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



Jeremy Werdell NASA Goddard Space Flight Center

UMaine Ocean Optics Summer Course Jul 7 – Aug 3, 2013

1

UMaine Ocean Optics Summer Course, PJW, NASA

### **rationale**

changes in the Earth's climate

can lead to changes in phytoplankton species composition

which can alter regional & global C budgets & food webs

large spatial & temporal scales required to study broad, long-term environmental changes on species assemblages

microscopic enumeration of phytoplankton cells alone insufficient

in practice, remote (including space-based) tools required

ocean color satellites provide daily, synoptic views of Earth SeaWiFS – 1997 to 2010 MERIS – 2002 to 2010 MODIS-Aqua – 2002 to present



UMaine Ocean Optics Summer Course, PJW, NASA



#### 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



# **measuring PSCs & PFTs in the field**

microscopy flow cytometry coulter counters video imaging continuous plankton recorder spectroscopy 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 Vidussi<sup>1</sup>, Hervé Claustre<sup>1</sup>, Beniamino B. Manca<sup>2</sup>, Anna Luchetta<sup>3</sup>, and Jean-Claude Marty<sup>1</sup>

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<sup>1, 2</sup>, D. J. Mackey<sup>2,\*</sup>, H. W. Higgins<sup>2</sup>, S. W. Wright<sup>3</sup>

<sup>1</sup>University Chemical Laboratory, Lensfield Rd, Cambridge CB2 1EW, United Kingdom <sup>2</sup>CSIRO Division of Oceanography, PO Box 1538, Hobart, Tasmania 7001, Australia <sup>3</sup> Australian 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.



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<sub>w</sub>  $f_{\text{nano}} = (1.27 \text{ Hex-fuco} + 0.35 \text{ But-fuco} + 0.60 \text{ Allo}) / \text{DP}_{w}$ adjusted chl-to-accessory  $f_{\text{pico}} = (1.01 \text{ TChl-b} + 0.86 \text{ Zea}) / \text{DP}_{w}$ pigment ratios – link to micro-Chl-a =  $f_{\text{micro}}$  Chl-a fractional chl for each PSC nano-Chl-a =  $f_{\text{nano}}$  Chl-a pico-Chl-a =  $f_{\text{pico}}$  Chl-a



# **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],  $b_b(\lambda)$ ,  $a_{\text{ph}}(\lambda)$ , 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<sub>bp</sub>( $\lambda$ ), a( $\lambda$ ), a<sub>ph</sub>( $\lambda$ ), combinations of these



# 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



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

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



### **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.



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



UMaine Ocean Optics Summer Course, PJW, NASA

### **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,<sup>1</sup> Hervé Claustre,<sup>1</sup> André Morel,<sup>1</sup> and Stanford B. Hooker<sup>2</sup>

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]<sub>surf</sub>, and the Associated Parameters<sup>a</sup>

		<b>Stratified Waters</b>									<b>Mixed Waters</b>				
	S1	S <sub>2</sub>	S3	S4	S5	S6	S7	S8	S9	M1	M <sub>2</sub>	M <sub>3</sub>	M <sub>4</sub>	M5	
[Chla] <sub>surf</sub> range, mg m <sup>-3</sup>	$< 0.04^b$	$0.04 - 0.08$	$0.08 - 0.12$	$0.12 - 0.2$	$0.2 - 0.3$	$0.3 - 0.4$	$0.4 - 0.8$	$0.8 - 2.2$	$2.2 - 4^c$	$\leq 0.4^d$	$0.4 - 0.8$	$0.8 - 1$	$1 - 4$	$>4^{\circ}$	
Number of profiles	109	268	269	320	287	180	260	110	18	155	153	53	182	55	
Average [Chla] <sub>surf</sub> , mg m <sup>-3</sup>	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 $\overline{\text{Chla}}_{\text{Zeu}}$ , mg m <sup>-3</sup>	0.0910	0.151	0.185	0.250	0.338	0.410	0.578	.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 $\langle \text{Chla} \rangle_{\text{Zeu}}$ , mg m <sup>-2</sup>	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 $\rangle$ <sub>1.5</sub> z <sub>cu</sub> , mg m <sup>-2</sup>	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 $Z_{\text{cu}}$ , 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)	

<sup>a</sup>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).

<sup>b</sup>Minimum value 0.015 mg m<sup>-3</sup>.

 $\mathrm{C}$ Maximum value 3.97 mg m<sup>-3</sup>

<sup>d</sup>Minimum value 0.047 mg m<sup>-3</sup>.

 $\mathrm{C}$ Maximum value 23.9 mg m<sup>-3</sup>.

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



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 – 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

lemote Sensinį<br>Environment

#### **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<sup>-3</sup>) 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**

b) 03/2004





f) 11/2004

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

# pico when  $a_{ph}(443) < 0.023$  m<sup>-1</sup>

nano otherwise

Longitude [deg.]

90

180

 $.90$ 

# 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



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 <sup>a,\*</sup>, Antonio Mannino <sup>a</sup>, Mary E. Russ <sup>a</sup>, Stanford B. Hooker <sup>a</sup>, Lawrence W. Harding Jr. <sup>b</sup>

<sup>a</sup> NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA

<sup>b</sup> 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

lemote Sensing<br>Environment



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

#### **Table 4**

Derived coefficients for pigment algorithms from Eq. (1):  $log[$  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.











**DEEP-SEA RESEARCH** PART II

**PERGAMON** 

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

www.elsevier.com/locate/dsr2

#### Detecting *Trichodesmium* blooms in SeaWiFS imagery

Ajit Subramaniam<sup>a,\*</sup>, Christopher W. Brown<sup>b</sup>, Raleigh R. Hood<sup>c</sup>, Edward J. Carpenter<sup>d</sup>, Douglas G. Capone<sup>a</sup>

#### 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  $(0.5-3.0 \,\text{mg/m}^3)$  in SeaWiFS imagery: A pixel was flagged as dominated by *Trichodesmium* if the following three criteria were satisfied:

1. nLw(490) > 1.3 mW cm<sup>2</sup>/µm/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





Available online at www.sciencedirect.com



**DEEP-SEA RESEARCH** PART I

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

www.elsevier.com/locate/dsr

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

S. Alvain<sup>a</sup>, C. Moulin<sup>a,\*</sup>, Y. Dandonneau<sup>b</sup>, F.M. Bréon<sup>a</sup>

provide estimate of dominant PFT for each pixel





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



Fig. 5. Spectral signatures of nLw<sup>\*</sup> 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<sup>\*</sup> defined in Table 5 to characterize phytoplankton groups.

#### $nL_w(\lambda)$  anomalies for each PFT





**LIMNOLOGY** and **OCEANOGRAPHY: METHODS** 

Limnol. Oceanogr.: Methods 4, 2006, 237-253 C 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. Ciotti<sup>1</sup> and Annick Bricaud<sup>2</sup>

<sup>1</sup>UNESP-CLP/SV, Campus do Litoral Paulista, Praça Infante Dom Henrique s/nº, São Vicente (SP), Brazil <sup>2</sup>CNRS, 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

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

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

where  $\bar{a}_{\text{spico}}(\lambda)_{\text{spico}}(\lambda)$  and  $\bar{a}_{\text{emico}}(\lambda)_{\text{smicro}}(\lambda)$  are the "basis" vectors" (or absorption spectra normalized by their own average over the visible spectrum) corresponding to picoplankton and microplankton, respectively, and  $a_{\text{obs}}(\lambda)$  is the scaling factor to be applied to the normalized absorption spectrum. The size parameter  $S<sub>f</sub>$  is a parameter constrained to vary between 0 and 1 and specifying the relative contributions of picoplankton and microplankton to



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,<sup>1,2</sup> D. A. Siegel,<sup>1,3</sup> and S. Maritorena<sup>1</sup>



#### estimate the relative fraction of 3 PSCs for each pixel



Figure 1. Results of the forward Mie model run with the default parameters as in Table 1. (a) The resulting  $b_{h\rho}(\lambda)$  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,  $\eta$ , 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,  $\xi$ , and  $\eta$  (left y axis), as well as the relationship between  $\xi$  and the value of  $\log_{10} (b_{bn}(440)/N_o)$  (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  $b_{bn}(\lambda)$  slope is also shown (scale on left  $y$  axis).









## **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. Roesler<sup>1</sup>, Stacey M. Etheridge<sup>2</sup>, and Grant C. Pitcher<sup>3</sup> 'Bigelow Laboratory for Ocean Sciences, PO Box 475, West Boothbay Harbor, ME 04575, USA; <sup>2</sup>Department. of Marine Science, University of Connecticut, 1084 Shennecossett Rd., Groton, CT 06340, USA; <sup>3</sup>Marine and Coastal Management, Private Bag X2, Rogge Bay 8012, Cape Town, South Africa

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

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

UMaine Ocean Optics Summer Course, PJW, NASA



### **algorithm sensitivites**

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 an inversion model to parameterization**



#### Werdell et al. 2013



# **measuring PSCs & PFTs in the field**

microscopy flow cytometry coulter counters video imaging continuous plankton recorder spectroscopy 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



# **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**









