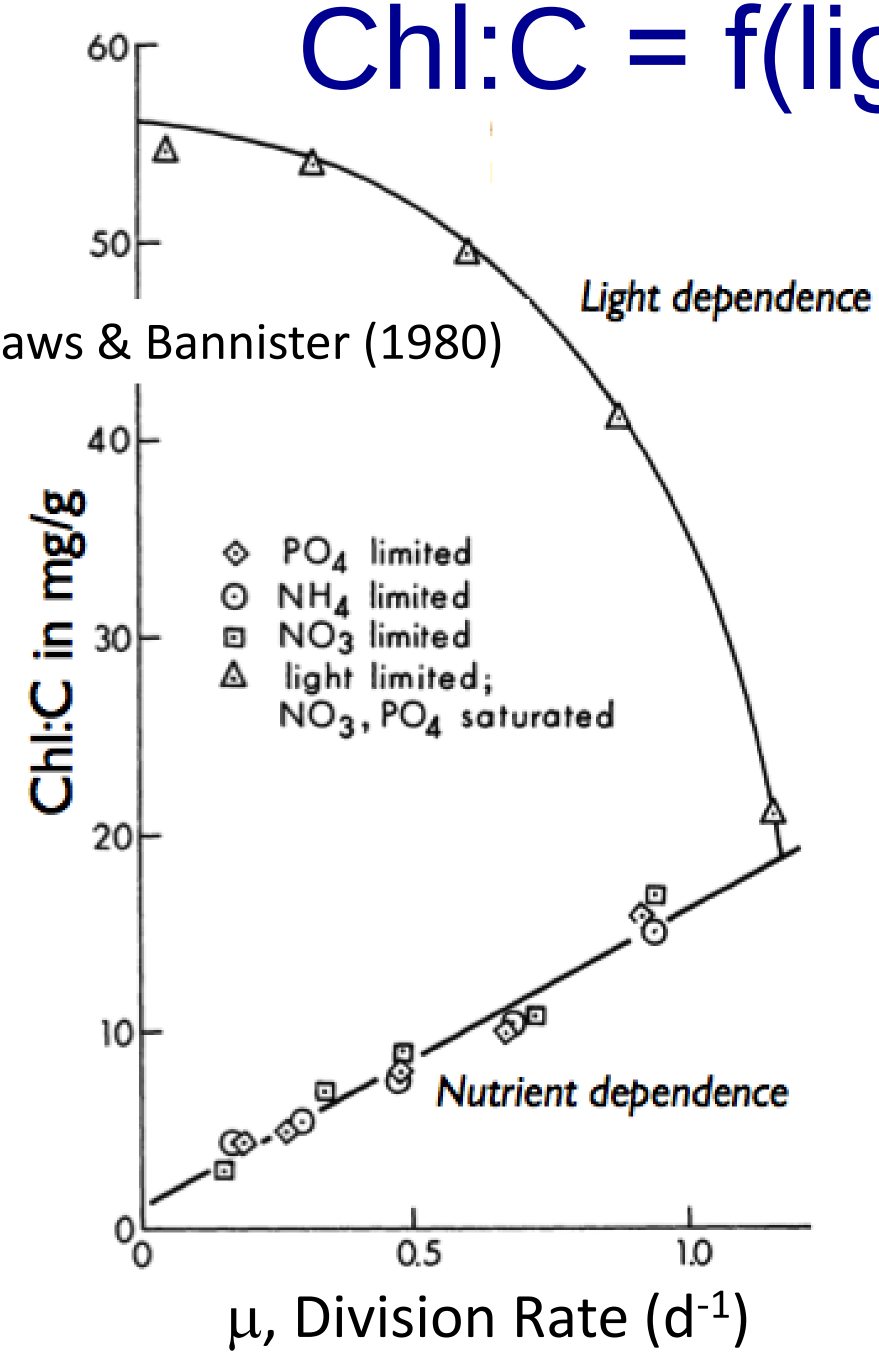
What About Trends in Time?

- SeaWiFS trends are negative for Chl_{OC4} in the warm ocean but are insignificant for Chl_{GSM}
- CDM trends in the warm ocean are negative (which likely explains the Chl_{OC4} trends)
- Global correlations with SST are greatest with CDM (CDM responds to physics closer than Chl)
- Interpreting trends and change using empirical Chl algorithms should be done very carefully

So, What is Chlorophyll Really?

- Chlorophyll = f(phytoplankton abundance, physiological adaptations, community composition, …)
- Global Chl patterns reflect abundance changes due to large-scale nutrient inputs
- But Chl/C’s can change more than five-fold
- Question: *Are changes in* Chl_{GSM} *due to changes in biomass or to physiology?*

Chl:C = f(light, nutrients, …)



Laws & Bannister (1980)

Lab studies of *T. fluviatilis* under various limitations

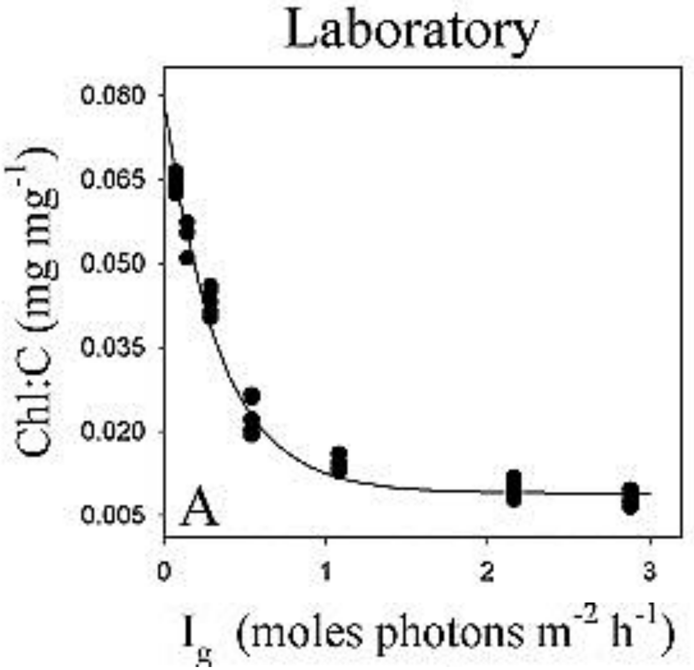
Provides envelope for expected Chl:C variations

Light limitation: Chl:C is big & inversely related to μ

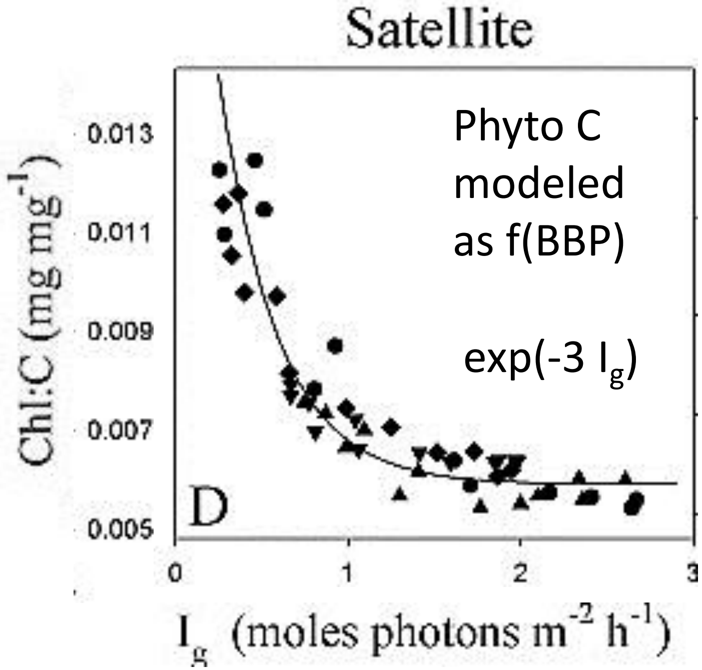
Nutrient limitation: Chl:C is small & linear with μ

Enables Chl variability to be diagnosed independent of changes of C biomass

Chl:C: Light Limitations



Chl:C vs. growth irradiance for *D. tertiolecta*



Phyto C modeled as f(BBP)

$\exp(-3\ I_g)$

Satellite Chl:C for four oceanic regions vs. ML light

Opens the door to modeling phytoplankton growth rates & carbon-based NPP

Behrenfeld et al. (2005) GBC

Biomass vs. Light-Induced Physiology?

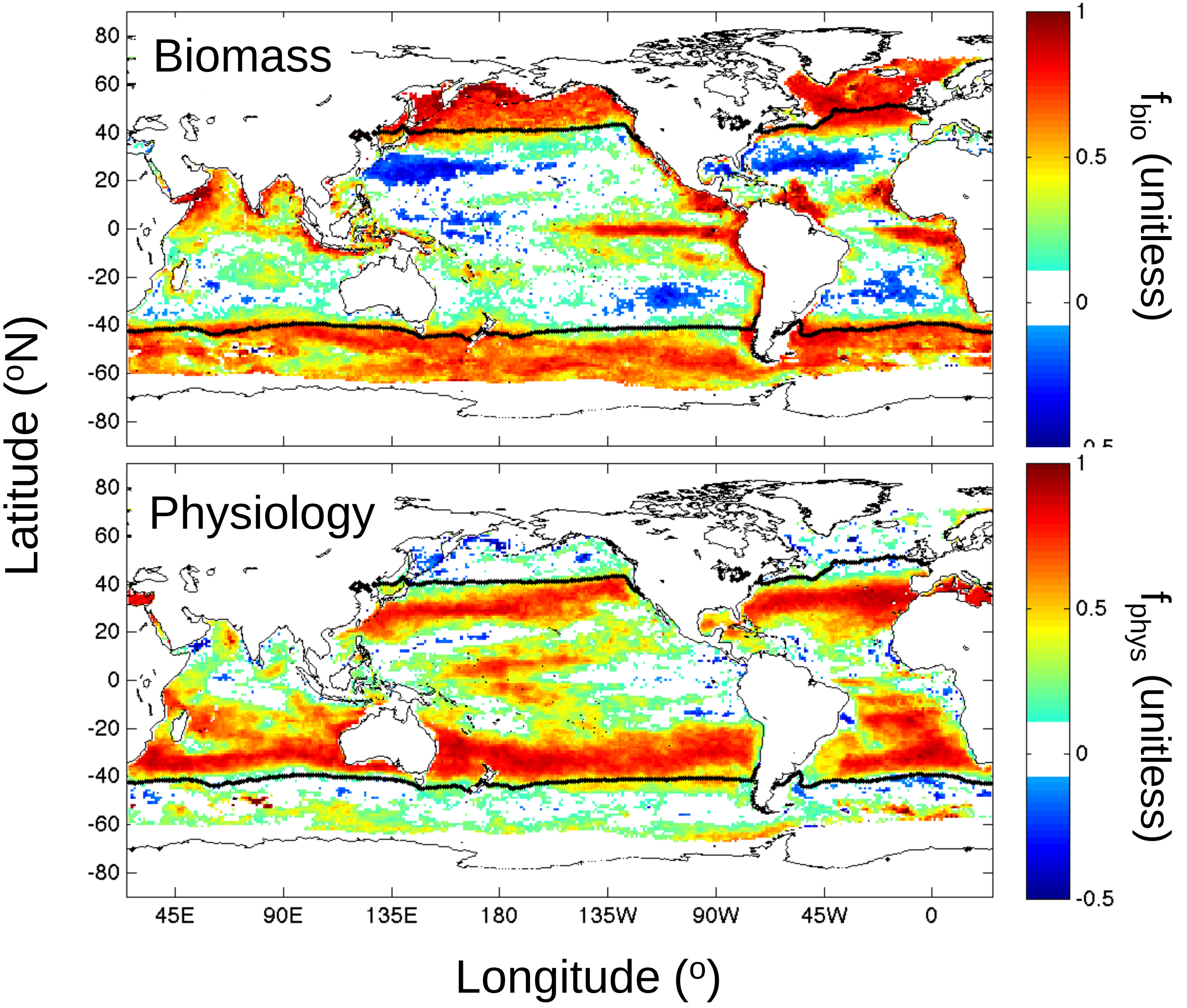
- Model changes in Chl_{GSM} as the sum of biomass & light-induced physiological components

$$\log(\hat{\mathrm{Chl}}_{GSM}) = \underbrace{f_{bio}\,(\mathrm{BBP})}_{\text{biomass}} + \underbrace{f_{phys}\,(\mathrm{BBP} * \exp(-3\,I_g))}_{\text{physiology}}$$

- $\mathrm{BBP} = b_{bp}(443)$ (used as proxy for phytoC)
- $\exp(-3\,I_g)$ represents Chl:C ratio (as before)
- Regression of standardized variables for each 1^o bin
- f_{bio} & f_{phys} measure importance of each process

Siegel et al. RSE (2013)

Chl is driven by Biomass AND Physiology



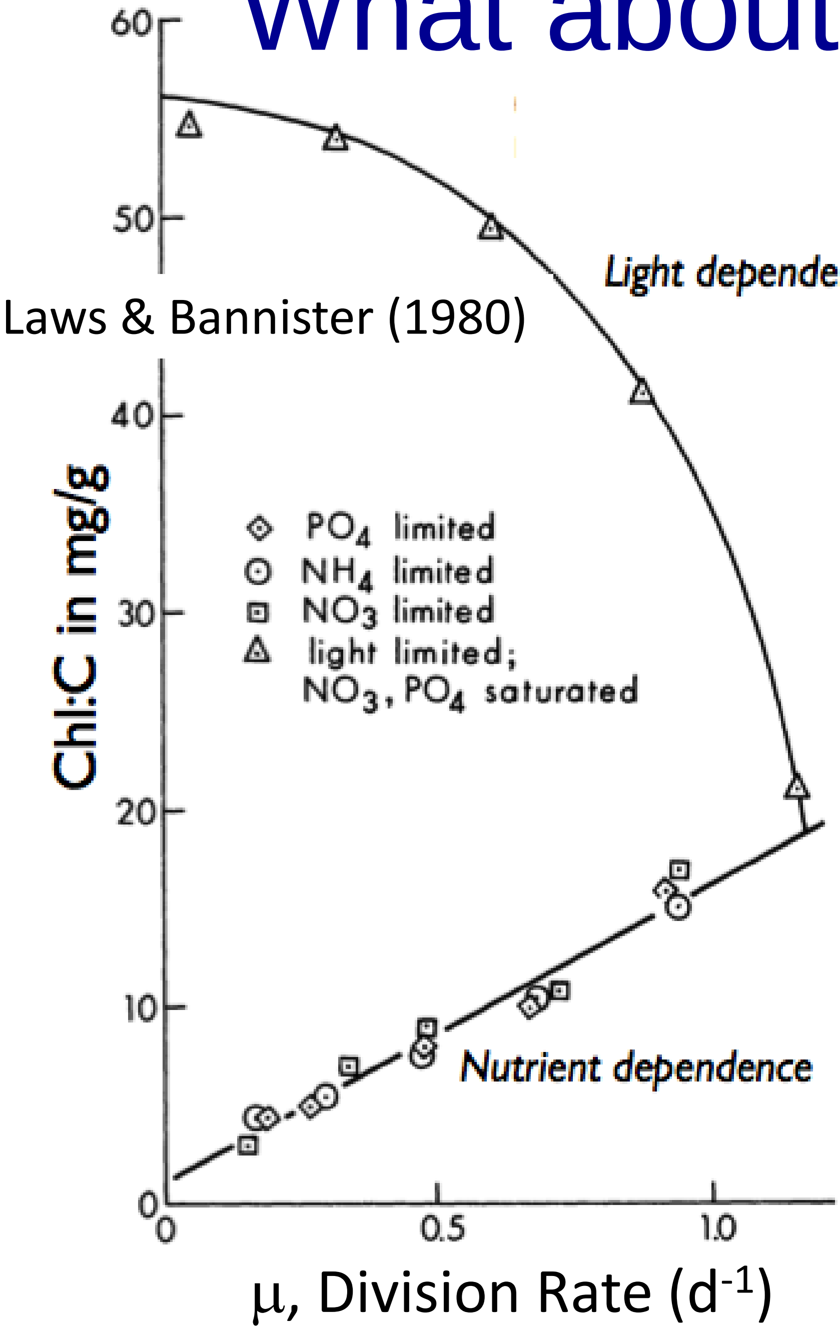
Upwelling regions & the perpetually cool oceans

Subtropics

Siegel et al. RSE (2013)

Only significant correlations shown

What about nutrient limitation?



Laws & Bannister (1980)

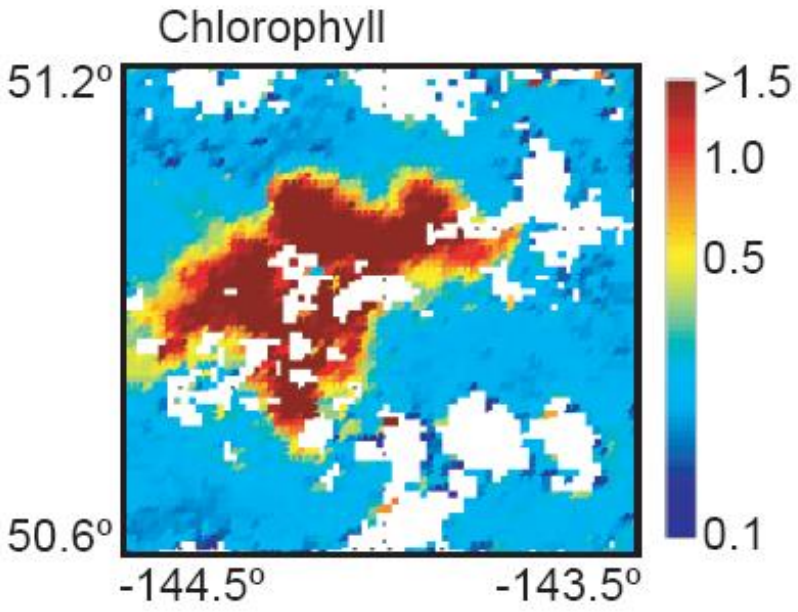
Lab studies of *T. fluviatilis* under various limitations

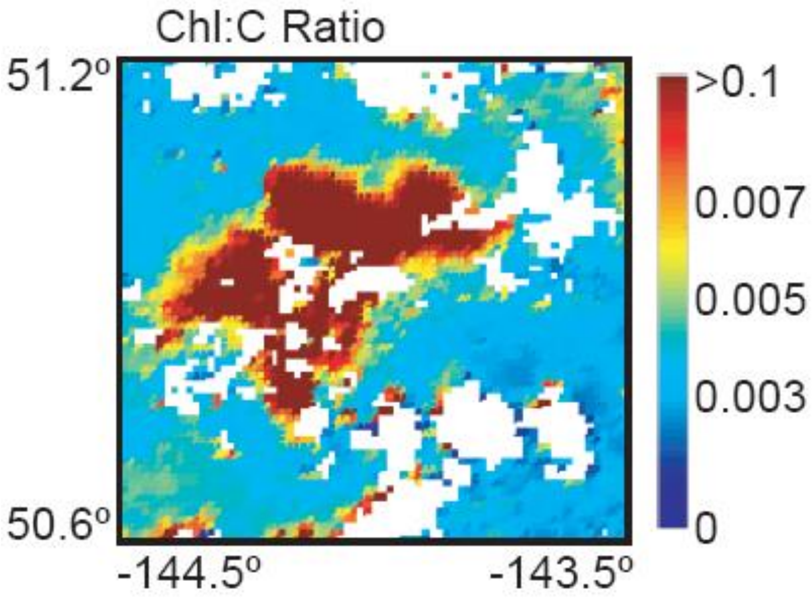
There is a minimum Chl:C under nutrient limitation

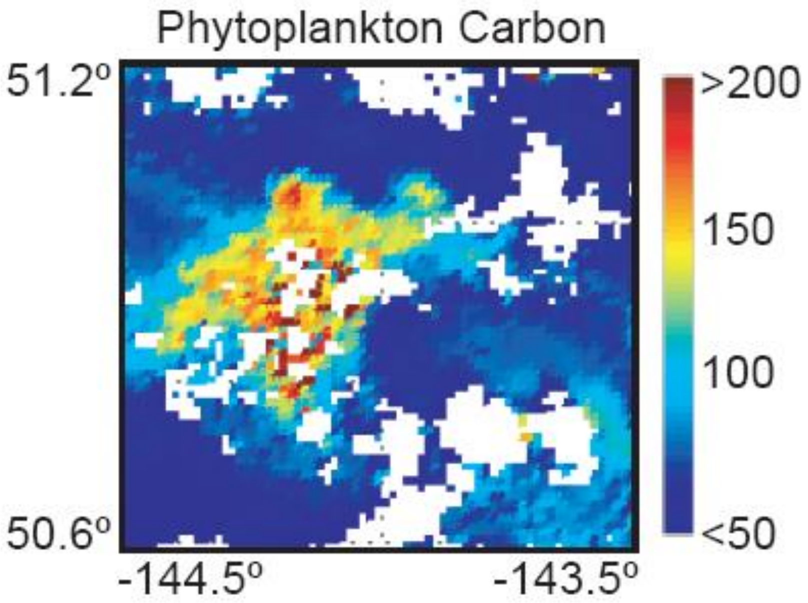
If nutrient limitations are released, an increase in Chl:C is expected

Iron addition experiments should be a good way to test this

SERIES (Station P) Fe Addition







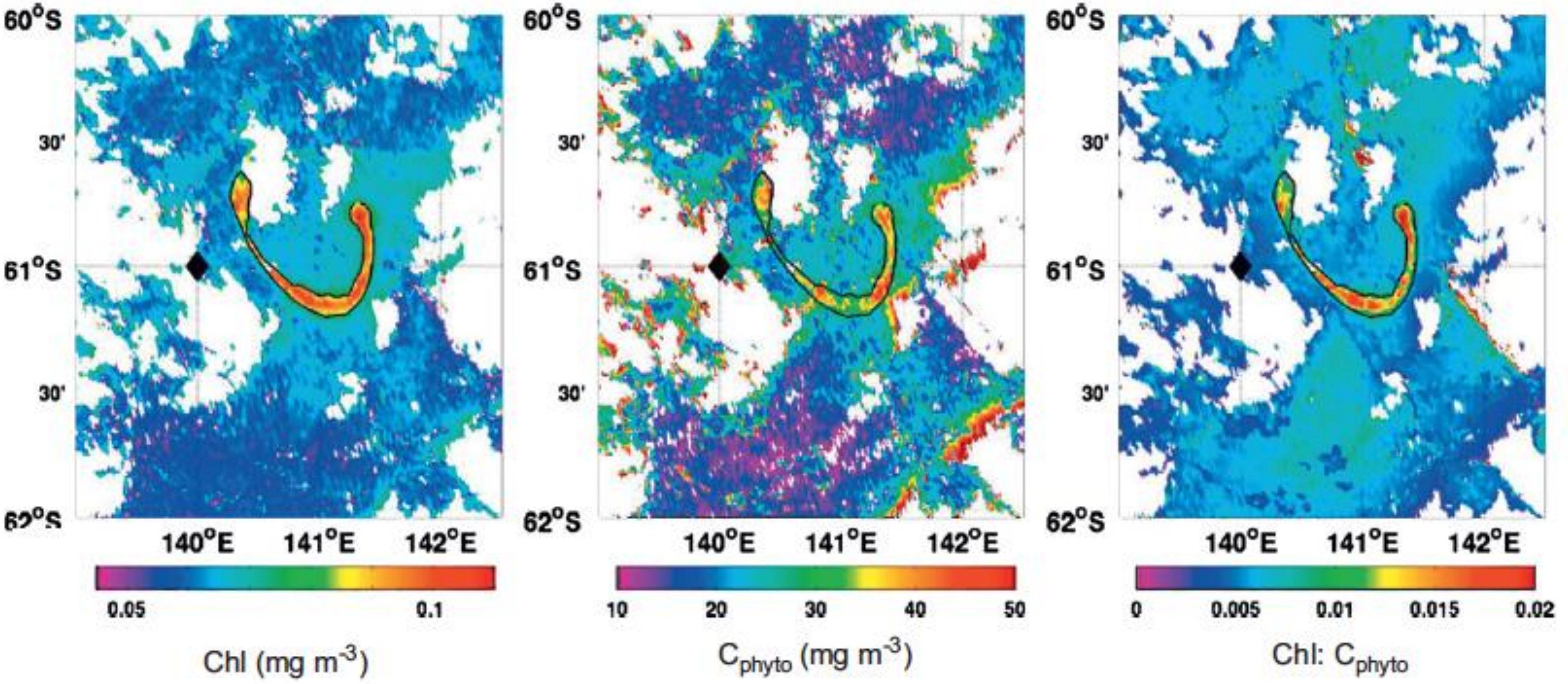
19 days after Fe addition

Chl:C increases following Fe addition as expected

Illustrates decoupling of Chl & C biomass

Following Westberry et al. [2013]

SOIRRE (Southern Ocean) Fe Addition



Only good image of SOIRRE - 46 days after the iron addition

Chl, PhytoC & Chl:C increase in the iron addition patch

Release of iron limitation creates differences in Chl & C

Westberry et al. [2013]

Chlorophyll is Biomass or Physiology?

- Temporal correlations with light show…
  - Biomass dominate high latitude & upwelling zones
  - Physiological responses dominate subtropics
- Iron addition experiments show…
  - Chl:C increases as nutrient limitation is released
- Retrieved Chl:C values reflect expectations from phytoplankton culture experiments
- Chlorophyll is very often **not** a good index for phytoplankton population variations

Need to Get Past Chlorophyll Already!

- CDOM signals are huge – bias empirical Chl signals & mask true phytoplankton signals
- Empirical algorithms are dangerous, especially for measuring small global change signals
- Chlorophyll itself is simply too plastic to be a useful global index for phytoplankton
  - Chl:C retrievals reflect environmental forcings
- However, Chl:C retrievals do provide new insights into phytoplankton physiological state

Need to Embrace Bio-Optical Complexity

- Must separate CDOM & phytoplankton signals
- Need to measure PhytoC **and** Chl

  Field data are needed to build & validate algorithms

  Remember other retrievals are useful (PFT, PSD, etc.)
- Future satellite missions must account for bio-optical complexity
- One example is NASA's planned Pre-Aerosol, Cloud and Ecosystems (PACE) mission

PACE Mission

The Fundamental PACE Science Drivers

WHY are ecosystems changing, **WHO** within an ecosystem are driving change, **WHAT** are the consequences & **HOW** will the future ocean look?

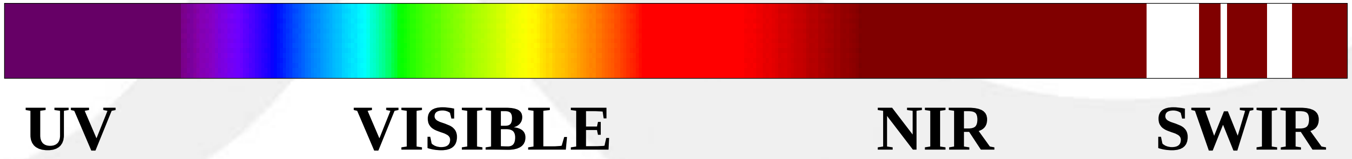
PACE will allow research into:

- Plankton Stocks– Distinguish living phytoplankton from other constituents and identify nutrient stressors from turbid coastal waters to the bluest ocean
- Plankton Diversity – Characterize phytoplankton functional groups, particle size distributions, and dominant species
- Ocean Carbon – Assess changes in carbon concentrations, primary production, net community production and carbon export to the deep sea
- Human Impacts – Evaluate changes in land-ocean interactions, water quality, recreation, and other goods & services
- Understanding Change – Provide superior data precision and accuracy, advanced atmospheric correction, inter-mission synergies
- Forecasting Futures – Resolve mechanistic linkages between biology and physics that support of process-based modeling of future changes

PACE Mission

PACE will improve our understanding of ocean ecosystems and carbon cycling through its…

- Spectral Resolution – 5 nm resolution to separate constituents, characterize phytoplankton communities & nutrient stressors
- Spectral Range – Ultraviolet to Near Infrared covers key ocean spectral features
- Atmospheric Corrections – UV bands allow ‘spectral anchoring‘, SWIR for turbid coastal systems, *polarimeter option for advanced aerosol characterization is TBD*
- Strict Data Quality Requirements – Reliable detection of temporal trends and assessments of ecological rates
- PACE mission and operations concept will be similar to the successful SeaWiFS mission.



PACE Threshold-mission Ocean Science Traceability Matrix (STM)

Science Questions

1. What are the standing stocks, compositions, and productivity of ocean ecosystems? How and why are they changing?
2. How and why are ocean biogeochemical cycles changing? How do they influence the Earth system?
3. What are the material exchanges between land & ocean? How do they influence coastal ecosystems and biogeochemistry? How are they changing?
4. How do aerosols influence ocean ecosystems & biogeochemical cycles? How do ocean biological & photochemical processes affect the atmosphere?
5. How do physical ocean processes affect ocean ecosystems & biogeochemistry? How do ocean biological processes influence ocean physics?
6. What is the distribution of both harmful and beneficial algal blooms and how is their appearance and demise related to environmental forcings? How are these events changing?
7. How do changes in critical ocean ecosystem services affect human health and welfare? How do human activities affect ocean ecosystems and the services they provide? What science-based management strategies need to be implemented to sustain our health and well-being?

Approach

Approach	Maps to Science Question
Quantify phytoplankton biomass, pigments, optical properties, key groups (functional/HABS), & estimate productivity using bio-optical models, chlorophyll fluorescence, & ancillary physical properties (e.g., SST, MLD)	1, 4, 2, 5, 3, 6
Measure particulate &dissolved carbon pools, their characteristics & optical properties	2, 3
Quantify ocean photobiochemical & photobiological processes	2, 4
Estimate particle abundance, size distribution (PSD), & characteristics	1, 3
Assimilate PACE observations in ocean biogeochemical model fields to evaluate key properties (e.g., air-sea CO_2 flux, carbon export, pH, etc.)	2, 4
Compare PACE observations with field- and model data of biological properties, land-ocean exchange, physical properties (e.g., winds, SST, SSH), and circulation (ML dynamics, horizontal divergence, etc)	3, 4, 5, 6
Combine PACE ocean & atmosphere observations with models to evaluate ecosystem-atmosphere interactions	4
Assess ocean radiant heating and feedbacks	5
Conduct field sea-truth measurements & modeling to validate retrievals from the pelagic to near-shore environments	1, 4, 2, 5, 3, 6
Link science, operational, & resource management communities. Communicate social, economic, & management impacts of PACE science. Implement strong education & capacity building programs.	7

Measurement Requirements

- water leaving radiance at 5 nm resolution from 355 to 800 nm
- 10 to 40 nm wide atmospheric correction bands at 350, 865, 1240, 1640, & 2130 nm, plus one additional NIR band
- characterization of instrument performance changes to ±0.2% in first 3 years & for remaining duration of the mission
- monthly characterization of instrument spectral drift to 0.3 nm accuracy
- daily measurement of dark current & a calibration target/source with its degradation known to ~0.2%
- Prelaunch characterization of linearity, RVVA, polarization sensitivity, radiometric & spectral temperature sensitivity, high contrast resolution, saturation, saturation recovery, crosstalk, radiometric & band-to-band stability, bidirectional reflectance distribution, & relative spectral response
- overall instrument artifact contribution to TOA radiance of < 0.5%
- characterization & correction for image striping to noise levels or below
- crosstalk contribution to radiance uncertainties of 0.1% at L_{typ}
- polarization sensitivity ≤ 1%
- knowledge of polarization sensitivity to ≤ 0.2%
- no detector saturation for any science measurement bands at L_{max}
- RVVA of < 5% for entire view angle range & < 0.5% for view angles differing by less than 1°
- Stray light contamination < 0.2% of L_{typ} 3 pixels away from a cloud
- Out-of-band contamination < 0.01 for all multispectral channels
- Radiance-to-counts characterized to 0.1% over full dynamic range
- Global spatial coverage of 1 km x 1 km (±0.1 km) along-track
- Multiple daily observations at high latitudes
- View zenith angles not exceeding ±60°
- Standard marine atmosphere, clear-water $[r_w(l)]_N$ retrieval with accuracy of max[5% , 0.001] over the wavelength range 400 – 710 nm
- SNR at L_{typ} for 1 km^2 aggregate bands of 1000 from 360 to 710 nm; 300 @ 350 nm; 600 @ NIR bands; 250, 180, and 50 @ 1240, 1640, & 2130 nm

Implementation Requirements

Vicarious Calibration: Ground-based R_{rs} data for evaluating post-launch instrument gains. Features: (1) Spectral range = 350 - 900 nm at ≤ 3 nm resolution, (2) Spectral accuracies ≤ 5%, (3) Spectral stability ≤ 1%, (4) Deploy = 1 yr prelaunch through mission lifetime, (5) Gain standard errors to ≤ 0.2% in 1 yr post-launch, (6) Maintenance & deploy centrally organized, & (7) Routine field campaigns to verify data quality & evaluate uncertainties

Product Validation: Field radiometric & biogeochemical data over broad possible dynamic range to evaluate PACE science products. Features: (1) Competed & revolving Ocean Science Teams, (2) PACE-supported field campaigns (2 per year), (3) Permanent/public archive with all supporting data

Ocean Biogeochemistry-Ecosystem Modeling

- Expand model capabilities by assimilating expanded PACE retrieved properties, such as NPP, IOPs, & phytoplankton groups & PSD's
- Extend PACE science to key fluxes: e.g., export, CO_2, land-ocean exchange

Platform Needs

2-day global coverage to solar zenith angle of 75°

Sun-synchronous polar orbit with equatorial crossing time between 11:00 and 1:00

Maintain orbit to ±10 minutes over mission lifetime

Mitigation of sun glint

Mission lifetime of 5 years

Storage and download of full spectral and spatial data

Monthly lunar observations at constant phase angle through Earth observing port

Pointing accuracy of 0.2° over full range of viewing geometries, with knowledge to 0.01°

Pointing jitter of 0.001° between adjacent scans or image rows

Spatial band-to-band registration of 80% of one IFOV between any two bands, without resampling

Simultaneity of 0.02 second

Other Requir'ts

Capability to reprocess full data set 1 – 2 times annually

Ancillary data sets from models missions, or field observations:

Measurement Requirements
(1) Ozone
(2) Water vapor
(3) Surface wind velocity and barometric pressure
(4) NO_2

Science Requirements
(1) SST
(2) SSH
(3) PAR
(4) UV
(5) MLD
(6) CO_2
(7) pH
(8) Ocean circulation
(9) Aerosol deposition
(10) run-off loading in coastal zone

eLecture 1

- Review satellite ocean color basics
- Highlight important findings from SeaWiFS
  - Interpret climate-relevant trends in chlorophyll

eLecture 2

- Introduce open ocean bio-optical complexity
  - Retrieve relevant inherent optical properties (IOPs)
  - Confront the trends with changes in IOPs
- Introduce steps forward (NASA’s PACE mission…)

Thank You for Your Attention!!

Special thanx to the
NASA Goddard Ocean Biology Processing Group
NRC Committee on Sustained Ocean Color Obs, and
NASA PACE Science Definition Team