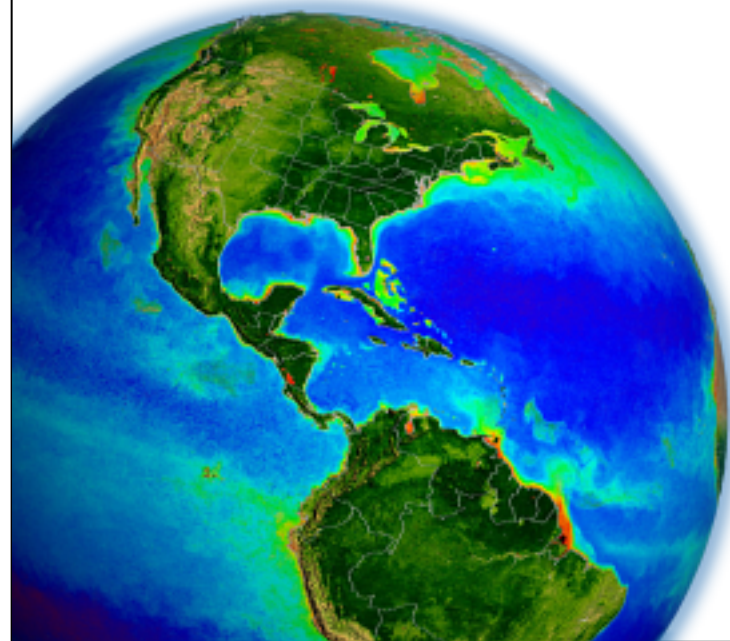


Estimating phytoplankton functional types & particle size classes from satellite ocean color

Jeremy Werdell

NASA Goddard Space Flight Center

UMaine Ocean Optics Summer Course
6 – 31 July 2015



QUESTIONNAIRE

Despite comprising < 1% of plant/algal biomass on Earth ...

(1) Do you like to breathe?

phytoplankton produce 50-70% of the oxygen we breath

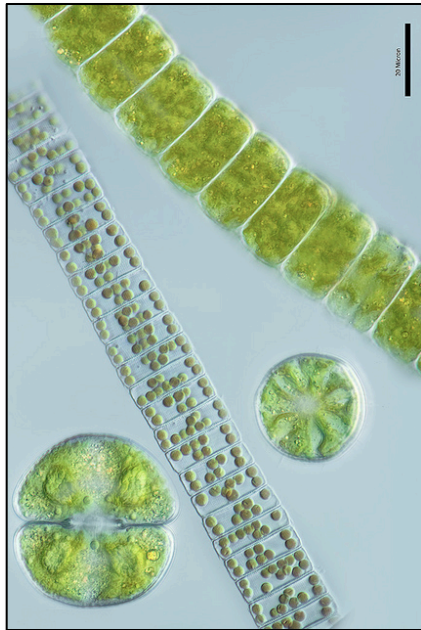
(2) Do you like to eat?

phytoplankton represent the first link in the marine food web & play key role in the ecology of the ecosystem

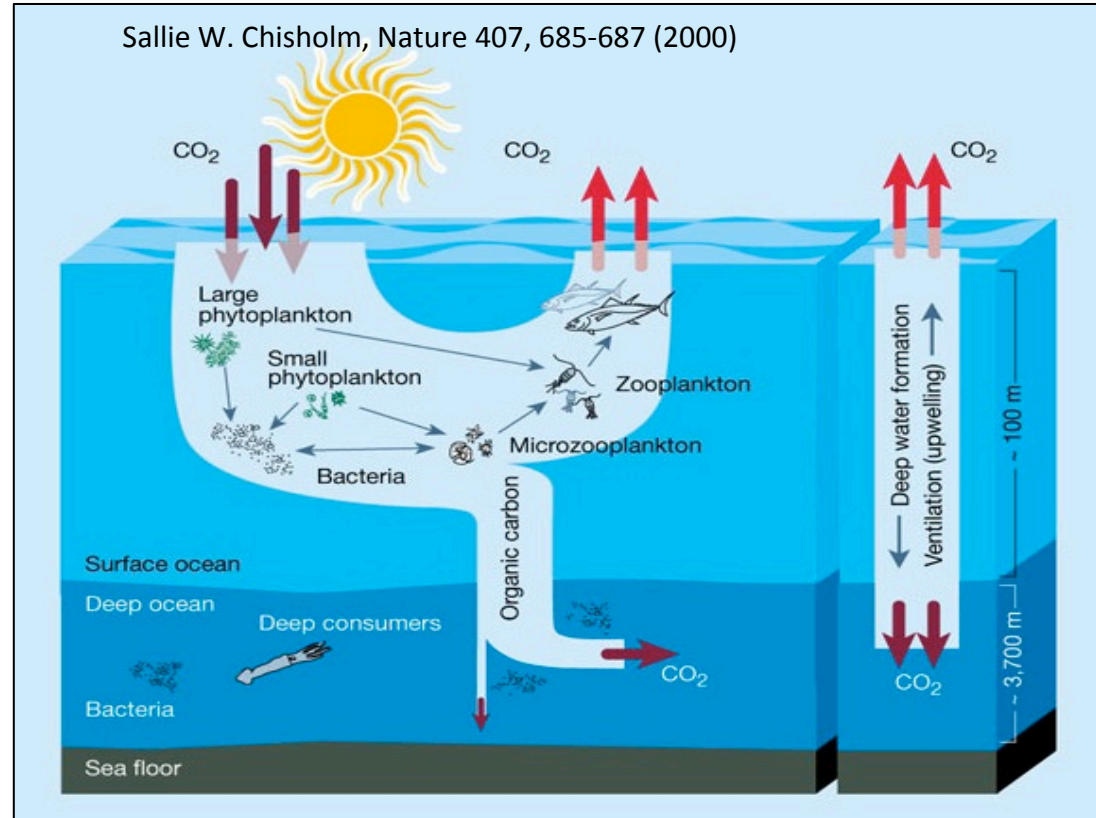
why phytoplankton? fun fact #2

phytoplankton fix* 100M tons of carbon / day
= 40B tons carbon / year (~40 Pg C each year)

> 99% of organic carbon resides in marine sediments



* fixing carbon is the process of converting CO_2 to organic matter



Pre-Aerosols, Clouds, and ocean Ecosystems (PACE) mission

Pre-Aerosol, Clouds, and ocean Ecosystem (PACE) Mission Science Definition Team Report

b.1. Threshold Ocean Science Questions

The threshold ocean science questions (SQ) addressed by the OCI option are listed below. The SQ are addressed by the ocean science instrument (OCI) and the mission requirements, as specified in Appendices I and II of this summary.

SQ-1: What are the standing stocks, compositions, and productivity of ocean ecosystems? How and why are they changing?

SQ-2: How and why are ocean biogeochemical cycles changing? How do they influence the Earth system?

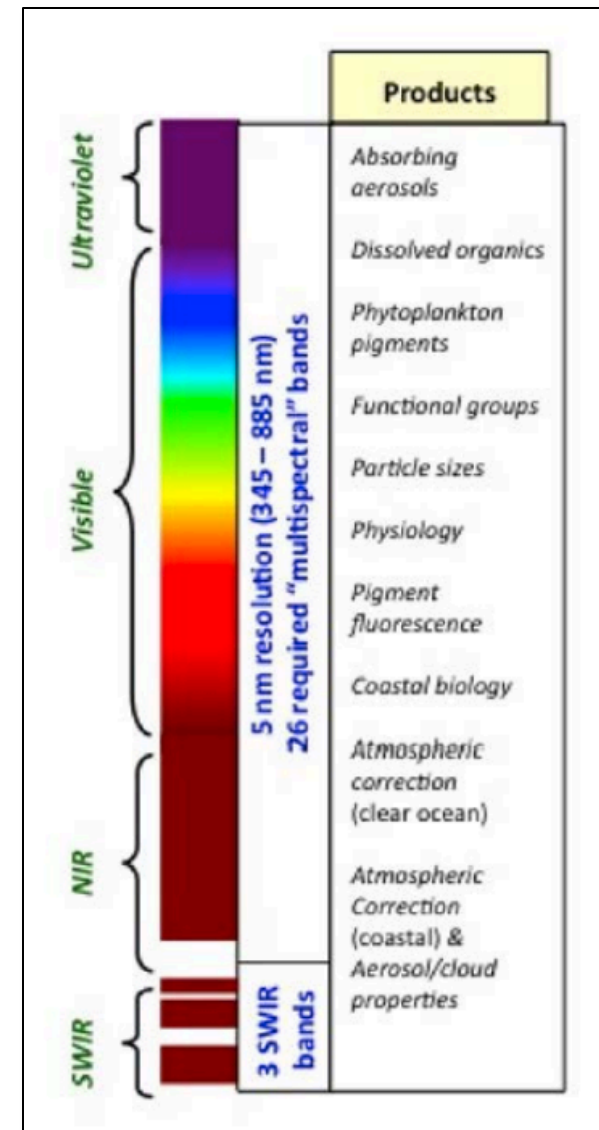
SQ-3: What are the material exchanges between land and ocean? How do they influence coastal ecosystems and biogeochemistry? How are they changing?

SQ-4: How do aerosols influence ocean ecosystems and biogeochemical cycles? How do ocean biological and photochemical processes affect the atmosphere?

SQ-5: How do physical ocean processes affect ocean ecosystems and biogeochemistry? How do ocean biological processes influence ocean physics?

SQ-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?

SQ-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?



summary & progress

NASA is invested in seeing phytoplankton community composition studied from space (satellites & 10+ years of OB&B investment into research & algorithm development)

the GSFC Ocean Biology Processing Group (OBPG) has begun preparing to support this:

- SeaBASS (data archive) support for *in situ* measurements
- algorithm implementation into l2gen/SeaDAS
- match-up system support for algorithm validation

much work remains to be done & challenges abound



www.archives.gov

terminology

PSC – particle size class

micro: > 20 μm

nano: 2 to 20 μm

pico: < 2 μm

← can describe either
phytoplankton or particles

PFT – phytoplankton functional type

“function” can mean many things (see Lecture 4 from week 1)

often class/genus-ish levels – diatom vs. dinoflagellate vs. cyano, etc.
sometimes functions like “nitrogen fixers” or “calcifiers”

perspective

the faithful & the skeptical surround us

this is pushing the limits of existing satellite instruments

many methods have been proposed, most fall into 2 classes

spatially, temporally diverse validation data are, um, ...

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

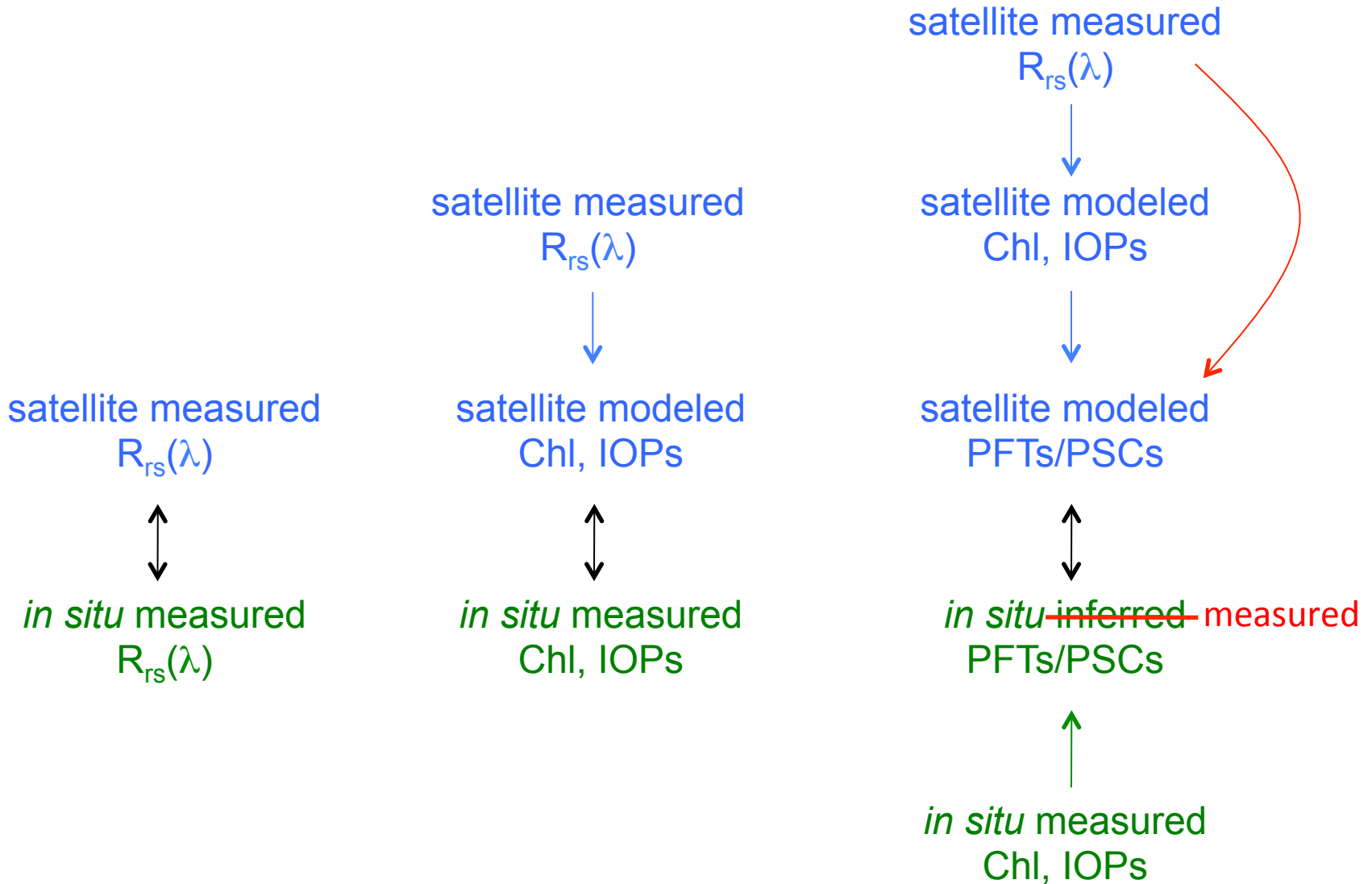
HUGE science driver for PACE (Pre-Aerosols, Clouds, and ocean Ecosystems)

this presentation will walk through methods & issues

why will it be more challenging to measure & validate PFTs than other ocean color products?

- (1) the (increased) degrees of separation between the satellite & *in situ* measurements
- (2) the (increased) number of satellite methods to model phytoplankton community composition
- (3) the (increased) number of *in situ* methods to infer phytoplankton community composition

degrees of separation in data products



outline

diverse bio-optical methods to estimate PSCs/PFTs exist

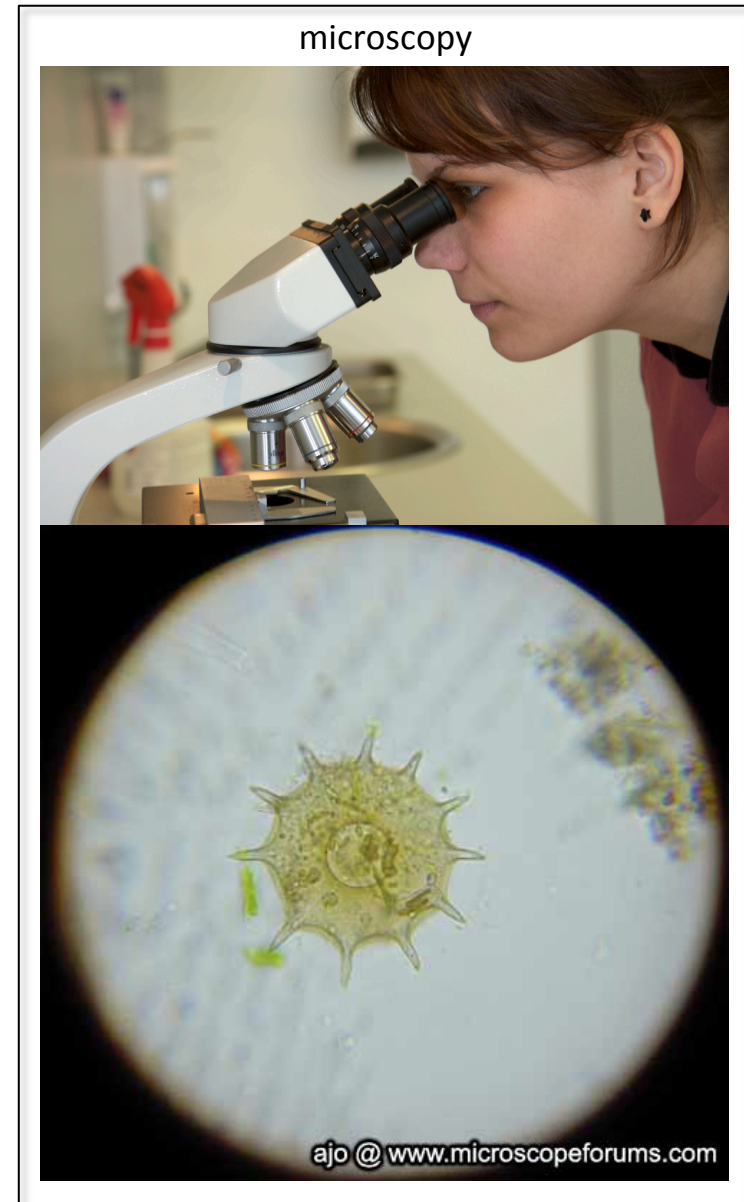
their sensitivities remain unexplored

most folks use proxy data sets for their validation

measuring PSCs & PFTs in the field

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

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



phytoplankton accessory pigments

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

DPA = Diagnostic
Pigment Analysis

Francesca Vidussi¹, Hervé Claustre¹, Beniamino B. Manca², Anna Luchetta³,
and Jean-Claude Marty¹

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. Higgins², S. W. Wright³

¹University Chemical Laboratory, Lensfield Rd, Cambridge CB2 1EW, United Kingdom

²CSIRO Division of Oceanography, PO Box 1538, Hobart, Tasmania 7001, Australia

³Australian Antarctic Division, Channel Highway, Kingston, Tasmania 7050, Australia

phytoplankton accessory pigments

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.

<u>Abbreviation</u>	<u>Name</u>	<u>Taxonomic Significance</u>	<u>Size</u>
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)

$DP = \text{Fuco} + \text{Perid} + \text{Hex-fuco} + \text{But-fuco} + \text{Allo} + \text{TChl-b} + \text{Zea}$

$\text{micro} = (\text{Fuco} + \text{Perid}) / DP$

$\text{nano} = (\text{Hex-fuco} + \text{But-fuco} + \text{Allo}) / DP$

$\text{pico} = (\text{TChl-b} + \text{Zea}) / DP$

Modifications by Uitz et al. (2006)

$DP_w = 1.41 \text{ Fuco} + 1.41 \text{ Perid} + 1.27 \text{ Hex-fuco} + 0.35 \text{ But-fuco} + 0.60 \text{ Allo} + 1.01 \text{ TChl-b} + 0.86 \text{ Zea}$

$f_{\text{micro}} = (1.41 \text{ Fuco} + 1.41 \text{ Perid}) / DP_w$

$f_{\text{nano}} = (1.27 \text{ Hex-fuco} + 0.35 \text{ But-fuco} + 0.60 \text{ Allo}) / DP_w$

$f_{\text{pico}} = (1.01 \text{ TChl-b} + 0.86 \text{ Zea}) / DP_w$

$\text{micro-Chl-a} = f_{\text{micro}} \text{ Chl-a}$

$\text{nano-Chl-a} = f_{\text{nano}} \text{ Chl-a}$

$\text{pico-Chl-a} = f_{\text{pico}} \text{ Chl-a}$

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

outline

diverse bio-optical methods to estimate PSCs/PFTs exist

their sensitivities remain unexplored

most folks use proxy data sets for their validation

methods

two flavors of algorithms:

abundance

- exploit observed relationships between the trophic status of the environment & the type of phytoplankton expected to be present
- assign empirically-derived thresholds on [chl], $b_b(\lambda)$, $a_{ph}(\lambda)$, etc.

spectral

- exploit variations realized in the spectral shape of $R_{rs}(\lambda)$ with varying community structure
- use unique optical signatures of specific PFTs or PSCs to distinguish between groups

varied inputs to the algorithms:

- $R_{rs}(\lambda)$, Chl, $b_{bp}(\lambda)$, $a(\lambda)$, $a_{ph}(\lambda)$, combinations of these

outline

model input

satellite-derived [chl]

satellite-derived IOPs

$a(\lambda)$
Ciotti (2006)
Devred (2006)
Hirata (2008)

$b_b(\lambda) + a(\lambda)$
Aiken (2007)

$b_b(\lambda)$
Kostadinov (2010)

Uitz (2006)
Hirata (2011)

data products

[accessory pigments]

PSC (size classes:
pico,nano,micro)

PFT (taxonomic
community)

model input

Pan (2010)

Mouw (2010)

Roesler (2004)
Westberry (2005)

Brown (1994)
Subramaniam (2002)
Sathyendranath (2004)
Alvain (2005, 2008)

satellite-measured
radiances & -derived IOPS

satellite-measured
radiances

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

satellite-derived [chl]

satellite-derived IOPs

$a(\lambda)$
Ciotti (2006)
Devred (2006)
Hirata (2008)

$b_b(\lambda) + a(\lambda)$
Aiken (2007)

$b_b(\lambda)$
Kostadinov (2010)

Uitz (2006)
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data products

[accessory pigments]

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Subramaniam (2002)
Sathyendranath (2004)
Alvain (2005, 2008)

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
© Author(s) 2011. CC Attribution 3.0 License.

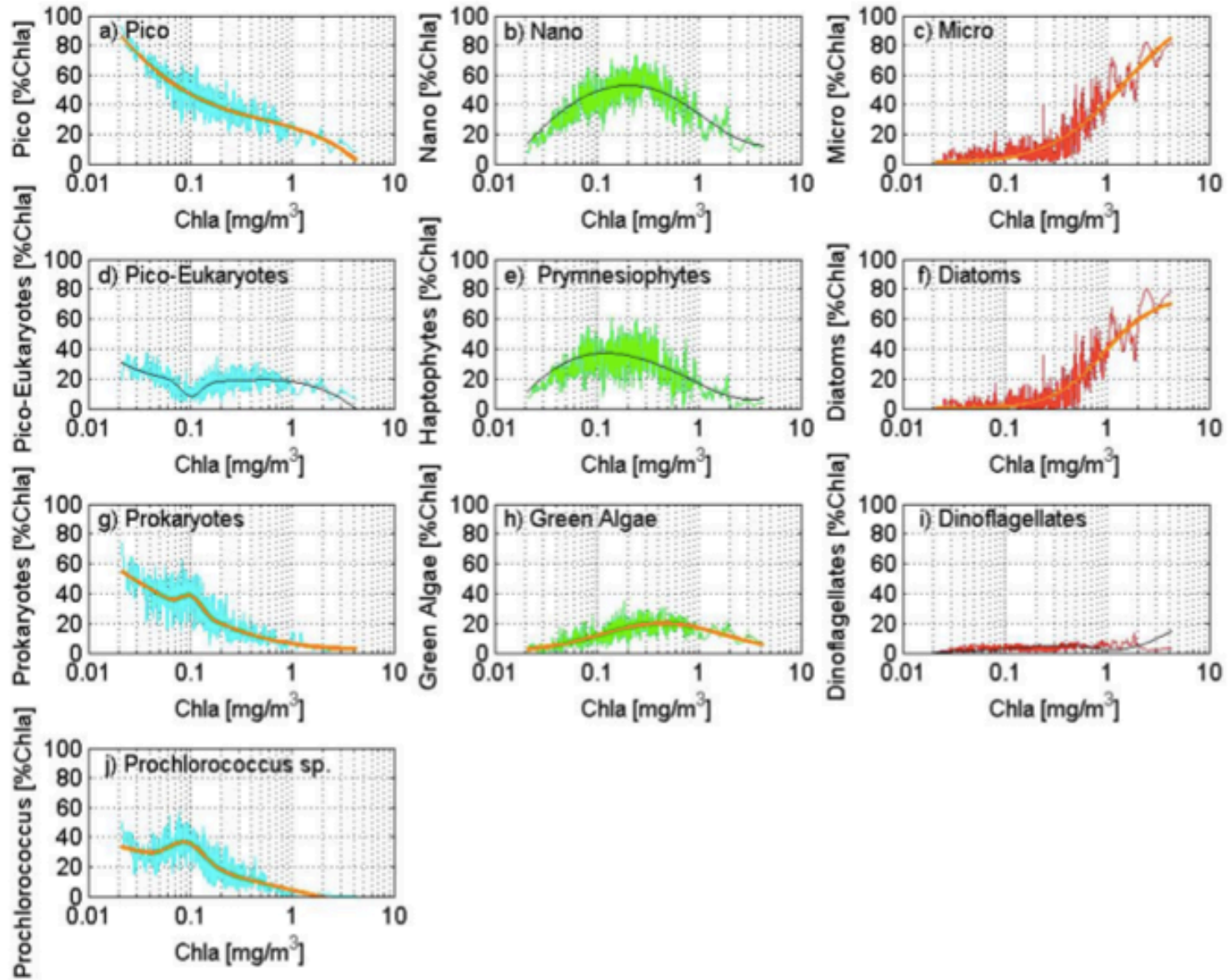


Synoptic relationships between surface Chlorophyll-*a* and diagnostic pigments specific to phytoplankton functional types

T. Hirata^{1,2,*,}, N. J. Hardman-Mountford^{1,2}, R. J. W. Brewin^{1,3}, J. Aiken¹, R. Barlow^{4,5}, K. Suzuki⁶, T. Isada⁷, E. Howell⁸, T. Hashioka^{9,10}, M. Noguchi-Aita^{7,10}, and Y. Yamanaka^{6,9,10}**

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

abundance – Chl as input



abundance – Chl as input

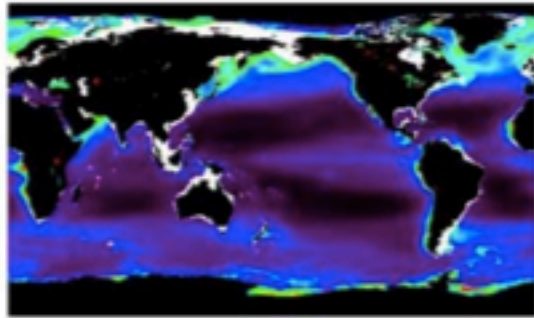
Table 2. Equations to estimate fractions [0.0–1.0] of PSCs (Micro-, Nano- and Picoplankton) and PFTs (other). Set PFT fraction to 1.0 if >1.0, and 0 if <0. To get % Chl-*a*, multiply 100 to the fractions derived.

PSCs/PFTs	Formula	a ₀	a ₁	a ₂	a ₃	a ₄	a ₅	a ₆
Microplankton	$[a_0 + \exp(a_1 x + a_2)]^{-1}$	0.9117	-2.7330	0.4003				
Diatoms	$[a_0 + \exp(a_1 x + a_2)]^{-1}$	1.3272	-3.9828	0.1953	-	-	-	-
Dinoflagellates	(= Micro-Diatoms)	-	-	-	-	-	-	-
Nanoplankton	(= 1-Micro-Pico)	-	-	-	-	-	-	-
Green Algae	$(a_0/y) \exp[a_1(x + a_2)^2]$	0.2490	-1.2621	-0.5523	-	-	-	-
Prymnesiophytes (Haptophytes)	(\simeq Nano-Green Algae)	-	-	-	-	-	-	-
Picoplankton	$-[a_0 + \exp(a_1 x + a_2)]^{-1} + a_3 x + a_4$	0.1529	1.0306	-1.5576	-1.8597	2.9954	-	-
Prokaryotes	$(a_0/a_1/y) \exp[a_2(x + a_3)^2/a_1^2]$ $+ a_4 x^2 + a_5 x + a_6$	0.0067	0.6154	-19.5190	0.9643	0.1027	-0.1189	0.0626
Pico-eukaryotes <i>Prochlorococcus sp.</i>	(= Pico-Prokaryotes)	-	-	-	-	-	-	-
	$(a_0/a_1/y) \exp[a_3(x + a_4)^2/a_1^2]$ $+ a_4 x^2 + a_5 x + a_6$	0.0099	0.6808	-8.6276	0.9668	0.0074	-0.1621	0.0436

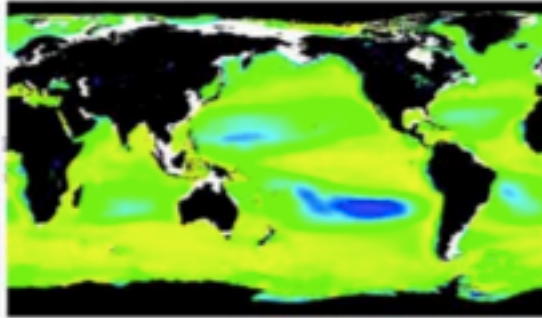
$x = \log_{10}(\text{Chl-}a)$; $y = \text{Chl-}a$

abundance – Chl as input

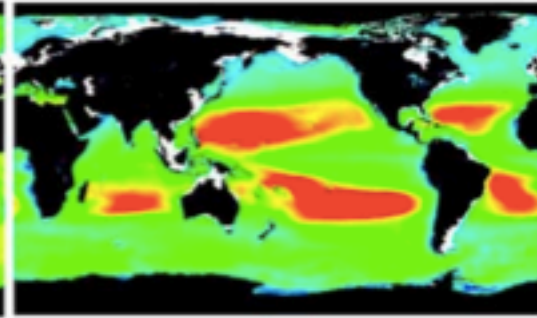
a) Micro



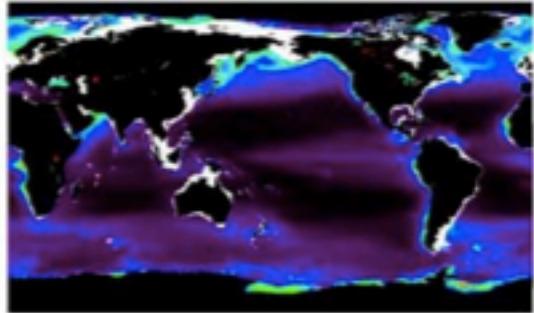
b) Nano



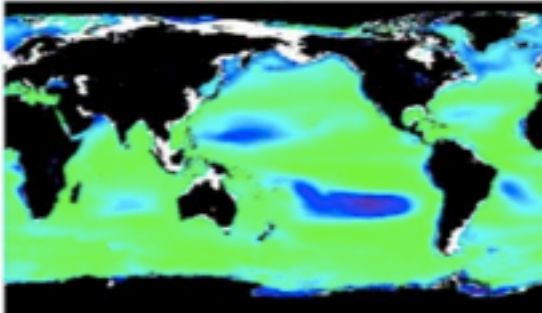
c) Pico



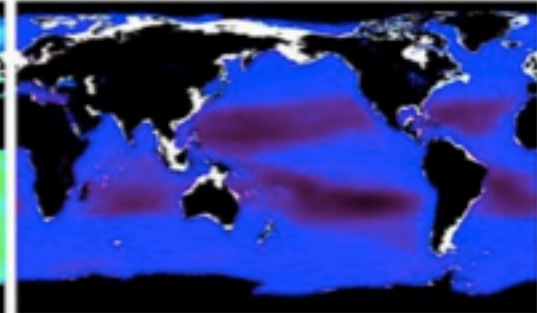
d) Diatoms



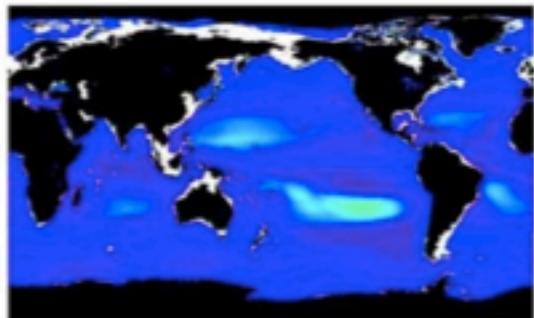
e) Prymnesiophytes



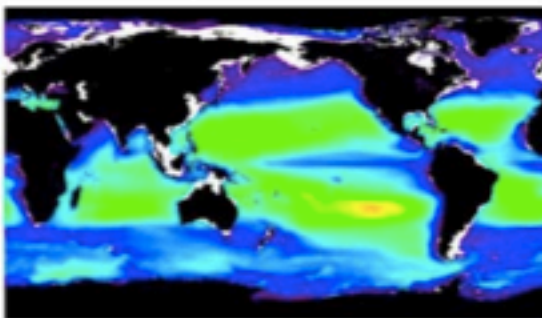
f) Green Algae



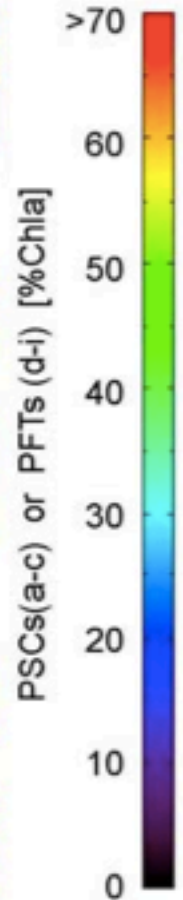
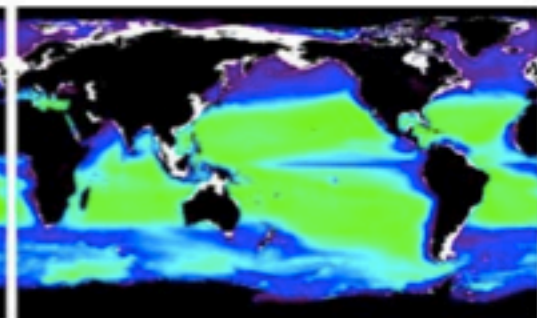
g) Pico-Eukaryotes



h) Prokaryotes



i) *Prochlorococcus* sp.



abundance – Chl as input

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



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. Hooker²

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, $[Chl]_{surf}$, and the Associated Parameters^a

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

^aThese parameters are derived from the calculations involving the complete database 1 and are presented as averages and standard deviations (the latter shown in parentheses).

^bMinimum value 0.015 $mg\ m^{-3}$.

^cMaximum value 3.97 $mg\ m^{-3}$.

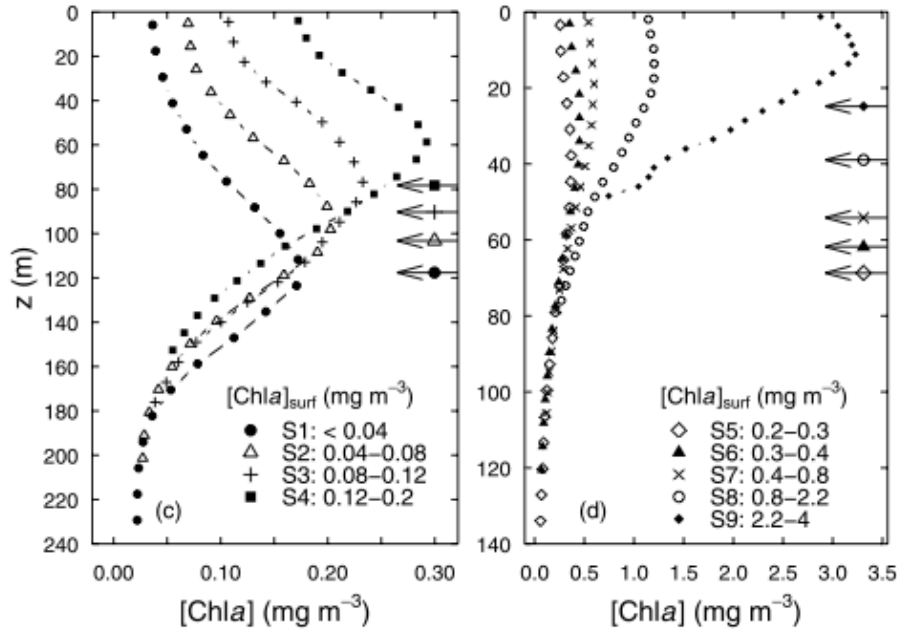
^dMinimum value 0.047 $mg\ m^{-3}$.

^eMaximum value 23.9 $mg\ m^{-3}$.

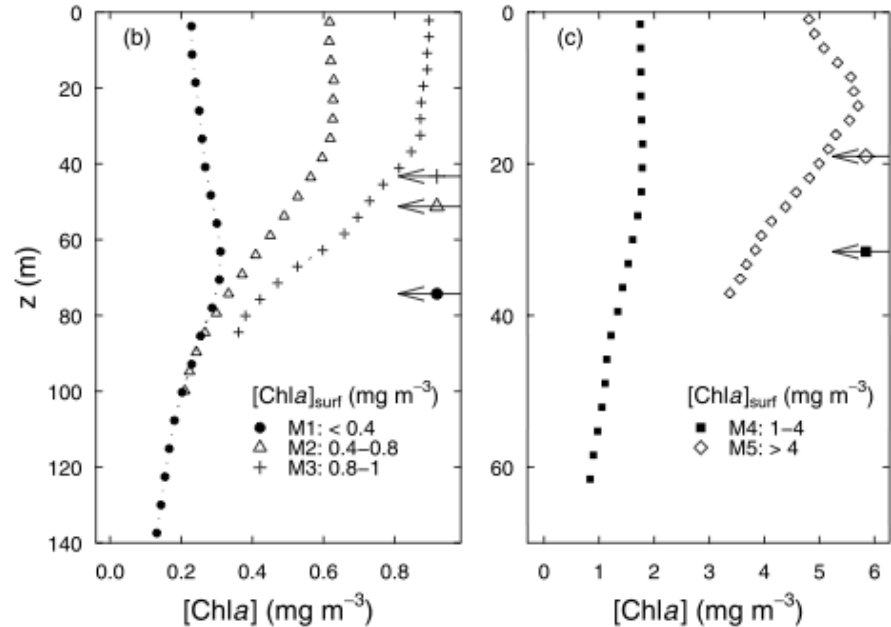
use range of Chl & estimate of mixed layer depth (MLD) to assign each pixel to 1 of 14 trophic categories

abundance – Chl as input

stratified water



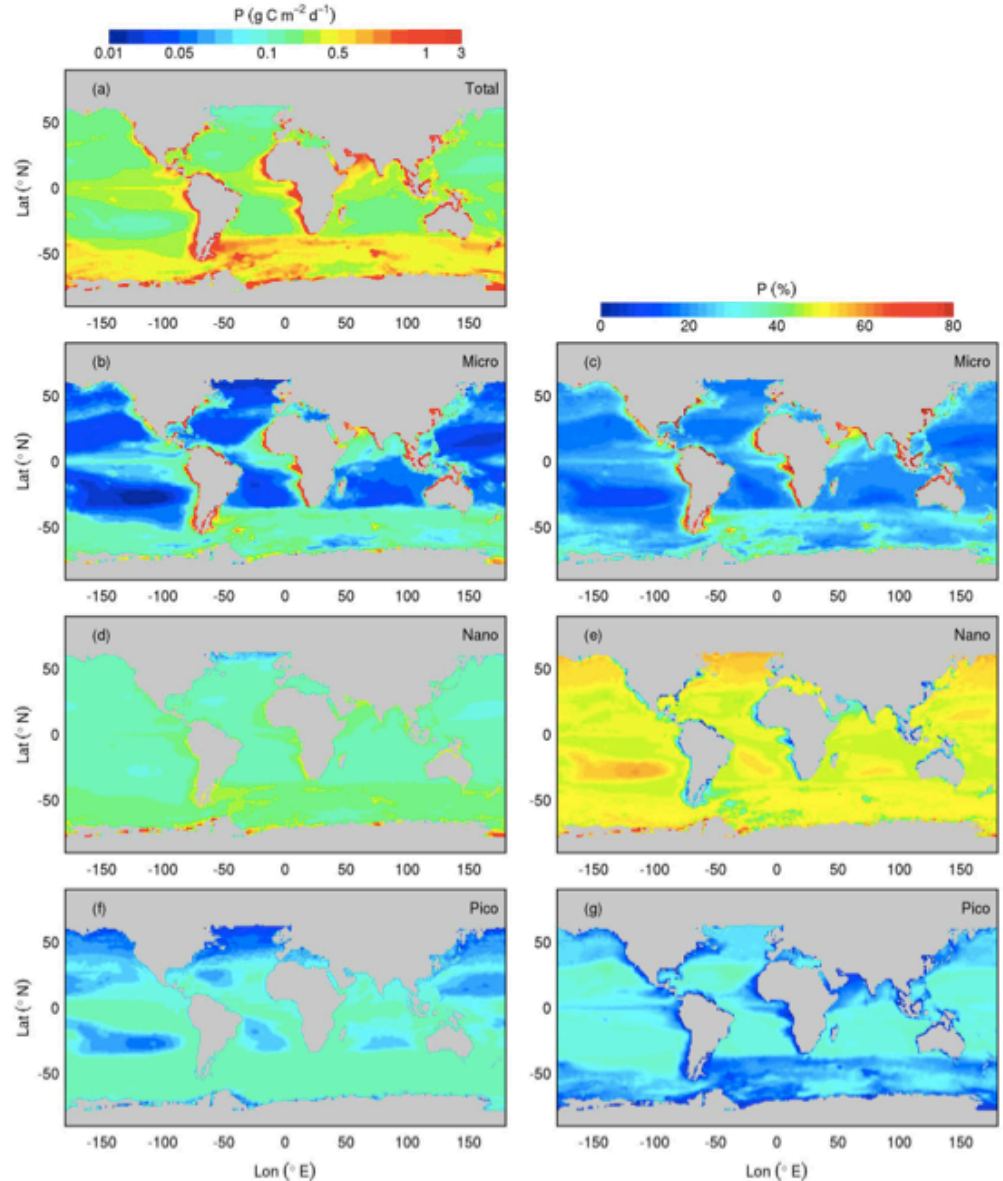
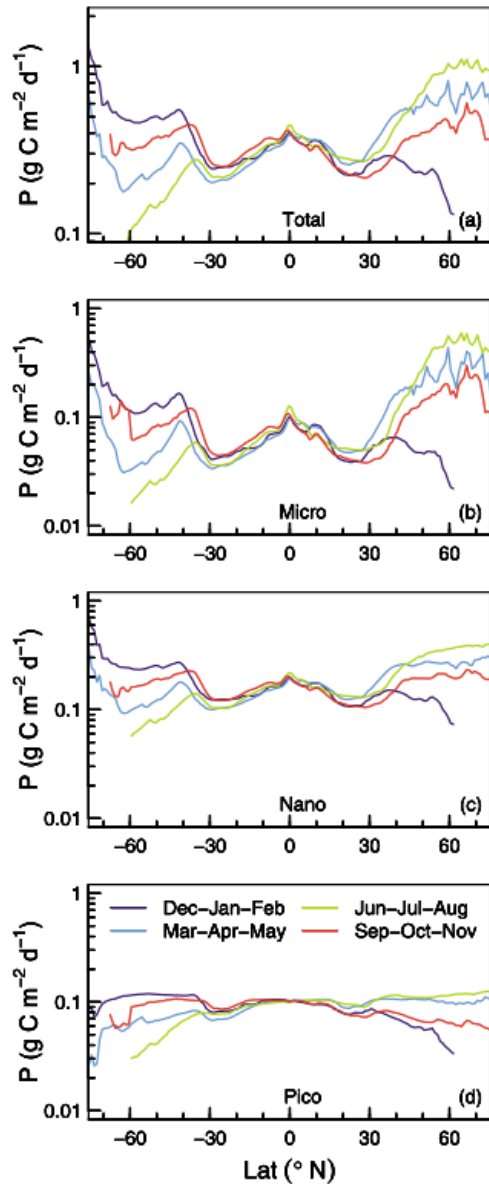
mixed water



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

outline

model input

satellite-derived [chl]

satellite-derived IOPs

$a(\lambda)$
Ciotti (2006)
Devred (2006)
Hirata (2008)

Uitz (2006)
Hirata (2011)

$b_b(\lambda) + a(\lambda)$
Aiken (2007)

$b_b(\lambda)$
Kostadinov (2010)

data products

[accessory pigments]

PSC (size classes: pico,nano,micro)

PFT (taxonomic community)

model input

Pan (2010)

Mouw (2010)

Roesler (2004)
Westberry (2005)

Brown (1994)
Subramaniam (2002)
Sathyendranath (2004)
Alvain (2005, 2008)

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

assign a dominant PSC to each satellite pixel

abundance – IOPs as input

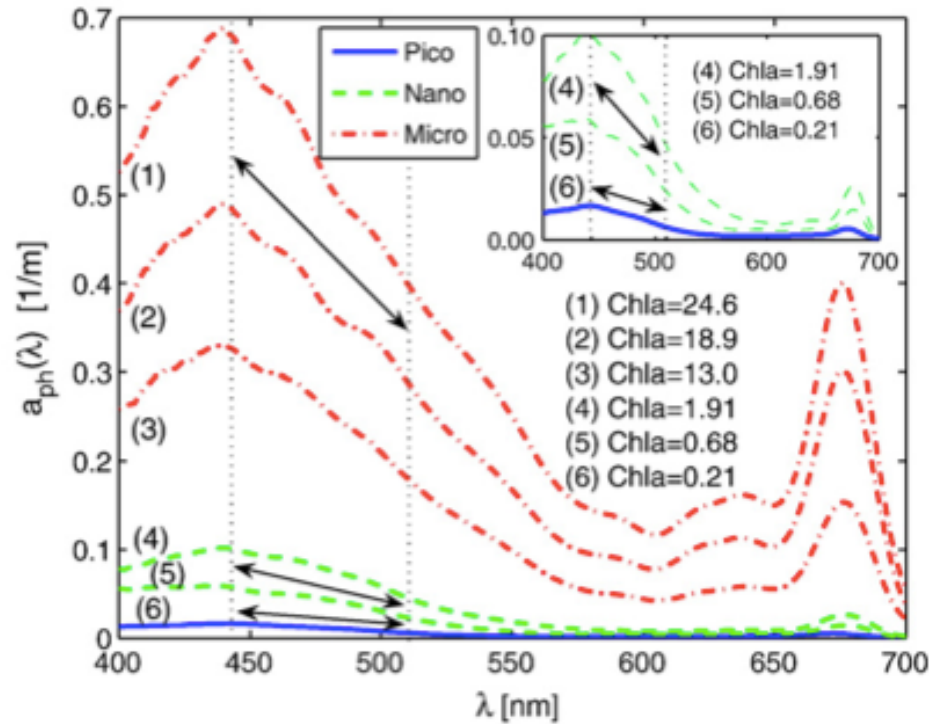
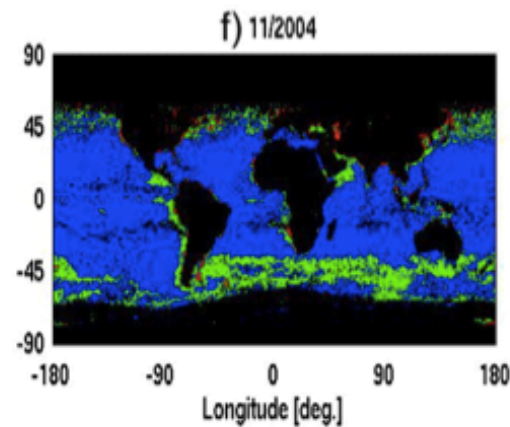
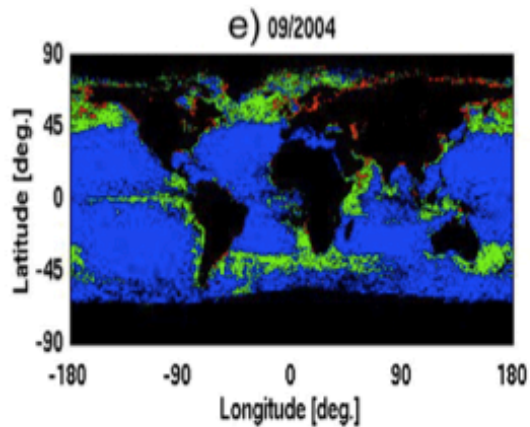
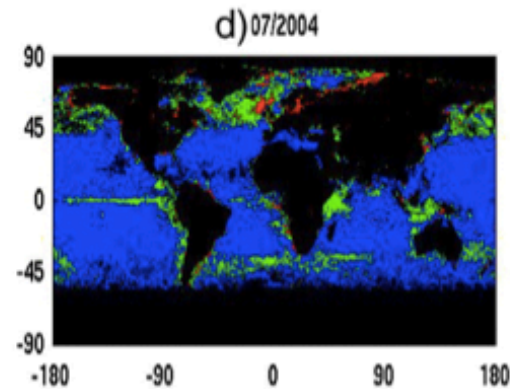
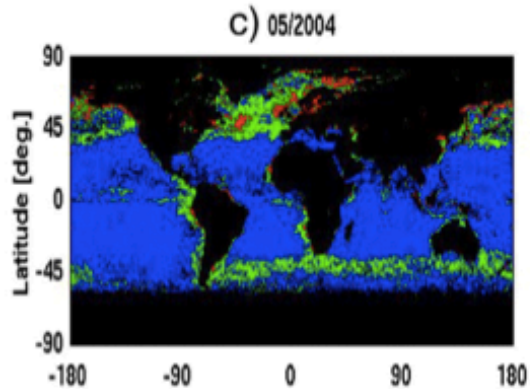
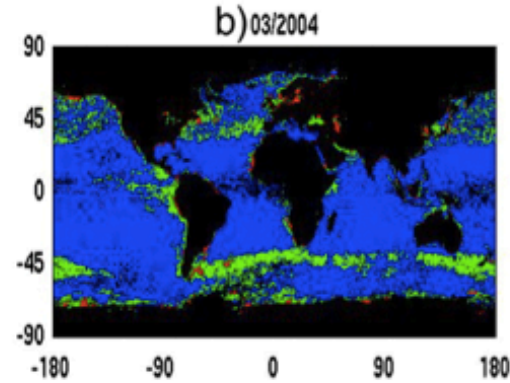
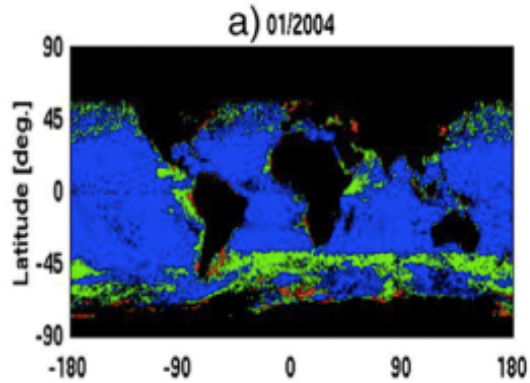


Fig. 1. Phytoplankton absorption spectra for a range of Chla (24.6, 18.9, 13.0, 1.91, 0.68, 0.21 mg m^{-3}) and taxonomic size classes (pico, nano and micro) with decreasing slope from high to low $a_{ph}(\lambda)$ and Chla; inset spectra of pico and nanoplankton at expanded range.

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

abundance – IOPs as input



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

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

nano otherwise

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

satellite-derived [chl]

satellite-derived IOPs

Uitz (2006)
Hirata (2011)

$a(\lambda)$
Ciotti (2006)
Devred (2006)
Hirata (2008)

$b_b(\lambda) + a(\lambda)$
Aiken (2007)

$b_b(\lambda)$
Kostadinov (2010)

data products

[accessory pigments]

PSC (size classes:
pico,nano,micro)

PFT (taxonomic
community)

model input

Pan (2010)

Mouw (2010)

Roesler (2004)
Westberry (2005)

Brown (1994)
Subramaniam (2002)
Sathyendranath (2004)
Alvain (2005, 2008)

satellite-measured
radiances & -derived IOPS

satellite-measured
radiances

spectral – $R_{rs}(\lambda)$ as input

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

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

spectral – $R_{rs}(\lambda)$ as input

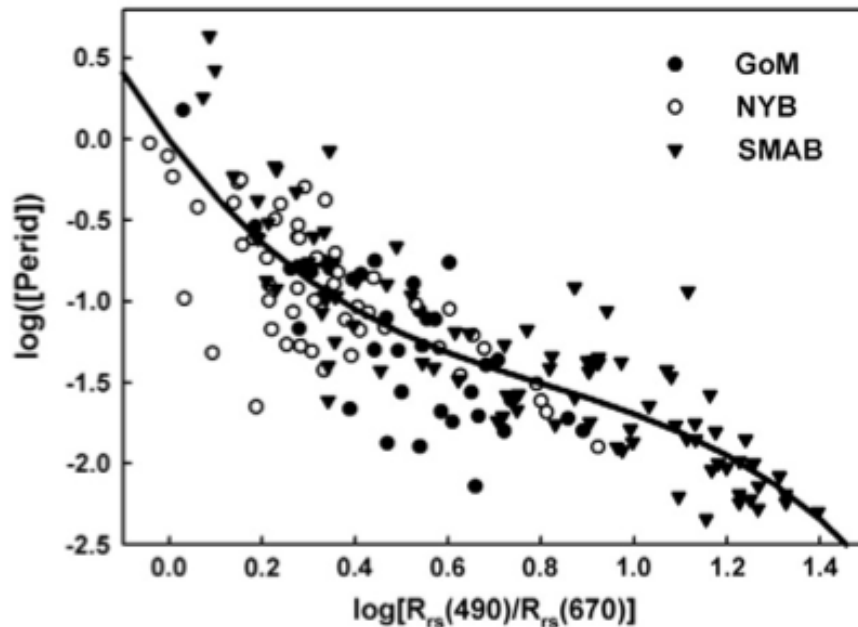


Fig. 4. Algorithm development for peridinin concentration ([Perid]). See Fig. 3 for detailed description.

Table 4

Derived coefficients for pigment algorithms from Eq. (1): $\log[\text{Pigment}] = A_0 + A_1X + A_2X^2 + A_3X^3$, where $X = \log[R_{rs}(\lambda_1)/R_{rs}(\lambda_2)] - 1.5\log(T_w)$ for Zea, but $X = \log[R_{rs}(\lambda_1)/R_{rs}(\lambda_2)]$ for other pigments. Total data points $N = 196$. A set of 2nd-order polynomial functions replaced the 3rd-order polynomial functions for Fuco due to their similar regression results and more reasonable performance.

Pigments	λ_1/λ_2	A_0	A_1	A_2	A_3	r^2	RMSE
<i>Group_A pigments</i>							
TChl_a	490/555	0.02534	-3.033	2.096	-1.607	0.86	0.244
	488/547	0.03664	-3.451	2.276	-1.096	0.83	0.261
	490/670	1.351	-2.427	0.9395	-0.2432	0.89	0.217
TChl_c	490/555	-0.7750	-3.071	0.7940	-1.559	0.81	0.302
	488/547	-0.7584	-3.511	0.4116	-0.4283	0.79	0.314
	490/670	0.4424	-2.291	1.190	-0.5307	0.82	0.293
Caro	490/555	-1.344	-2.604	3.050	-3.351	0.84	0.232
	488/547	-1.341	-2.952	3.802	-4.256	0.82	0.245
	490/670	-0.01909	-2.775	1.703	-0.5496	0.86	0.212
Fuco	490/555	-0.6334	-3.533	1.317	-	0.77	0.356
	488/547	-0.6208	-3.928	1.339	-	0.75	0.373
	490/670	0.6908	-2.053	0.2658	-	0.77	0.346
<i>Group_B pigments</i>							
TChl_b	490/555	-1.101	-1.993	0.9228	-7.980	0.70	0.294
	488/547	-1.097	-2.348	0.9633	-9.374	0.69	0.299
Allo	490/555	-1.402	-4.114	-0.9104	0.9988	0.72	0.384
	488/547	-1.401	-4.816	-1.264	5.838	0.71	0.391
	490/670	0.04234	-2.747	1.562	-0.8771	0.77	0.345
Dia	490/555	-1.001	-2.626	1.501	-3.736	0.74	0.310
	488/547	-0.9963	-3.113	1.635	-2.164	0.72	0.318
Perid	490/555	-1.416	-2.363	2.565	-4.186	0.64	0.352
	488/547	-1.401	-2.817	2.634	-2.396	0.62	0.365
	490/670	-0.01038	-3.807	3.612	-1.489	0.70	0.327
Lut	490/555	-2.196	-1.935	2.042	-3.601	0.53	0.314
	488/547	-2.188	-2.037	2.179	-10.16	0.53	0.313
Neo	490/555	-1.984	-1.790	1.610	-11.31	0.73	0.239
	488/547	-1.983	-2.151	2.134	-12.67	0.70	0.251
Viola	490/555	-1.950	-1.285	2.595	-14.65	0.67	0.273
	488/547	-1.947	-1.601	3.258	-17.31	0.63	0.285
<i>Group_C pigment</i>							
Zea	490/555	-11.58	-17.94	-11.02	-2.323	0.65	0.293
	488/547	-9.885	-14.84	-9.230	-1.998	0.64	0.296

outline

model input

satellite-derived [chl]

satellite-derived IOPs

$a(\lambda)$
Ciotti (2006)
Devred (2006)
Hirata (2008)

$b_b(\lambda) + a(\lambda)$
Aiken (2007)

$b_b(\lambda)$
Kostadinov (2010)

Uitz (2006)
Hirata (2011)

data products

[accessory pigments]

PSC (size classes: pico,nano,micro)

PFT (taxonomic community)

model input

satellite-measured radiances & -derived IOPS

satellite-measured radiances

Pan (2010)

Mouw (2010)

Roesler (2004)
Westberry (2005)

Brown (1994)
Subramaniam (2002)
Sathyendranath (2004)
Alvain (2005, 2008)



PERGAMON

Deep-Sea Research II 49 (2002) 107–121

DEEP-SEA RESEARCH
PART II

www.elsevier.com/locate/dsr2

Detecting *Trichodesmium* blooms in SeaWiFS imagery

Ajit Subramaniam^{a,*}, Christopher W. Brown^b, Raleigh R. Hood^c,
Edward J. Carpenter^d, Douglas G. Capone^a

3.4. Classification scheme

Based upon these empirical observations and model results, we propose the following classification scheme to identify the presence of *Trichodesmium* at moderate chlorophyll concentrations (0.5–3.0 mg/m³) in SeaWiFS imagery: A pixel was flagged as dominated by *Trichodesmium* if the following three criteria were satisfied:

1. $nLw(490) > 1.3 \text{ mW cm}^2/\mu\text{m/sr}$ and $nLw(490) > nLw(412), nLw(443), nLw(555)$
2. $nLw(510) > nLw443$
3. $0.4 < [nLw(490) - nLw(443)] / [nLw(490) - nLw(555)] < 0.6$

Criteria #1 and #2 represent absolute and relative magnitude thresholds, while criterion #3 depends on spectral shape. The threshold for $nLw(490)$ was employed because it was a

outline

model input

satellite-derived [chl]

satellite-derived IOPs

$a(\lambda)$
Ciotti (2006)
Devred (2006)
Hirata (2008)

$b_b(\lambda) + a(\lambda)$
Aiken (2007)

$b_b(\lambda)$
Kostadinov (2010)

Uitz (2006)
Hirata (2011)

data products

[accessory pigments]

PSC (size classes:
pico,nano,micro)

PFT (taxonomic
community)

model input

Pan (2010)

Mouw (2010)

Roesler (2004)
Westberry (2005)

Brown (1994)
Subramaniam (2002)
Sathyendranath (2004)
Alvain (2005, 2008)

satellite-measured
radiances & -derived IOPS

satellite-measured
radiances

spectral – $R_{rs}(\lambda)$ as input



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Deep-Sea Research I 52 (2005) 1989–2004

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

provide estimate of dominant PFT for each pixel

spectral – $R_{rs}(\lambda)$ as input

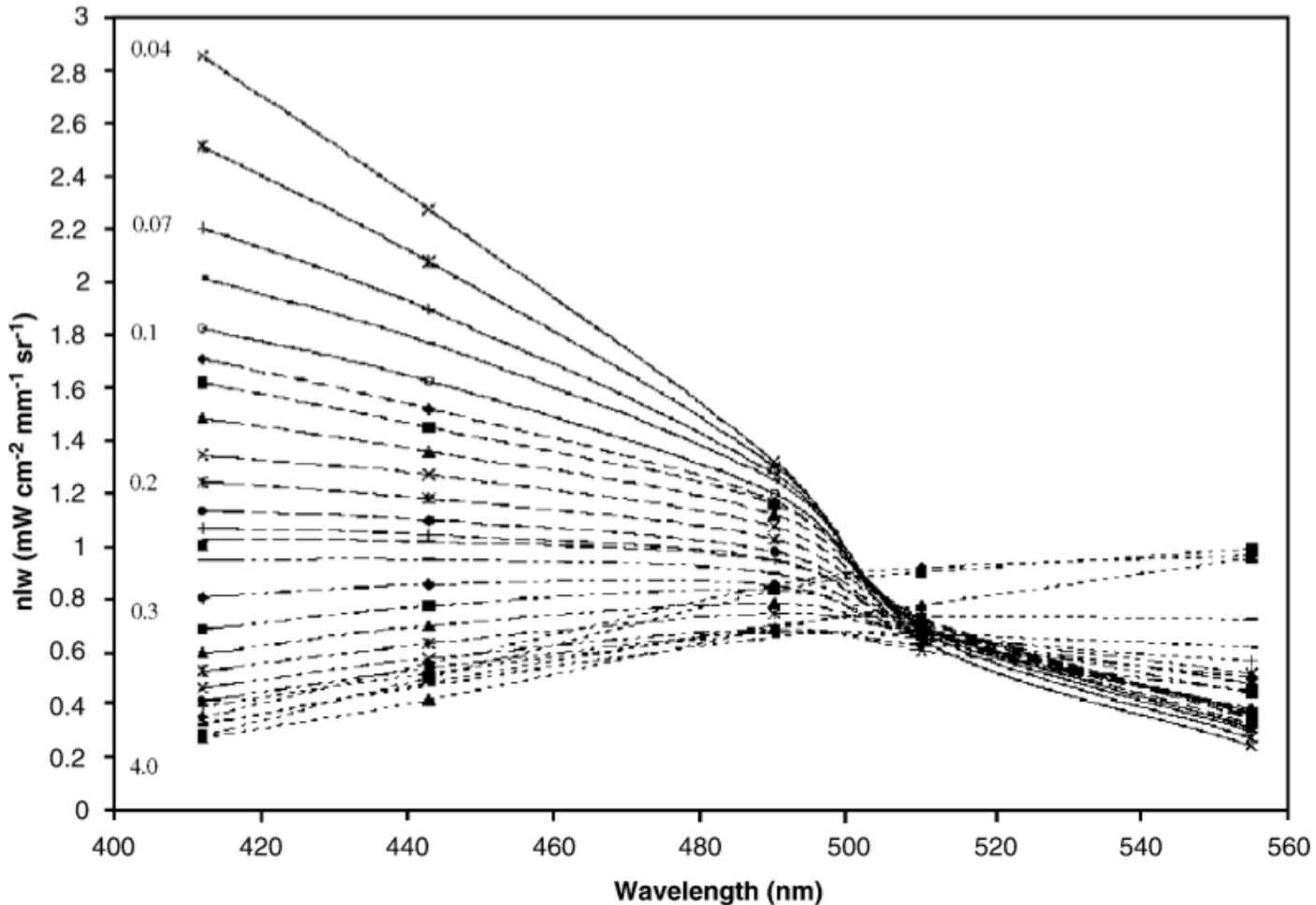


Fig. 1. Normalized water-leaving radiance nL_w as a function of wavelength for various chlorophyll- a . Average spectra were obtained from 28 800 coincident SeaWiFS chlorophyll a concentration and nL_w spectra located in the vicinity of the GeP&CO ship tracks.

average satellite $nL_w(\lambda)$ for a range of Chl

spectral – $R_{rs}(\lambda)$ as input

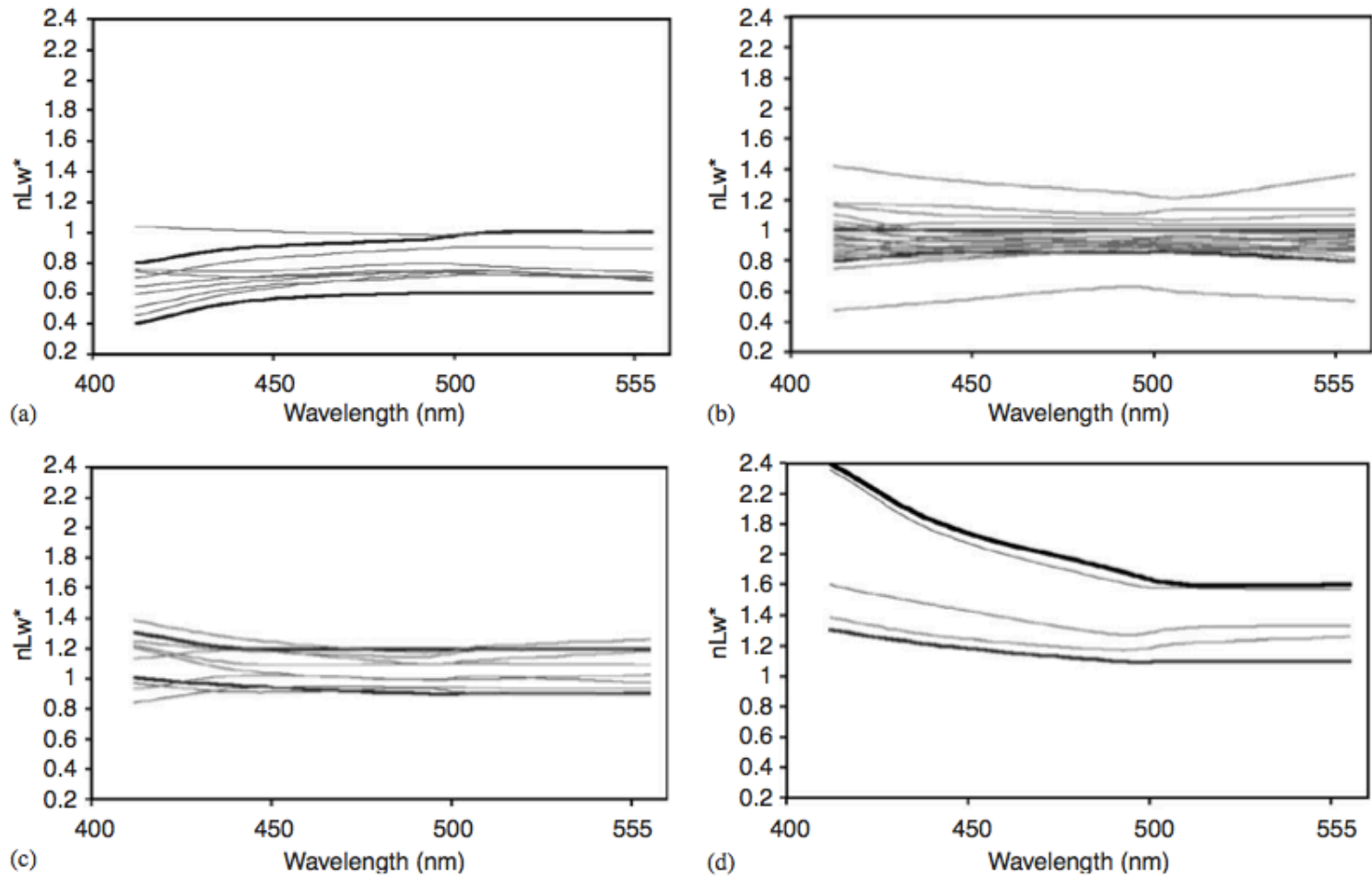


Fig. 5. Spectral signatures of nLw^* of the four different phytoplankton assemblages, dominated by (a) haptophytes, (b) *Prochlorococcus*, (c) SLC and (d) diatoms. Individual SeaWiFS nLw^* are depicted by the grey lines. Bold plain lines show the minimum and maximum spectral values of nLw^* defined in Table 5 to characterize phytoplankton groups.

$nL_w(\lambda)$ anomalies for each PFT

outline

model input

satellite-derived [chl]

satellite-derived IOPs

$a(\lambda)$
Ciotti (2006)
Devred (2006)
Hirata (2008)

Uitz (2006)
Hirata (2011)

$b_b(\lambda) + a(\lambda)$
Aiken (2007)

$b_b(\lambda)$
Kostadinov (2010)

data products

[accessory pigments]

PSC (size classes: pico,nano,micro)

PFT (taxonomic community)

model input

Pan (2010)

Mouw (2010)

Roesler (2004)
Westberry (2005)

Brown (1994)
Subramaniam (2002)
Sathyendranath (2004)
Alvain (2005, 2008)

satellite-measured radiances & -derived IOPS

satellite-measured radiances

spectral – $a_{ph}(\lambda)$ as input

LIMNOLOGY and OCEANOGRAPHY: METHODS

Limnol. Oceanogr.: Methods 4, 2006, 237–253
© 2006, by the American Society of Limnology and Oceanography, Inc.

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. Ciotti¹ and Annick Bricaud²

¹UNESP–CLP/SV, Campus do Litoral Paulista, Praça Infante Dom Henrique s/nº, São Vicente (SP), Brazil

²CNRS, Laboratoire d'Océanographie de Villefranche, Villefranche-sur-Mer; Université Pierre et Marie Curie-Paris, Laboratoire d'Océanographie de Villefranche, Villefranche-sur-Mer, France

estimate the relative fraction of 2 PSCs for each pixel

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

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

$$a_{\phi}(\lambda) = a_{\langle\phi\rangle}(\lambda) \cdot \{[S_f \cdot \bar{a}_{\langle\text{pico}\rangle}(\lambda)] + [(1 - S_f) \cdot \bar{a}_{\langle\text{micro}\rangle}(\lambda)]\} \quad (1)$$

where $\bar{a}_{\langle\text{pico}\rangle}(\lambda)$ and $\bar{a}_{\langle\text{micro}\rangle}(\lambda)$ are the “basis vectors” (or absorption spectra normalized by their own average over the visible spectrum) corresponding to picoplankton and microplankton, respectively, and $a_{\langle\phi\rangle}(\lambda)$ is the scaling factor to be applied to the normalized absorption spectrum. The size parameter S_f is a parameter constrained to vary between 0 and 1 and specifying the relative contributions of picoplankton and microplankton to

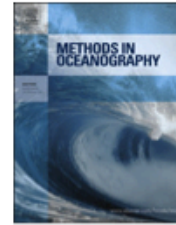
spectral – $a_p(\lambda)$ as input



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Full length article

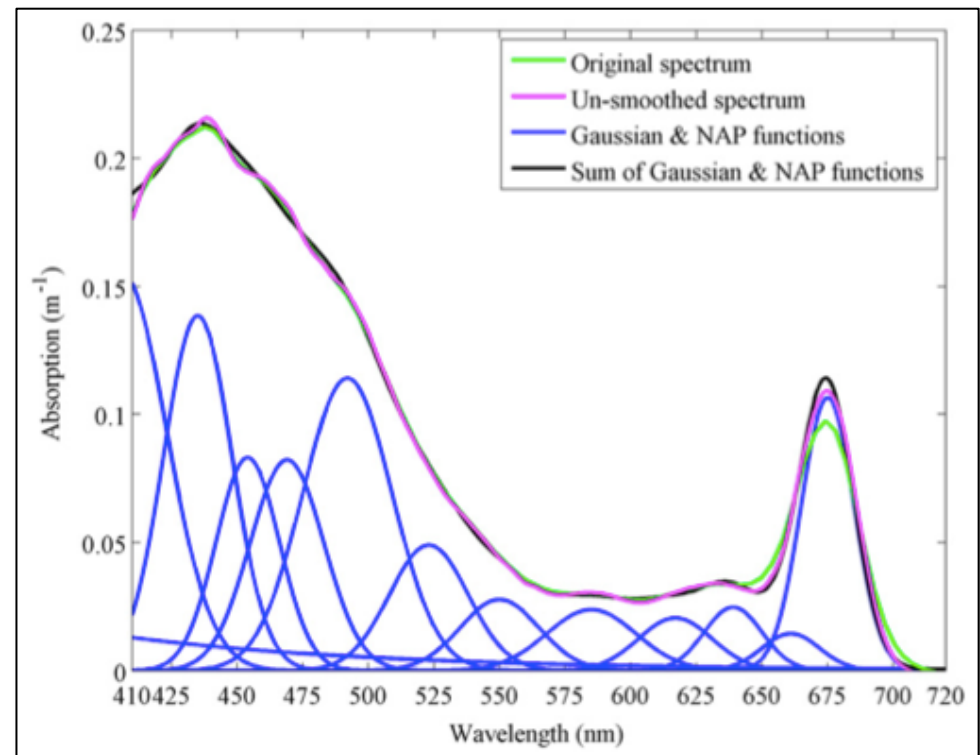
Decomposition of in situ particulate absorption spectra



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

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

correlate with HPLC pigment concentrations



outline

model input

satellite-derived [chl]

satellite-derived IOPs

$a(\lambda)$
Ciotti (2006)
Devred (2006)
Hirata (2008)

$b_b(\lambda) + a(\lambda)$
Aiken (2007)

$b_p(\lambda)$
Kostadinov (2010)

Uitz (2006)
Hirata (2011)

data products

[accessory pigments]

PSC (size classes:
pico,nano,micro)

PFT (taxonomic
community)

model input

Pan (2010)

Mouw (2010)

Roesler (2004)
Westberry (2005)

Brown (1994)
Subramaniam (2002)
Sathyendranath (2004)
Alvain (2005, 2008)

satellite-measured
radiances & -derived IOPS

satellite-measured
radiances

spectral – $b_{bp}(\lambda)$ as input

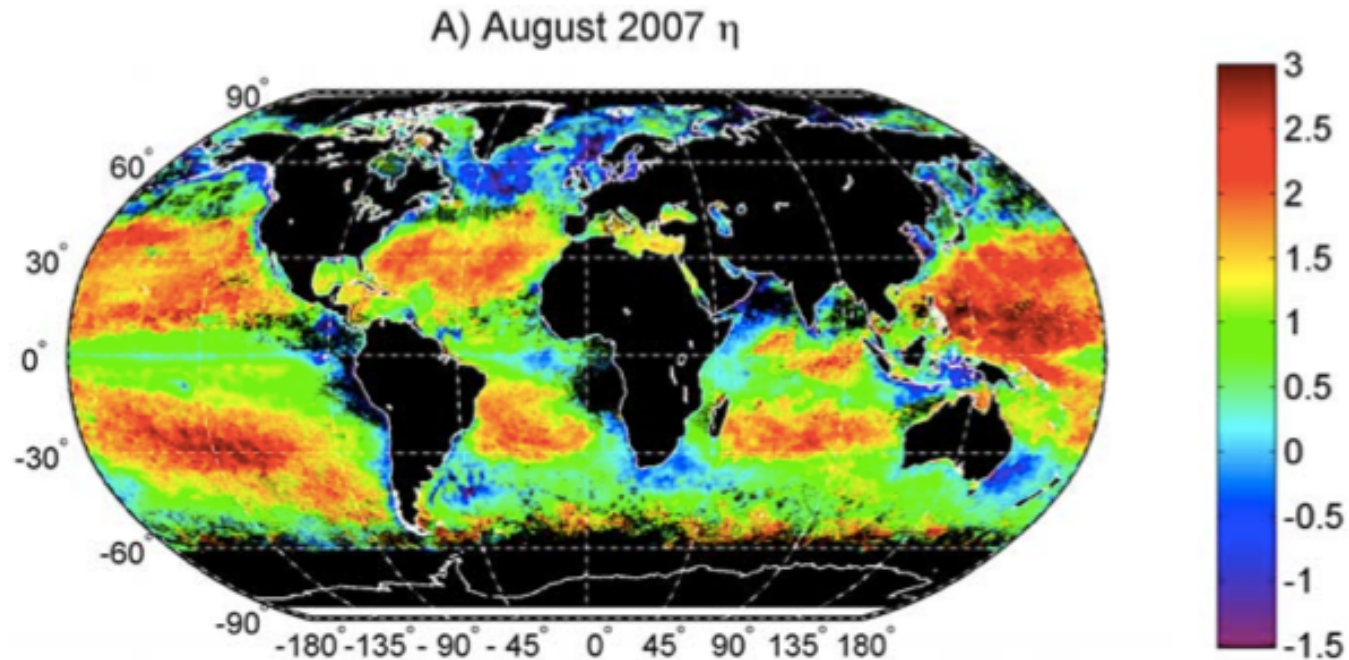
JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 114, C09015, doi:10.1029/2009JC005303, 2009



η from Loisel & Stramski 2000

Retrieval of the particle size distribution from satellite ocean color observations

T. S. Kostadinov,^{1,2} D. A. Siegel,^{1,3} and S. Maritorena¹



estimate the relative fraction of 3 PSCs for each pixel

spectral – $b_{bp}(\lambda)$ as input

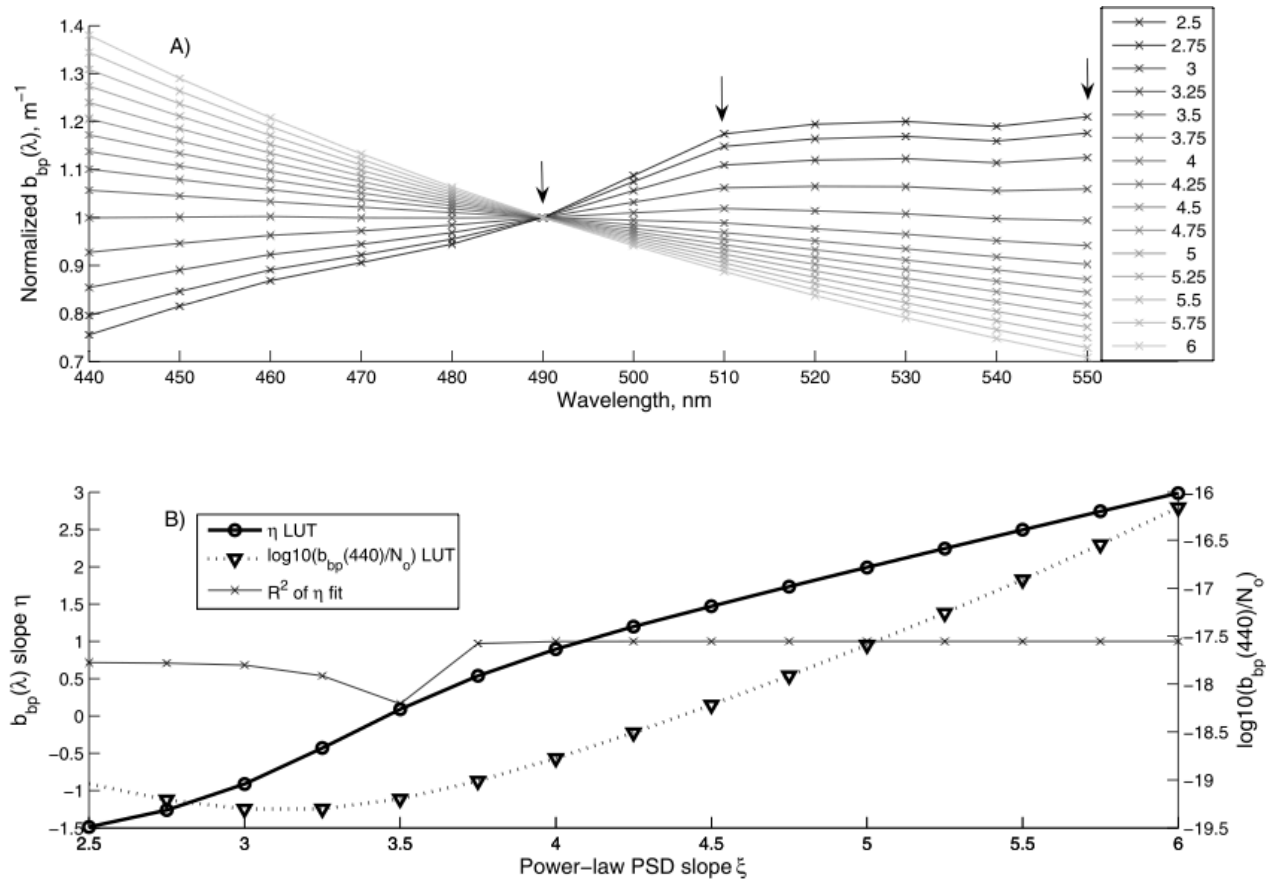
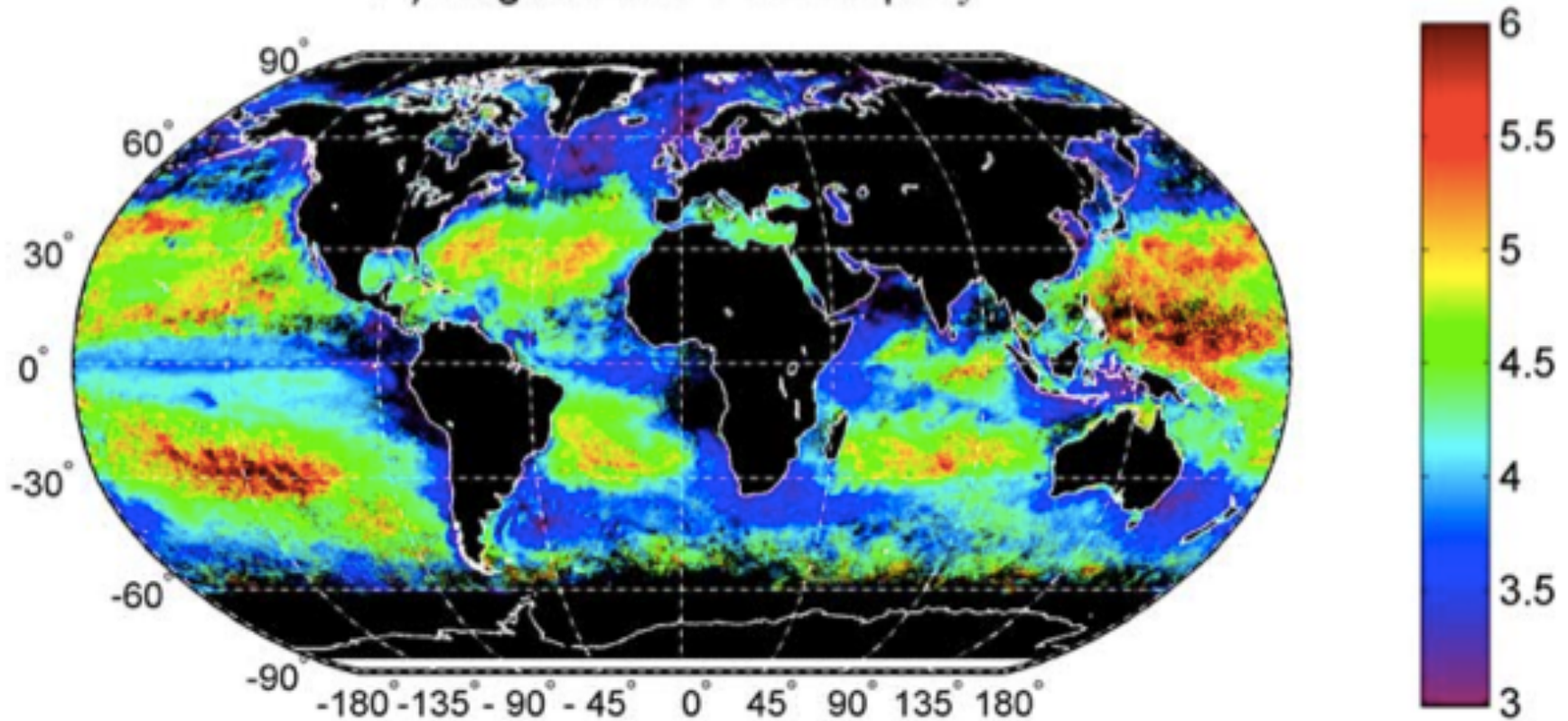


Figure 1. Results of the forward Mie model run with the default parameters as in Table 1. (a) The resulting $b_{bp}(\lambda)$ spectra are shown for different PSD slopes, as in the legend, from lowest ($\xi = 2.5$, black curve) to highest ($\xi = 6$, lightest shade of gray). The wavelengths at which Mie calculations were performed are marked with crosses. The particulate backscattering slope, η , was calculated using only the three wavelengths marked with arrows, both for modeled and SeaWiFS-retrieved spectra (see section 2.1 for details). (b) The resulting relationship between the power law slope of the PSD, ξ , and η (left y axis), as well as the relationship between ξ and the value of $\log_{10}(b_{bp}(440)/N_o)$ (right y axis). These relationships are the basis of the look-up tables (LUTs) presented in the text. The determination coefficient, R^2 , of the linear regression used to calculate the $b_{bp}(\lambda)$ slope is also shown (scale on left y axis).

spectral – $b_{bp}(\lambda)$ as input

A) August 2007 PSD slope ξ



spectral – $b_{bp}(\lambda)$ as input

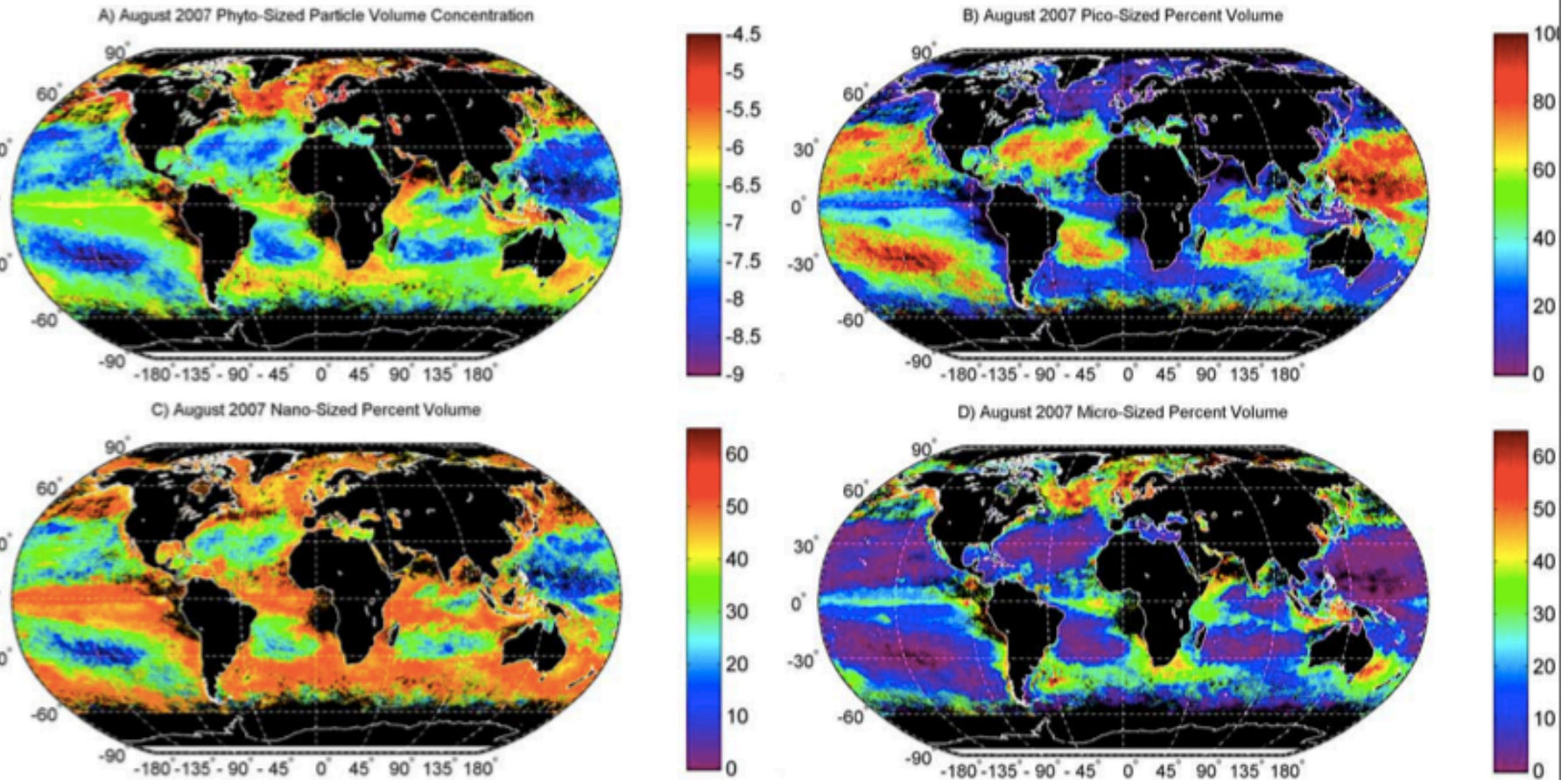


Figure 11. Global maps of (a) volume concentration of phytoplankton-sized (0.5 and 50 μm) particles, a dimensionless quantity, $\log_{10}(\text{volume of particles}/\text{volume of seawater})$; (b) percent volume due to picoplankton-sized particles (0.5–2 μm); (c) percent volume due to nanoplankton-sized particles (2–20 μm); and (d) percent volume due to microplankton-sized particles (20–50 μm).

outline

model input

satellite-derived [chl]

satellite-derived IOPs

$a(\lambda)$
Ciotti (2006)
Devred (2006)
Hirata (2008)

$b_b(\lambda) + a(\lambda)$
Aiken (2007)

$b_b(\lambda)$
Kostadinov (2010)

Uitz (2006)
Hirata (2011)

data products

[accessory pigments]

PSC (size classes:
pico,nano,micro)

PFT (taxonomic
community)

model input

Pan (2010)

Mouw (2010)

Roesler (2004)
Westberry (2005)

Brown (1994)
Subramaniam (2002)
Sathyendranath (2004)
Alvain (2005, 2008)

satellite-measured
radiances & -derived IOPS

satellite-measured
radiances

spectral – inversion modeling

inversion modeling as described in Lectures 19 & 20, except ...

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

Collin S. Roesler¹, Stacey M. Etheridge², and Grant C. Pitcher³

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

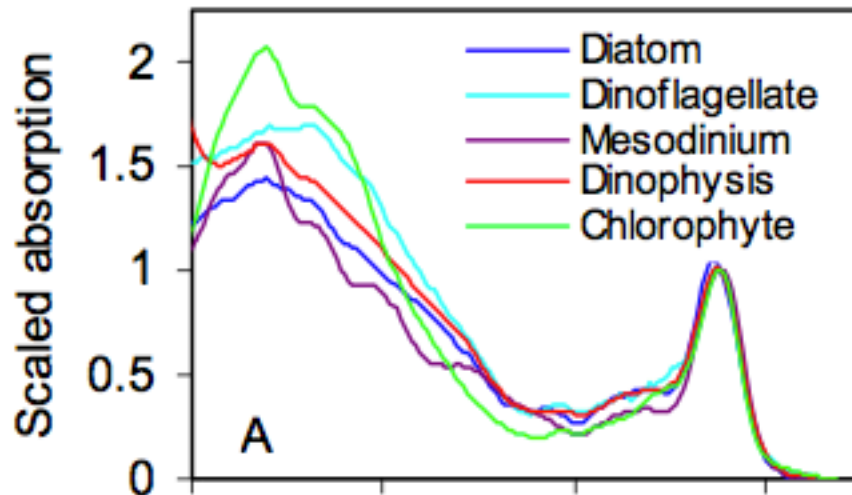
Emmanuel Boss

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

... solve for slope of beam-c

spectral – $a_{ph}(\lambda)$ as input

$$a(\lambda) = a_w(\lambda) + \sum_{i=1}^{N_\phi} A_{\phi_i} a_{\phi_i}^*(\lambda) \\ + \sum_{i=1}^{N_d} A_{d_i} a_{d_i}^*(\lambda) + \sum_{i=1}^{N_g} A_{g_i} a_{g_i}^*(\lambda),$$



Roesler et al. 2004

outline

diverse bio-optical methods to estimate PSCs/PFTs exist

their sensitivities remain unexplored

most folks use proxy data sets for their validation

algorithm sensitivities

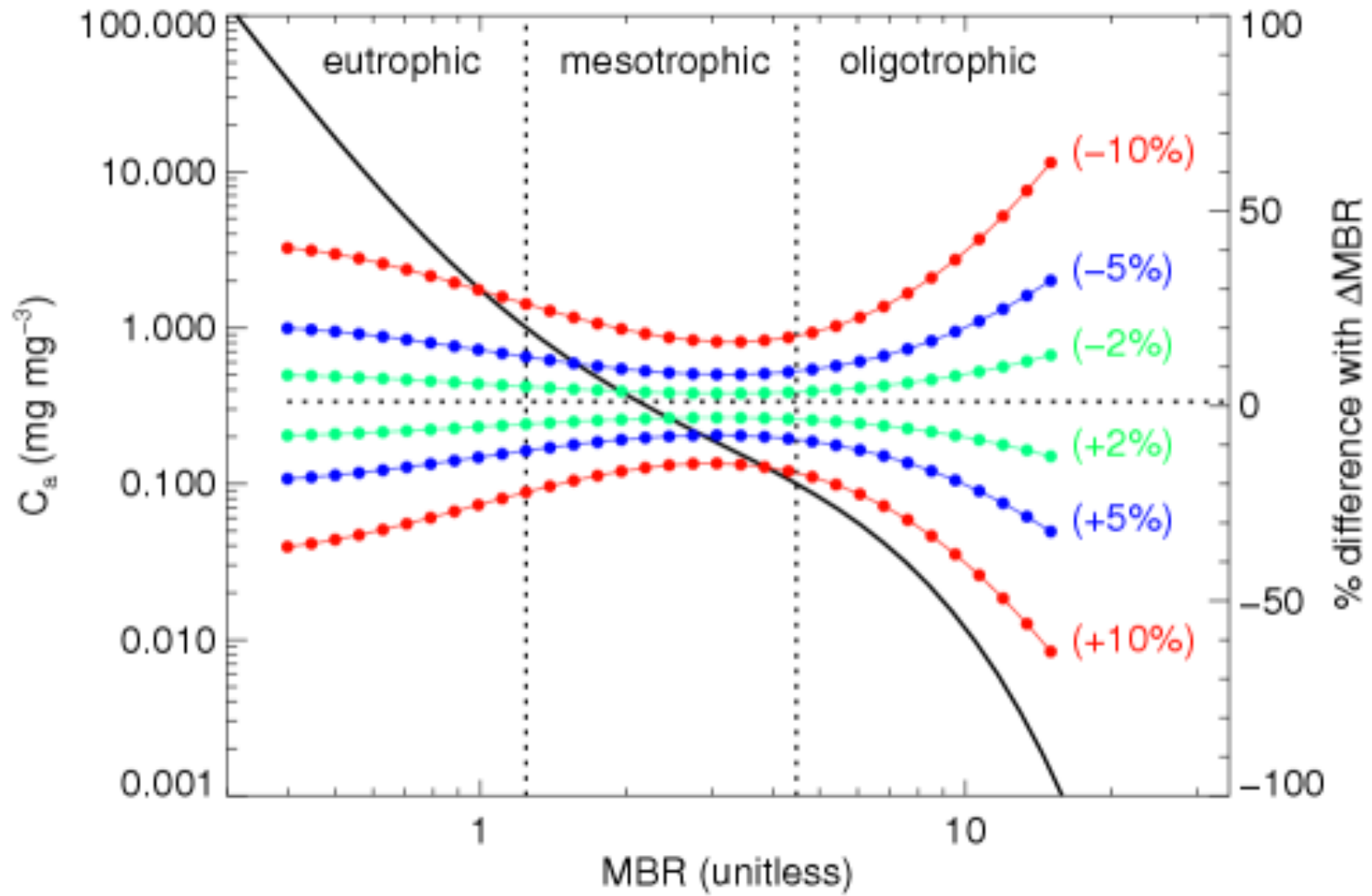
all PFT algorithms use derived products (e.g., Chl & IOPs) or make *a priori* environmental assumptions

unfortunately, few PFT/PSC modeling papers include robust analysis of the sensitivity of the model outputs to the model inputs

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 $a_{ph}(\lambda)$?

sensitivity of the operational chl algorithm



sensitivity of an inversion model to parameterization

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
α_{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
$400 \leq \lambda \leq 600$ nm	424	0.23	0.21	0.08	0.38

Werdell et al. 2013

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.

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

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

IOCCG workshop participant feedback

what do you consider to be the 3 biggest problems you've faced or think need to be overcome with regards to validating remote sensing PFT algorithms?

sample size: 5 (not including myself)

- (5) availability of global datasets for algorithm development & satellite validation; need to rely on HPLC (thus, DPA & CHEMTAX); limitations of HPLC as a proxy
- (2) mismatch between spatial & temporal scales of satellite & *in situ* measurements
- (1) satellite uncertainties & sensitivities to algorithm inputs
- (1) satellite limits of PFT detectability
- (1) *in situ* methods & their differences & uncertainties
- (1) differences in algorithm outputs (size, taxonomic groups or species, fraction of Chl vs fraction of absorption, etc.)
- (1) PSC definitions

outline

diverse bio-optical methods to estimate PSCs/PFTs exist

their sensitivities remain unexplored

most folks use proxy data sets for their validation

measuring PSCs & PFTs in the field

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

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

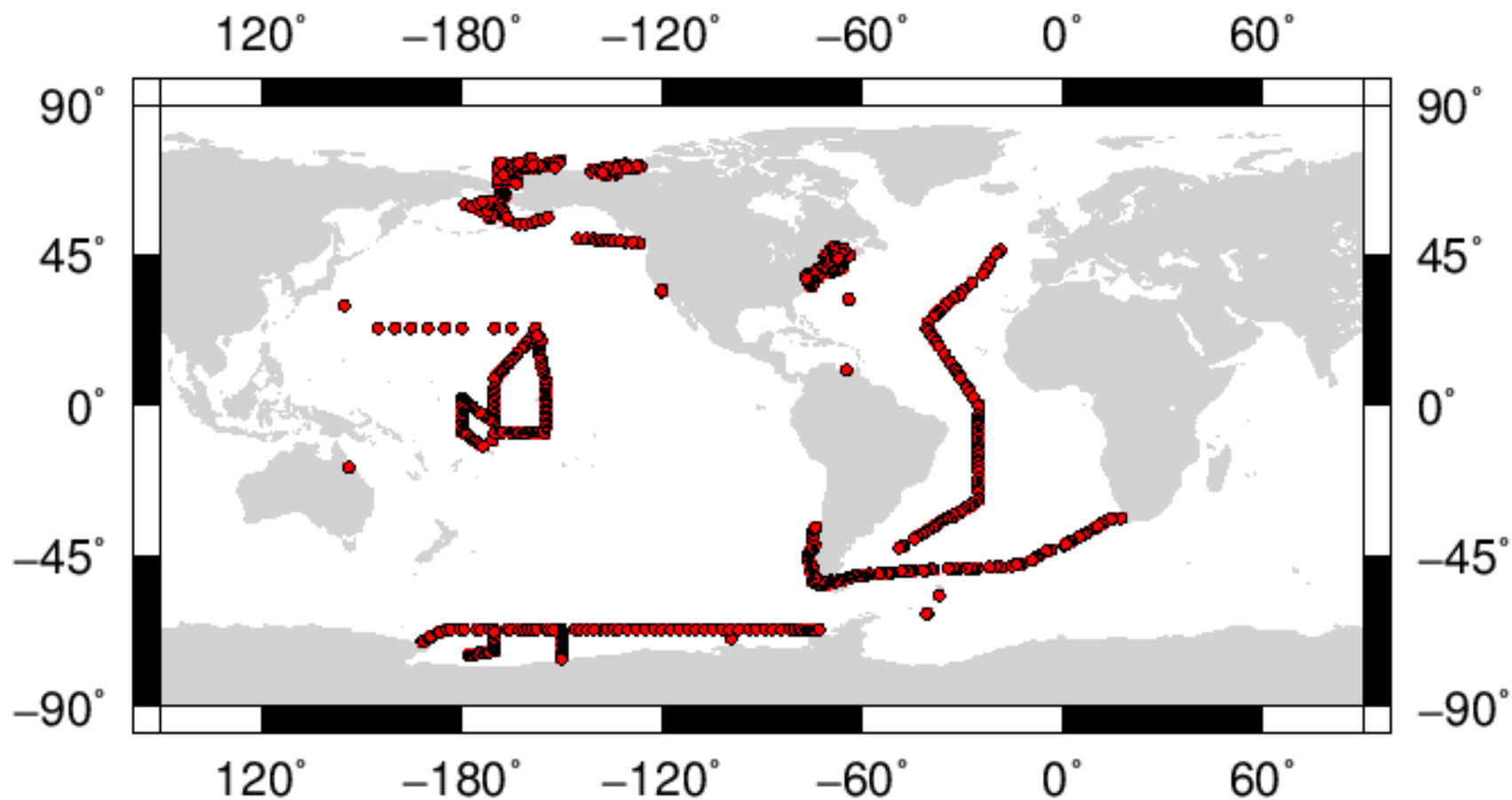


HPLC measurements as proxy PFT/PSC data

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

these measurements are scarce, whereas HPLC pigment data are now abundant & globally distributed

NASA HPLC measurements since 2009



HPLC measurements as proxy PFT/PSC data

weaknesses in DPA:

various phytoplankton groups share some taxonomic pigments (e.g., fucoxanthin in diatoms, plus dinoflagellates & Phaeocystis)

some phytoplankton groups encompass wide size ranges (e.g., most diatoms are micro, but some are nano)

requires a priori knowledge of accessory pigment ratios

validation via visual inspection

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

example validation exercises

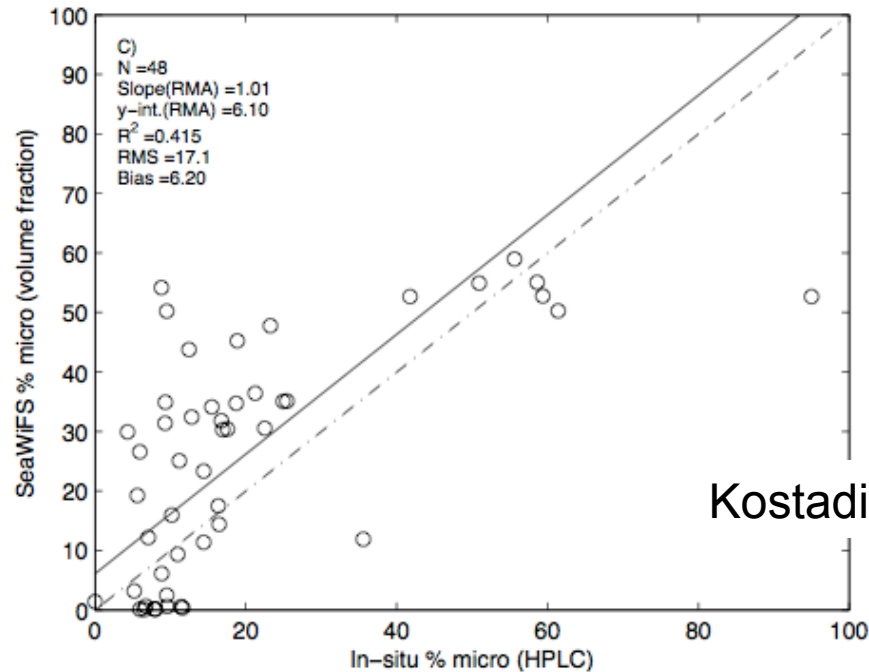
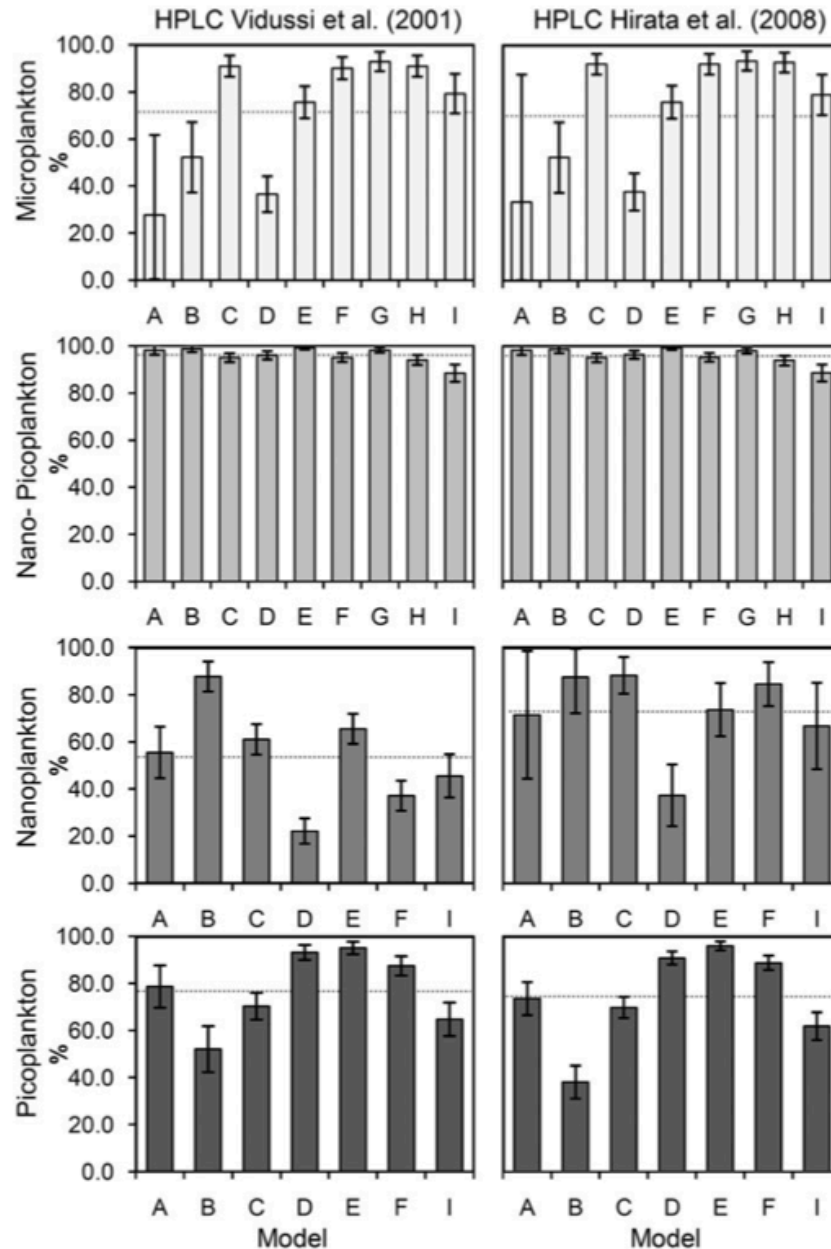


Fig. 3. PFT algorithm validation regressions for (A) percent picoplankton, (B) percent nanoplankton and (C) percent microplankton. The in-situ PFT's (x-axes) were calculated using the Vidussi et al. (2001) diagnostic phytoplankton pigment ratio method. Global HPLC surface data were matched to Level-3 daily SeaWiFS imagery in order to calculate a satellite PFT estimate using the PSD algorithm (y-axes). Type II regressions were used. RMS (Root Mean Square) and bias statistics are independent of the regression lines.

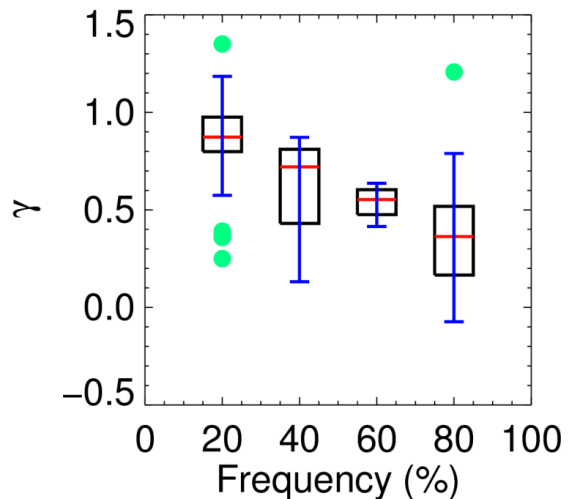
example validation exercises



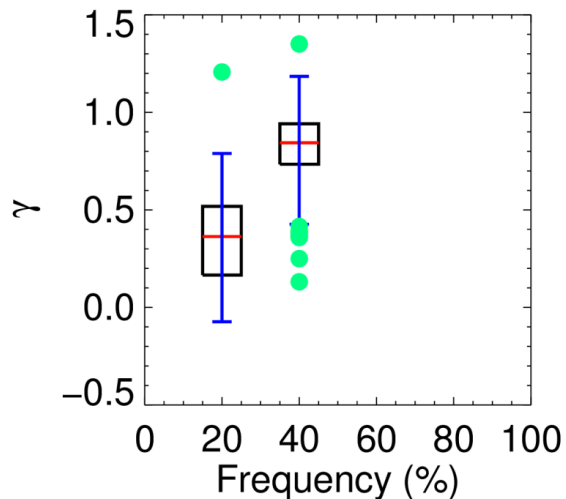
Brewin et al. 2010

example validation exercises

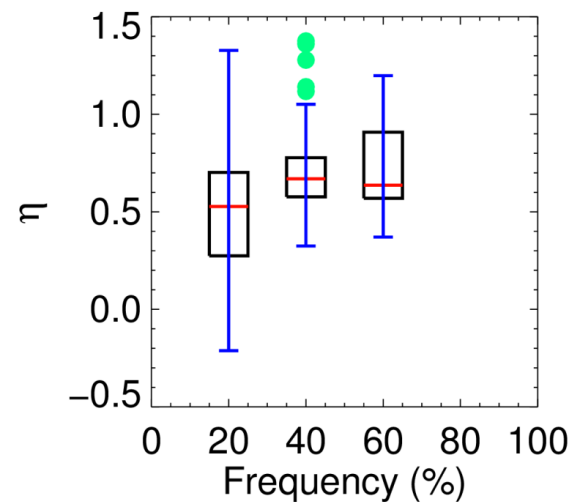
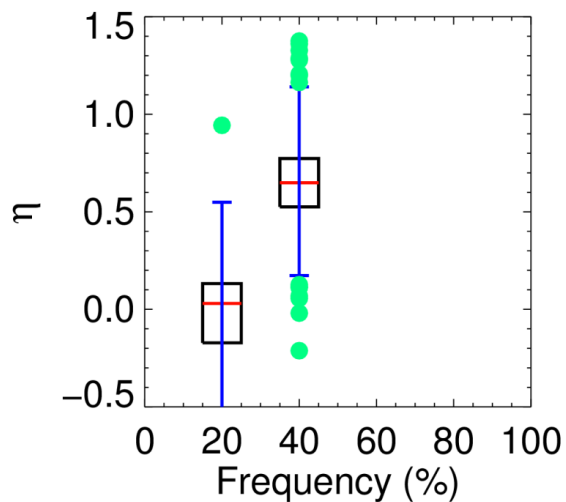
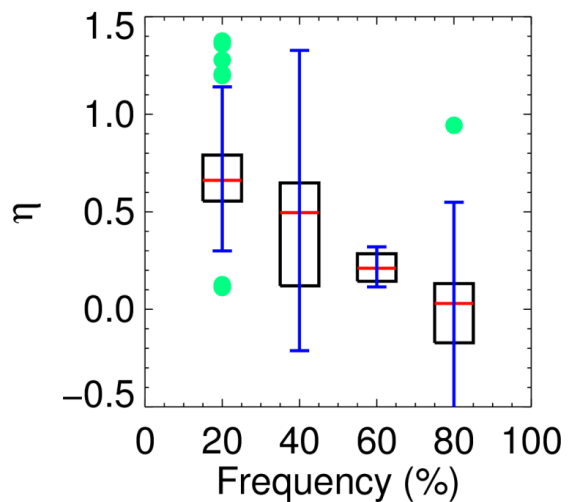
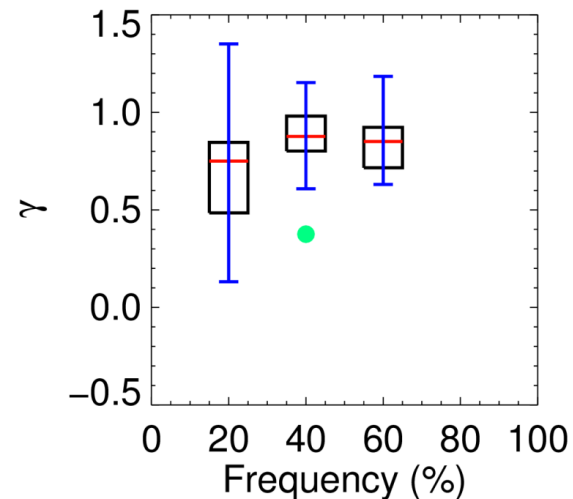
Micro



Nano



Pico



discussion

thoughts?