# Your in situ data and you

Alternative title: *How* in situ *data are used informs on how a remote sensing product should be interpreted* 

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2024 IOCCG CETT training course



## sharing experiences with *in situ* and satellite data with the goals of you ...

leaving with an appreciation for the interconnectedness of *in situ* and remote sensing data (*in situ* data are pervasive!)

keeping this interconnectedness in mind when interpreting your results



In situ data inform empirical relationships

In situ data inform semi-analytic retrievals

empirical (adjective): based on, concerned with, or verifiable by observation or experience rather than theory or pure logic

## Rrs maximum band ratio

 $X = \log_{10}[ \frac{\text{Rrs}(443 > 490 > 510)}{\text{Rrs}(555)}]$  $\log_{10}(\text{chl}) = a_0 + a_1X + a_2X^2 + a_3X^3 + a_4X^4$ 

**O'Reilly & Werdell 2019, Rem. Sens. Environ.** [after O'Reilly et al. 1998, J. Geophys. Res.; O'Reilly et al. 2002, NASA TM, Werdell 2005, NASA OceanColor Web, others]



Valente et al. 2022, Earth Syst. Sci. Data

### developed using a "global" dataset of in situ $Rrs(\lambda)$ and chl



# SeaBASS (NASA in situ archive) holdings by year: 2006-2009





Szeto et al. 2011, J. Geophys. Res.

## Rrs line height (baseline subtraction)

Chlorophyll Index (CI) from Hu et al. 2012, J. Geophys. Res. and Hu et al. 2019, J. Geophys. Res.

 $CI = R_{rs,555} - \left[ \frac{R_{rs,443}}{43} + \frac{(555 - 443)}{(670 - 443)} x \left( \frac{R_{rs,670}}{R_{rs,443}} \right) \right]$ 



original

### modified

### difference



inverse (adjective): opposite or contrary in position, **direction**, **order**, or effect

**one sentence summary of this inversion paradigm**: How much of each absorbing and backscattering component is needed (in a least squares sense) to reconstruct the measured reflectance spectrum?

 $Rrs(\lambda) \leftarrow forward model \leftarrow IOP(\lambda)[chl, whatever]$ 

$$r_{rs}(\lambda) = G(\lambda) \frac{b_{bw}(\lambda) + B_{bp}b_{bp}^{*}(\lambda)}{a_{w}(\lambda) + A_{ph}a_{ph}^{*}(\lambda) + A_{dg}a_{dg}^{*}(\lambda)}$$

 $\operatorname{Rrs}(\lambda) \rightarrow inverse \mod \rightarrow \operatorname{IOP}(\lambda)$ , chl, whatever

**one sentence summary of this inversion paradigm**: How much of each absorbing and backscattering component is needed (in a least squares sense) to reconstruct the measured reflectance spectrum?

... can reconstruct this?

what combination of these ...





$$b_{bw}(\lambda) + B_{bp}b_{bp}^*(\lambda)$$

$$r_{rs}(\lambda) = G(\lambda) \frac{1}{a_w(\lambda) + A_{ph}a_{ph}^*(\lambda) + A_{dg}a_{dg}^*(\lambda)}$$

Reference	Uses measured data (Y/N)	Input data required	Description			
Prieur and Sathyendranath (1981)	Y	$C_a$	Single $a_{ph}^{*}(\lambda)$ vector			
Roesler et al. (1989)	Y	Ca	Single $a_{ph}^{*}(\lambda)$ shape			
Lee et al. (1996a, b)	N	Ca	Blends two Gaussian basis vectors			
Bricaud et al. (1995)	Y	Ca	Blends two basis vectors			
Bricaud et al. (1998)	Y	Ca	Blends two basis vectors			
Hoge and Lyon (1996)	N	Ca	Single Gaussian basis vector (Hoepffner and Sathyendranath, 1993)			
Sathyendranath et al. (2001)	Y	Ca	Blends $a_{ph}^{*}(\lambda)$ basis vectors for two phytoplankton populations			
Ciotti et al. (2002)	Y	Size parameter, $S_f$	Blends $a_{ph}^{*}(\lambda)$ basis vectors for micro- and picophytoplankton			

#### Werdell et al. 2018, Prog. Oceanography

$$b_{bw}(\lambda) + B_{bp}b_{bp}^*(\lambda)$$

$$r_{rs}(\lambda) = G(\lambda)$$

$$a_w(\lambda) + A_{ph}a_{ph}^*(\lambda) + A_{dg}a_{dg}^*(\lambda)$$

Method	Uses measured data (Y/N)	Input data required	Description
Morel and Maritorena (2001)	Y	Ca	• $S_{bp}$ defined in terms of $\tilde{b}$
Gordon et al. (1988)	Ν	Ca	<ul> <li>Defines b<sub>p</sub>(λ) from C<sub>a</sub></li> <li>Assumes b̃ = F(Ca)</li> </ul>
Ciotti et al. (1999)	Y	Ca	• Logarithmic function from $-2$ where $C_a = 0.05 \text{ mg m}^{-3}$ to 0 where $C_a = 20 \text{ mg m}^{-3}$
Lee et al. (2002)	Y	$r_{rs}(\lambda)$	Empirical relationship
Roesler and Boss (2003)	Ν	$\widetilde{b}$ ( $\lambda$ ), $c_p(\lambda)$ , $a_p(\lambda)$	• Solves for for $b_{bp}(\lambda)$ and $S_c$
Antoine et al. (2011)	Y	$C_a$ or $b_b(555)$	Empirical relationship
Brewin et al. (2012)	Y	Ca	• Empirical relationship for $b_{bp}(\lambda)$

Table 2

 $b_{bw}(\lambda) + B_{bp}b_{bp}^*(\lambda)$ 

$r_{rs}(\lambda)$	=	$G(\lambda)$
10		

(1)		-11 $-*$ (1)
$(I \cap (A))$	$+(A_{n}, A_{n}, A_{n})$	$+ + A_{J_{n}} (I_{n} (A))$
	' pn~pn(~)	
		0 - 0

Reference	Method and assumptions for parameterizing $a_{ph}(\lambda)$ and $a_{dg}(\lambda)$	Additional input data	Applied to ocean color data? (Y/N) N	
Roesler et al. (1989)	<ul> <li>a<sub>dg</sub>(λ) has fixed exponential slope, S<sub>dg</sub></li> <li>a<sub>ph</sub>(λ) blue-to-red absorption peak defined using pigment data</li> <li>Solves for a<sub>dg</sub>(λ) and a<sub>ph</sub>(λ)</li> </ul>	<ul> <li><i>C<sub>a</sub></i></li> <li>Phaeophytin-a concentration</li> </ul>		
Lee et al. (2002)	<ul> <li>a<sub>dg</sub>(λ) has fixed exponential slope, S<sub>dg</sub></li> <li>Empirical relationship uses r<sub>rs</sub>(λ) to parameterize band ratio of a<sub>ph</sub>(λ)</li> <li>Solves for a<sub>dg</sub>(λ) and a<sub>ph</sub>(λ)</li> </ul>	• None	Y	
Ciotti and Bricaud (2006) Method 1	<ul> <li><i>a</i><sub>dg</sub>(λ) assumed to be exponential</li> <li>Empirical relationships uses <i>C<sub>a</sub></i> to parameterize band ratios of <i>a</i><sub>ph</sub>(λ)</li> <li>Solves for <i>M</i><sub>dg</sub>, <i>S</i><sub>dg</sub>, <i>a</i><sub>dg</sub>(λ), and <i>a</i><sub>ph</sub>(λ) algebraically (Bricaud and Stramski 1990)</li> </ul>	• <i>C</i> <sub>a</sub>	Y	
Ciotti and Bricaud (2006) Method 2	<ul> <li>a<sub>dg</sub>(λ) assumed to be exponential</li> <li>a<sub>ph</sub>(λ) parameterized through mixing of pico- and microphytoplankton contributions (Ciotti et al. 2002)</li> <li>Solves for M<sub>dg</sub>, S<sub>dg</sub>, M<sub>ph</sub>, and the size parameter of phytoplankton (S<sub>f</sub>) via nonlinear optimization</li> </ul>	• <i>C</i> <sub>a</sub>	Y	
Zheng and Stramski (2013b)	<ul> <li>a<sub>dg</sub>(λ) assumed to be exponential</li> <li>a<sub>ph</sub>(λ) shape expressed through band ratios of 412:443 and 510:490</li> <li>Searches multiple speculative (feasible) solutions of M<sub>dg</sub>, S<sub>dg</sub>, a<sub>dg</sub>(λ), and a<sub>ph</sub>(λ) (Bricaud and Stramski, 1990)</li> <li>Computes candidate and selects optimal solution for a<sub>dg</sub>(λ) and a<sub>ph</sub>(λ) using stacked inequality contstraints</li> </ul>	<ul> <li>Pre-determined bounds of inequality constraints</li> </ul>	Y	
Zhang et al. (2015)	<ul> <li><i>a</i><sub>dg</sub>(λ) assumed to be exponential</li> <li><i>a</i><sub>ph</sub>(λ) parameterized as the sum of mixing of pico-, nano-, and microphytoplankton contributions</li> <li>Solves for <i>M</i><sub>dg</sub>, <i>S</i><sub>dg</sub>, <i>a</i><sub>dg</sub>(λ), and <i>a</i><sub>ph</sub>(λ) including contributions of pico-, nano-, and microphytoplankton using constrained least-squares optimization</li> </ul>	<ul> <li><i>C<sub>a</sub></i>-specific <i>a<sup>*</sup><sub>ph</sub></i>(λ) for pico-, nano-, and micro-phytoplankton</li> </ul>	Ν	

Werdell et al. 2018, Prog. Oceanography

 $b_{bw}(\lambda) + B_{bp}b^*_{bp}(\lambda)$ 

 $r_{rs}(\lambda) = G(\lambda)$ 

$a_w(\lambda)$	$+A_{nh}a$	$u_{nh}^{*}(\lambda)$	$++A_{da}$	$a_{da}^*$	$(\lambda)$
	· pr	$pn < \gamma$	- uy	uy	

Run	Ν	MPD			Median					
		$b_{bp}$	a	$a_{dg}$	$a_{\phi}$	$\Delta R_{ m rs}$	$\Delta b_{bp}$	$\Delta a$	$\Delta a_{dg}$	$\Delta a_{\phi}$
GIOP-DC	437	NA	NA	NA	NA	1.04	8.52	8.56	27.25	35.83
$S_{bp} - 33\%$	440	5.19	5.17	7.58	2.98	0.99	11.23	11.70	32.14	34.69
$S_{bp} + 33\%$	436	5.65	5.70	8.82	2.90	1.14	11.40	10.70	23.51	39.12
$S_{dg} - 33\%$	448	18.96	33.44	101.73	46.59	1.61	16.27	19.08	32.94	31.95
$S_{dg} + 33\%$	399	3.77	8.41	40.10	32.92	1.23	9.44	8.95	79.90	59.32
$S_{dg}$ from [7]	439	3.20	5.33	20.40	14.58	1.10	8.65	9.80	22.25	34.42
$C_a - 33\%$ in [14]	419	2.02	2.92	1.48	7.25	1.19	8.79	8.83	28.62	31.10
$C_a + 33\%$ in [14]	437	1.56	2.28	1.14	5.90	1.10	8.12	9.17	26.79	40.09
Fixed $C_a$ in [14]	369	4.57	7.89	2.60	21.68	1.46	11.30	11.53	30.97	26.70
$a_{\phi}^*$ from [17]	357	8.33	12.72	7.04	22.23	1.20	14.26	16.75	38.30	23.13
$\vec{G}$ from [22]	422	9.99	6.15	7.49	14.12	1.16	11.50	13.64	37.49	36.24
Matrix inversion	475	4.60	3.68	2.24	7.41	1.73	9.15	9.43	24.79	36.82
$400 \le \lambda \le 600 \text{ nm}$	424	0.23	0.21	0.08	0.38	0.92	8.76	8.78	31.94	36.55

Table 5. Delta Statistics for the Sensitivity Analyses\*

<sup>*a*</sup>N is the sample size. MPD is the average spectral median percent difference between GIOP-DC and each alternate run, as calculated in Tables 2 and 3. Medians of the  $\Delta$ IOP frequency distributions are also presented, as presented in Table 4.

*In situ* data inform empirical relationships

In situ data inform semi-analytic retrievals

Degrees of separation between *in situ* and satellite data vary by product suite

one algorithm or dataset CANNOT always represent all conditions (and this is ok)

# degrees of separation in data products



# consider a 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<sub>b</sub>, c spectral slopes) HPLC pigment analyses etc.







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Atmospheric correction is riddled with *in situ data* 

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meaningfully relating *in situ* and satellite variables is an area of ongoing research (and this is ok)

#### NASA/TM-2016-217551



Atmospheric Correction for Satellite Ocean Color Radiometry

Curtis D. Mobley, Jeremy Werdell, Bryan Franz, Ziauddin Ahmad, and Sean Bailey

National Aeronautics and Space Administration

Goddard Space Flight Center Greenbelt, Maryland 20771

June 2016

aerosol lookup tables (AERONET) NIR correction (black pixel assumption) out-of-band correction pure seawater foam and whitecap mask/correction BRDF correction ( others I'm forgetting )

<u>ancillary data</u>

atmospheric pressure water vapor relative humidity wind speed ozone NO2 SST, SSS sea ice In situ data inform empirical relationships

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Data treatment / compositing changes the answer

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*in situ* data are embedded into almost 100% of ocean color

- horizontal resolution
- temporal resolution
- vertical resolution





### one MODIS scan at ~45 degrees scan angle



### two MODIS scans showing overlap of pixels



## multiple MODIS scans showing pixel overlap



### bin boundaries overlaid on pixel locations



- horizontal resolution
- temporal resolution
- vertical resolution







- horizontal resolution
- temporal resolution
- vertical resolution







- horizontal resolution
- temporal resolution
- vertical resolution







- horizontal resolution
- temporal resolution
- vertical resolution







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Consideration of scales and resolution is critical to interpret differences

Question:

Based on horizontal distance (*D*) between the blue and red dots, which pair(s) below would you consider to be different: 1, 2, or 3?

Answer: D is the same for all (stop wasting our time!)



# Question:

Based on horizontal distance (*D*) between the blue and red dots, which pair(s) below would you consider to be different: 1, 2, or 3?

*This time, we'll consider measurement uncertainty and draw a probability density function around each point ...* 

Answer: (a) yes, (b) no, (c) somewhat.



# Validation metrics

$$mean \ bias = \frac{1}{N} \sum_{i=0}^{N} M_i - O_i$$

$$MAE = \frac{1}{N} \sum_{i=0}^{N} |M_i - O_i|$$

MAE: mean absolute error

# A method to account for overlapping PDFs

For mean bias and MAE, we compute the difference between the satellite observed ( $O_i$ ) and in situ measurement ( $M_i$ ) data pairs:

 $D_i = M_i - O_i$ 

We correct difference with correction factor (CF):  $CF_i = 1 - DO_i$ 

 $(DO_i)$  is the *degree of overlap metric* proposed by Harmel et al (2010) (see paper for calculus).

Corrected difference is:

 $D'_i = CF_iD_i$ 



# A method to account for overlapping PDFs For mean bias and MAE, we compute the difference • Less weight is applied when DO<sub>i</sub> approaches 1 between the satellite observed $(O_i)$ and in situ • For completely overlapping $P_0(o_i)$ and $P_m(m_i)$ , where $Do_i = 1$ , no $p_m(m_i)$ difference can be discerned $M_i$ ected difference is: O<sub>i,min</sub> O<sub>i,max</sub> $M_{i.min}$ $D'_i = CF_iD_i$ M<sub>i,max</sub>

# Validation metrics



#### MAE: mean absolute error

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Move beyond scatter plots

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#### population statistics: long-term distributions and time series



Fig. 4. In situ C, distributions (thick lines) in the Lower, Middle, and Upper Bays compared to OC and GSM retrievals for SeaWiFS (thin solid) and MODIS-Aqua (thin dashed). OC4 was used for SeaWiFS and OC3 for MODIS-Aqua. Samples sizes (in million pixels) for satellite retrievals are provided in each panel, with SeaWiFS indicated by S and MODIS-Aqua indicated by A. In situ sample sizes are 7204, S814, and 3660 for the Lower, Middle, and Upper Bay, respectively. Data from all four seasons are included.



Fig. 5. Monthly averages of *in situ* C<sub>a</sub> (thin lines) in the Upper, Middle, and Lower Bays compared to OC retrievals for SeaWiPS (OC4; empty squares) and MODIS-Aqua (OC3; filled circles). The grey shaded area represents one standard deviation about the *in situ* averages. The RPD reported in the text was calculated as 100% · (median(C<sub>a</sub><sup>estrelit</sup>/C<sub>a</sub><sup>b situ</sup>) - 1) using each monthly satellite and *in situ* pair.

residual histograms and scatter plots



Fig. 3.  $Log_{10}$  residuals histograms and scatterplots the SeaWiFS-to-*in situ Chl* match-ups. The top row are histograms of  $log_{10}$  summarizing the error distribution of GSM, OC3, and OCI algorithms. The bottom panels are residual plots of the difference between model satellite *Chl* and the reference *in situ* values versus reference values. The plots were created with  $log_{10}$  values, but the axes are in *Chl* units (mg m<sup>-3</sup>).

Zeta-score plots





Figure 4. Zeta score plots comparing modeled and observed  $b_{bp}(555)$  varying with the method average values of  $b_{bp}(555)$ . Subplots (a)–(c) correspond to LH, GIOP, and Huot models, respectively. Subplots (d)–(f) use corrected zeta scores for the LH, GIOP, and Huot models, respectively.

#### Taylor and target diagrams



Fig. 5. Taylor and Target diagrams for IOPs at 412 nm from the IOCCG data set for the 12 alternate parameterizations of GIOP compared to GIOP-DC. *uRMSD* is the unbiased root mean square difference. Symbols indicate the following: blue cross =  $S_{dg} - 33\%$  (= 0.012 nm<sup>-1</sup>); red cross =  $S_{dg} + 33\%$  (= 0.024 nm<sup>-1</sup>); green circle =  $S_{dg}$  dynamically calculated using Lee *et al.* [7]; blue square =  $S_{bp}$  from Lee *et al.* [7] -33%; black square =  $S_{bp}$  from Lee *et al.* [7] +33%; red circle = OC-derived  $C_a - 33\%$  prior to input into Bricaud *et al.* [14]; black circle = OC-derived  $C_a + 33\%$  prior to input into Bricaud *et al.* [14]; green square  $= a_{\phi}^*(\lambda)$  from Bricaud *et al.* [12]; with a size fraction of 0.5; black cross =  $G(\lambda)$  from Morel *et al.* [22]; orange cross = optimization using linear matrix inversion; and green cross = optimization considering only  $400 \le \lambda \le 600$  nm.

#### confusion matrices



Fig. 3. Confusion matrix from the algorithm validation with (A) MC only, and (B) MC and cyanobacteria cell density as field CyanoHAB reference data. Numbers in the confusion matrix represent the sample count in each scenario. CyanoHAB dass and the no-bloom classes were coded as 'Presence' and 'Absence' class.



Fig. 6. Comparison of the metrics results of bias, MAE, pairwise percent wins and coefficient of variation summarized in star plots across all water types. The plot center represents values that indicate poor algorithm performance, while farthest from center represents the best performance. The numbers represent the value of the best performing algorithm value for each metric.

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any one figure CANNOT reveal all meaningful information

# 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<sup>1</sup>, Audrey B. Ciochetto<sup>1</sup>, and James A. Yoder<sup>1</sup>

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**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





#### 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



Remote Sensing of Environment Volume 240, April 2020, 111689



Incorporating environmental data in abundancebased algorithms for deriving phytoplankton size classes in the Atlantic Ocean

#### Timothy S. Moore <sup>a, b</sup> 옷 쩓, Christopher W. Brown <sup>c</sup> 쩓

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