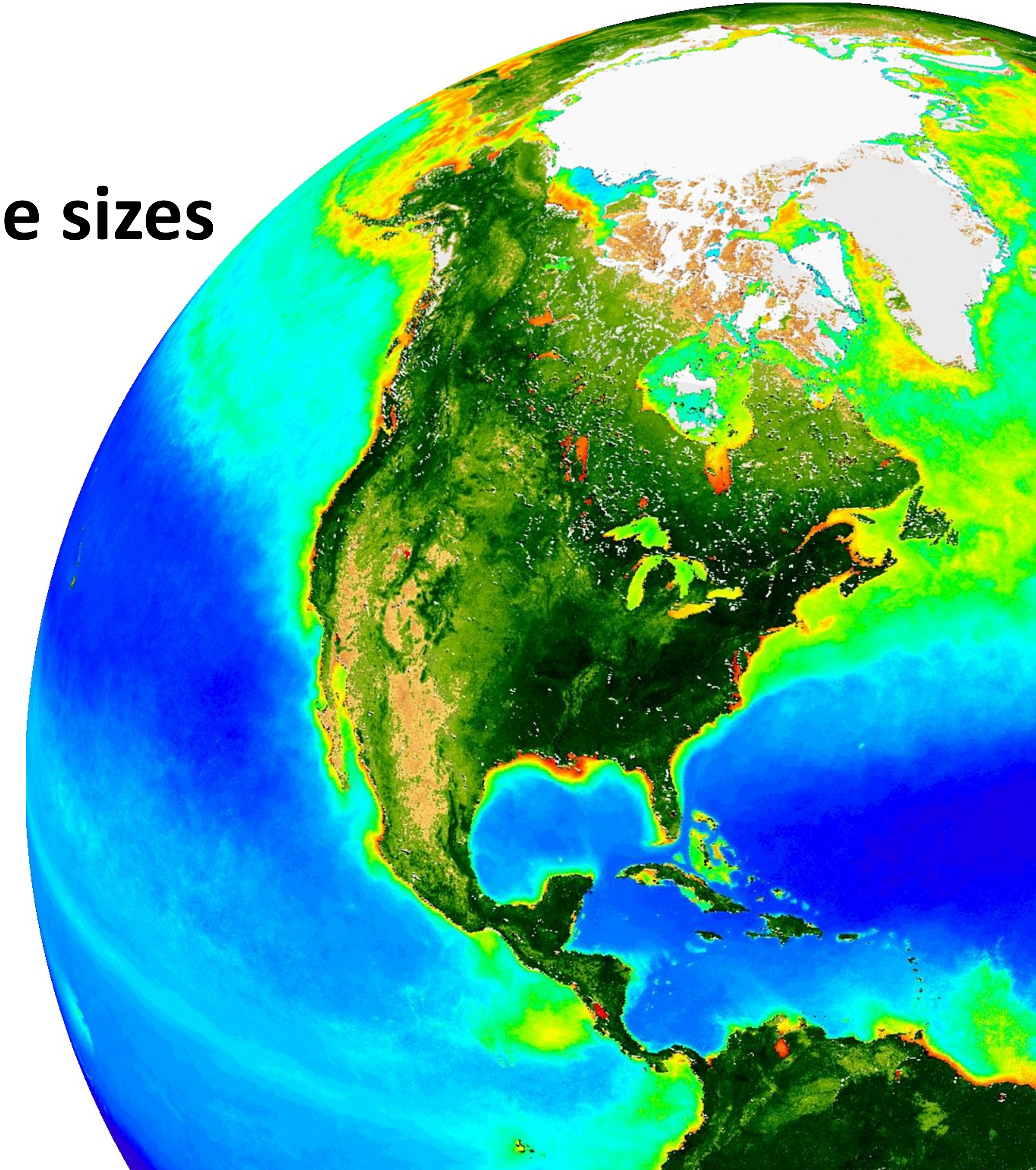
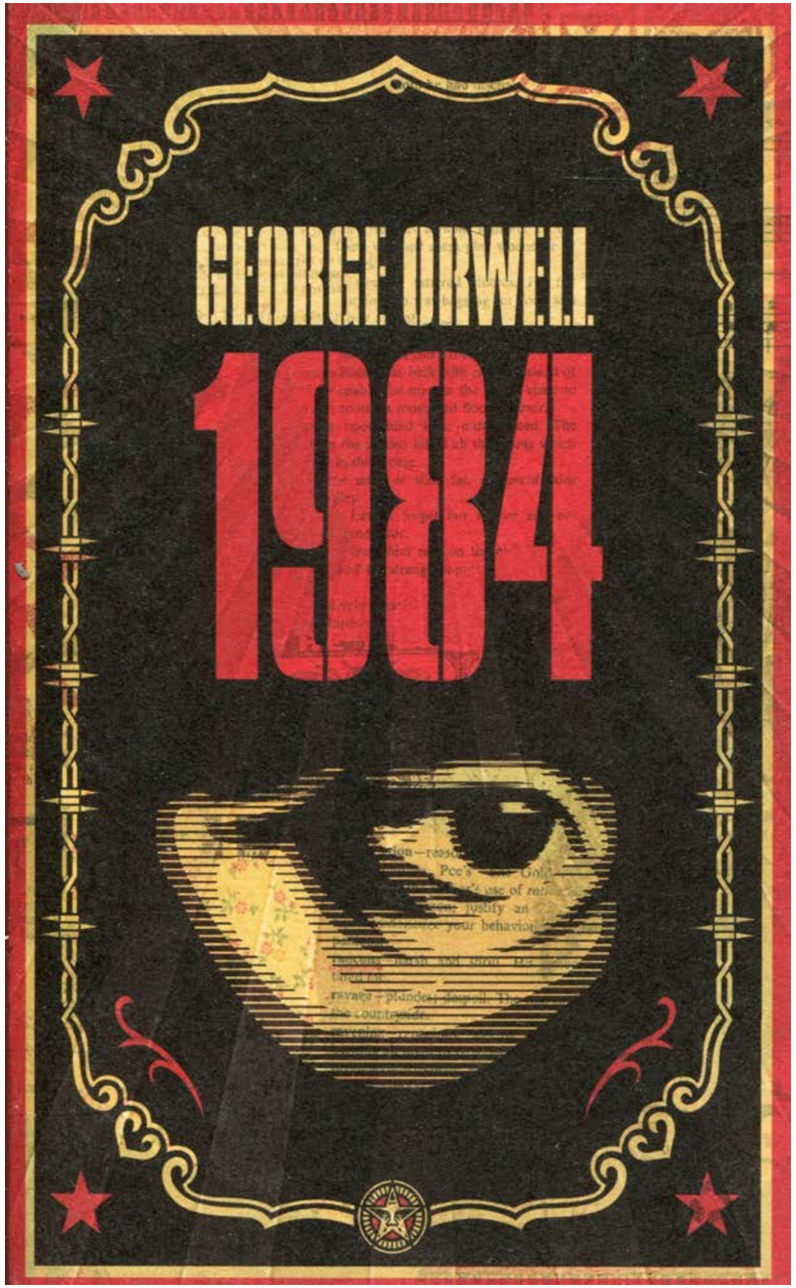
Estimating phytoplankton community structure & particle sizes from satellite ocean color

Jeremy Werdell
NASA Goddard Space Flight Center

2021 Ocean Optics Summer Course





doublethink

the act of simultaneously accepting two mutually contradictory beliefs as correct

example:

“advanced ocean color missions will finally enable us to identify phytoplankton community composition from space”

”ocean color approaches to identify phytoplankton community composition are limited in their abilities and performance”

resources: IOCCG PFT working group

Reports and Monographs of the International Ocean-Colour Coordinating Group

An Affiliated Program of the Scientific Committee on Oceanic Research (SCOR)
An Associated Member of the (CEOS)

IOCCG Report Number 15, 2014

Phytoplankton Functional Types from Space

Edited by:
Shubha Sathyendranath (Plymouth Marine Laboratory)

Report of an IOCCG working group on Phytoplankton Functional Types, chaired by Shubha Sathyendranath and based on contributions from (in alphabetical order):

Jim Aiken, Séverine Alvain, Ray Barlow, Heather Bouman, Astrid Bracher, Robert J. W. Brewin, Annick Bricaud, Christopher W. Brown, Aurea M. Ciotti, Lesley Clementson, Susanne E. Craig, Emmanuel Devred, Nick Hardman-Mountford, Takafumi Hirata, Chuanmin Hu, Tihomir S. Kostadinov, Samantha Lavender, Hubert Loisel, Tim S. Moore, Jesus Morales, Cyril Moulin, Colleen B. Mouw, Anitha Nair, Dionysios Raitsos, Collin Roesler, Shubha Sathyendranath, Jamie D. Shutler, Heidi M. Sosik, Inia Soto, Venetia Stuart, Ajit Subramaniam and Julia Uitz.

http://www.ioccg.org/groups/PFT.html

NASA/TM–2015-217528

Report on IOCCG Workshop

Phytoplankton Composition from Space: Towards a validation strategy for satellite algorithms

Astrid Bracher, Nick Hardman-Mountford, Takafumi Hirata, Stewart Bernard, Emmanuel Boss, Robert Brewin, Annick Bricaud, Vanda Brotas, Alison Chase, Aurea Ciotti, Jong-Kuk Choi, Lesley Clementson, Emmanuel Devred, Paul DiGiacomo, Cécile Dupouy, Toru Hirawake, Wonkook Kim, Tihomir Kostadinov, Ewa Kwiatkowska, Samantha Lavender, Tiffany Moisan, Colleen Mouw, Seunghyun Son, Heidi Sosik, Julia Uitz, Jeremy Werdell, and Guangming Zheng

The International Ocean-Colour Coordinating Group (IOCCG)
25–26 October 2014
Portland, Maine, USA

http://ioccg.org/groups/PFT-TM_2015-217528_01-22-15.pdf

resources: recent articles in Frontiers in Marine Science

frontiers in Marine Science

REVIEW
published: 21 February 2017
doi: 10.3389/fmars.2017.00041

Check for updates

A Consumer's Guide to Satellite Remote Sensing of Multiple Phytoplankton Groups in the Global Ocean

Colleen B. Mouw[1], Nick J. Hardman-Mountford[2], Séverine Alvain[3], Astrid Bracher[4,5], Robert J. W. Brewin[6,7], Annick Bricaud[8], Aurea M. Ciotti[9], Emmanuel Devred[10], Amane Fujiwara[11], Takafumi Hirata[12,13], Toru Hirawake[14], Tihomir S. Kostadinov[15], Shovonlal Roy[16] and Julia Uitz[8]*

frontiers in Marine Science

REVIEW
published: 03 March 2017
doi: 10.3389/fmars.2017.00055

Check for updates

Obtaining Phytoplankton Diversity from Ocean Color: A Scientific Roadmap for Future Development

Astrid Bracher[1,2], Heather A. Bouman[3], Robert J. W. Brewin[4,5], Annick Bricaud[6,7], Vanda Brotas[8], Aurea M. Ciotti[9], Lesley Clementson[10], Emmanuel Devred[11], Annalisa Di Cicco[12], Stephanie Dutkiewicz[13], Nick J. Hardman-Mountford[14], Anna E. Hickman[15], Martin Hieronymi[16], Takafumi Hirata[17,18], Svetlana N. Losa[1], Colleen B. Mouw[19], Emanuele Organelli[4], Dionysios E. Raitsos[4], Julia Uitz[6,7], Meike Vogt[20] and Aleksandra Wolanin[1,2,21]*

major gaps identified as:

- mismatch between satellite, *in situ*, and model data
- lack of quantitative uncertainty estimates
- spectral limitation of current sensors
- limited applicability in regional waters

recommended actions:

- increase communication & round robin exercises
- launch higher spectrally sensors
- launch higher spatially resolved sensors
- develop hyperspectral algorithms
- develop synergistic satellite + *in situ* data algorithms

perspective

the faithful & the skeptical surround you

this is pushing the limits of existing (& future?) satellite instruments

many methods have been proposed, most fall into 2 classes

spatially, temporally diverse validation data are historically unavailable

like it or not, this is our future – already big in our community

HUGE science driver for PACE

this presentation will walk through general methods & issues

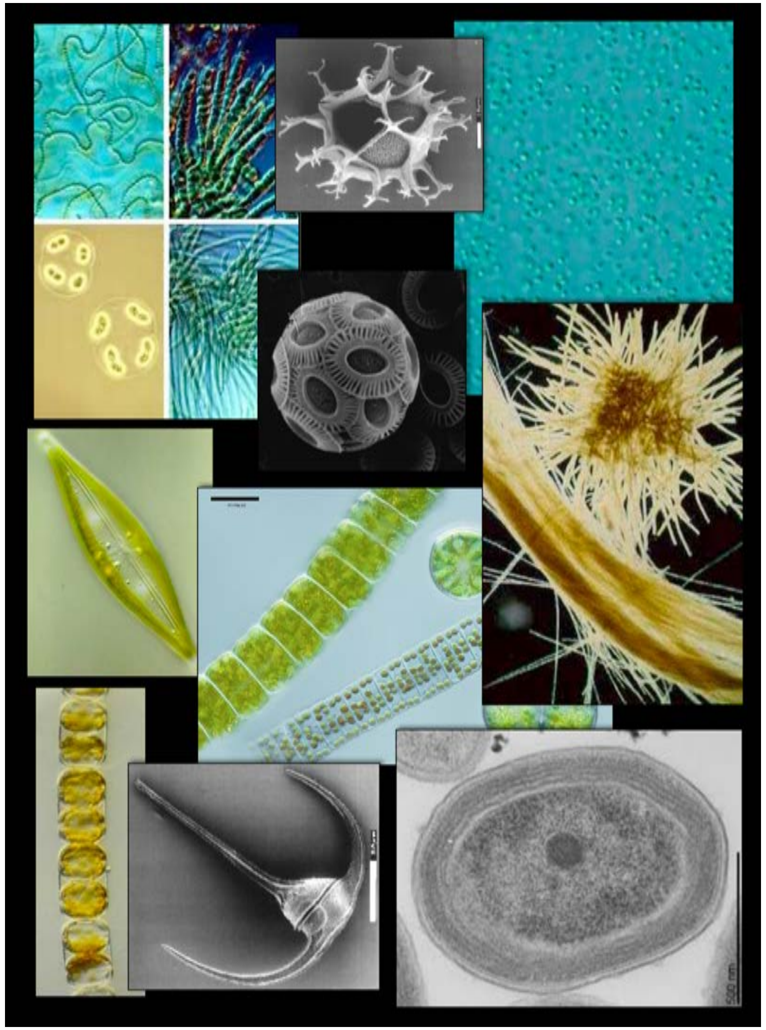
why is it more challenging to measure & validate metrics of phytoplankton community composition than other ocean color products?

(1) the (increased) number of satellite methods to model phytoplankton community composition

(2) the (increased) number of *in situ* methods to infer phytoplankton community composition

(3) the (increased) degrees of separation between the satellite & *in situ* measurements

terminology for the diverse array of satellite approaches



PSC – particle size class ← describes either particles or phytoplankton

- micro: > 20 μm
- nano: 2 to 20 μm
- pico: < 2 μm

PFT – phytoplankton functional type

- "function" can mean many things
- often class/genus-ish levels – diatom vs. dinoflagellate, etc.
- sometimes functions like "nitrogen fixers" or "calcifiers"

degrees of separation in data products

satellite measured $R_{rs}(\lambda)$

↕

in situ measured $R_{rs}(\lambda)$

---

satellite measured $R_{rs}(\lambda)$

↓

satellite modeled Chl, IOPs

↕

in situ measured Chl, IOPs

---

satellite measured $R_{rs}(\lambda)$

↓

satellite modeled Chl, IOPs

↓

satellite modeled PFTs/PSCs

↕

in situ inferred PFTs/PSCs

↑

in situ measured Chl, IOPs

in situ measured PFTs/PSCs

key points for our exploration of satellite methods to derive phytoplankton community composition

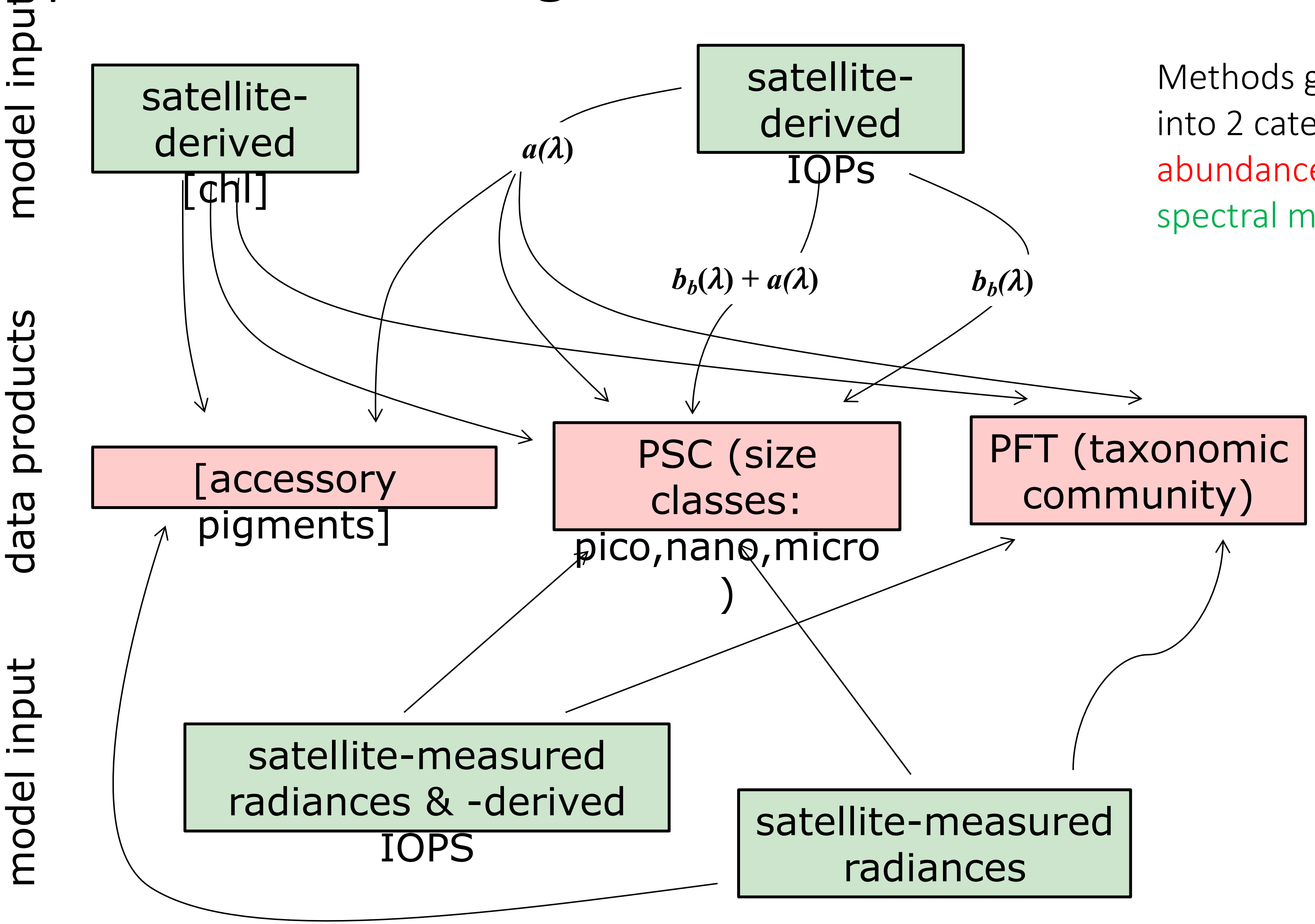
→ diverse bio-optical methods to estimate PSCs/PFTs exist

their sensitivities remain unexplored

most folks use proxy data sets for their validation

satellite data compositing matters

roadmap: 2 flavors of algorithms with varied in/outputs



Methods generally fall into 2 categories:
abundance methods
spectral methods

Google Scholar searches:

”phytoplankton function type” yielded 473 results

ocean color “phytoplankton community structure” & ocean color “phytoplankton community composition” both yielded >4,000 results

this is an exploding field … so,we will only cover several heritage examples

take home messages:

a diverse array of methods exists

you need a critical eye to select or derive the best approach for your application(s)

2 major categories: abundance-based & spectral

TABLE 2 | A compilation of global algorithms to retrieve phytoplankton composition from satellite data.

Approach		Phytoplankton composition product		References
ABUNDANCE		Size classes		Uitz et al., 2006; Brewin et al., 2010, 2015
		Size classes and multiple taxa		Hirata et al., 2011
SPECTRAL	REFLECTANCE	Multiple taxa		Alvain et al., 2005, 2008; Li et al., 2013; Ben Mustapha et al., 2014
		Single taxon	Coccolithophores	Brown and Yoder, 1994; Moore et al., 2012
			Trichodesmium	Subramaniam et al., 2002; Westberry et al., 2005
	ABSORPTION	Size index		Ciotti and Bricaud, 2006; Mouw and Yoder, 2010; Bricaud et al., 2012
		Size classes		Devred et al., 2006, 2011; Hirata et al., 2008; Fujiwara et al., 2011; Roy et al., 2013
		Multiple taxa		Bracher et al., 2009; Sadeghi et al., 2012a; Werdell et al., 2014
	BACK-SCATTERING	Size classes		Kostadinov et al., 2009, 2016; Fujiwara et al., 2011
ECOLOGICAL		Taxonomic groups		Palacz et al., 2013

Obtaining Phytoplankton Diversity from Ocean Color: A Scientific Roadmap for Future Development

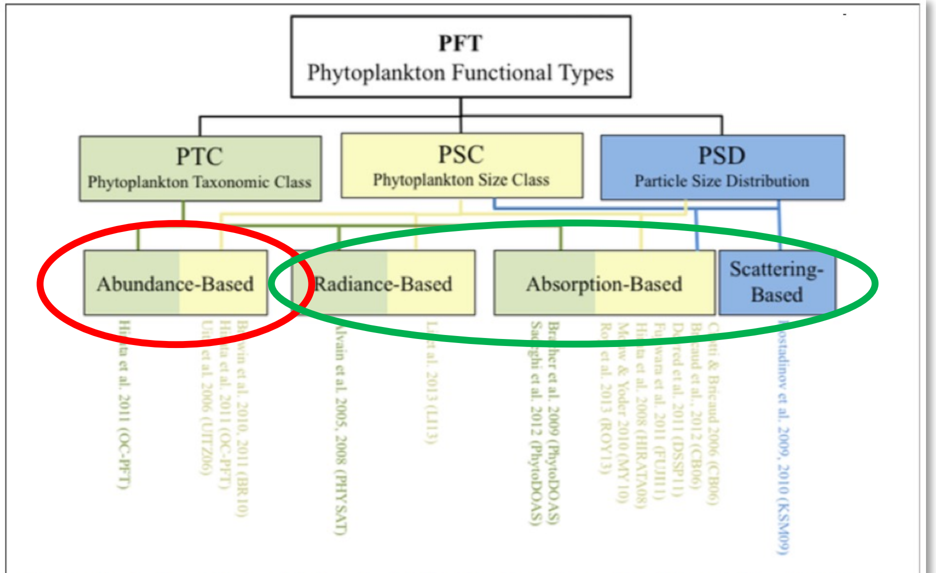


FIGURE 1 | Schematic of various phytoplankton functional type (PFT) algorithms grouped according to their output classification (PTC, PSC, or PSD) and algorithm development types (abundance-, radiance-, absorption-, and scattering-based). Color indicates the output classification of phytoplankton taxonomic class (PTC, green), phytoplankton size class (PSC, yellow) or particle size distribution (PSD, blue).

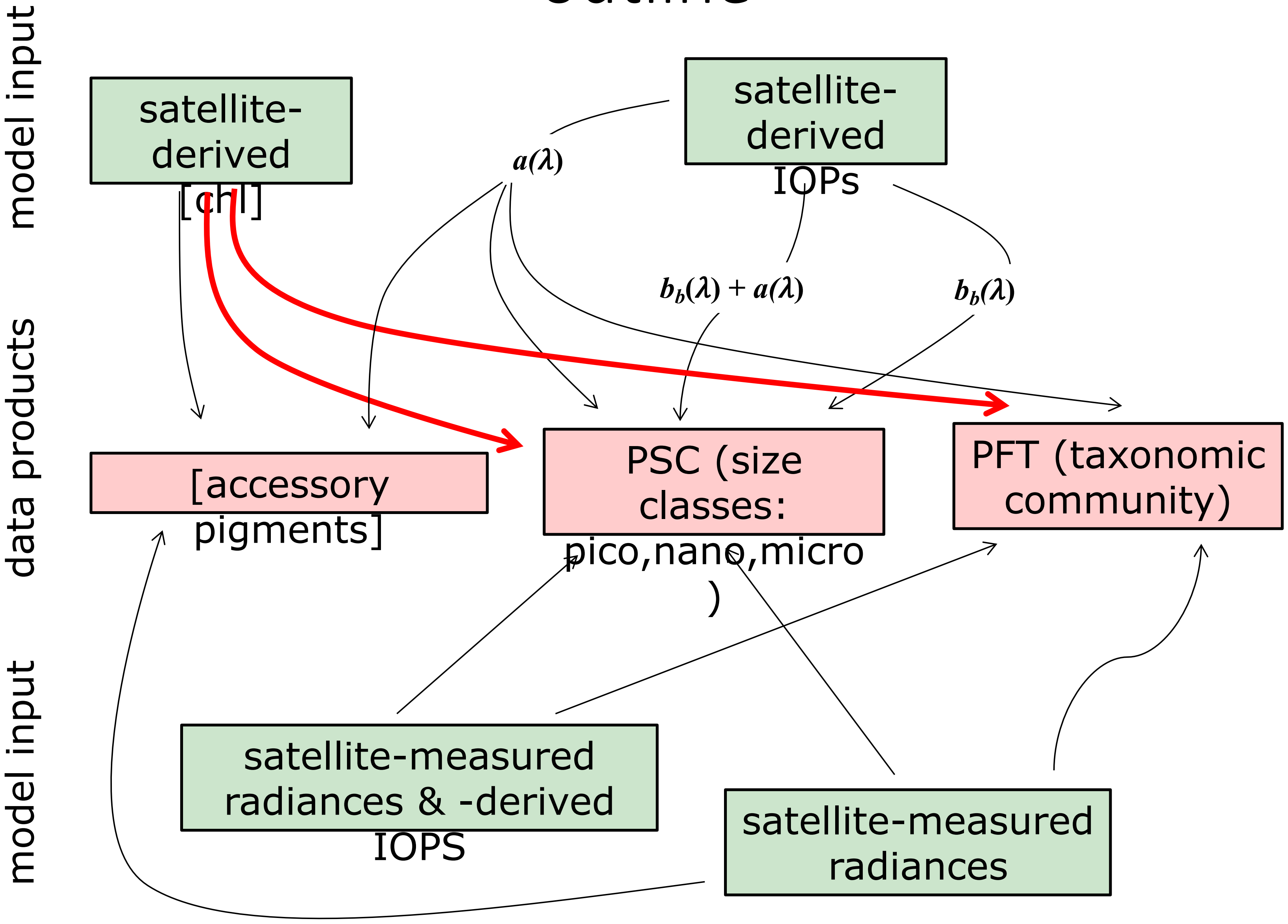
A Consumer's Guide to Satellite Remote Sensing of Multiple Phytoplankton Groups in the Global Ocean

these tables provide references to approaches, at least as of 2017 …

abundance methods

assume that **a given phytoplankton biomass**, defined by either Chl or IOPs – in particular, $a_{ph}(\lambda)$ – **covaries with the dominance** of or fraction of a particular PFT or PSC

outline


model input
data products
model input
satellite-derived [chl]
satellite-derived IOPs
$a(\lambda)$
$b_b(\lambda) + a(\lambda)$
$b_b(\lambda)$
[accessory pigments]
PSC (size classes: pico,nano,micro)
PFT (taxonomic community)
satellite-measured radiances & -derived IOPS
satellite-measured radiances

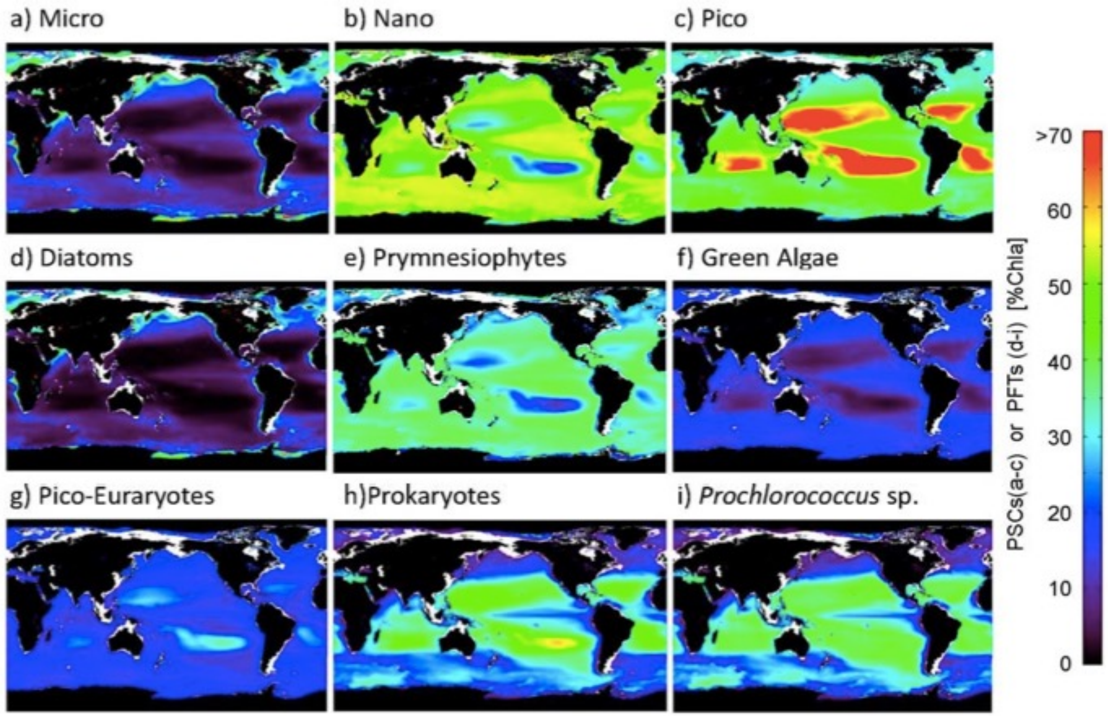
abundance – Chl as input

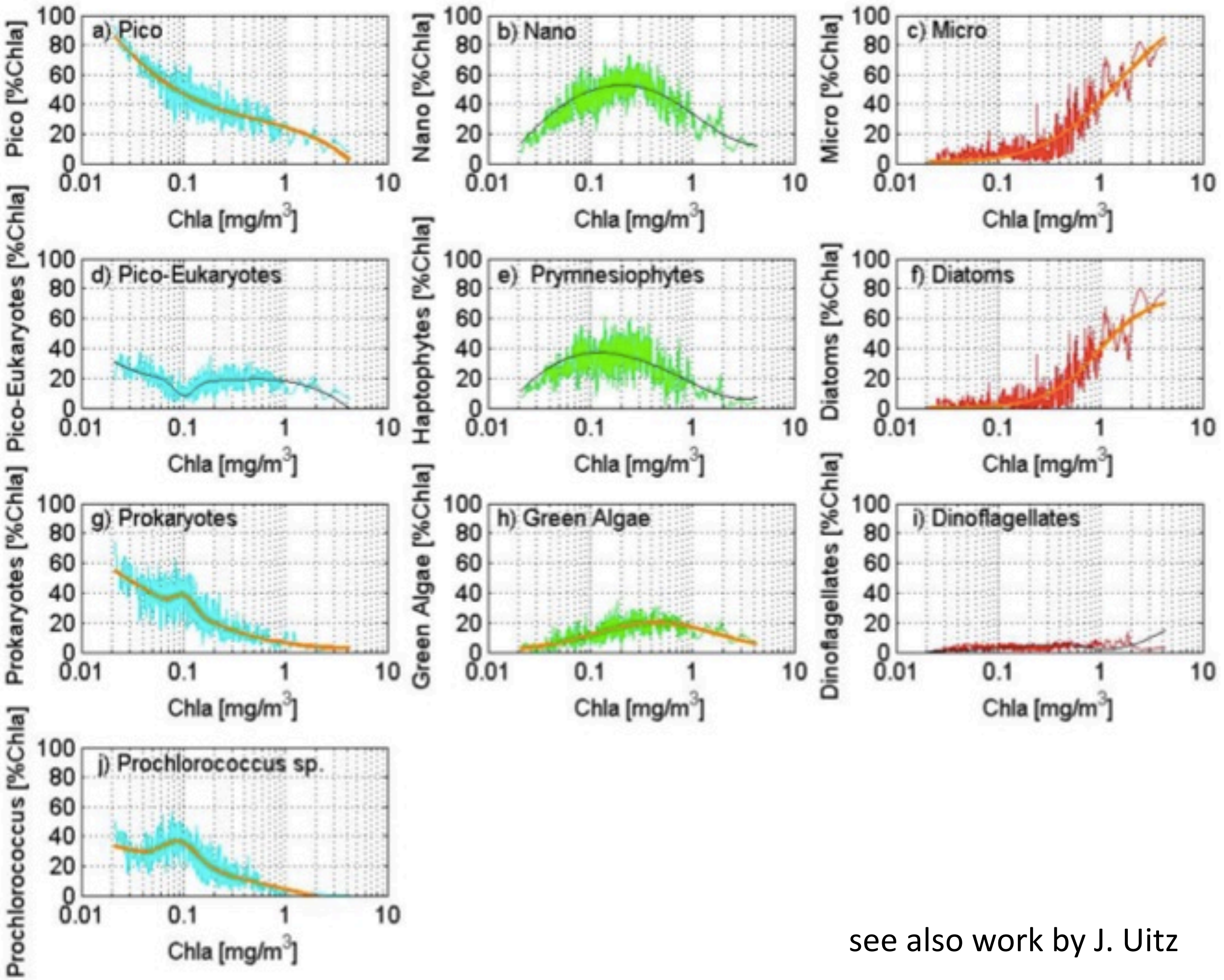
Biogeosciences, 8, 311–327, 2011
www.biogeosciences.net/8/311/2011/
doi:10.5194/bg-8-311-2011

Biogeosciences

Synoptic relationships between surface Chlorophyll-*a* and diagnostic pigments specific to phytoplankton functional types

T. Hirata[1,2,*,**], N. J. Hardman-Mountford[1,2], R. J. W. Brewin[1,3], J. Aiken[1], R. Barlow[4,5], K. Suzuki[6], T. Isada[7], E. Howell[8], T. Hashioka[9,10], M. Noguchi-Aita[7,10], and Y. Yamanaka[6,9,10]

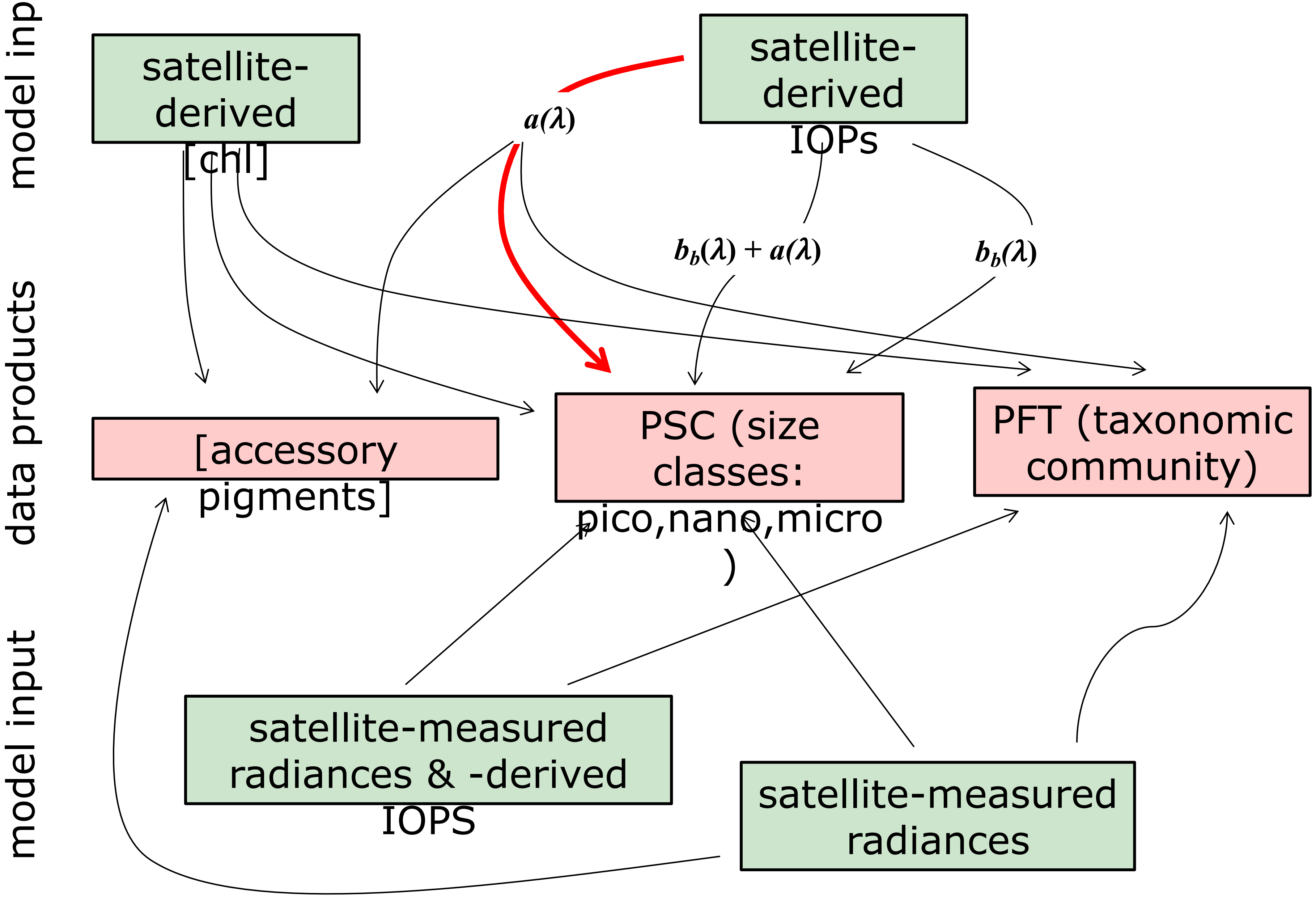




see also work by J. Uitz

purpose: provide an estimate of %Chl for each PFT/PSC in a pixel

outline


model input
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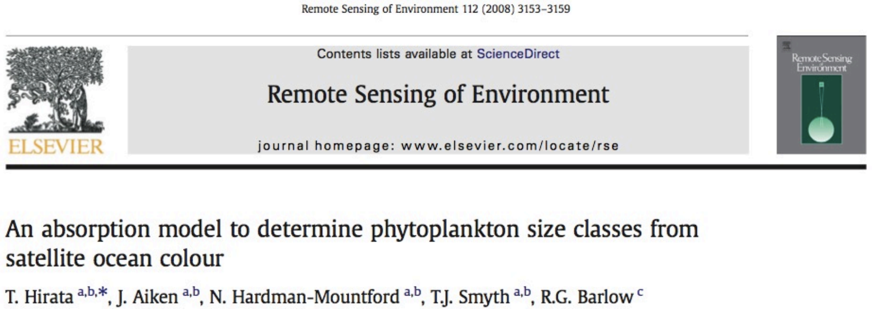
$b_b(\lambda)$
[accessory pigments]
PSC (size classes: pico,nano,micro)
PFT (taxonomic community)
satellite-measured radiances & -derived IOPS
satellite-measured radiances

abundance – IOPs as input


Remote Sensing of Environment 112 (2008) 3153–3159

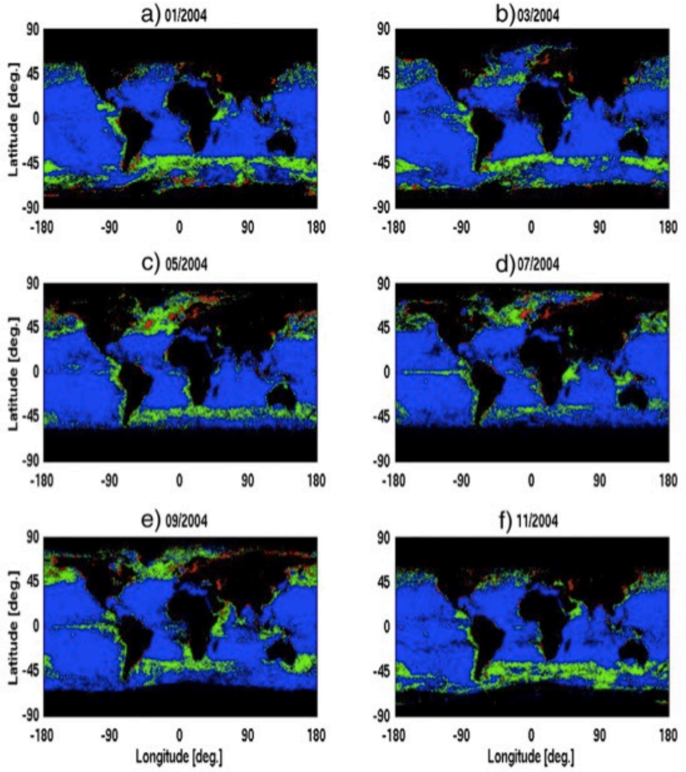
Contents lists available at ScienceDirect

Remote Sensing of Environment

journal homepage: www.elsevier.com/locate/rse

An absorption model to determine phytoplankton size classes from satellite ocean colour

T. Hirata [a,b,*], J. Aiken [a,b], N. Hardman-Mountford [a,b], T.J. Smyth [a,b], R.G. Barlow [c]



micro when

$a_{ph}(443) > 0.069\ m^{-1}$

pico when

$a_{ph}(443) < 0.023\ m^{-1}$

nano otherwise

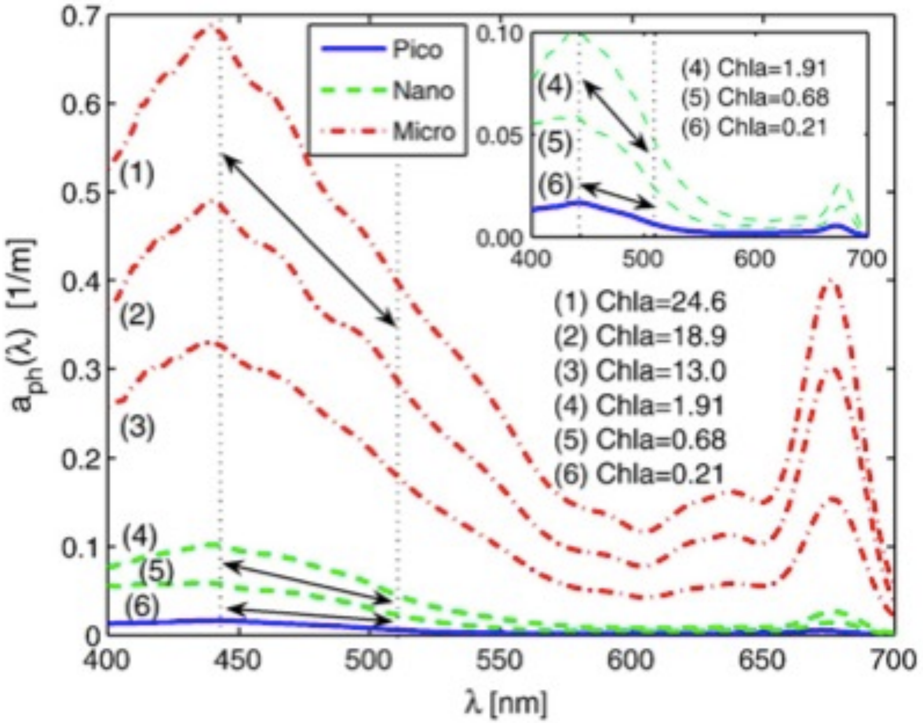


Fig. 1. Phytoplankton absorption spectra for a range of Chla (24.6, 18.9, 13.0, 1.91, 0.68, 0.21 mg m^{-3}) and taxonomic size classes (pico, nano and micro) with decreasing slope from high to low $a_{ph}(\lambda)$ and Chla; inset spectra of pico and nanoplankton at expanded range.

premise – slope of $a_{ph}(443)$ to $a_{ph}(510)$ & magnitude of $a_{ph}(443)$ vary with PSC

purpose: assign a dominant PSC to each satellite pixel

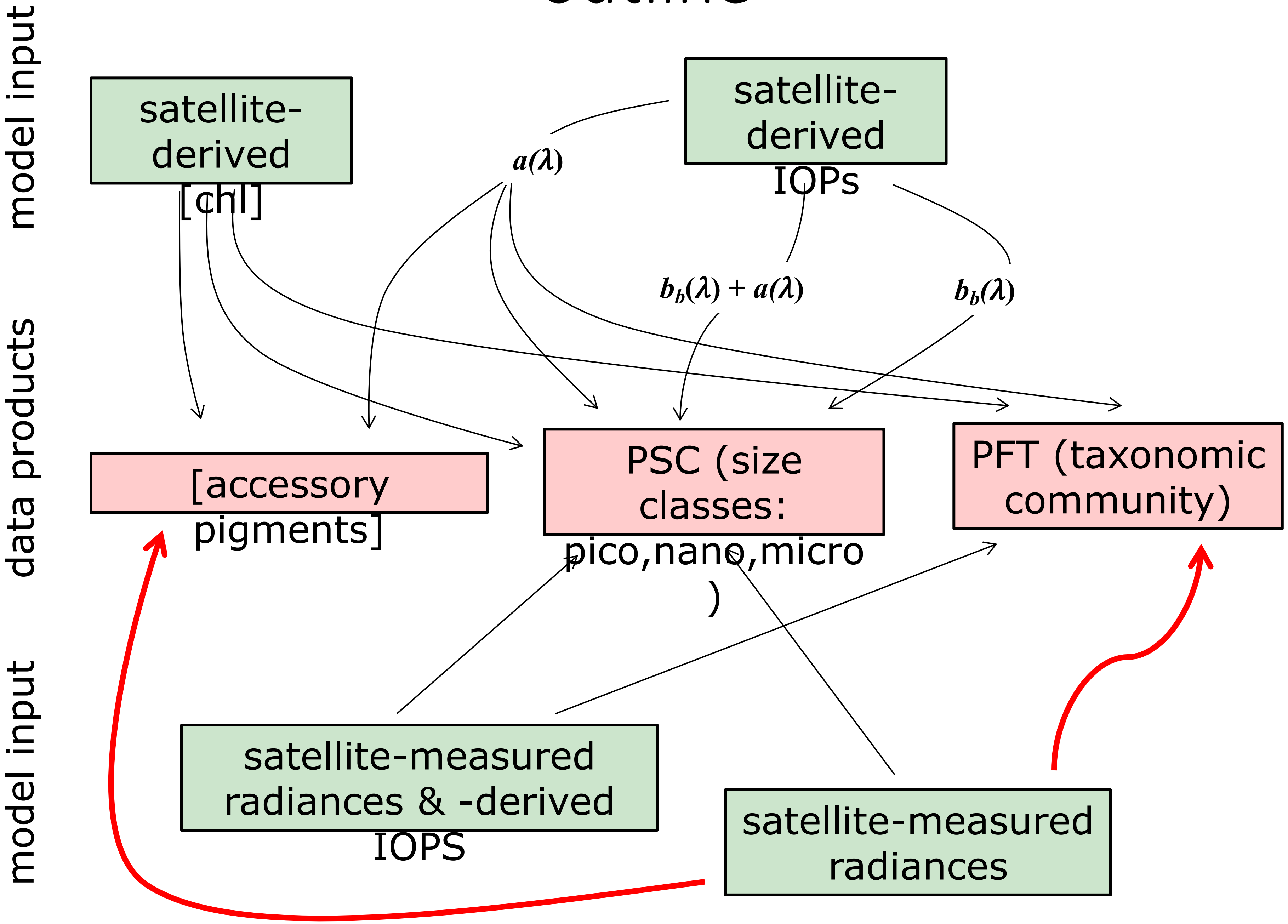
spectral methods

exploit variations realized in the spectral shape of $R_{rs}(\lambda)$ or IOPs with varying phytoplankton community structure

unlike abundance approaches, these can **detect different PFTs/PSCs with common total biomass, provided the groups have contrasting optical signatures**

but, often **confounded by variations of spectral characteristics of the same PFT/PSC** due to growth conditions, nutrient availability, & ambient light regimes

outline


model input
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model input
satellite-derived [chl]
satellite-derived IOPs
$a(\lambda)$
$b_b(\lambda) + a(\lambda)$
$b_b(\lambda)$
[accessory pigments]
PSC (size classes: pico,nano,micro)
PFT (taxonomic community)
satellite-measured radiances & -derived IOPS
satellite-measured radiances

spectral – $R_{rs}(\lambda)$ as input (1)

Remote Sensing of Environment 114 (2010) 2403–2416
Contents lists available at ScienceDirect
Remote Sensing of Environment
journal homepage: www.elsevier.com/locate/rse

Remote sensing of phytoplankton pigment distribution in the United States northeast coast

Xiaoju Pan [a,*], Antonio Mannino [a], Mary E. Russ [a], Stanford B. Hooker [a], Lawrence W. Harding Jr. [b]
[a] NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA
[b] Horn Point Laboratory, University of Maryland Center for Environmental Science, Box 775, Cambridge, MD 21613, USA

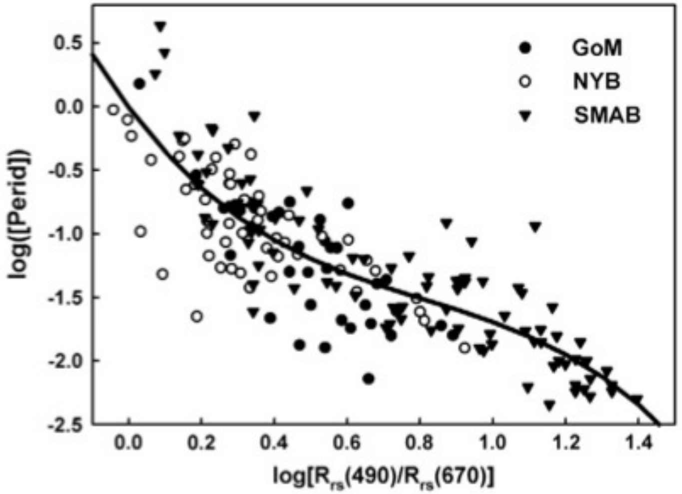


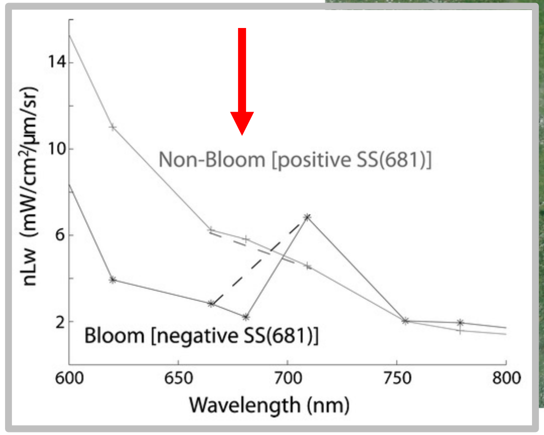
Fig. 4. Algorithm development for peridinin concentration ([Perid]). See Fig. 3 for detailed description.

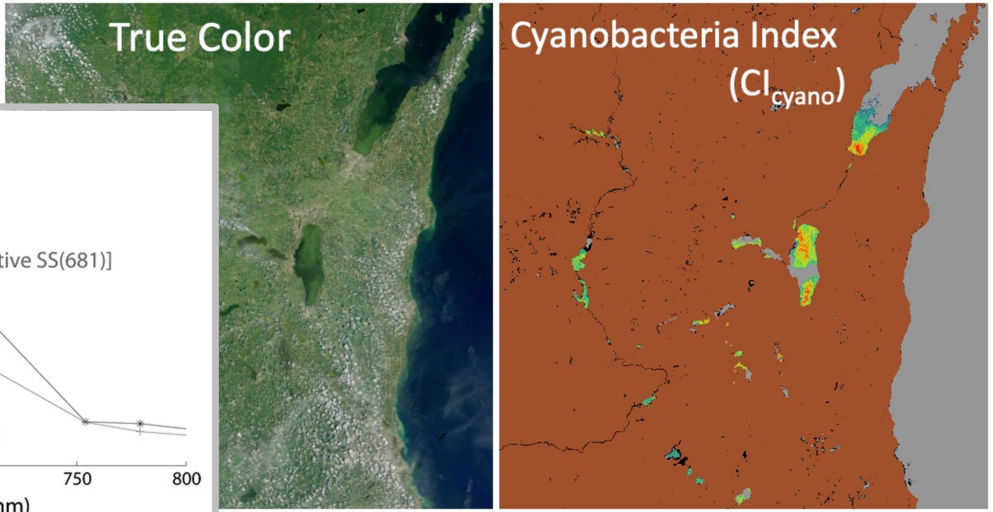
Remote Sensing Letters

Relating spectral shape to cyanobacterial blooms in the Laurentian Great Lakes

T. T. Wynne, R. P. Stumpf, M. C. Tomlinson, R. A. Warner, P. A. Tester, J. Dyble & ...show all

Pages 3665-3672 | Received 15 Aug 2007, Accepted 06 Feb 2008, Published online: 16 May 2008





purpose: provide estimate of phytoplankton accessory pigment concentration (mg m^{-3}) for each satellite pixel

purpose: identify the presence of cyanobacteria in freshwater lakes; assign severity levels

spectral – $R_{rs}(\lambda)$ as input (2)

Available online at www.sciencedirect.com
SCIENCE DIRECT
Deep-Sea Research I 52 (2005) 1989–2004
ELSEVIER
DEEP-SEA RESEARCH PART I
www.elsevier.com/locate/dsr

Remote sensing of phytoplankton groups in case 1 waters from global SeaWiFS imagery

S. Alvain[a], C. Moulin[a,*], Y. Dandonneau[b], F.M. Bréon[a]

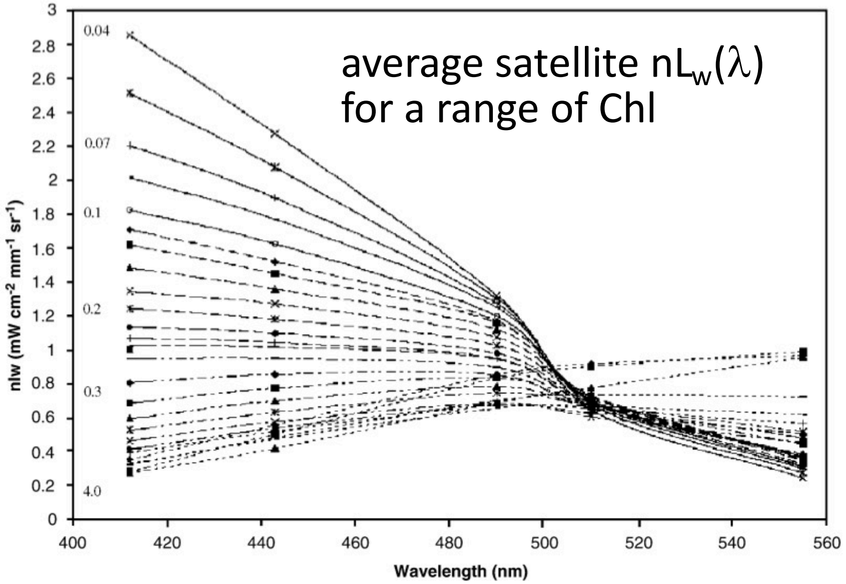
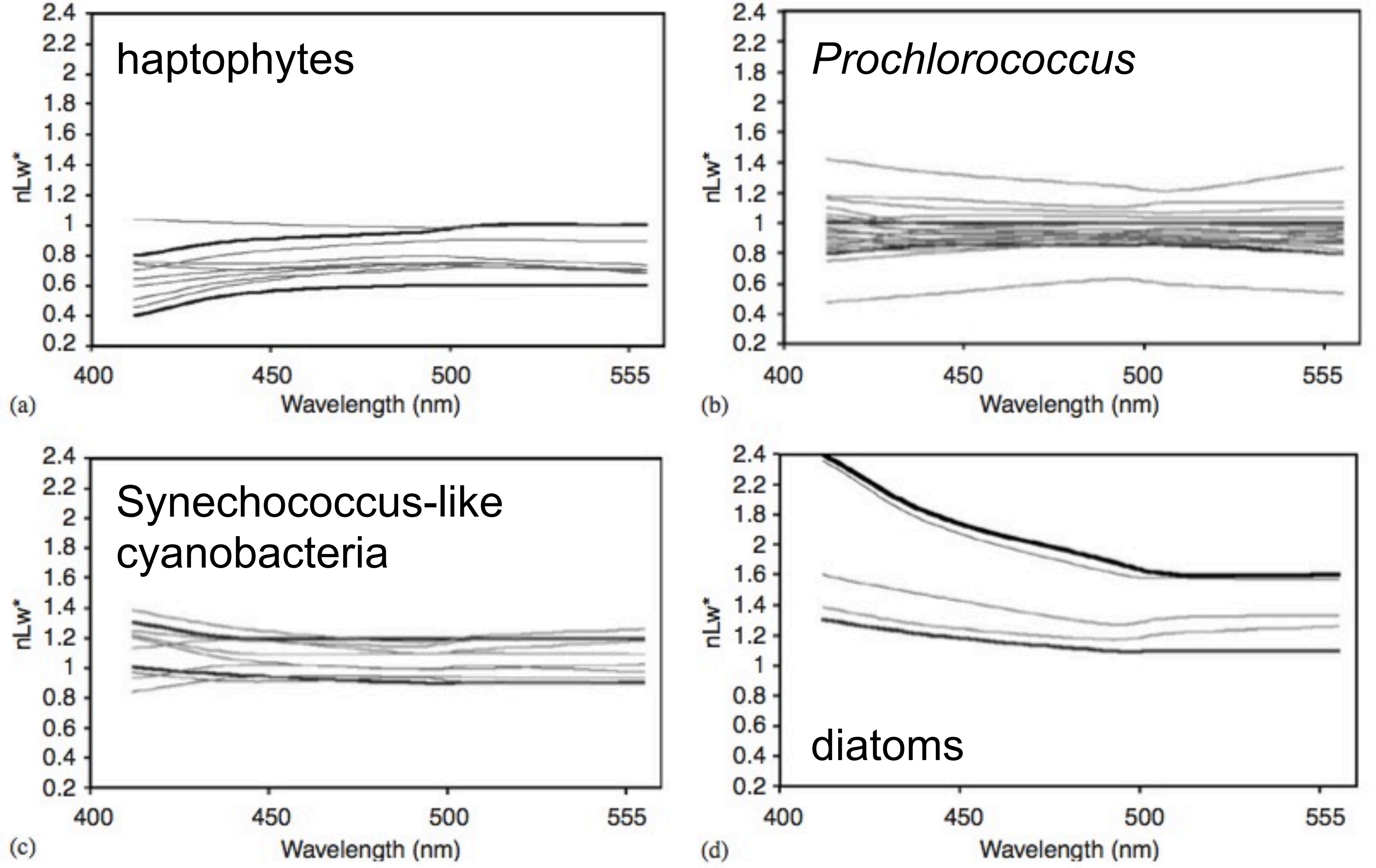


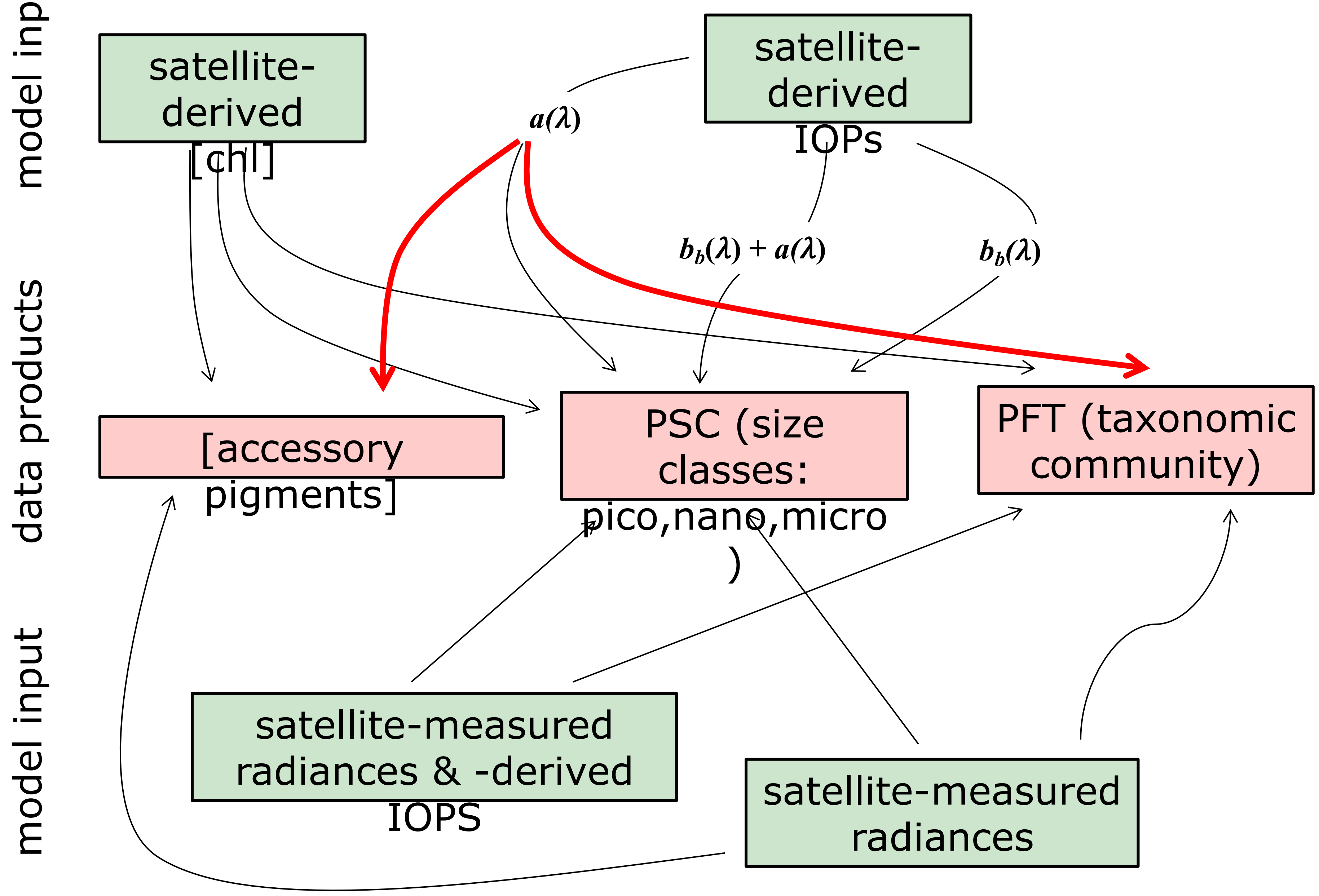
Fig. 1. Normalized water-leaving radiance nLw as a function of wavelength for various chlorophyll-*a*. Average spectra were obtained from 28 800 coincident SeaWiFS chlorophyll *a* concentration and nLw spectra located in the vicinity of the GeP&CO ship tracks.



$nL_w(\lambda)$ anomalies for each PFT

purpose: provide estimate of dominant PFT for each pixel

outline



model input
data products
model input
satellite-derived [chl]
satellite-derived IOPs
$a(\lambda)$
$b_b(\lambda) + a(\lambda)$
$b_b(\lambda)$
[accessory pigments]
PSC (size classes: pico,nano,micro)
PFT (taxonomic community)
satellite-measured radiances & -derived IOPS
satellite-measured radiances

spectral – $a_p(\lambda)$, $a_{ph}(\lambda)$ as input


Contents lists available at ScienceDirect

Methods in Oceanography

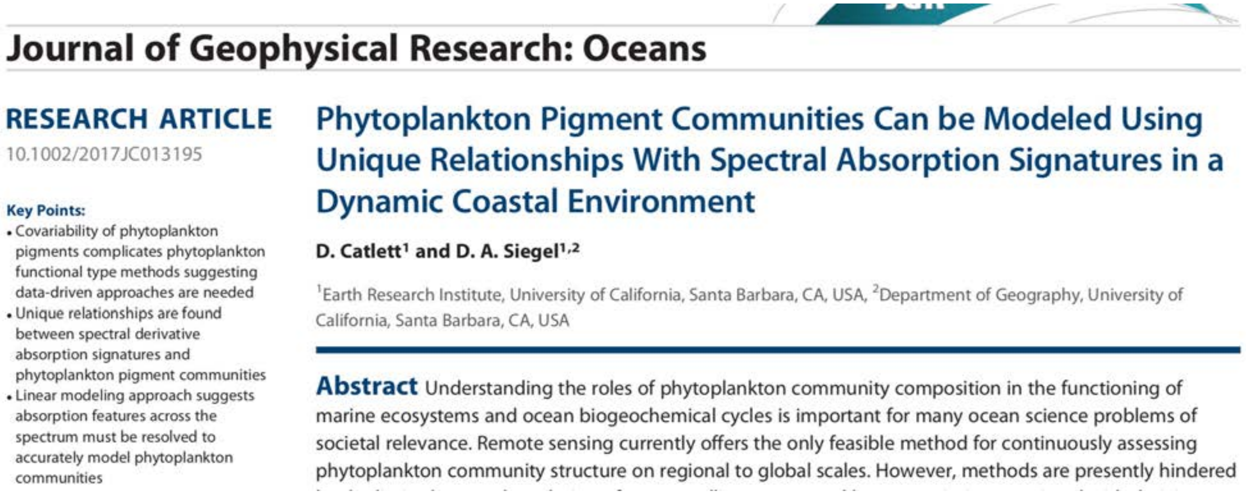
journal homepage: www.elsevier.com/locate/mio

ELSEVIER

Full length article

Decomposition of in situ particulate absorption spectra

Alison Chase[a,*], Emmanuel Boss[a], Ronald Zaneveld[b], Annick Bricaud[c], Herve Claustre[c], Josephine Ras[c], Giorgio Dall'Olmo[d], Toby K. Westberry[e]


Journal of Geophysical Research: Oceans

RESEARCH ARTICLE

10.1002/2017JC013195

Key Points:

- Covariability of phytoplankton pigments complicates phytoplankton functional type methods suggesting data-driven approaches are needed
- Unique relationships are found between spectral derivative absorption signatures and phytoplankton pigment communities
- Linear modeling approach suggests absorption features across the spectrum must be resolved to accurately model phytoplankton communities

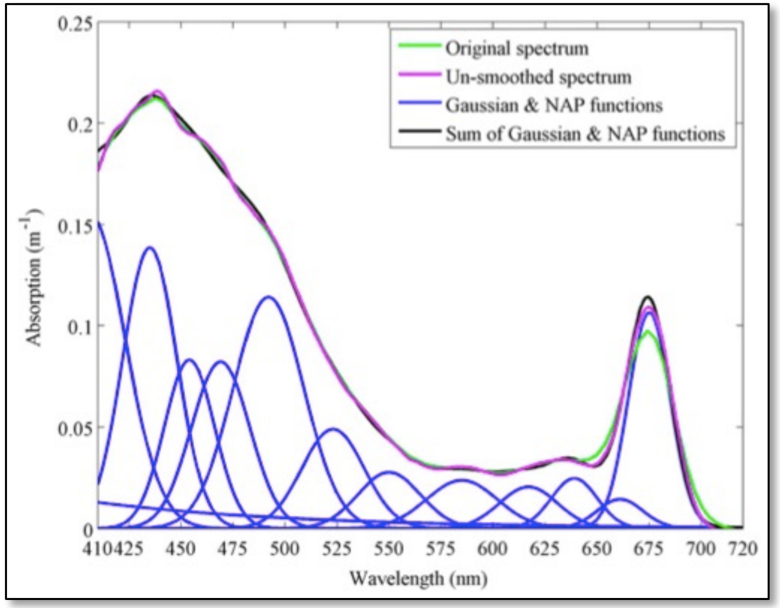
Phytoplankton Pigment Communities Can be Modeled Using Unique Relationships With Spectral Absorption Signatures in a Dynamic Coastal Environment

D. Catlett[1] and D. A. Siegel[1,2]

[1]Earth Research Institute, University of California, Santa Barbara, CA, USA, [2]Department of Geography, University of California, Santa Barbara, CA, USA

Abstract Understanding the roles of phytoplankton community composition in the functioning of marine ecosystems and ocean biogeochemical cycles is important for many ocean science problems of societal relevance. Remote sensing currently offers the only feasible method for continuously assessing phytoplankton community structure on regional to global scales. However, methods are presently hindered

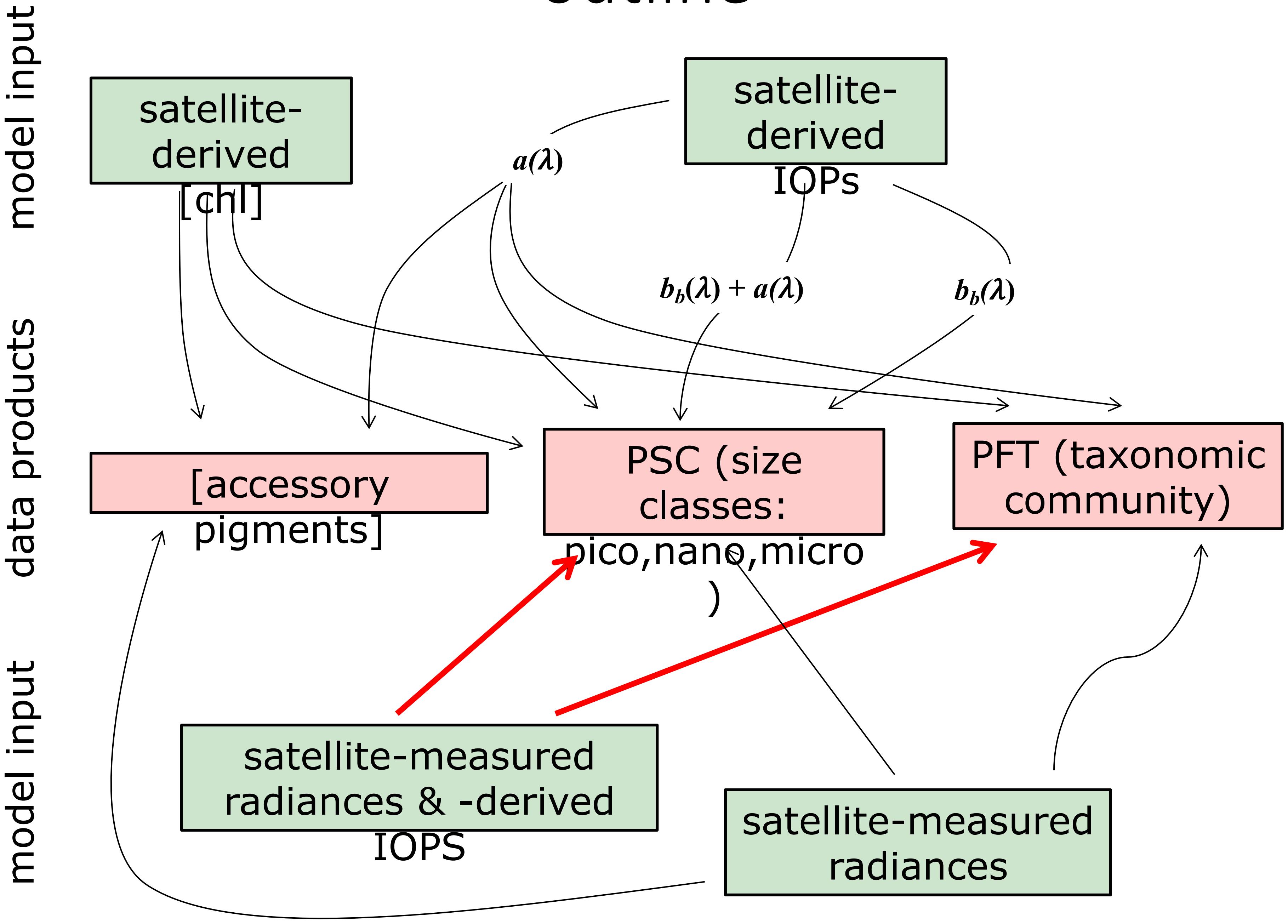
relationships between spectral derivative absorption signatures & phytoplankton pigment communities



use component Gaussian functions to represent absorption by individual or groups of pigments

purpose: relate pigment absorption features to their presence

outline



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b_b(λ)
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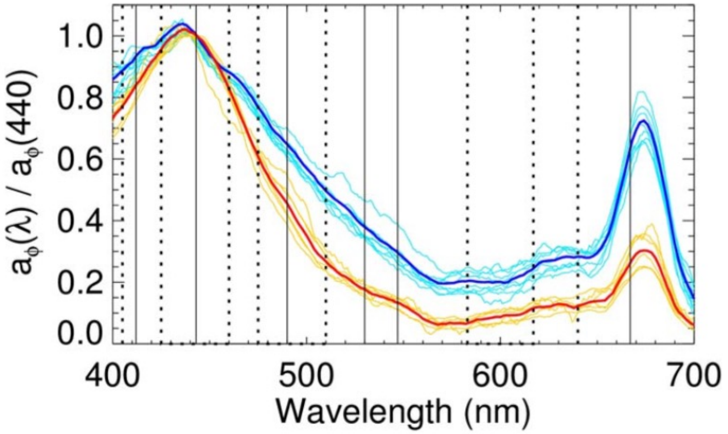
PFT (taxonomic community)
satellite-measured radiances & -derived IOPS
satellite-measured radiances

spectral – inversion modeling

Discrimination of phytoplankton functional groups using an ocean reflectance inversion model

P. Jeremy Werdell,[1,2,*] Collin S. Roesler,[3] and Joaquim I. Goes[4]
[1]NASA Goddard Space Flight Center, Code 616, Greenbelt, Maryland 20771, USA
[2]School of Marine Sciences, University of Maine, Orono, Maine 04469, USA
[3]Department of Earth and Ocean Sciences, Bowdoin College, Brunswick, Maine 04011, USA
[4]Lamont Doherty Earth Observatory, Columbia University, Palisades, New York 10964, USA
*Corresponding author: jeremy.werdell@nasa.gov

Received 6 January 2014; revised 4 April 2014; accepted 8 May 2014; posted 10 June 2014 (Doc. ID 204088); published 21 July 2014



Absorption spectra for *N. miliaris* and diatoms,

$$a(\lambda) = a_w(\lambda) +$$

$$M_{\phi D} a^*_{\phi D}(\lambda) + M_{\phi N} a^*_{\phi N}(\lambda)$$

$$+ M_{dg} a^*_{dg}(\lambda)$$

see also Chase et al. 2017

LIMNOLOGY and OCEANOGRAPHY: METHODS

Limnol. Oceanogr.: Methods 4, 2006, 237–253

Retrievals of a size parameter for phytoplankton and spectral light absorption by colored detrital matter from water-leaving radiances at SeaWiFS channels in a continental shelf region off Brazil

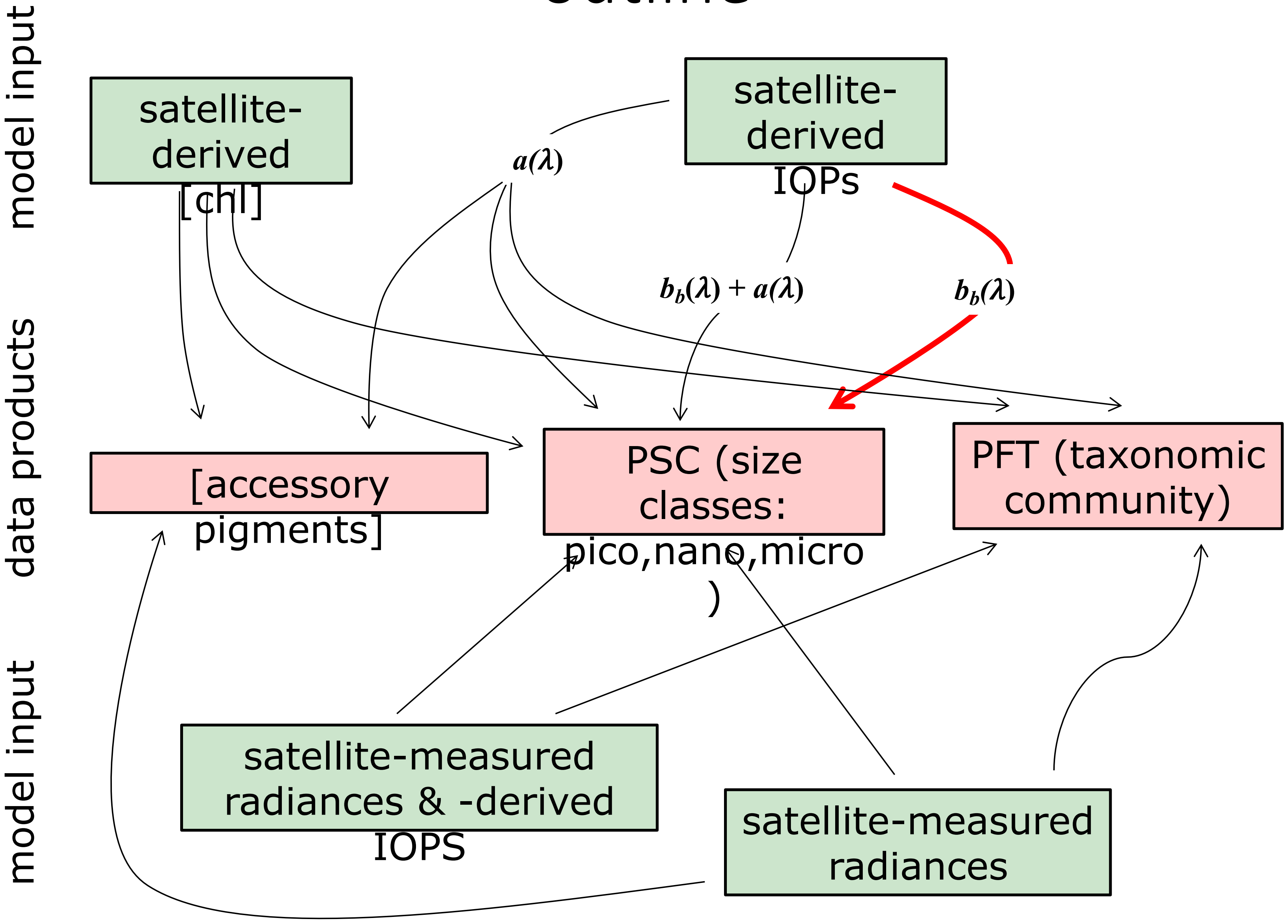
Aurea M. Ciotti[1] and Annick Bricaud[2]
[1]UNESP–CLP/SV, Campus do Litoral Paulista, Praça Infante Dom Henrique s/nº, São Vicente (SP), Brazil
[2]CNRS, Laboratoire d'Océanographie de Villefranche, Villefranche-sur-Mer; Université Pierre et Marie Curie-Paris, Lab d'Océanographie de Villefranche, Villefranche-sur-Mer, France

deconvolve $a_{ph}(\lambda)$ from a stepwise inversion algorithm into contributions by two size classes

$$a_\phi(\lambda) = a_{<\phi>}(\lambda) \cdot \{[S_f \cdot \bar{a}_{<pico>}(\lambda)] + [(1 - S_f) \cdot \bar{a}_{<micro>}(\lambda)]\}$$

purpose: use inversion modeling (e.g., Lectures 23) to solve for multiple $a_{ph}(\lambda)$

outline



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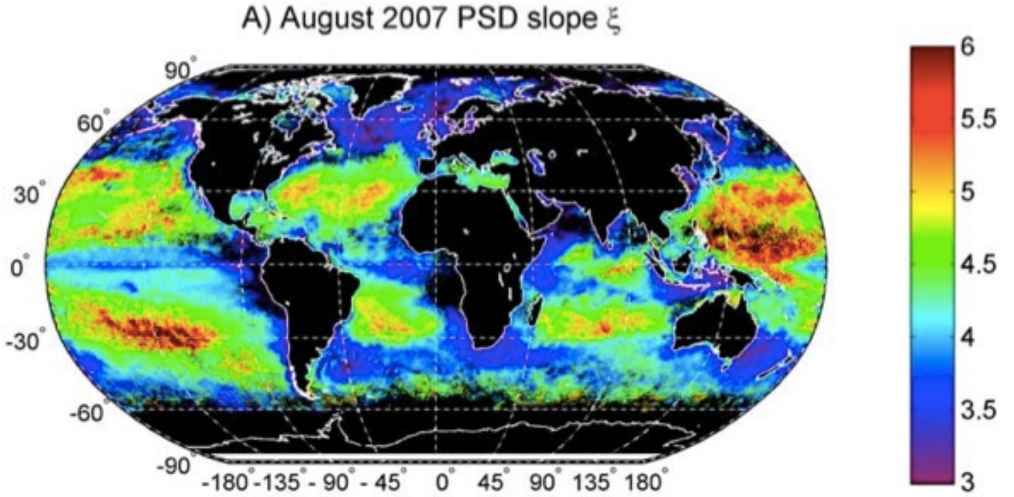
$b_b(\lambda)$
[accessory pigments]
PSC (size classes: pico,nano,micro)
PFT (taxonomic community)
satellite-measured radiances & -derived IOPS
satellite-measured radiances

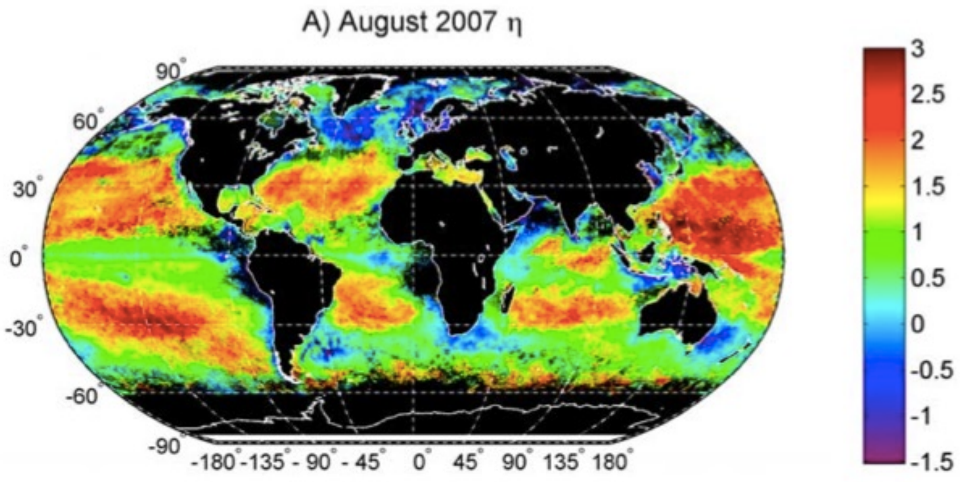
spectral – $b_{bp}(\lambda)$ as input

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 114, C09015, doi:10.1029/2009JC005303, 2009

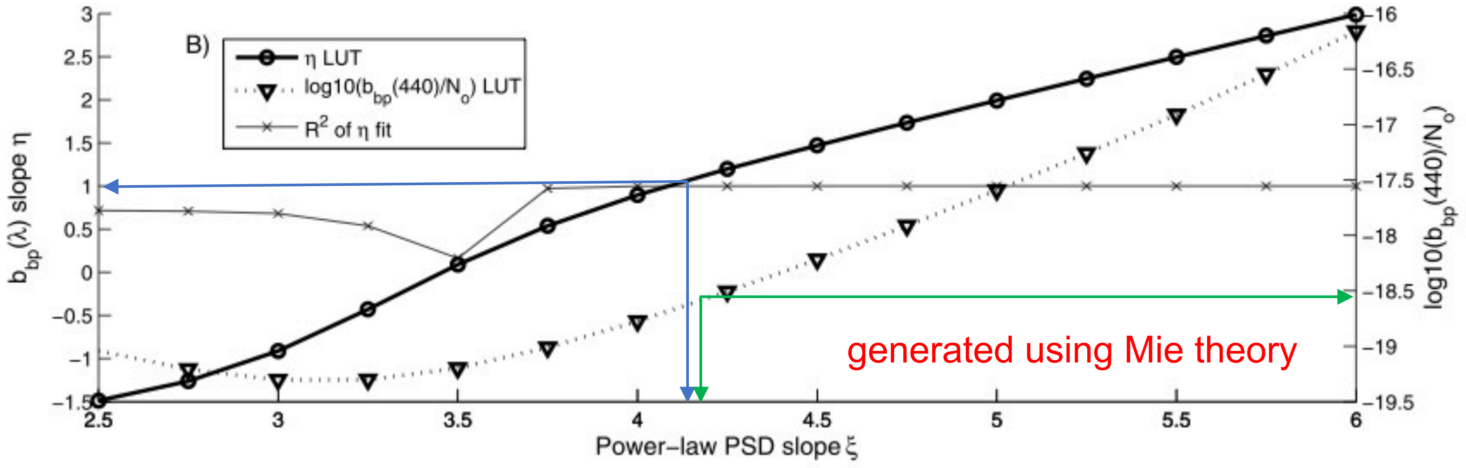
Retrieval of the particle size distribution from satellite ocean color observations

T. S. Kostadinov,[1,2] D. A. Siegel,[1,3] and S. Maritorena[1]





$b_{bp}(\lambda)$ & η from Loisel & Stramski 2000



purpose: estimate the relative fraction of 3 PSCs for each pixel


JUDGE ROY BEAN
NOTARY PUBLIC
JUSTICE OF THE PEACE
ICE BEER.
LAW WEST OF THE PECOS
THE JERSEY

what about environmental conditions?

SPACE SCIENCE

Global Biogeochemical Cycles

RESEARCH ARTICLE
10.1029/2018GB006118

Key Points:
- Globally, light availability in the water column is the most important parameter for phytoplankton size distribution
- Regionally, phytoplankton size distributions vary, responding to variable light and modes of nutrient delivery
- Cell size is increasing in the cold ocean and the dynamic regions in the warm ocean and declining in the warm ocean

A Satellite Assessment of Environmental Controls of Phytoplankton Community Size Structure

Colleen B. Mouw[1], Audrey B. Ciochetto[1], and James A. Yoder[1]

[1]Graduate School of Oceanography, University of Rhode Island, Narragansett, RI, USA

Abstract Phytoplankton play a key role as the base of the marine food web and a crucial component in the Earth's carbon cycle. There have been a few regional studies that have utilized satellite-estimated phytoplankton functional type products in conjunction with other environmental metrics. Here we expand to a global perspective and ask, what are the physical drivers of phytoplankton composition variability? Using a variety of satellite-observed ocean color products and physical properties spanning 1997–2015, we characterize spatial and temporal variability in phytoplankton community size structure in relation to

LIMNOLOGY AND OCEANOGRAPHY

ASLO
Association for the Sciences of Limnology and Oceanography

Article | Free Access

Identifying four phytoplankton functional types from space: An ecological approach

Dionysios E. Raitsos, Samantha J. Lavender, Christos D. Maravelias, John Haralabous, Anthony J. Richardson, Philip C. Reid

First published: 31 March 2008 | https://doi.org/10.4319/lo.2008.53.2.0605 | Citations: 75

ELSEVIER

Remote Sensing of Environment
Volume 240, April 2020, 111689

Incorporating environmental data in abundance-based algorithms for deriving phytoplankton size classes in the Atlantic Ocean

Timothy S. Moore [a, b], Christopher W. Brown [c]

Show more

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https://doi.org/10.1016/j.rse.2020.111689   Get rights and content

emerging mathematical & computation methods: what about EOFs, NNs, Bayes, AI, machine learning, etc?

Remote Sensing of Environment
Volume 252, January 2021, 112154

Biogeographical trends in phytoplankton community size structure using adaptive sentinel 3-OLCI chlorophyll *a* and spectral empirical orthogonal functions in the estuarine-shelf waters of the northern Gulf of Mexico

Bingqing Liu [a, b], Eurico J. D'Sa [a], Kanchan Maiti [a], Victor H. Rivera-Monroy [a], Zuo Xue [a]

Remote Sensing of Environment
Volume 253, February 2021, 112200

Hyperspectral retrievals of phytoplankton absorption and chlorophyll-*a* in inland and nearshore coastal waters

Nima Pahlevan [a, b], Brandon Smith [a, b], Caren Binding [c], Daniela Gurlin [d], Lin Li [e], Mariano Bresciani [f], Claudia Giardino [f]

6902 Vol. 59, No. 23 / 10 August 2020 / *Applied Optics* Research Article
applied optics

Bayesian retrieval of optically relevant properties from hyperspectral water-leaving reflectances

Zachary K. Erickson,[1,*] P. Jeremy Werdell,[2] and Ivona Cetinić[2,3]
[1]Ocean Ecology Laboratory, NASA Goddard Space Flight Center, Greenbelt, Maryland 21077, USA
[2]Ocean Ecology Laboratory, NASA Goddard Space Flight Center, Greenbelt, Maryland 21077, USA
[3]GESTAR/University Space Research Associates (USRA), 7178 Columbia Gateway Dr., Columbia, Maryland 21046, USA
*Corresponding author: zachary.k.erickson@nasa.gov

Received 21 May 2020; revised 10 July 2020; accepted 10 July 2020; posted 10 July 2020 (Doc. ID 398043); published 4 August 2020

Research Article Vol. 28, No. 18 / 31 August 2020 / *Optics Express* 25682
Optics EXPRESS

Radiometric approach for the detection of picophytoplankton assemblages across oceanic fronts

Priscila Kienteca Lange,[1,2,3,*] P. Jeremy Werdell,[1] Zachary K. Erickson,[1,4] Giorgio Dall'Olmo,[5] Robert J. W. Brewin,[6] Mikhail V. Zubkov,[7] Glen A. Tarran,[5] Heather A. Bouman,[8] Wayne H. Slade,[9] Susanne E. Craig,[1,2] Nicole J. Poulton,[10] Astrid Bracher,[11,12] Michael W. Lomas,[10] and Ivona Cetinić[1,2]

key points for our exploration of satellite methods to derive PSCs/PFTs

diverse bio-optical methods to estimate PSCs/PFTs exist

→ their sensitivities remain unexplored

most folks use proxy data sets for their validation

satellite data compositing matters

algorithm sensitivities (a.k.a. your future work)

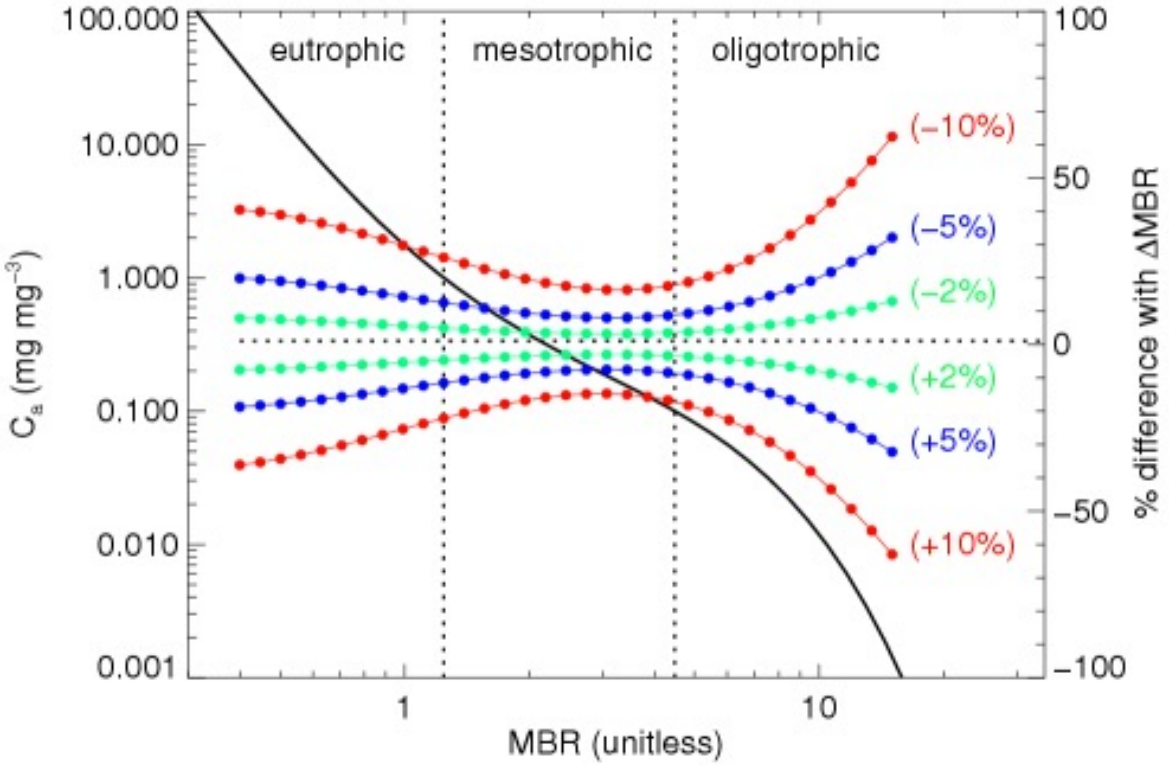
what we know:

- all PFT algorithms use derived products (e.g., Chl & IOPs) or make *a priori* environmental assumptions
- few PFT/PSC modeling papers include robust analysis of the sensitivity of the model outputs to the model inputs

what we don't know:

- how sensitive are the abundance methods to uncertainties in derived Chl & IOPs?
- how sensitive are the spectral methods to uncertainties in $R_{rs}(\lambda)$ & derived $a_{ph}(\lambda)$ & other parameters?

sensitivity of chl & inversion algorithms



Run	N	MPD			
		b_{bp}	a	a_{dg}	a_ϕ
GIOP-DC	437	NA	NA	NA	NA
S_{bp} − 33%	440	5.19	5.17	7.58	2.98
S_{bp} + 33%	436	5.65	5.70	8.82	2.90
S_{dg} − 33%	448	18.96	33.44	101.73	46.59
S_{dg} + 33%	399	3.77	8.41	40.10	32.92
S_{dg} from [7]	439	3.20	5.33	20.40	14.58
C_a − 33% in [14]	419	2.02	2.92	1.48	7.25
C_a + 33% in [14]	437	1.56	2.28	1.14	5.90
Fixed C_a in [14]	369	4.57	7.89	2.60	21.68
a^*_ϕ from [17]	357	8.33	12.72	7.04	22.23
G from [22]	422	9.99	6.15	7.49	14.12
Matrix inversion	475	4.60	3.68	2.24	7.41
$400 \le \lambda \le 600$ nm	424	0.23	0.21	0.08	0.38

Werdell et al. 2013, Applied Optics

key points for our exploration of satellite methods to derive PSCs/PFTs

diverse bio-optical methods to estimate PSCs/PFTs exist

their sensitivities remain unexplored

→ most folks use proxy data sets for their validation

satellite data compositing matters

measuring PFTs and PSCs in the field

microscopy
genetic/molecular methods
flow cytometry
coulter counters
video imaging (IFCB, FlowCam)
continuous plankton recorder
spectroscopy
optics (b_b, c spectral slopes)
HPLC pigment analyses
etc.

most heritage ocean color PFT/PSC algorithms tuned & validated using this proxy method

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 106, NO. C9, PAGES 19,939–19,956, SEPTEMBER 15, 2001

Phytoplankton pigment distribution in relation to upper thermocline circulation in the eastern Mediterranean Sea during winter

Francesca Vidussi[1], Hervé Claustre[1], Beniamino B. Manca[2], Anna Luchetta[3], and Jean-Claude Marty[1]

diagnostic pigment analyses (DPA)

Vol. 144: 265–283, 1996 | MARINE ECOLOGY PROGRESS SERIES Mar Ecol Prog Ser | Published December 5

CHEMTAX—a program for estimating class abundances from chemical markers: application to HPLC measurements of phytoplankton

M. D. Mackey[1,2], D. J. Mackey[2,*], H. W. Higgins[2], S. W. Wright[3]

[1]University Chemical Laboratory, Lensfield Rd, Cambridge CB2 1EW, United Kingdom
[2]CSIRO Division of Oceanography, PO Box 1538, Hobart, Tasmania 7001, Australia
[3]Australian Antarctic Division, Channel Highway, Kingston, Tasmania 7050, Australia

summary of validation exercises

TABLE 3 | Algorithm retrieval parameters and validation metrics.

Type	Algorithm	Type of retreival	Retreival parameters and units	Validation data source	Information source within reference	Validation measure	Strategy
Abundance	Brewin et al., 2010—BR10	PSC	Chla (mg m^{-3}): micro, nano, pico	HPLC pigments	Figure 6	pico: ME = 0.039	Semi-empirical
						nano: ME = 0.076	
						micro: ME = 0.149	
	Brewin R. J. et al., 2011—BR10	PSC	Absorption (m^{-1}): micro, nano, pico	Absorption	Figure 7	All at 443 nm: RMSE = 52.5% (size fractions not validated)	Empirical
	Hirata et al., 2011—OC-PFT	PSC, PTC	% Chl: pico, nano, micro diatom, dino, green hapto, prok, pico-euk prochlor	HPLC pigments	Table 4; Figure 4	pico: r^2 = 0.72, RMSE = 7.12	Empirical
						nano: r^2 = 0.56, RMSE = 8.55	
						micro: r^2 = 0.72, RMSE = 8.28	
						diatom: r^2 = 0.73, RMSE = 7.98	
						dino: r^2 = 0, RMSE = 1.87	
						green: r^2 = 0.40, RMSE = 4.71	
						hapto: r^2 = 0.37, RMSE = 10	
						prok: r^2 = 0.65, RMSE = 7.71	
						pico-euk: r^2 = 0.31, RMSE = 5.25	
						prochlor: r^2 = 0.72, RMSE = 6.25	
	Uitz et al., 2006—UITZ06	PSC	fractionated Chla (mg m^{-3}): micro, nano, pico	HPLC pigments	Figure 12A	$\log_{10}$ (predicted/measured)	Empirical
						median = 0.02	
						mean = −0.012	
						std. dev. = 0.883	
Radiance	Alvain et al., 2005, 2008—PHYSAT	PTC	Dominance (presence over time): nanoeuk, prochlor, syn, diatom, phaeo	HPLC pigments	Figure 6	Classification success	Empirical
					Alvain et al. (2008)	nanoeuc: 83%	
						prochlor: 51%	
						syn: 54%	
						diatom: 57%	
	Li et al., 2013—LI13	PSC	Fractionated: pico, nano, micro	HPLC pigments	Figure 7	pico: r^2 = 0.587, RMSE = 15.2	Empirical
						nano: r^2 = 0.475, RMSE = 12	Spectral features
						micro: r^2 = 0.617, RMSE = 17	
Absorption	Bracher et al., 2009 —PhytoDOAS	PTC	Chla (mg m^{-3}): cyano, diatom	HPLC pigments	Figure 8	diatom: r^2 = 0.92	Differential optical
						cyano: r^2 = 0.81	Absorption spectroscopy
	Sadeghi et al., 2012a —PhytoDOAS	PTC	Chla (mg m^{-3}): diatom, cocco, dino	Model and satellite	Figure 9	diatom: –	Differential optical
					Product comparison*	cocco: r^2 = 0.66 (MODIS PIC)	Absorption spectroscopy
						dino: –	

A Consumer's Guide to Satellite Remote Sensing of Multiple Phytoplankton Groups in the Global Ocean

summary of validation exercises

TABLE 3 | Continued

Type	Algorithm	Type of retreival	Retreival parameters and units	Validation data source	Information source within reference	Validation measure	Strategy
	Ciotti and Bricaud, 2006—CB06	PSC	S_f	Absorption	Table 4	RMSE all data = 17.2	Semi-analytical
							Non-linear optimization
	Bricaud et al., 2012—CB06	PSC	S_f	HPLC pigments	Table 1; Figure 4 in Brewin R. J. et al., 2011	52.0 ± 9.8% accuracy	Semi-analytical
	Validation in Brewin R. J. et al., 2011						Non-linear optimization
	Devred et al., 2011—DSSP11	PSC	% pico, % nano, % micro	HPLC pigments	Devred et al., 2011	pico: %diff = 3.4%, bias = 2.2%	Non-linear optimization
						nano: %diff = 11%, bias = −1.1%	
						micro: %diff = 12%, bias = −1.1%	
	Fujiwara et al., 2011—FUJI11	PSC	% Chla > 5μm	Size fractionated Chla	Figure 3	r^2 = 0.45, RMSE 22.7	Empirical
						Classification success = 69%	
	Hirata et al., 2008—HIRATA08	PSC	Dominance: pico, nano, micro	HPLC pigments	Table 3	Classification success	Empirical
						All data from AMT-07 = 73%	
	Mouw and Yoder, 2010b—MY10	PSC	S_{fm}	HPLC pigments	Table 2; Figure 13	micro: r^2 = 0.6, RMSE = 12.64	Look-up-table
	Roy et al., 2013—ROY13	PSD, PSC	PSD: exponent (unitless) and % Chl: micro, nano, pico	HPLC pigments absorption and error analysis	Figures 4, 5	pico: r^2 = 0.4	Semi-analytical
						nano: r^2 = 0.02	Non-linear optimization
						micro: r^2 = 0.42	
Scattering	Kostadinov et al., 2009—KSM09	PSD	PSD slope (unitless)	Coulter counter PSD	Figure 14	r^2 = 0.21 for PSD slope	Look-up-table
			PSD: pico, nano, micro [$\log_{10}(m^{-4})$]			r^2 = 0.26 for log10 (N_0)	
	Kostadinov et al., 2010—KSM09	PSC	% biovolume: pico, nano, micro	HPLC pigments	Figure 3	pico: r^2 = 0.34, RMSE = 24.1	Look-up-table
						nano: r^2 = 0.11, RMSE = 19.8	
						micro: r^2 = 0.42, RMSE = 17.1	

The four algorithm types are indicated by color: abundance (green), radiance (red), absorption (yellow), scattering (blue). The validation measure is as reported in the original algorithm publication and in units of the retrieval parameter, unless noted otherwise. Caution should be taken in comparing validation measures of differing units. ME is mean error, RMSE is root mean square error. A single asterisk indicates the validation data source is not a true validation; coccolithophores and diatoms are compared with numerical model output while coccolithophores are additionally compared with a satellite particulate inorganic carbon product and dinoflagellates are not compared. All algorithms with the exception of CB06 (Brazil continental shelf) and FUJI11 (Arctic and sub-Arctic) were developed for global extent. CB06 was later verified for global use by Bricaud et al. (2012).

HPLC measurements as proxy PFT/PSC data

all authors acknowledged the need for rigorous validation via **microscopic, imaging,** or **flow cytometric enumeration of cells**

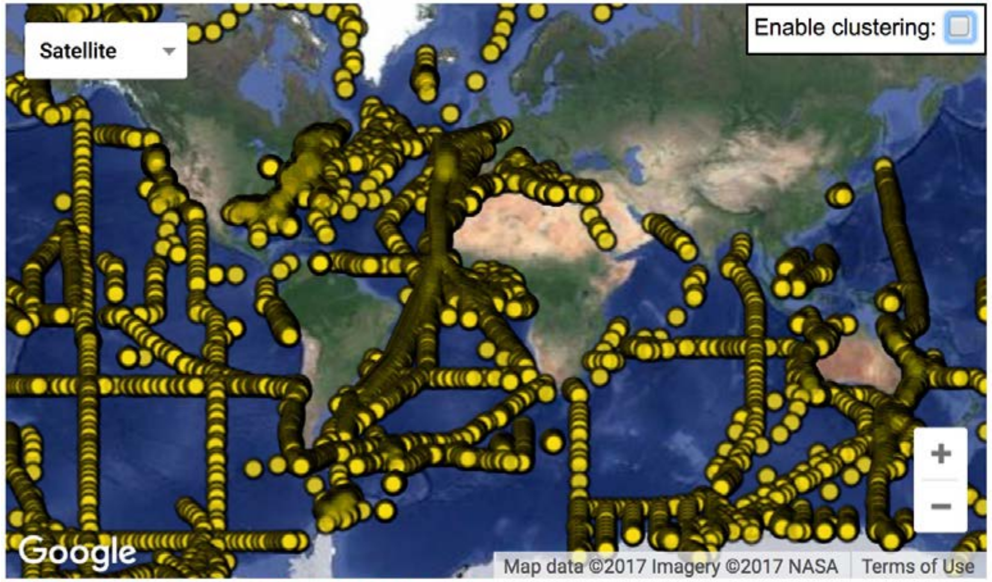
these measurements are [were] scarce, whereas HPLC pigment data are **abundant & globally distributed**

weaknesses in DPA / CHEMTAX:

- phytoplankton groups share taxonomic pigments (e.g., fucoxanthin in diatoms, dinoflagellates, & Phaeocystis)
- phytoplankton groups encompass wide size ranges (e.g., most diatoms are micro, but some are nano)
- methods require a priori knowledge of accessory pigment ratios

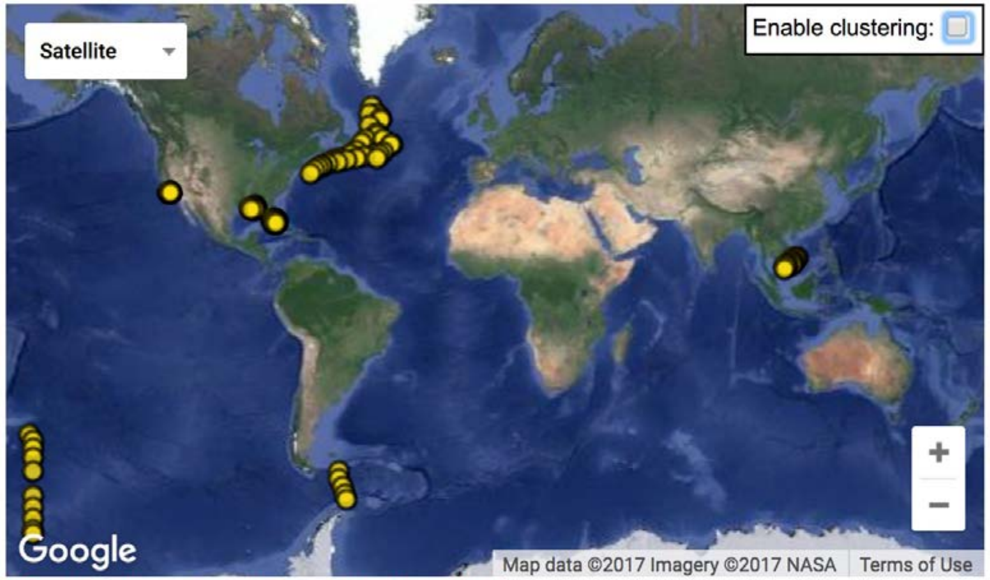
NASA SeaBASS HPLC holdings

through 2019



* Points displayed are subsampled and rounded.

Jan 2016 – Jul 2017

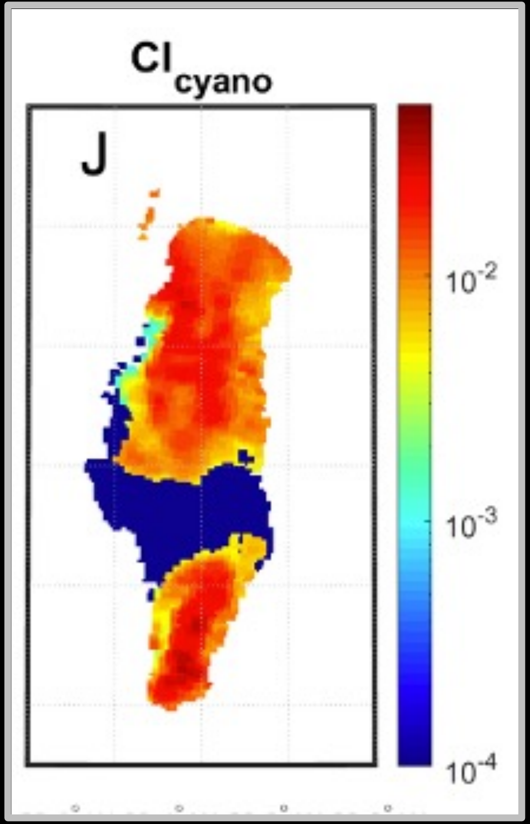


* Points displayed are subsampled and rounded.

take home question

Given what you know about the in situ methods and the satellite algorithms, how would you prepare the in situ data for a validation satellite exercise to get as close to apples-to-apples comparisons as possible (e.g., common units, observational space, etc.)?

- microscopy
- genetic/molecular methods
- flow cytometry
- coulter counters
- video imaging (IFCB, FlowCam)
- continuous plankton recorder
- spectroscopy
- optics (b_b, c spectral slopes)
- HPLC pigment analyses
- etc.



satellite measured
$R_{rs}(\lambda)$

↓

satellite modeled
Chl, IOPs

↓

satellite modeled
PFTs/PSCs

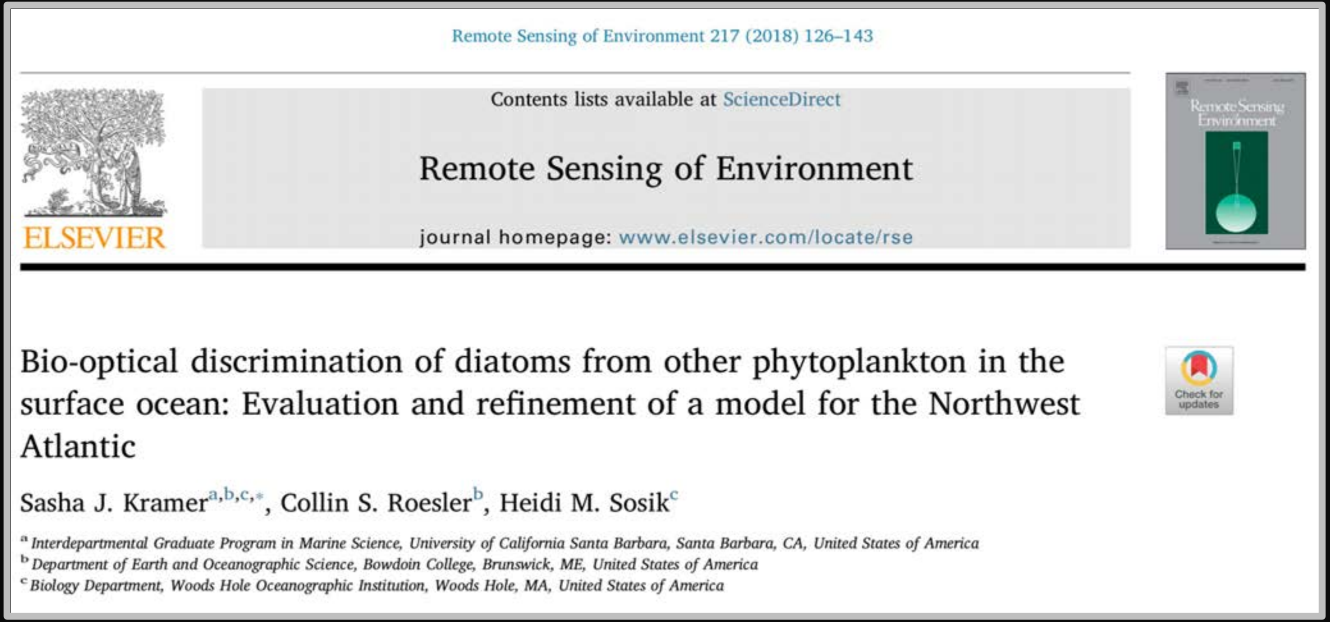
↕ ↕

in situ inferred PFTs/PSCs | *in situ* measured PFTs/PSCs

↑

in situ measured
Chl, IOPs

rigorous validation & metrics of performance assessment


Remote Sensing of Environment 217 (2018) 126–143

Contents lists available at ScienceDirect

Remote Sensing of Environment

journal homepage: www.elsevier.com/locate/rse

ELSEVIER

Bio-optical discrimination of diatoms from other phytoplankton in the surface ocean: Evaluation and refinement of a model for the Northwest Atlantic

Sasha J. Kramer[a,b,c,*], Collin S. Roesler[b], Heidi M. Sosik[c]

[a] Interdepartmental Graduate Program in Marine Science, University of California Santa Barbara, Santa Barbara, CA, United States of America
[b] Department of Earth and Oceanographic Science, Bowdoin College, Brunswick, ME, United States of America
[c] Biology Department, Woods Hole Oceanographic Institution, Woods Hole, MA, United States of America

extensive review & re-parameterization of an approach to distinguish diatoms from a mixed population of phytoplankton

conscientious review of strategies for validation & algorithm application

key points for our exploration of satellite methods to derive PSCs/PFTs

diverse bio-optical methods to estimate PSCs/PFTs exist

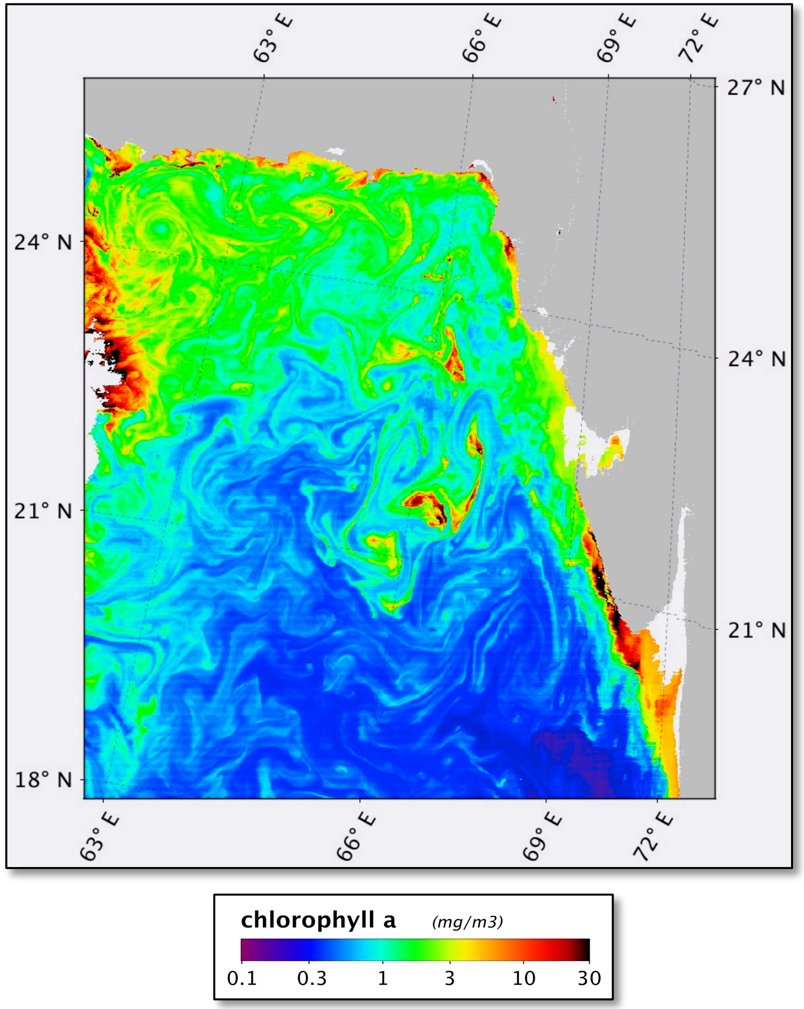
their sensitivities remain unexplored

most folks use proxy data sets for their validation

→ satellite data compositing matters

understand how data processing changes the "answers"

For your consideration:
- horizontal resolution
- temporal resolution
- vertical resolution



understand how data processing changes the “answers”

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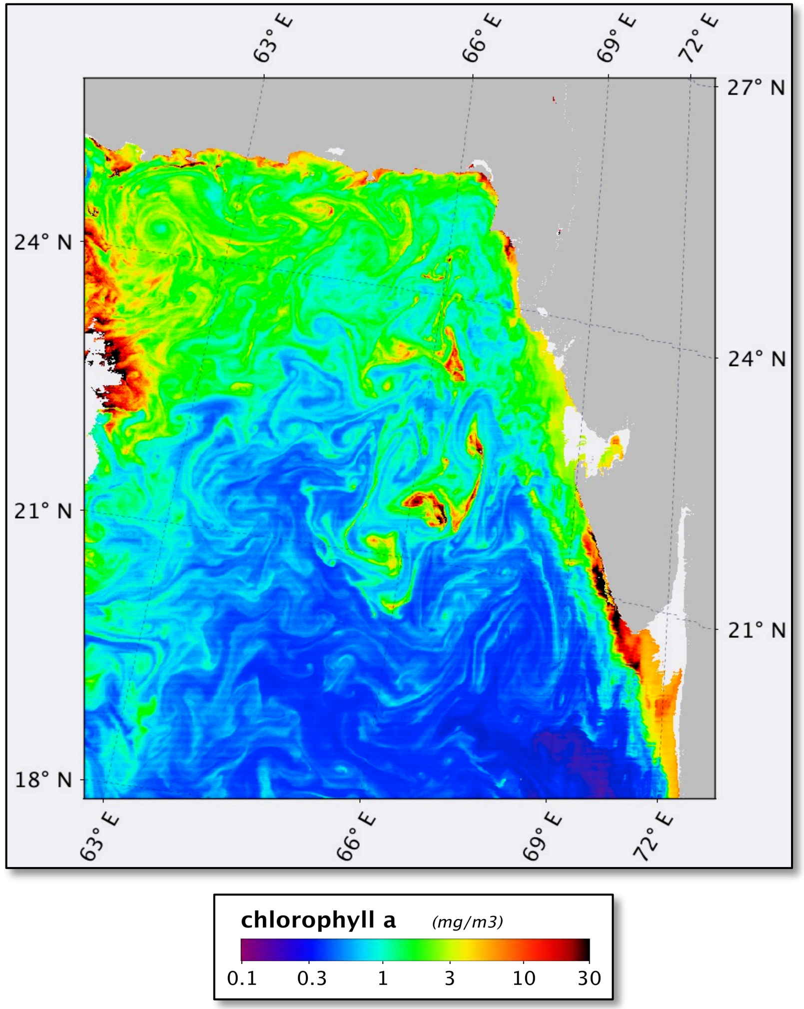

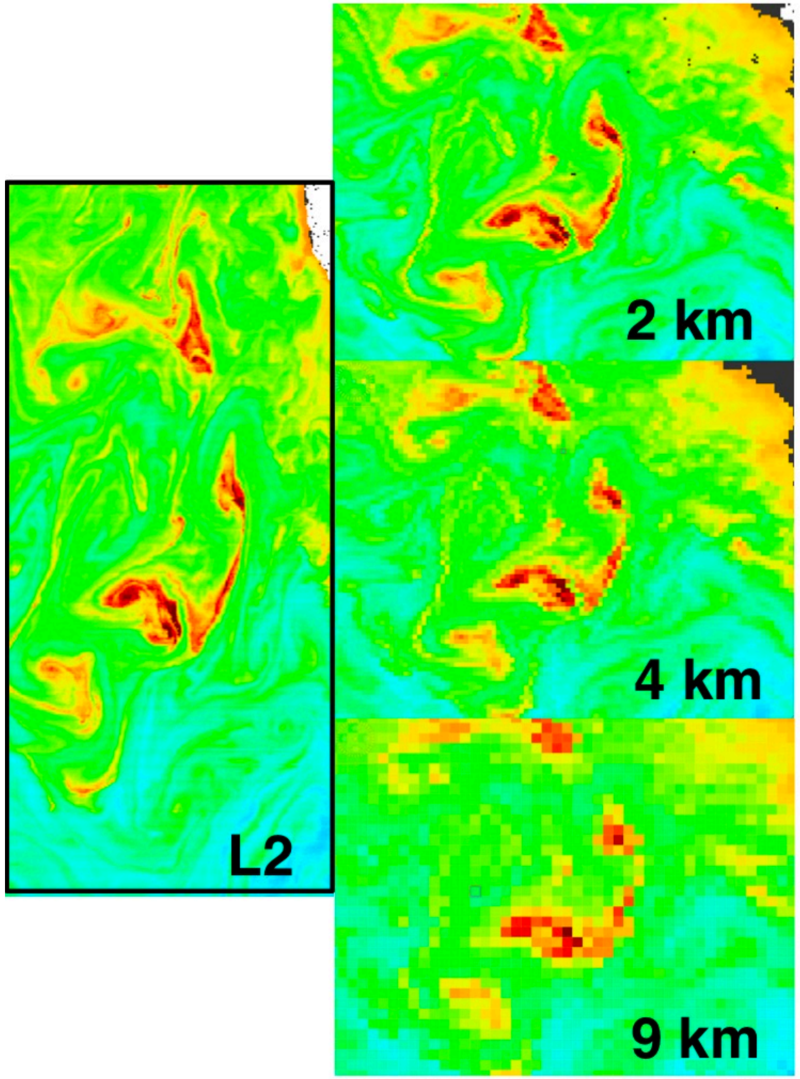

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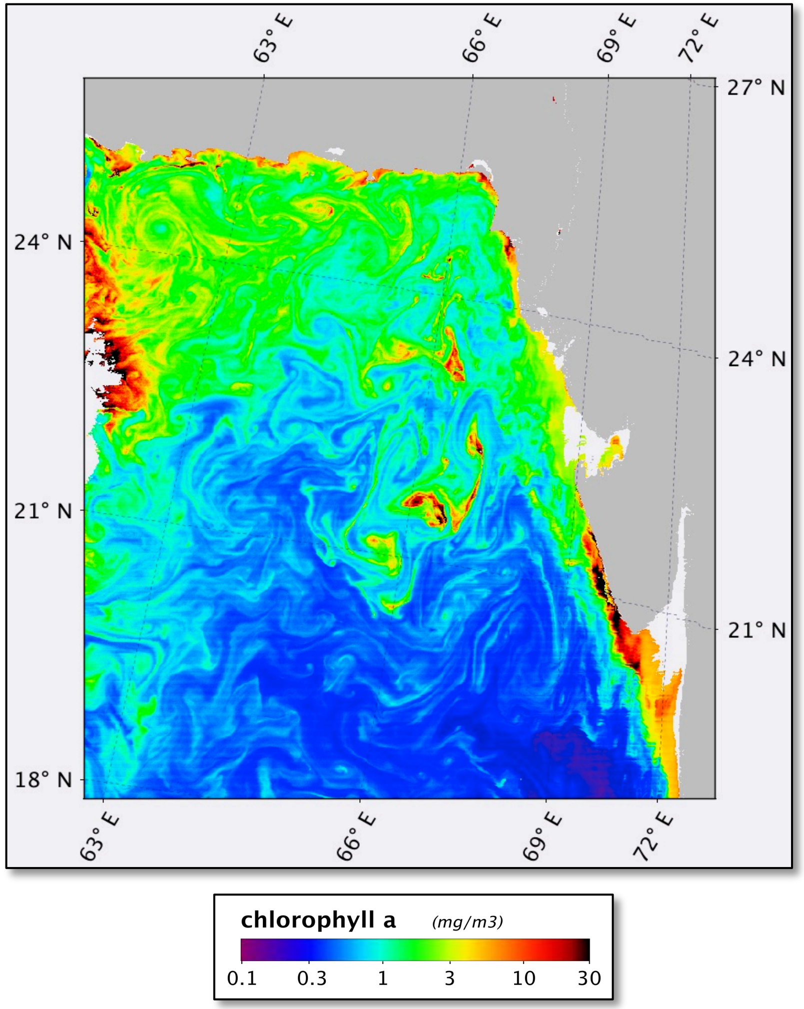

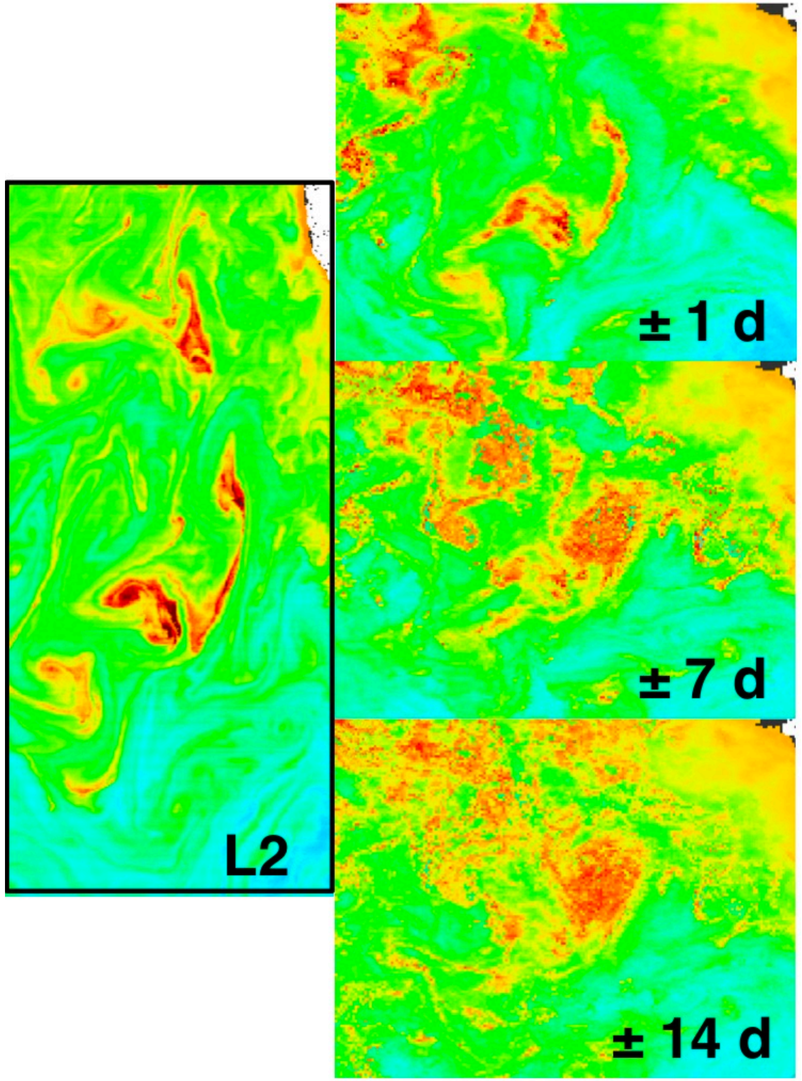

understand how data processing changes the "answers"

For your consideration:
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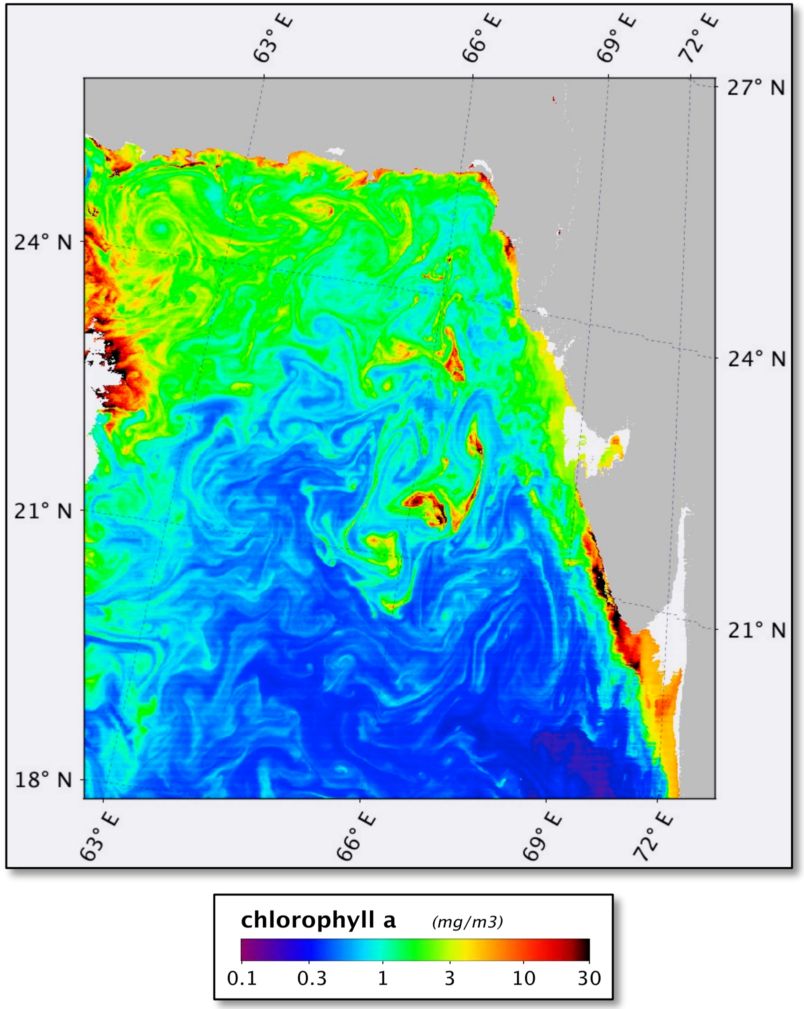
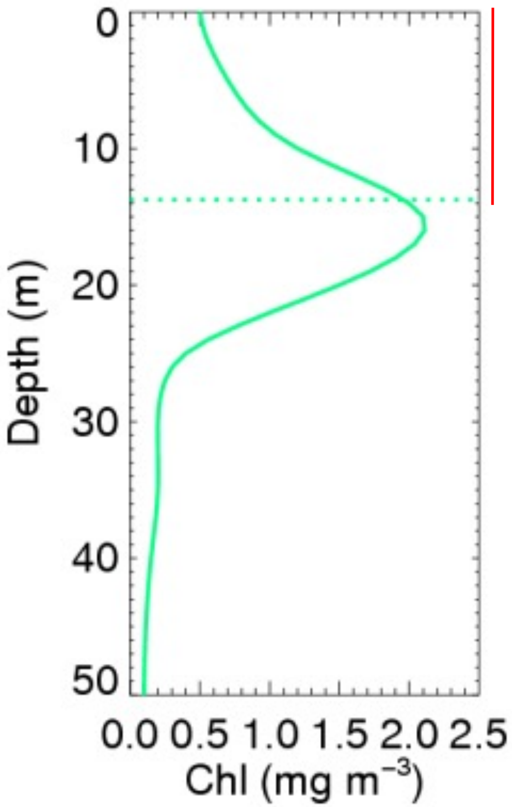
- vertical resolution





first optical depth
$0.37 = \exp(-K_d z)$
$-1 = -K_d z$

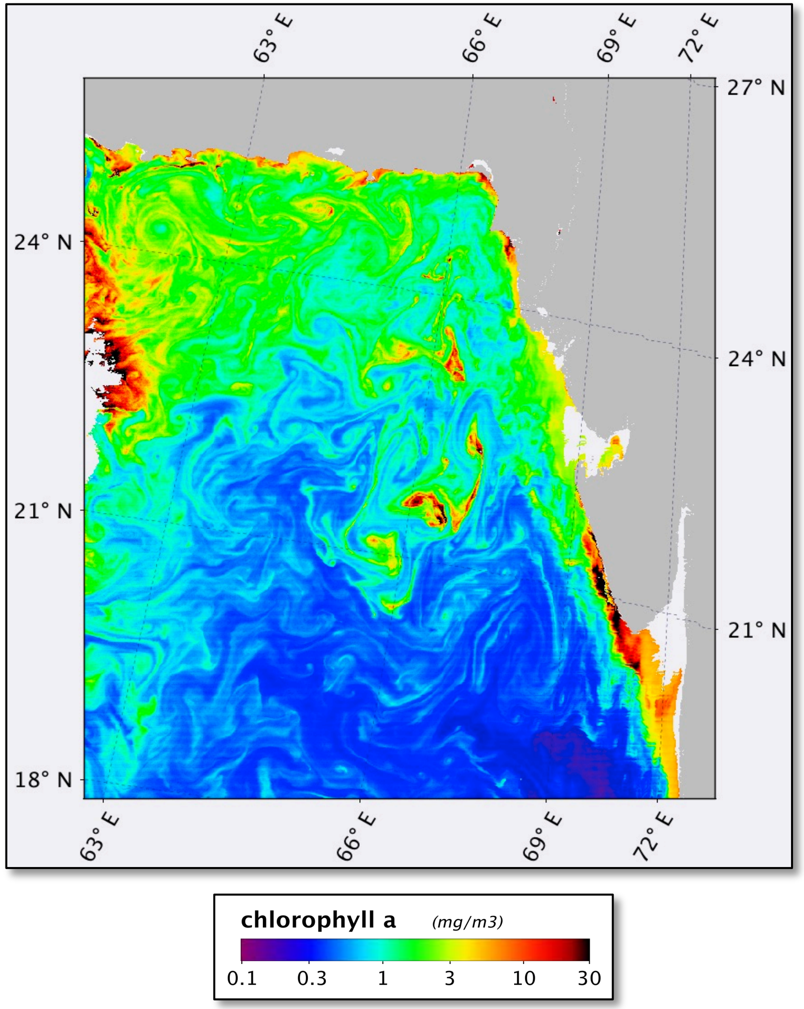
Estimation of the Depth of Sunlight Penetration in the Sea for Remote Sensing

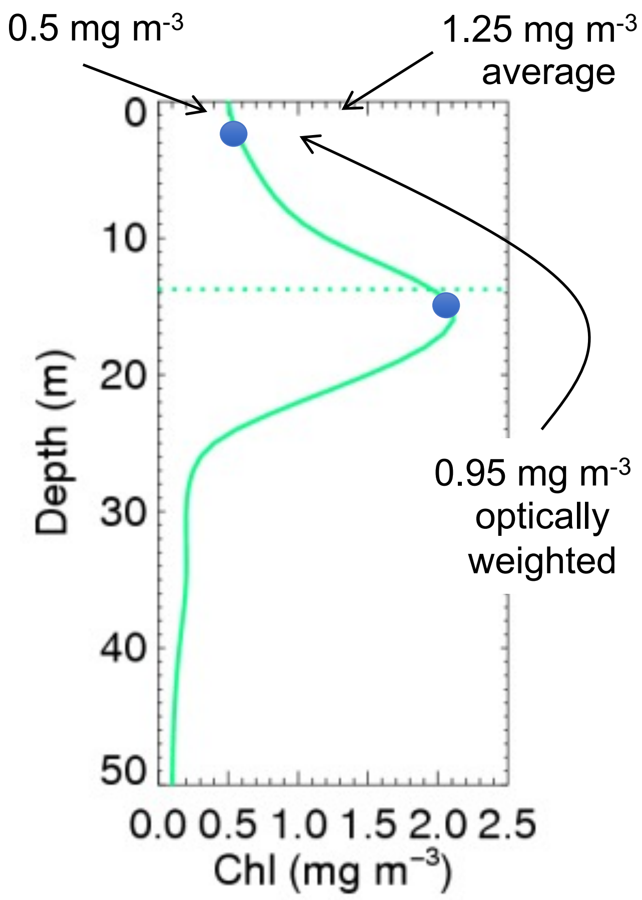
Howard R. Gordon and W. R. McCluney

February 1975 / Vol. 14, No. 2 / APPLIED OPTICS 413

understand how data processing changes the “answers”

For your consideration:
- horizontal resolution
- temporal resolution
- vertical resolution





Theoretical derivation of the depth average of remotely sensed optical parameters

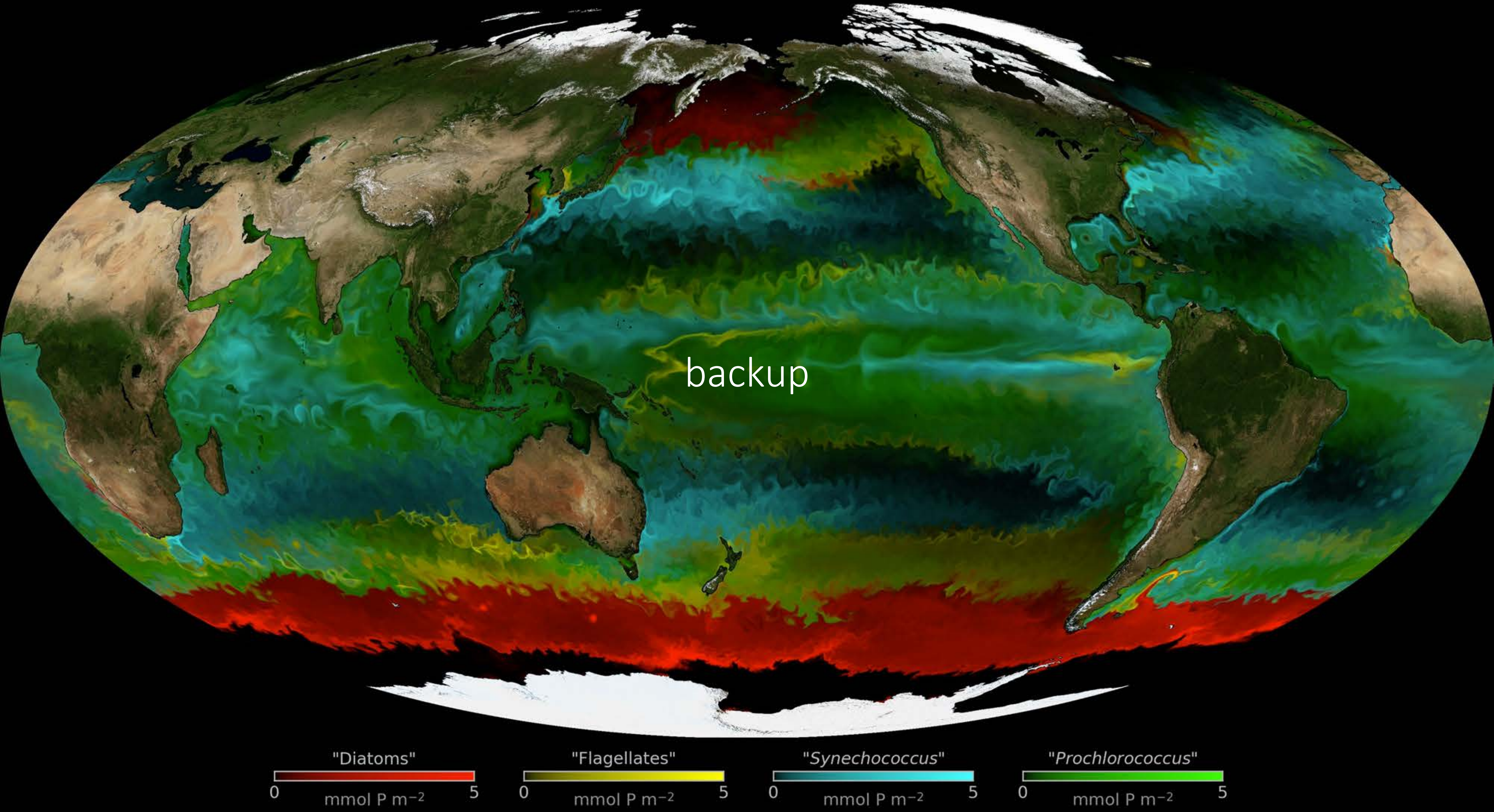
J. Ronald V. Zaneveld[1], Andrew H. Barnard[1] and Emmanuel Boss[2]
[1] WET Labs, Inc. P.O. Box 518, 620 Applegate Street, Philomath, OR 97370
[2] University of Maine, 5741 Libby Hall, Orono, ME 04469
ron@wetlabs.com

#8803 - $15.00 USD
Received 15 September 2005; revised 20 October 2005; accepted 24 October 2005

31 October 2005 / Vol. 13, No. 22 / OPTICS EXPRESS 9052

NEVER GIVE UP

NEVER STOP TRYING TO EXCEED YOUR LIMITS. WE NEED THE ENTERTAINMENT.


backup
"Diatoms"
0
mmol P m−2
5
"Flagellates"
0
mmol P m−2
5
"*Synechococcus*"
0
mmol P m−2
5
"*Prochlorococcus*"
0
mmol P m−2
5

using phytoplankton accessory pigments to determine the dominate PSC

Appendix A. Diagnostic Pigment Analyses

Vidussi et al. (2001) described a common method for diagnostic pigment analyses. Uitz et al. (2006) updated this method. Dominant phytoplankton groups are always assigned to the most significant contributor (often >45 or >50% relative presence required). A list of the biomarker pigments is provided below, as well as the sums and ratios suggested by both authors.

Abbreviation	Name	Taxonomic Significance	Size
Fuco	Fucoxanthin	diatoms	micro
Perid	Peridinin	dinoflagellates	micro
Hex-fuco	19'-hexanoyloxyfucoxanthin	chromophytes, nanoflagellates	nano
But-fuco	19'-butanoyloxyfucoxanthin	chromophytes, nanoflagellates	nano
Allo	Alloxanthin	cryptophytes	nano
TChl-b	Chl-b + Divinyl Chl-b	green flagellates, prochlorophytes	pico
Zea	Zeaxanthin	cyanobacteria, prochlorophyte	pico

Vidussi et al. (2001)

DP = Fuco + Perid + Hex-fuco + But-fuco + Allo + TChl-b + Zea
micro = (Fuco + Perid) / DP
nano = (Hex-fuco + But-fuco + Allo) / DP
pico = (TChl-b + Zea) / DP

Modifications by Uitz et al. (2006)

DP_w = 1.41 Fuco + 1.41 Perid + 1.27 Hex-fuco + 0.35 But-fuco + 0.60 Allo + 1.01 TChl-b +0.86 Zea
f_{micro} = (1.41 Fuco + 1.41 Perid) / DP_w
f_{nano} = (1.27 Hex-fuco + 0.35 But-fuco + 0.60 Allo) / DP_w
f_{pico} = (1.01 TChl-b + 0.86 Zea) / DP_w
micro-Chl-a = f_{micro} Chl-a
nano-Chl-a = f_{nano} Chl-a
pico-Chl-a = f_{pico} Chl-a

adjusted chl-to-accessory pigment ratios – link to fractional chl for each PSC

abundance – Chl as input

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 111, C08005, doi:10.1029/2005JC003207, 2006

Click Here for Full Article

Vertical distribution of phytoplankton communities in open ocean: An assessment based on surface chlorophyll

Julia Uitz,[1] Hervé Claustre,[1] André Morel,[1] and Stanford B. Hooker[2]

GLOBAL BIOGEOCHEMICAL CYCLES, VOL. 24, GB3016, doi:10.1029/2009GB003680, 2010

Phytoplankton class-specific primary production in the world's oceans: Seasonal and interannual variability from satellite observations

Julia Uitz,[1] Hervé Claustre,[2] Bernard Gentili,[2] and Dariusz Stramski[1]

provide estimate of relative presence (%) of 3 PSCs

abundance – Chl as input

Table 3. Trophic Categories Defined With Respect to the Chlorophyll *a* Concentration Within the Surface Layer, $[Chla]_{surf}$, and the Associated Parameters[a]

	Stratified Waters									Mixed Waters				
	S1	S2	S3	S4	S5	S6	S7	S8	S9	M1	M2	M3	M4	M5
$[Chla]_{surf}$ range, mg m^{-3}	<0.04[b]	0.04–0.08	0.08–0.12	0.12–0.2	0.2–0.3	0.3–0.4	0.4–0.8	0.8–2.2	2.2–4[c]	<0.4[d]	0.4–0.8	0.8–1	1–4	>4[e]
Number of profiles	109	268	269	320	287	180	260	110	18	155	153	53	182	55
Average $[Chla]_{surf}$, mg m^{-3}	0.032	0.062	0.098	0.158	0.244	0.347	0.540	1.235	2.953	0.244	0.592	0.885	1.881	6.320
	(0.005)	(0.012)	(0.012)	(0.023)	(0.030)	(0.028)	(0.106)	(0.403)	(0.520)	(0.092)	(0.112)	(0.051)	(0.753)	(2.916)
Average $\overline{Chla}_{Zeu}$, mg m^{-3}	0.0910	0.151	0.185	0.250	0.338	0.410	0.578	1.206	2.950	0.280	0.591	0.872	2.059	7.574
	(0.025)	(0.067)	(0.088)	(0.144)	(0.152)	(0.153)	(0.229)	(0.526)	(1.191)	(0.130)	(0.175)	(0.189)	(0.996)	(3.700)
Average $\langle Chla \rangle_{Zeu}$, mg m^{-2}	10.54	14.15	15.98	18.79	22.09	24.70	29.72	44.05	71.98	19.90	30.27	37.57	58.64	120.00
	(1.84)	(3.31)	(3.29)	(4.08)	(4.99)	(4.64)	(5.88)	(10.46)	(15.28)	(4.70)	(4.73)	(4.44)	(15.30)	(26.75)
Average $\langle Chla \rangle_{1.5\ Zeu}$, mg m^{-2}	18.27	22.13	24.74	27.19	29.42	31.83	38.22	58.18	101.33	28.46	40.22	51.49	85.42	178.37
	(3.97)	(5.18)	(6.35)	(8.29)	(8.58)	(8.76)	(9.57)	(19.9)	(26.59)	(7.52)	(8.17)	(8.13)	(26.80)	(44.55)
Average Z_{eu}, m	119.1	99.9	91.0	80.2	70.3	63.4	54.4	39.8	26.1	77.1	53.2	44.0	31.5	16.9
	(12.2)	(15.4)	(11.8)	(12.6)	(11.9)	(9.3)	(8.2)	(8.0)	(4.5)	(14.3)	(6.8)	(4.6)	(6.8)	(2.4)

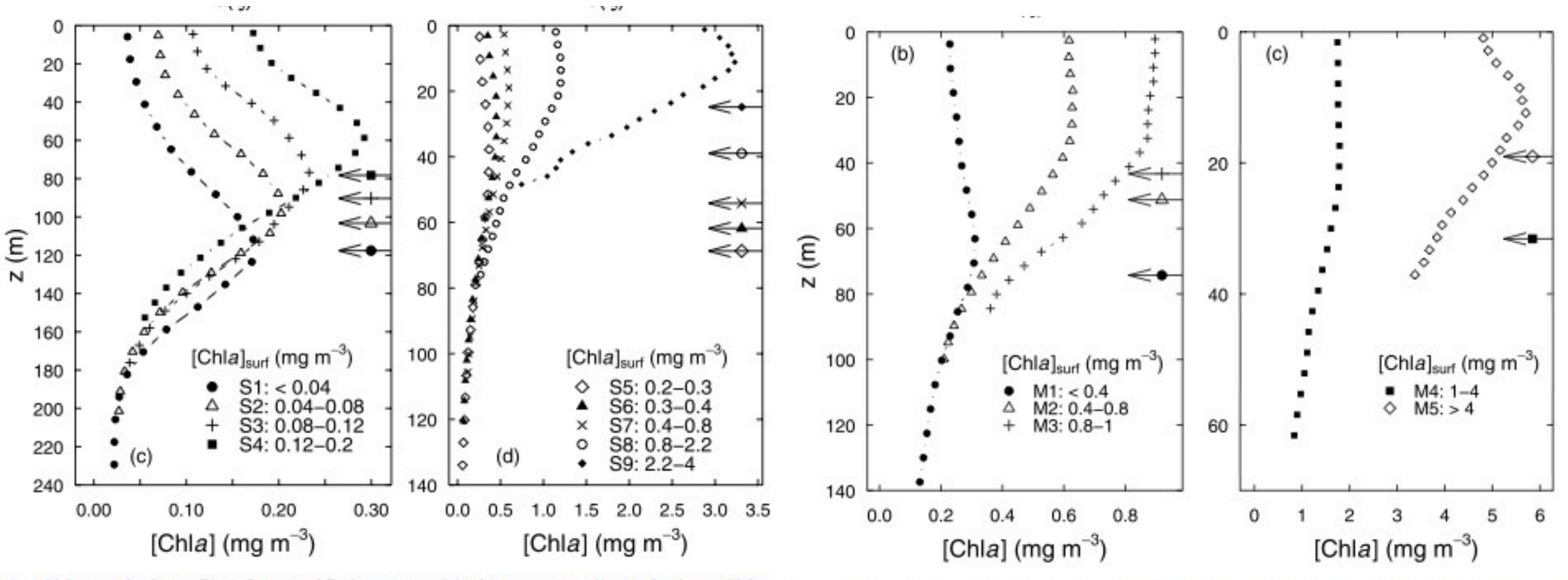
[a]These parameters are derived from the calculations involving the complete database 1 and are presented as averages and standard deviations (the latter shown in parentheses).
[b]Minimum value 0.015 mg m^{-3}.
[c]Maximum value 3.97 mg m^{-3}.
[d]Minimum value 0.047 mg m^{-3}.
[e]Maximum value 23.9 mg m^{-3}.

use range of Chl & estimate of mixed layer depth (MLD) to assign each pixel to 1 of 14 trophic categories

abundance – Chl as input

stratified water

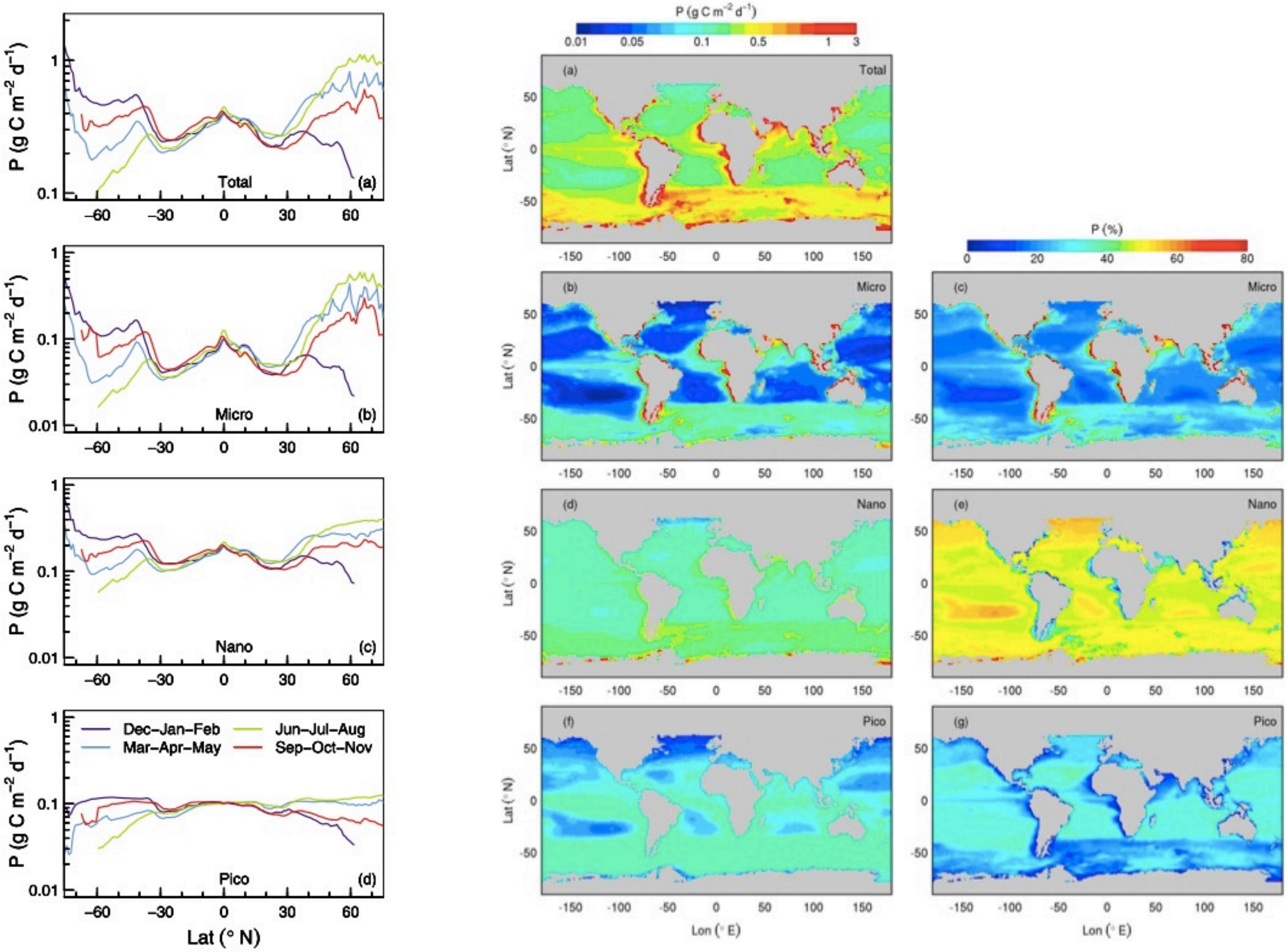
mixed water



empirically parameterized vertical profiles of PSCs for 9 stratified & 5 mixed water categories

used to infer column-integrated phytoplankton biomass, its vertical distribution, & community size composition

abundance – Chl as input



estimates of marine productivity

spectral – inversion modeling

inversion modeling as described in Lectures 21 & 22, except …

Application of an Ocean Color Algal Taxa Detection Model to Red Tides in the Southern Benguela

Collin S. Roesler[1], Stacey M. Etheridge[2], and Grant C. Pitcher[3]

[1]*Bigelow Laboratory for Ocean Sciences, PO Box 475, West Boothbay Harbor, ME 04575, USA;*
[2]*Department. of Marine Science, University of Connecticut, 1084 Shennecossett Rd., Groton, CT 06340, USA;*
[3]*Marine and Coastal Management, Private Bag X2, Rogge Bay 8012, Cape Town, South Africa*

… solve for multiple $a_{ph}(\lambda)$

GEOPHYSICAL RESEARCH LETTERS, VOL. 30, NO. 9, 1468, doi:10.1029/2002GL016185, 2003

Spectral beam attenuation coefficient retrieved from ocean color inversion

Collin S. Roesler
Bigelow Laboratory for Ocean Sciences, West Boothbay Harbor, Maine, USA

Emmanuel Boss
School of Marine Sciences, University of Maine, Orono, Maine, USA

… solve for slope of beam-c

spectral – $L_t(\lambda)$ as input

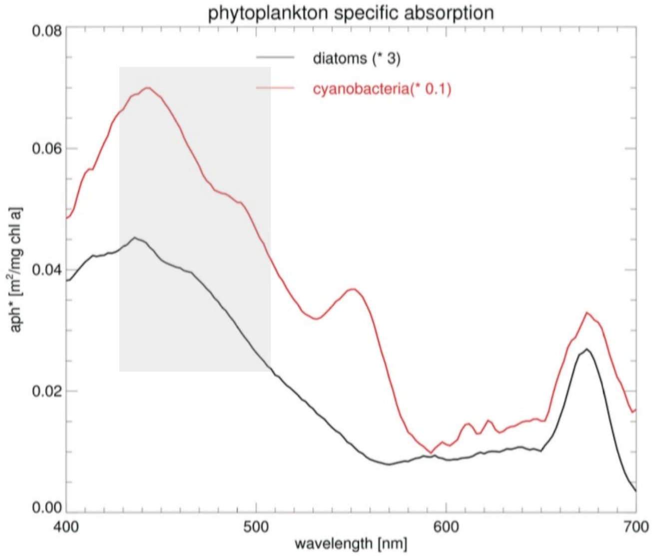
Biogeosciences, 6, 751–764, 2009
www.biogeosciences.net/6/751/2009/

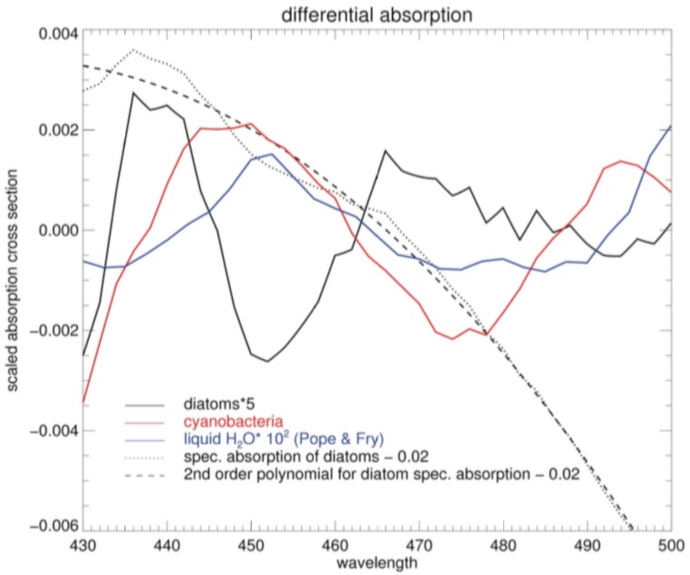
Biogeosciences

Quantitative observation of cyanobacteria and diatoms from space using PhytoDOAS on SCIAMACHY data

A. Bracher[1,2], M. Vountas[2], T. Dinter[2], J. P. Burrows[2,3], R. Röttgers[4], and I. Peeken[5,1]

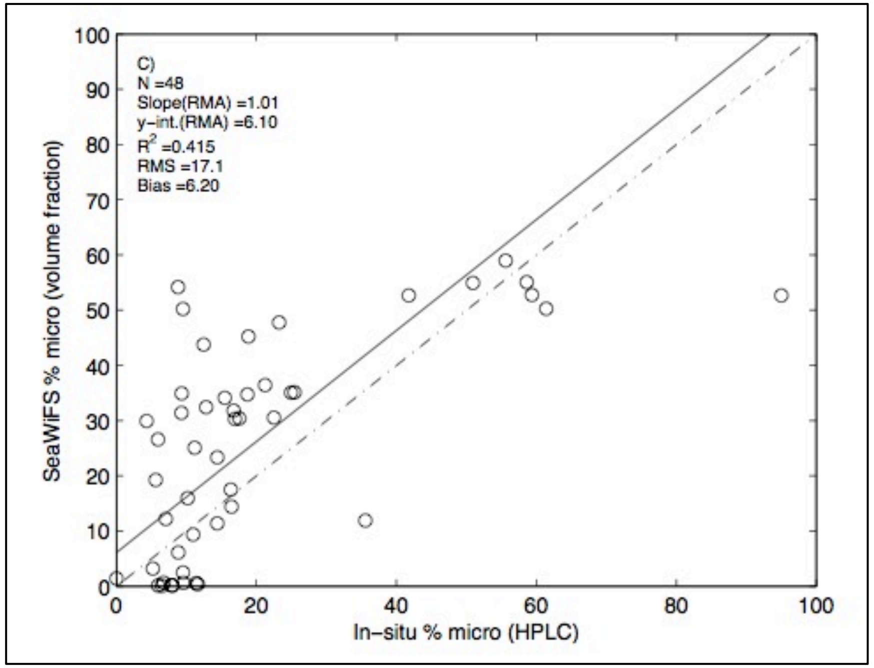
purpose: provide pixel-by-pixel estimates of cyanos & diatoms



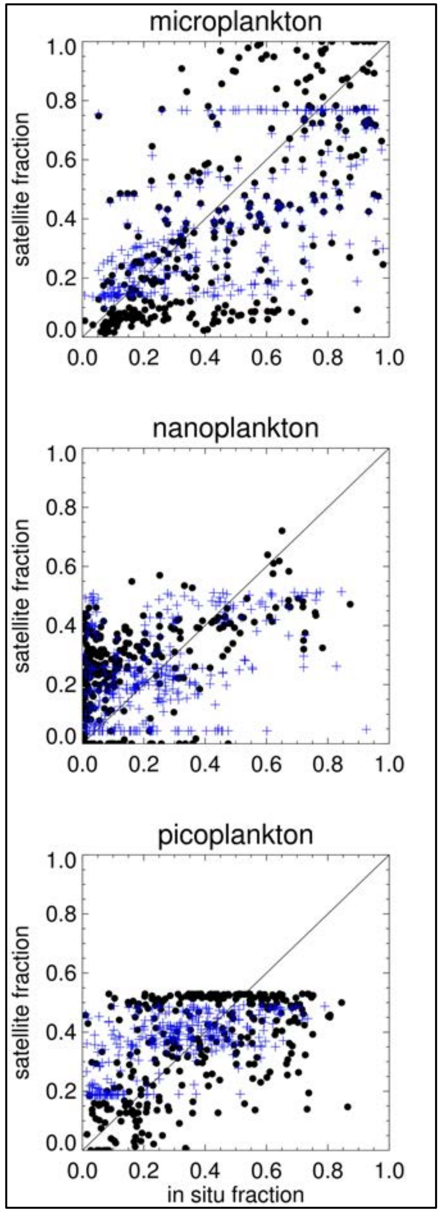


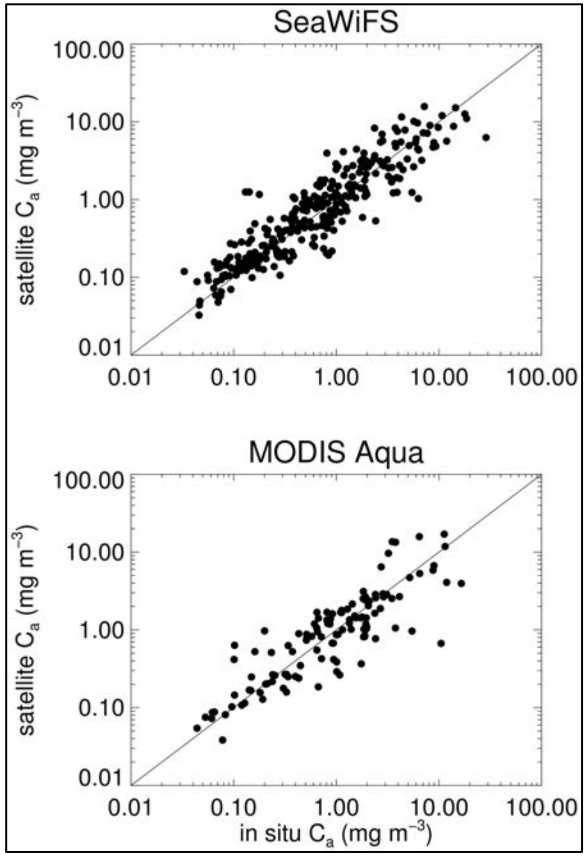
- uses differential optical absorption spectroscopy (DOAS)
- fits (non-linear optimization) differential absorptions
- exploits sharp spectral features
- requires hyperspectral data (applied to SCIAMACHY)

methods of validation: HPLC & scatter plots



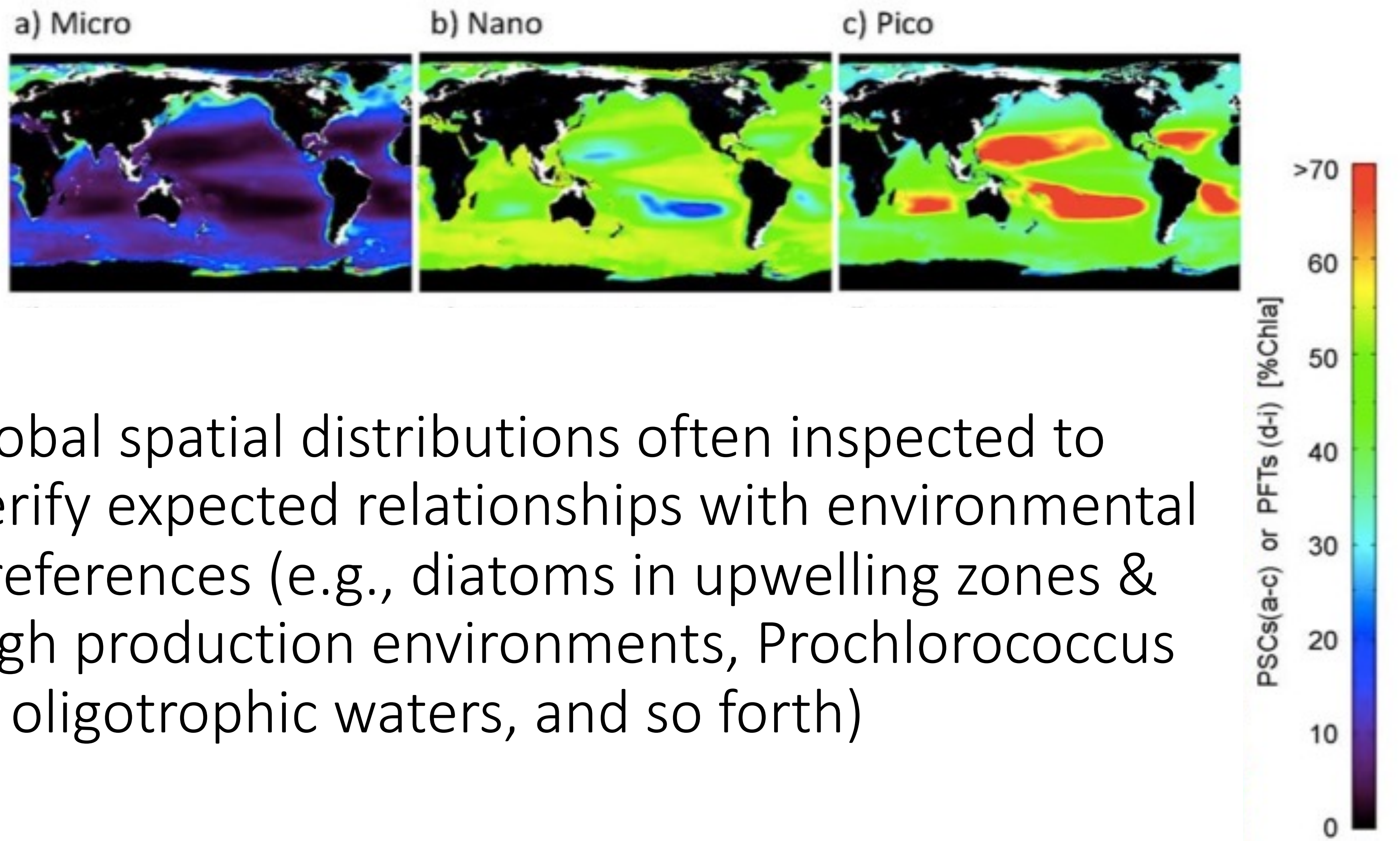
Kostadinov et al. 2010





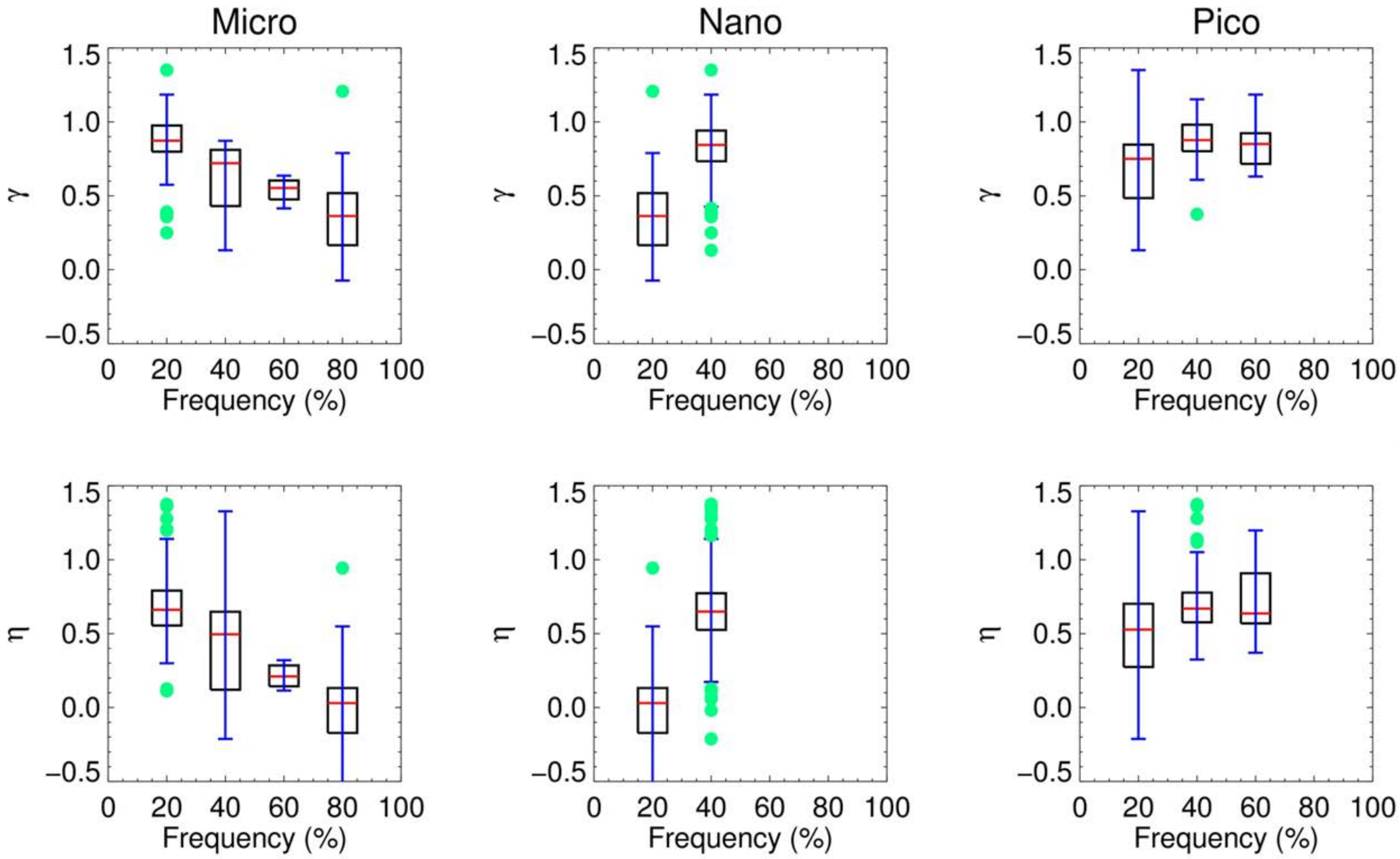
SeaWiFS global match-ups for 2 popular algorithms versus HPLC/DPA (province-tuned following Vichi et al. 2005)

other methods of validation: visual inspection



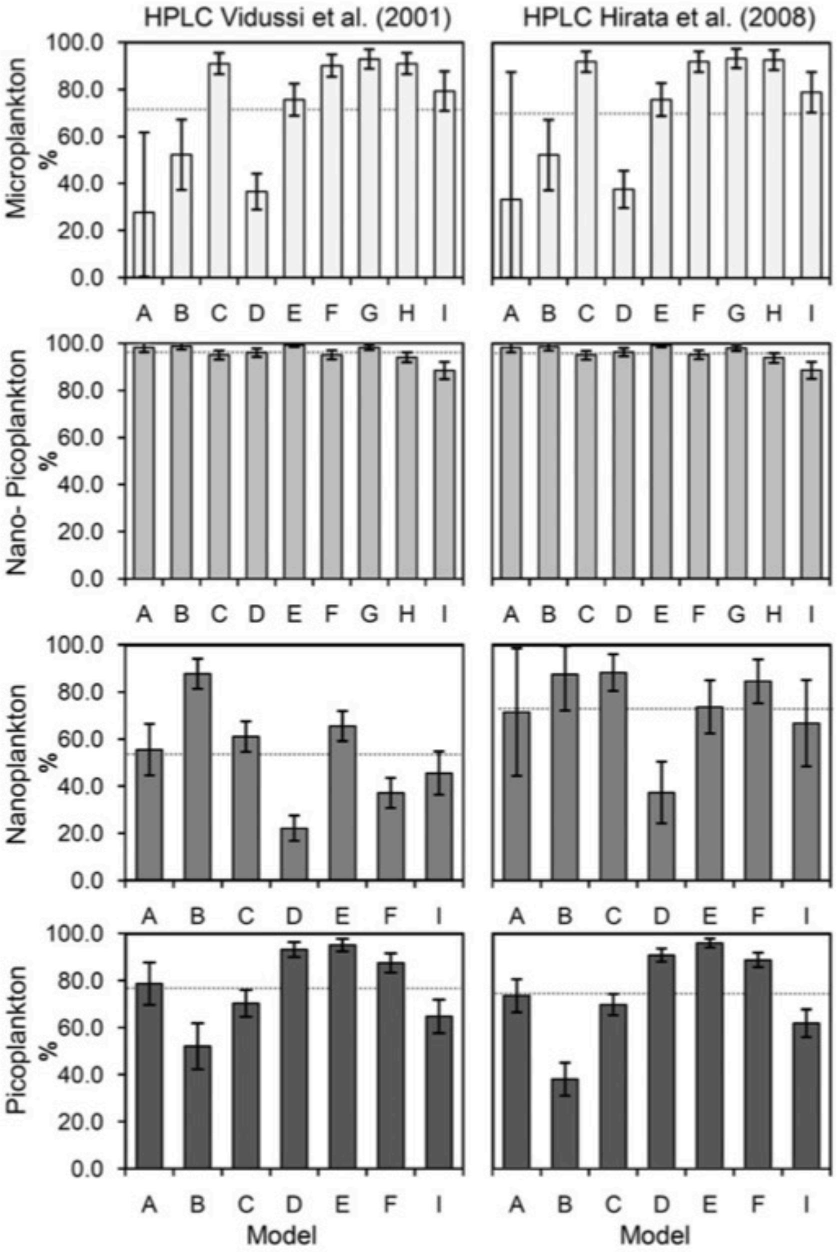
global spatial distributions often inspected to verify expected relationships with environmental preferences (e.g., diatoms in upwelling zones & high production environments, Prochlorococcus in oligotrophic waters, and so forth)

other methods of validation: spectral slopes



Werdell et al. 2013, Methods in Oceanography

other methods of validation: algorithm intercomparisons



Brewin et al. 2010