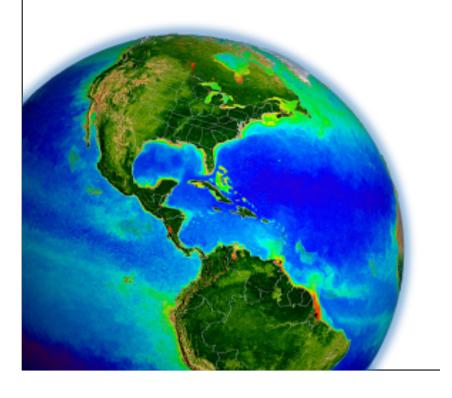
In situ data support for ocean color satellite calibration & validation



Jeremy Werdell

NASA Goddard Space Flight Center

UMaine Ocean Optics Summer Course July 10 – Aug 4 2017

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"cal/val"

cal/val = calibration & validation

cal/val has become the catch-all phrase in our community for all activities related to the:

- on-orbit calibration of a satellite instrument
- execution of field programs
- validation of biogeophysical satellite data records
- development of related atmospheric & bio-optical algorithms

outline

the purpose of this presentation is to:

- provide an overview of how in situ data are used in an operational cal/val environment
- describe some of the issues we wrestle with within this environment

outline

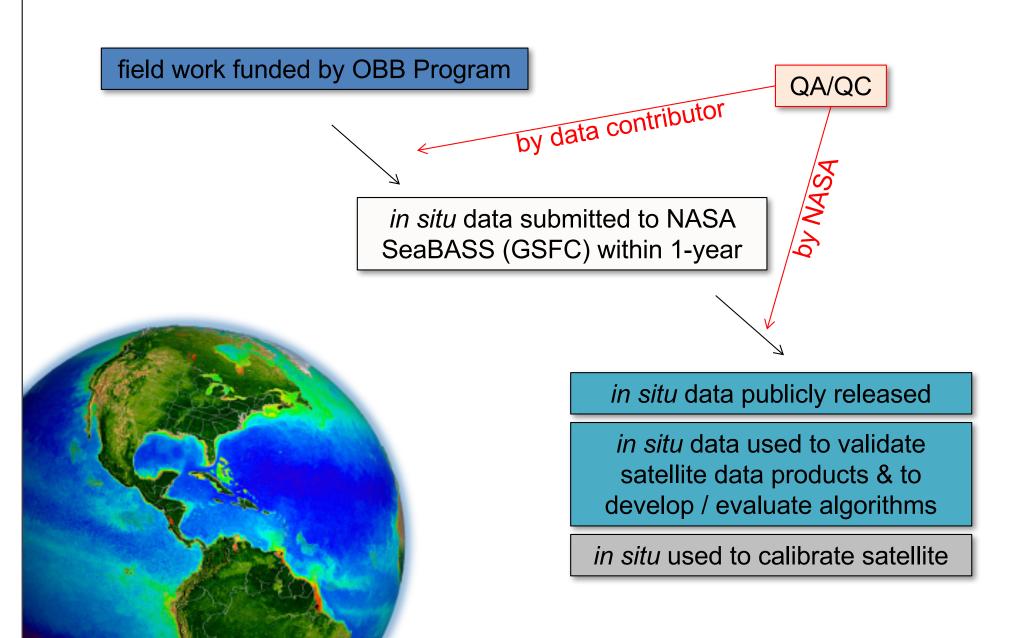
great field data enable great satellite data products

an abundance of field data is hard to come by

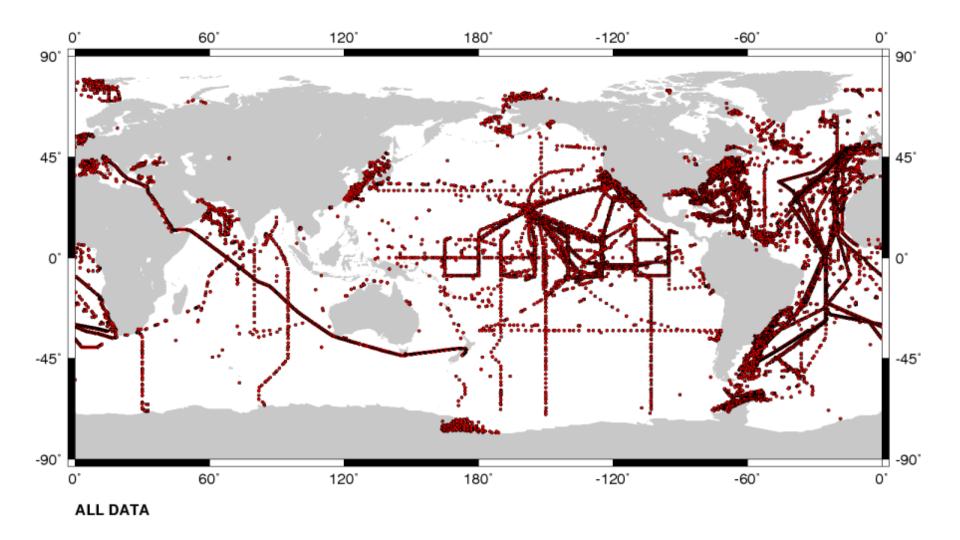
emerging technologies can provide rich data streams

QA/QC metrics are essential (or this all falls apart) = quality assurance & quality control

NASA Ocean Biology & Biogeochemistry Program



SeaBASS @ seabass.gsfc.nasa.gov



AOPs, IOPs, carbon stocks, CTD, pigments, aerosols, etc. continuous & discrete profiles; some fixed observing or along-track

outline

great field data enable great satellite data products

an abundance of field data is hard to come by

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QA/QC metrics are essential (or this all falls apart)

great field data enable great satellite data products

satellite vicarious calibration (instrument + algorithm adjustment)

satellite data product validation

bio-optical algorithm development, tuning, & evaluation

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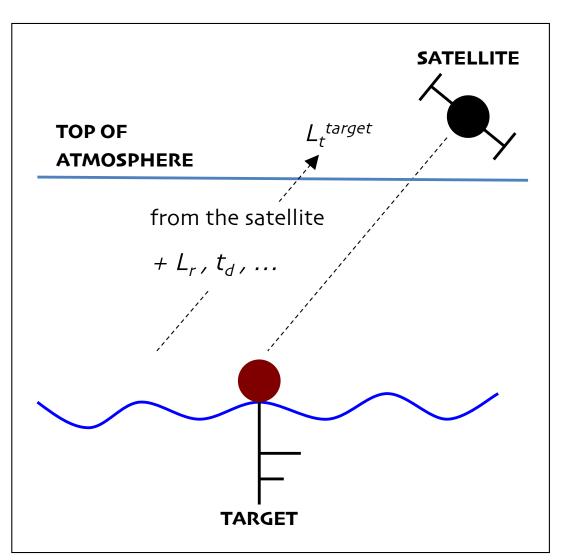
vicarious calibration

what is vicarious calibration?

spectral on-orbit calibrations

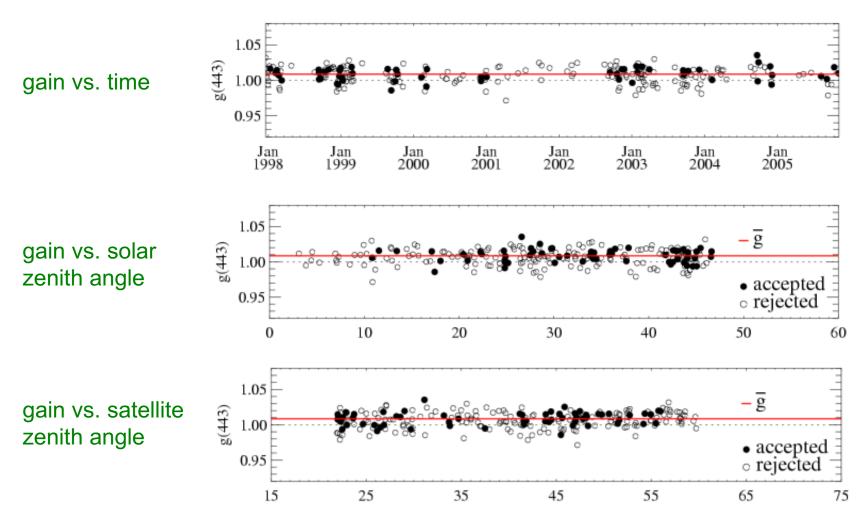
- 1. pre-launch instrument calibration
 - e.g., focal plane temperature
- 2. temporal calibration
 - reference Sun or Moon
- 3. absolute (vicarious) calibration
 - reference Earth surface
 - final, single gain adjustment
 - calibration of the combined instrument + algorithm system

$$g = L_t^{target} / L_t^{satellite}$$



vicarious calibration

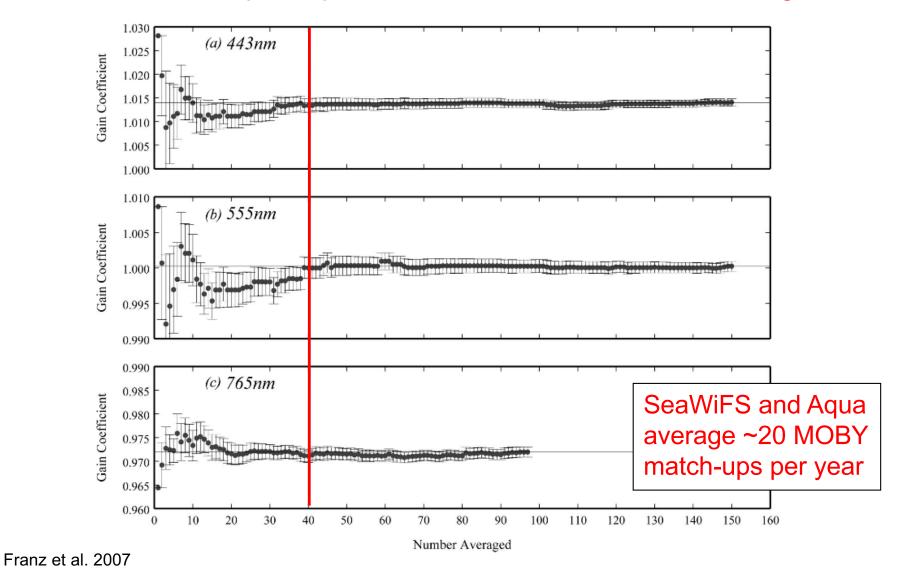
a single, spectral radiometric adjustment



Franz et al. 2007

vicarious calibration

~40 match-ups required to achieve "stable" vicarious gain



operational vicarious calibration

MOBY - the Marine Optical BuoY

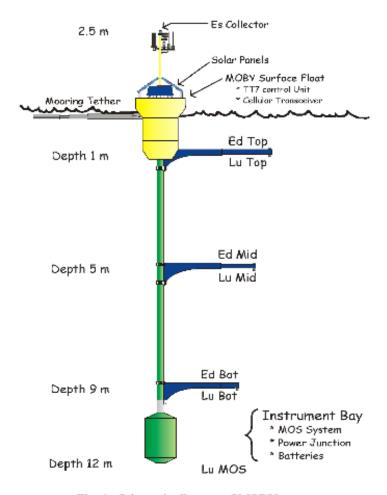


Fig. 1. Schematic diagram of MOBY.

maintained by UMiami, NOAA, NIST, & Moss Landing Marine Laboratory

20 miles west of Lanai, Hawaii

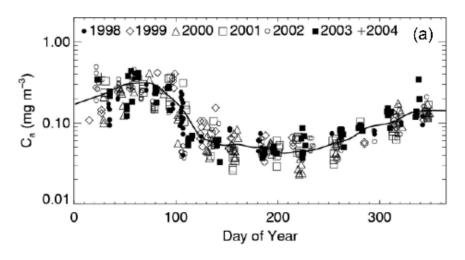
 $L_u(\lambda)$ and $E_d(\lambda)$ at nominal depths of 1, 5, and 9 meters, plus $E_s(\lambda)$

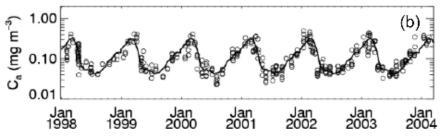
spectral range is 340-955 nm & spectral resolution is 0.6 nm

hyperspectral data convolved to specific bandpasses of each satellite

model-based vicarious calibration

build a climatology using a long-term Chl record (this is for BATS, near Bermuda) ...





$$L_{wn}(\lambda) = F(ChI)$$

... then, develop a $L_{wn}(\lambda)$ or $R_{rs}(\lambda)$ climatology using an ocean reflectance model (e.g., Morel & Maritorena 2001)

Werdell et al. 2007

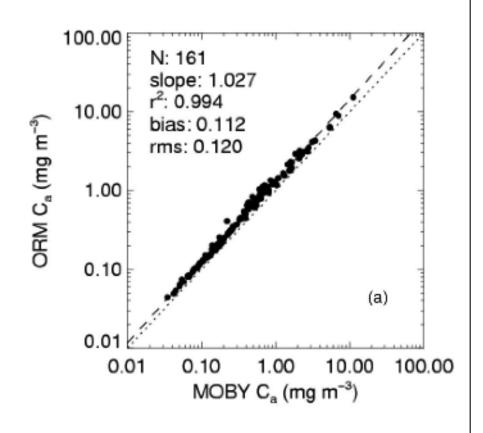
model-based vicarious calibration

Table 3. Percent Differences^a Between the MOBY and ORM g

	412	443	490	510	555	670
BATS	-0.31	-1.18	-1.14	-0.52	0.14	-0.07
HOTS	-0.74	-0.53	-0.48	-0.14	0.44	-0.21
BATS + HOTS	-0.52	-0.86	-0.81	-0.33	0.29	-0.13

^aCalculated using $(\bar{g}_{\text{ORM}} - \bar{g}_{\text{MOBY}}) \times 100\%/\bar{g}_{\text{MOBY}}$.

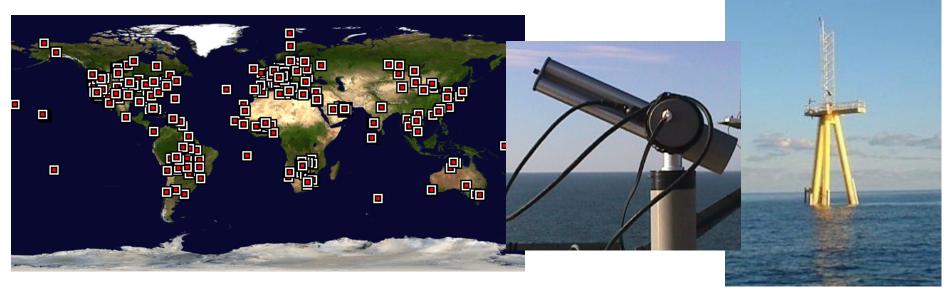
model-based gains typically differ from MOBY gains by < 1%



Werdell et al. 2007

alternative data for vicarious calibration

AERONET (fixed-above water platforms)



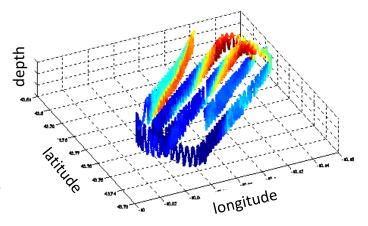


buoy networks



gliders, drifters, & other autonomous platforms

towed & underway sampling



alternative data for vicarious calibration

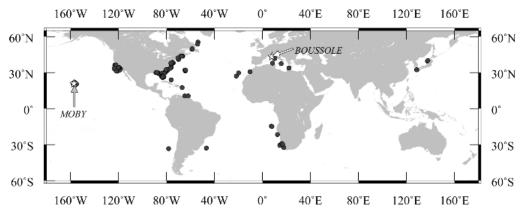


Fig. 1. Map showing the locations for the *in situ* data used in this study.

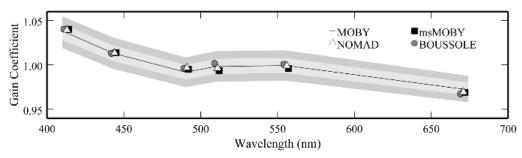


Fig. 3. Vicarious calibration coefficients as a function of wavelength. The standard MOBY-derived \bar{g}_{λ}' (solid curve) are overplotted by the msMOBY-, NOMAD-, and BOUSSOLE-derived \bar{g}_{λ}' . The shaded regions indicate the ranges for the first (light-gray) and second (dark-gray) standard deviations of the mean for \bar{g}_{λ}' .

Bailey et al. 2008

gains calculated using alternative *in situ* data typically differ from MOBY by < 0.3%

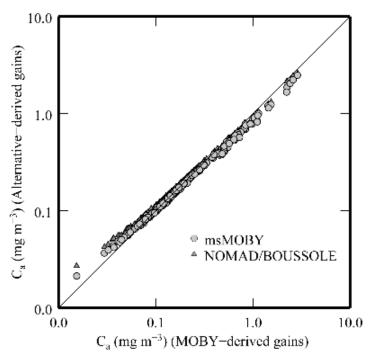


Fig. 7. Satellite-derived chlorophyll estimated from the two alternative \bar{g}' gain sets (msMOBY and NOMAD/BOUSSOLE) plotted versus the corresponding chlorophyll estimated from the standard MOBY \bar{g} .

selecting vicarious calibration sources

the gains shown previously for the multiple "ground-truth" targets differ only from 0.3 to 1%, but there are spectral dependencies in their differences ...

spectral differences impart changes in derived products

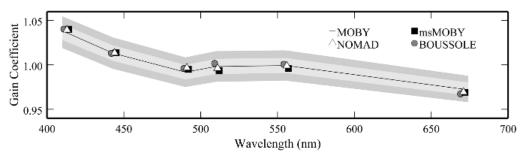


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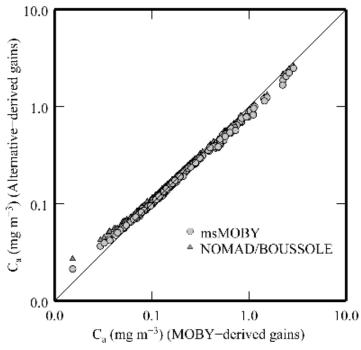


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great field data enable great satellite data products

satellite vicarious calibration (instrument + algorithm adjustment)

satellite data product validation

bio-optical algorithm development, tuning, & evaluation

Level-2 match-ups

general flow of match-up process, with exclusion criteria

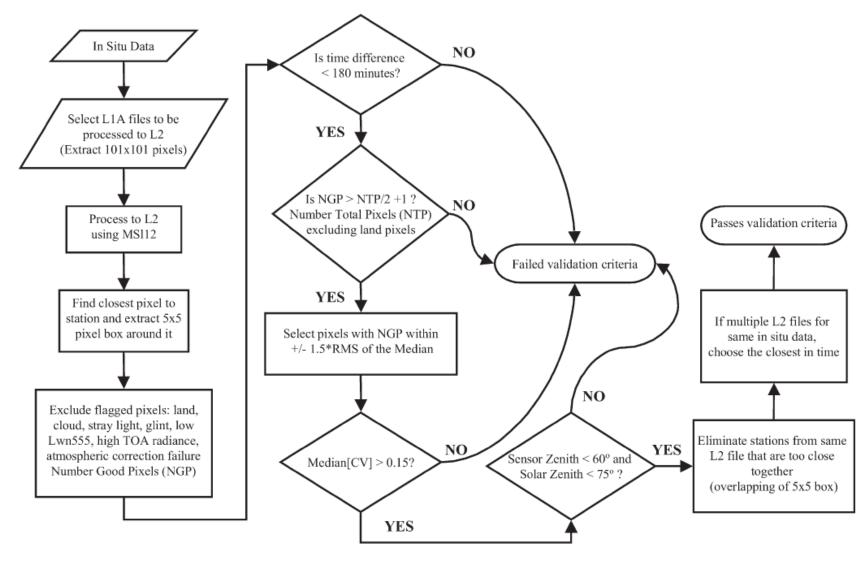


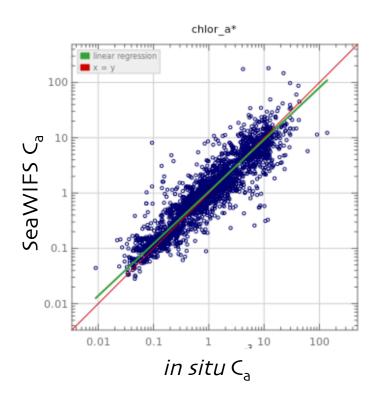
Fig. 1. Flowchart of the validation process highlighting the applied exclusion criteria.

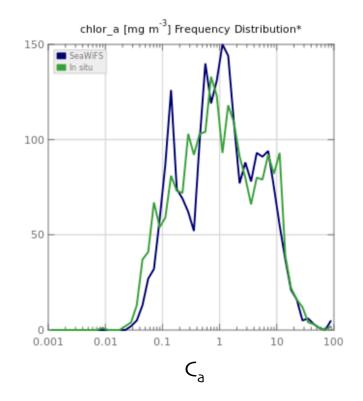
Level-2 match-ups

comparison of "coincident" in situ & satellite measurements

Product Name	SeaWiFS Range	In situ Range	#	Best Fit Slope*	Best Fit Intercept*	R ² *	Median Ratio	Median % Difference	RMSE*
chlor_a	0.02818 - 181.40287	0.00900 - 138.04700	2244	0.94136	0.02518	0.82849	1.07149	36.78435	0.29550

^{*} statistical calculations based on log10 (implies ignoring values of zero)



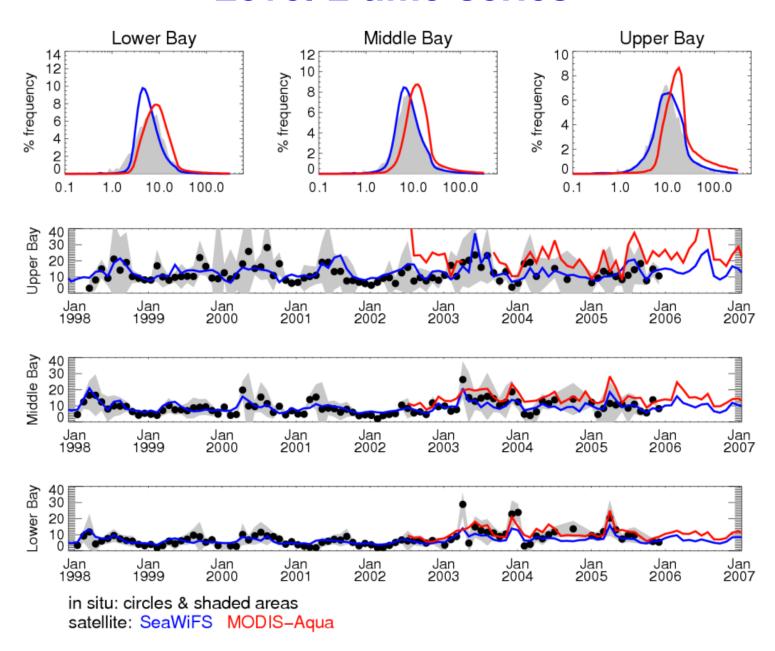


Bailey & Werdell 2006

https://seabass.gsfc.nasa.gov/search

Chesapeake Bay

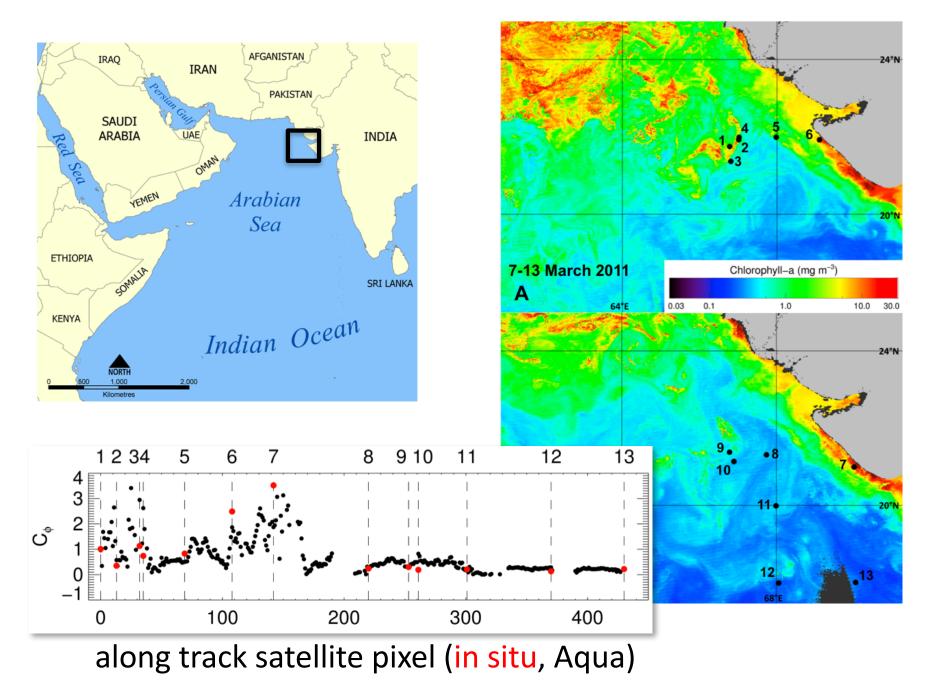
Level-2 time-series



Werdell et al. 2009

Chl-a (mg m⁻³)

along-track comparisons

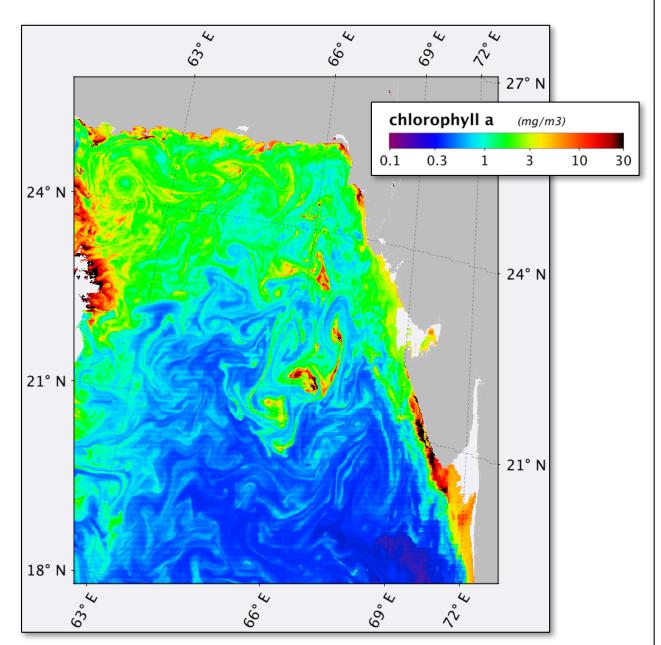


common limitations

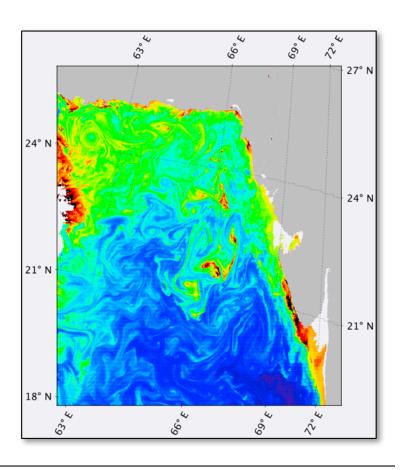
quality of *in situ* data is highly variable & difficult to assess *in situ* data coverage is limited, both geographically & temporally availability of *in situ* data in future is unknown highly localized (~meters) measurements represent pixel (>km) area satellite-to-*in situ* comparisons require expertise to prepare & evaluate generally useful only for assessing static biases in final products

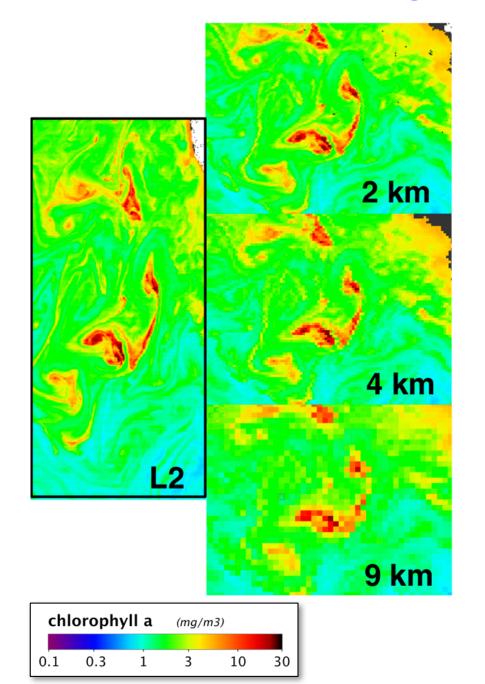
- horizontal resolution
- temporal resolution
- vertical resolution



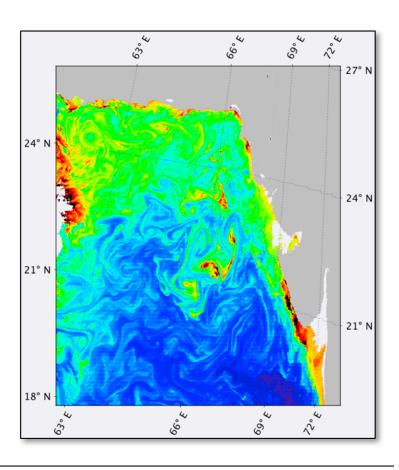


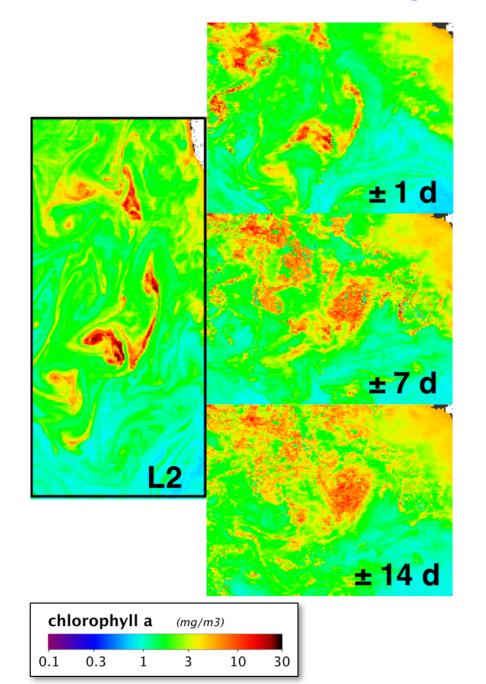
- horizontal resolution
- temporal resolution
- vertical resolution



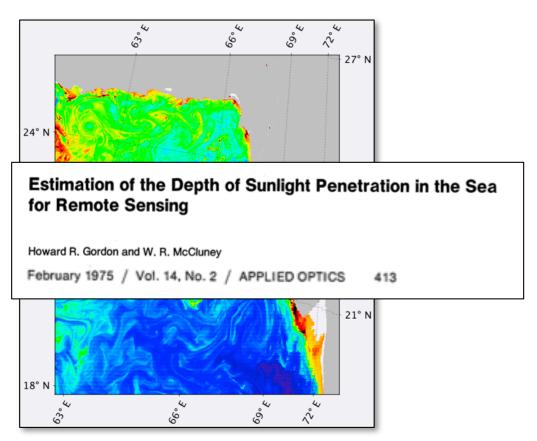


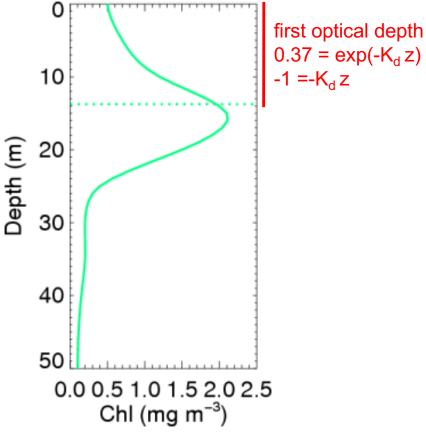
- horizontal resolution
- temporal resolution
- vertical resolution





- horizontal resolution
- temporal resolution
- vertical resolution

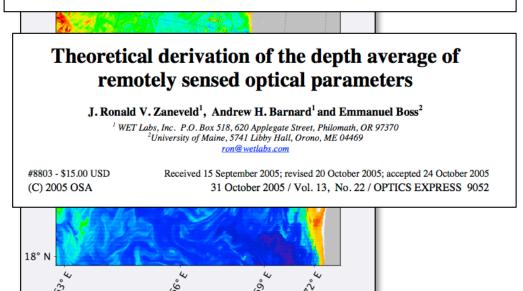


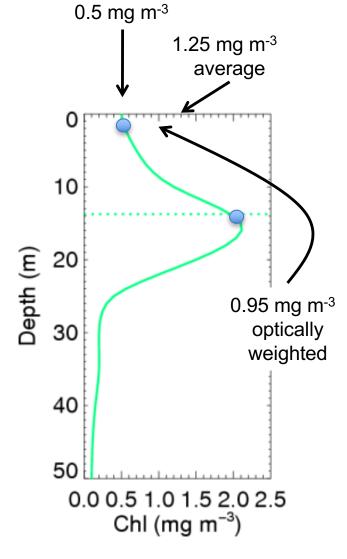


data collection

- horizontal resolution
- temporal resolution
- vertical resolution

not only is the resolution of vertical sampling important, but we must also understand (accept & ultimately consider) what the satellite sees & does not see





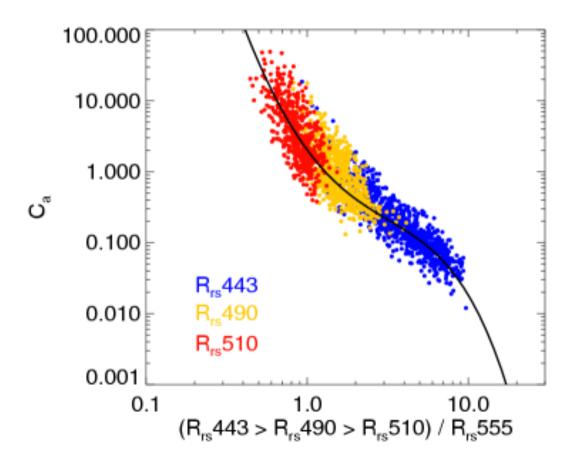
great field data enable great satellite data products

satellite vicarious calibration (instrument + algorithm adjustment)

satellite data product validation

bio-optical algorithm development, tuning, & evaluation

in-water algorithms



R_{rs} related to pigments, IOPs, carbon stocks, etc.

what satellite sees what you might want to study

atmospheric correction

in situ data are used in the development of:

aerosol tables (via AERONET)

the correction for non-zero $R_{rs}(NIR)$

the correction for bidirectional effects (f/Q)

the correction for spectral bandpass effects

outline

great field data enable great satellite data products

an abundance of field data is hard to come by

emerging technologies can provide rich data streams

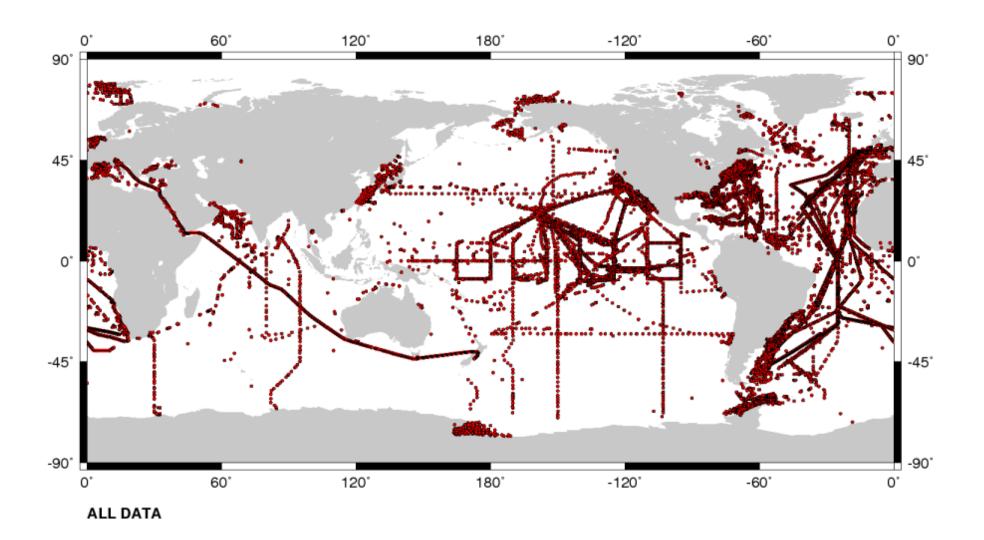
QA/QC metrics are essential (or this all falls apart)

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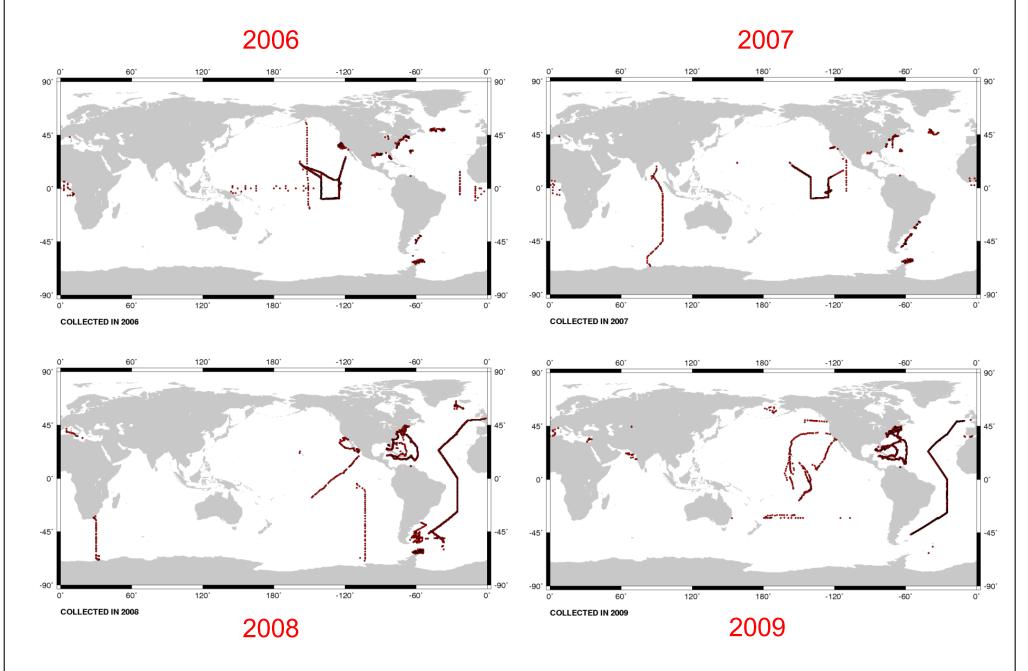
spatial & temporal distributions

"complete" suites of measurements (R_{rs}, IOPs, biogeochemistry)

SeaBASS @ seabass.gsfc.nasa.gov



SeaBASS holdings by year: 2006-2009



Level-2 match-ups

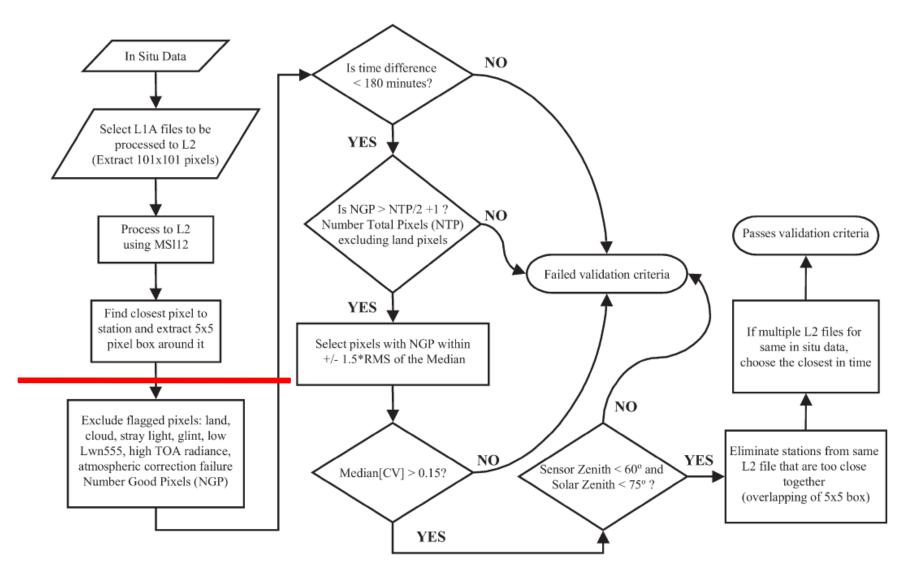
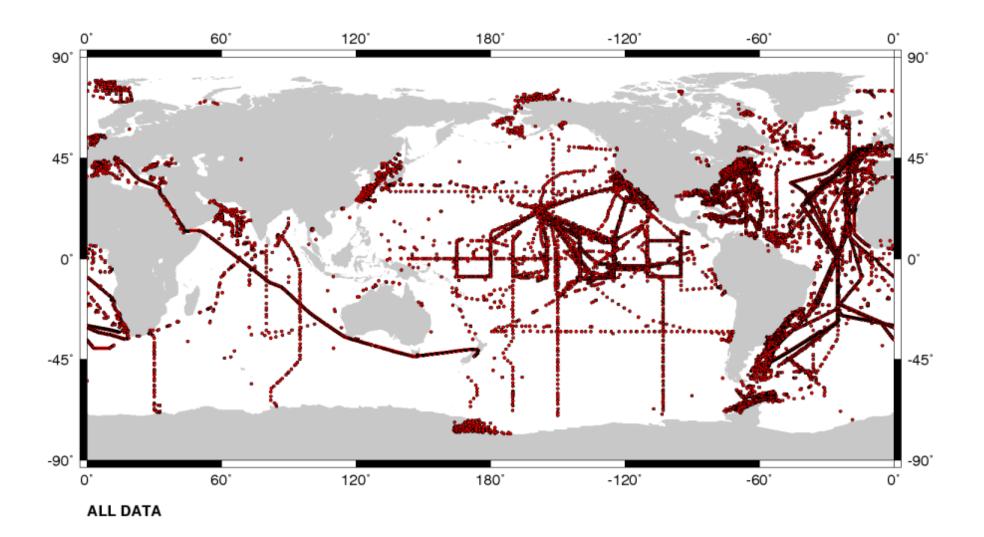


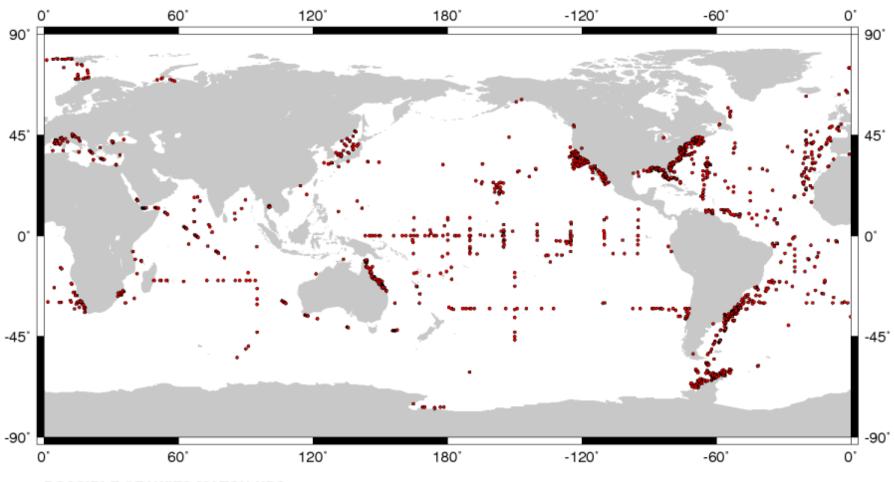
Fig. 1. Flowchart of the validation process highlighting the applied exclusion criteria.

S.W. Bailey and P.J. Werdell, "A multi-sensor approach for the on-orbit validation of ocean color satellite data products," Rem. Sens. Environ. 102, 12-23 (2006).

all available SeaBASS data

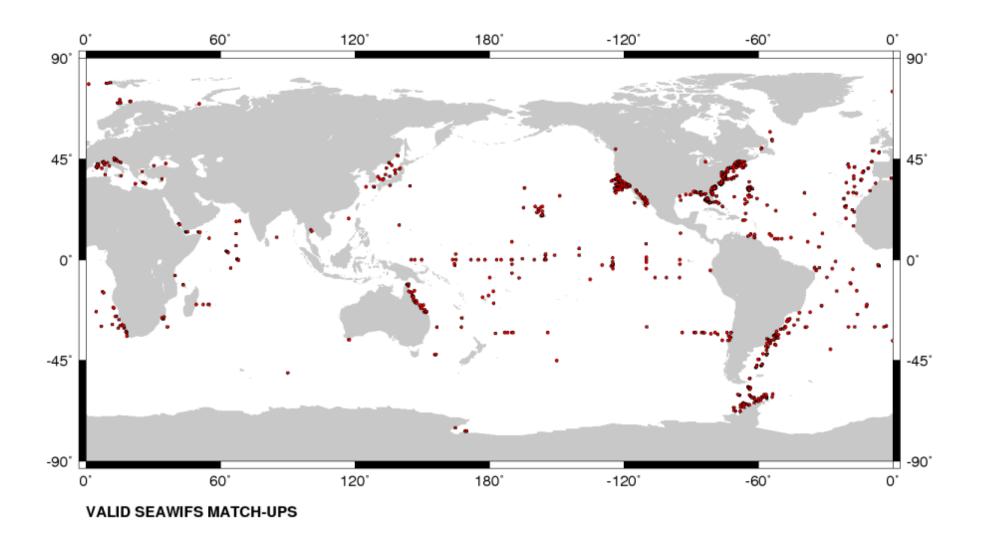


coincident SeaWiFS & in situ data

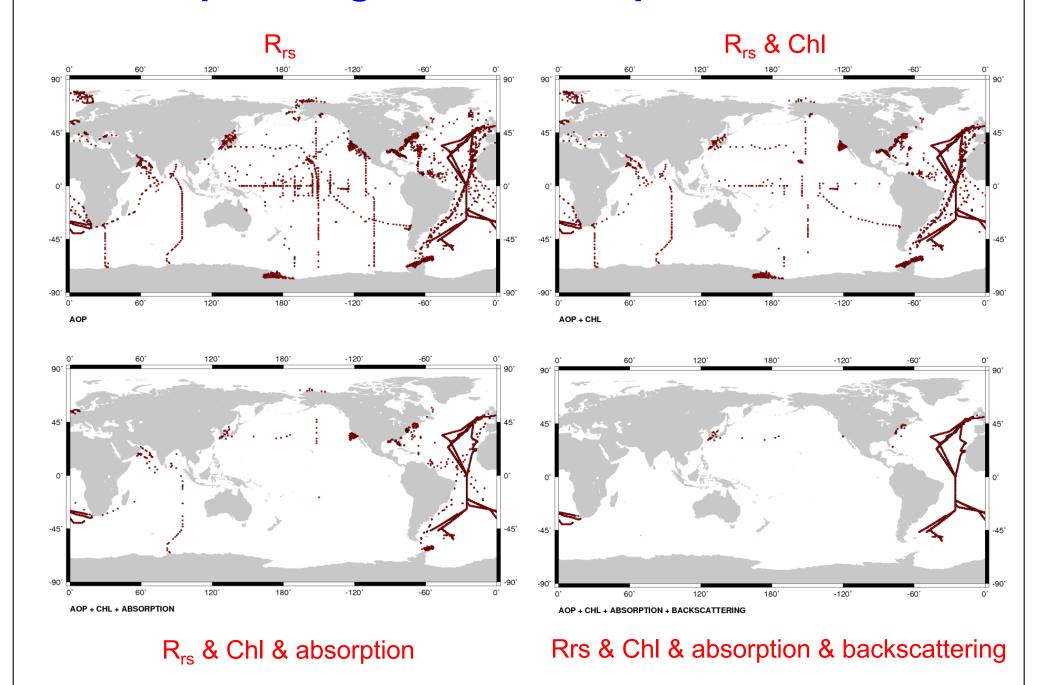


POSSIBLE SEAWIFS MATCH-UPS

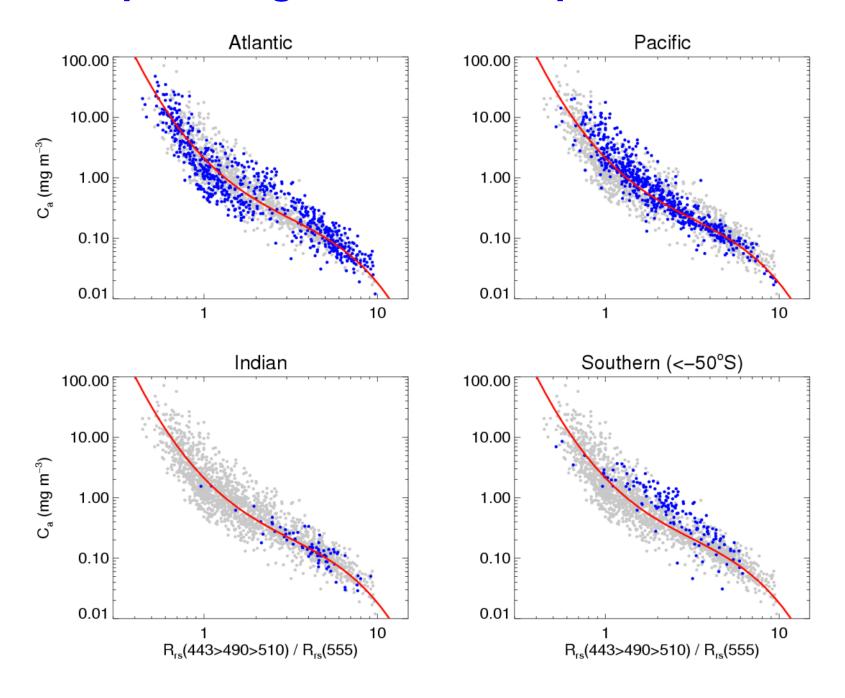
valid SeaWiFS match-ups



bio-optical algorithm development data sets



bio-optical algorithm development data sets



outline

great field data enable great satellite data products

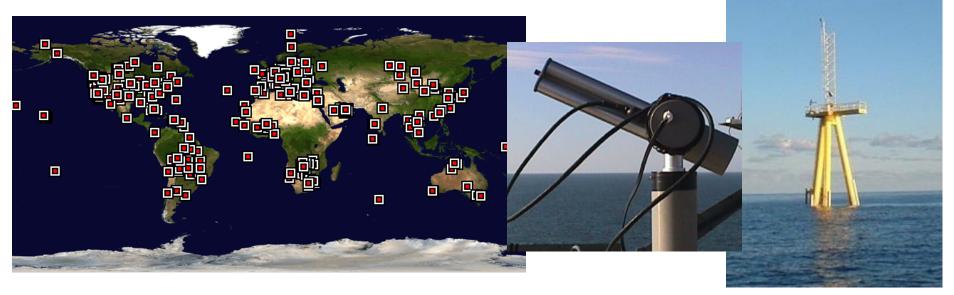
an abundance of field data is hard to come by

emerging technologies can provide rich data streams

QA/QC metrics are essential (or this all falls apart)

moving forward – community innovations

AERONET (fixed-above water platforms)



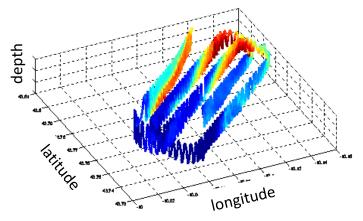


buoy networks



gliders, drifters, & other autonomous platforms

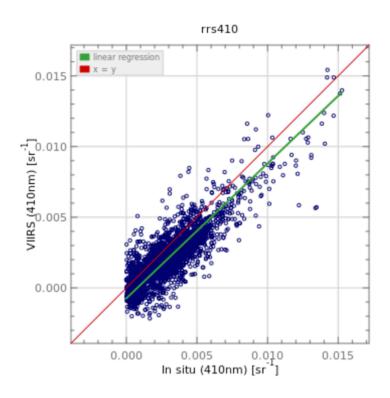
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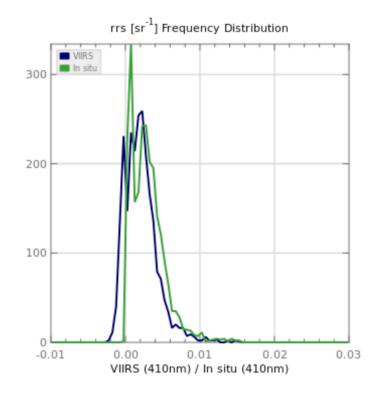


validation exercises using autonomous data

AERONET-OC match-ups with VIIRS (satellite data since Feb 2012)

Product Name	VIIRS Range	In situ Range	#	Best Fit Slope	Best Fit Intercept	R ²	Median Ratio	Median % Difference	RMSE
rrs410	-0.00216 - 0.01543	-0.00000 - 0.01527	2381	0.95545	-0.00074	0.73282	0.66572	47.77592	0.00148
rrs443	-0.00075 - 0.02072	0.00017 - 0.01871	2385	1.01295	-0.00055	0.85972	0.81181	28.55564	0.00110
rrs486	0.00045 - 0.02578	0.00058 - 0.02530	2387	0.90566	-0.00030	0.91740	0.81652	21.65905	0.00127
rrs551	0.00087 - 0.02462	0.00128 - 0.02633	2385	0.91013	-0.00023	0.93221	0.84637	17.41917	0.00121
rrs671	-0.00024 - 0.00985	-0.00000 - 0.01048	2384	0.96901	-0.00014	0.86795	0.82075	24.85650	0.00043



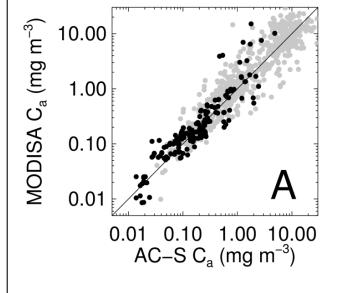


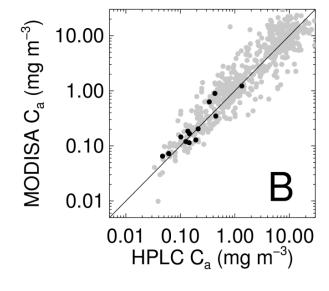
validation exercises using autonomous data

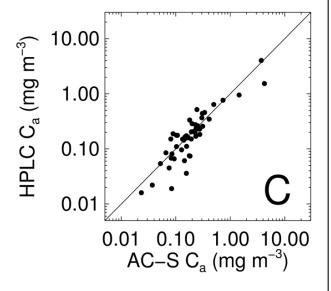
Tara Oceans expedition (2009-2012) AC-S products vs. MODISA







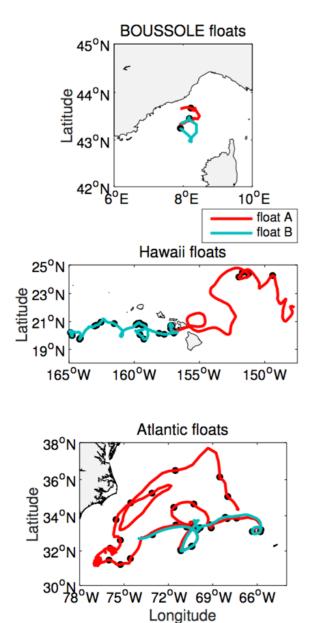


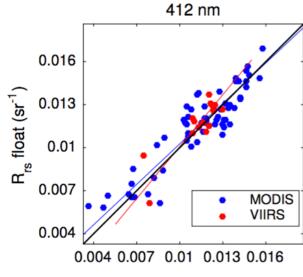


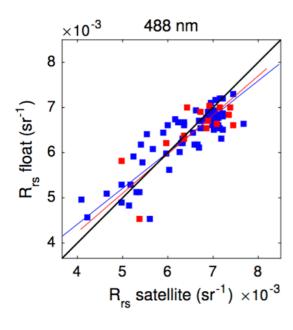
validation exercises using autonomous data

Autonomous profiling float radiometry vs. MODISA & VIIRS









outline

great field data enable great satellite data products

an abundance of field data is hard to come by

emerging technologies can provide rich data streams

QA/QC metrics are essential (or this all falls apart)

QA/QC metrics are essential

a single entity (e.g., NASA or equivalent) cannot collect sufficient volumes of *in situ* data to satisfy its operational calibration & validation needs

following, flight projects rely on multiple entities to collect in situ data

protocols for data collection & QA/QC ensures measurements are of the highest possible quality – well calibrated & understood, properly & consistently acquired, within anticipated ranges

robust QA/QC provides confidence in utility & quality of data

QA/QC metrics are essential

QA/QC methods vary in maturity – exist for many established instruments & platforms, but not always for newer or autonomous systems

QA/QC methods are ideal when:

they accommodate routine time-series reprocessing they are well documented they consistently maintain consensus from vendor → institution → end user revisited by subject matter experts routinely

recommend invested agencies/institutions facilitate routine activities (workshops, round robins, inter-comparisons) to revisit QA/QC protocols

consider, e.g., variance in AOP data sets

AOP instrumentation in SeaBASS or available commercially:

- many companies & instruments
 Biospherical, Satlantic, HOBI, Trios/Ramses, DALEC, SIMBAD-A, ASD, Spectron, custom
- many platforms & deployment strategies
 profilers, buoys, above-water (ship, permanent, hand-held), gliders, AUVs

dynamic range of problem set is growing:

- new missions emphasize research in shallow, optically complex water
- spectral domain stretching to UV and SWIR
- new missions have immediate, operational requirements





IOCCG Ocean Optics & Biogeochemical Protocols for Satellite Ocean Colour Sensor Validation Home » What We Do » IOCCG Publications » IOCCG Ocean Optics & Biogeochemical Protocols for Satellite Ocean-Colour Sensor Validation

In situ optical and biogeochemical in- and above-water measurements are critical for calibration and validation of satellite ocean colour radiometry data products, and for refinement of ocean colour algorithms. During the SeaWiFS era, NASA commissioned the development of a series of ocean optical measurement protocols (see NASA Ocean Optics Protocols for Satellite Ocean Color Sensor Validation) which have served as international reference standards ever since, and have promoted the collection and assembly of climate quality, ocean optical datasets by the global ocean colour community. Since publication of the last revision in 2004, there have been major advances in instrumentation and observing capability, so these community-vetted protocols need to be revised to account for new, emerging, and planned capabilities and modes of deployment.

Over the past few years NASA has sponsored several international workshops with experts (including breakout workshops at the International Ocean Colour Science meetings), to update and develop new community consensus protocols for ocean colour sensor validation. The newly drafted protocols will be made available to the international user community on this webpage for a period of time for testing, public comment and review, before they are accepted as international reference standards. Once accepted, the protocols will receive a publication date and version number (e.g., v1.0), and will also have a digital object identifier (doi). These revised protocols will be revisited periodically to determine if enough changes have taken place to warrant a significant update, in which case a new version number will be assigned.

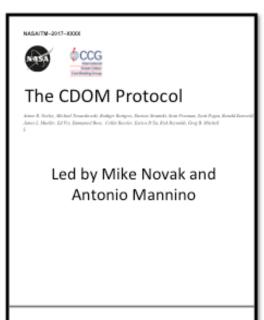
http://ioccg.org/what-we-do/ioccg-publications/ocean-optics-protocols-satellite-ocean-colour-sensor-validation/

- NASA resumed efforts in 2013 (last effort 2003)
- IOCCG joined as a collaborator
- NASA T/M style
- 30-60 days for public comment
- digital updates ~1-3 years as appropriate
- reprinting ~10-15 years with accumulated or major updates

online for public comment (end of June 2017)

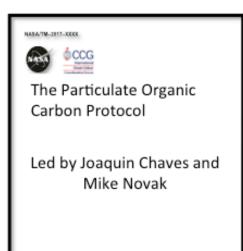
online for public comment (Fall 2017)

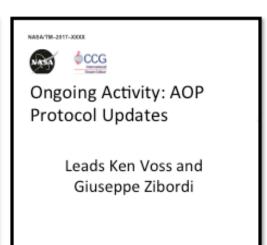


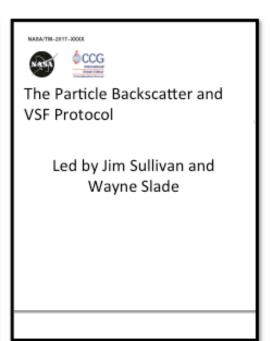




ongoing and in development









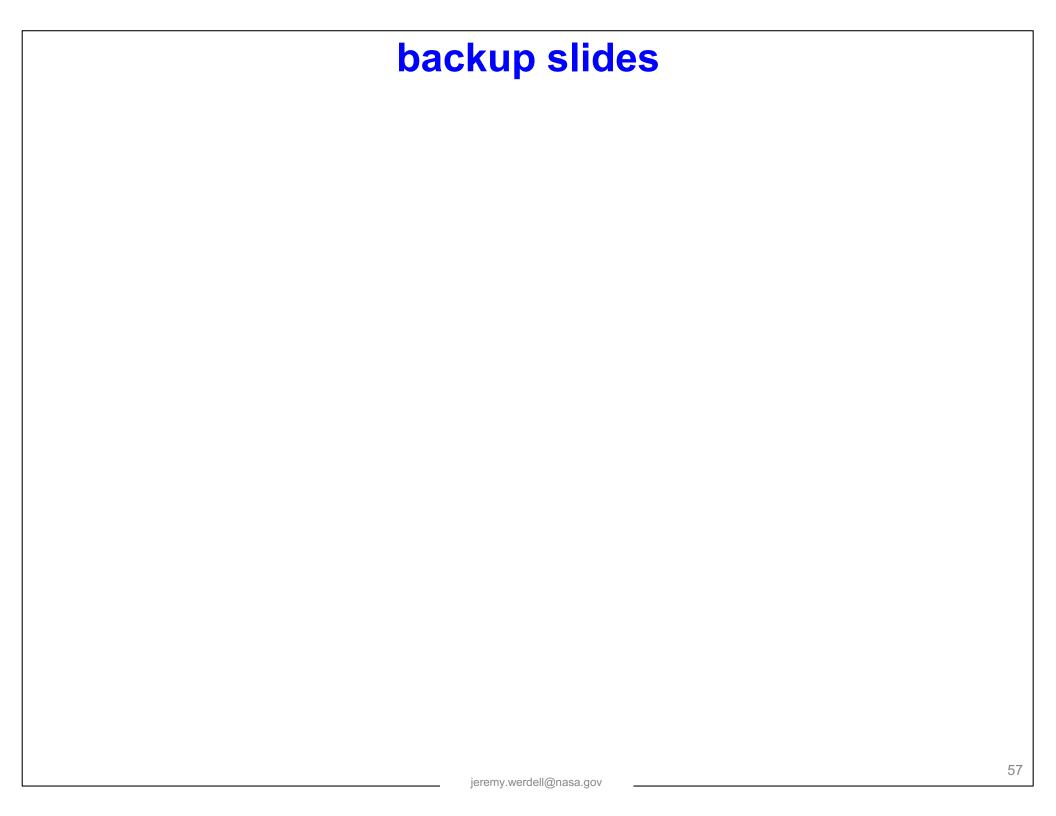
Phytoplankton Taxonomy Working Group

Working group to establish data standards and practices for taxon-resolved phytoplankton observations - Pls: Heidi Sosik (WHOI), Christopher Proctor (NASA GSFC/SSAI), Aimee Neeley (NASA GSFC/SSAI), Ivona Cetinić (NASA GSFC/USRA)

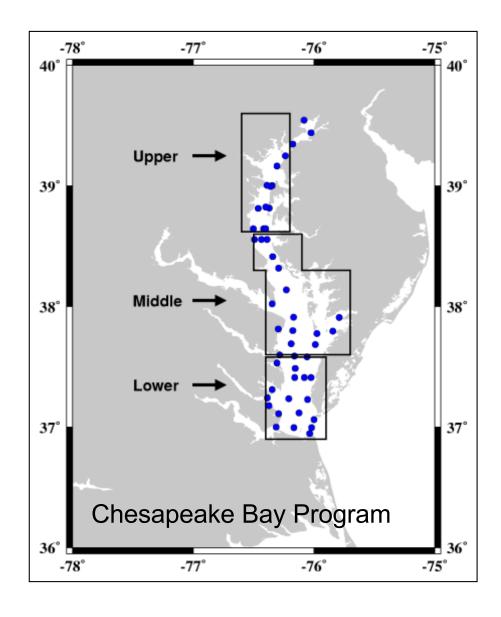
Objective: In an effort to facilitate community-wide access to phytoplankton data products that support critical satellite algorithm development and validation, this working group will convene relevant expertise (e.g., phytoplankton ecology and taxonomy, data systems, informatics, etc.) to develop a set of standards and best practices for phytoplankton taxonomy data.

For the future:
Particle sizes
Productivity





Level-2 time-series





http://www.chesapeakebay.net

routine data collection since 1984 12-16 cruises / year

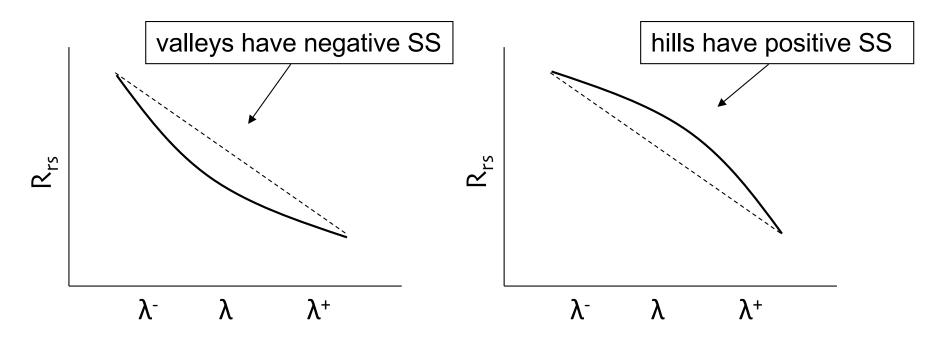
49 stations19 hydrographic measurements

algal biomass water clarity dissolved oxygen others

population statistics for vicarious calibration

compare spectral shapes of in situ & satellite populations

$$SS(\lambda) = R_{rs}(\lambda) - R_{rs}(\lambda^{-}) - \left[R_{rs}(\lambda^{+}) - R_{rs}(\lambda^{-})\right] \left(\frac{\lambda - \lambda^{-}}{\lambda^{+} - \lambda^{-}}\right)$$

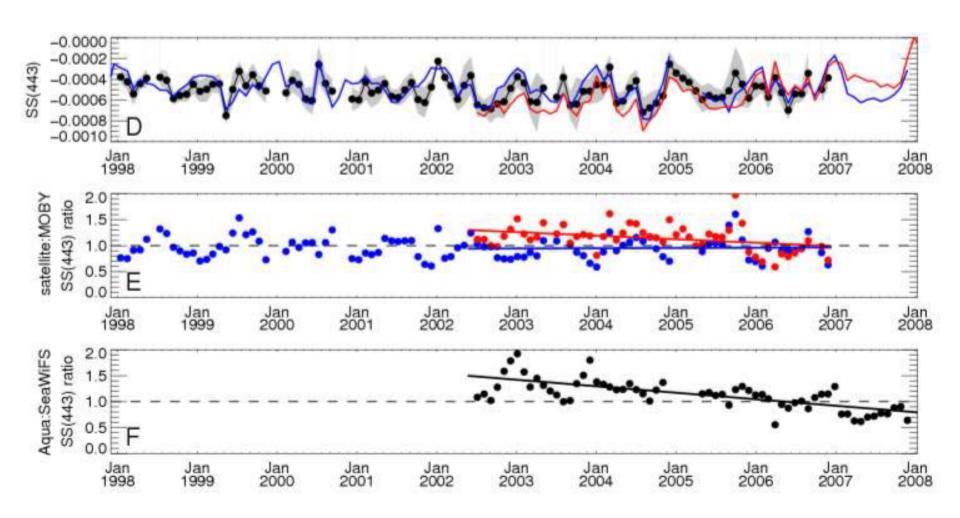


spectral shape @ 443 nm, SS(443), uses R_{rs}(412), R_{rs}(443), & R_{rs}(490)

Stumpf & Werdell 2010

population statistics for vicarious calibration

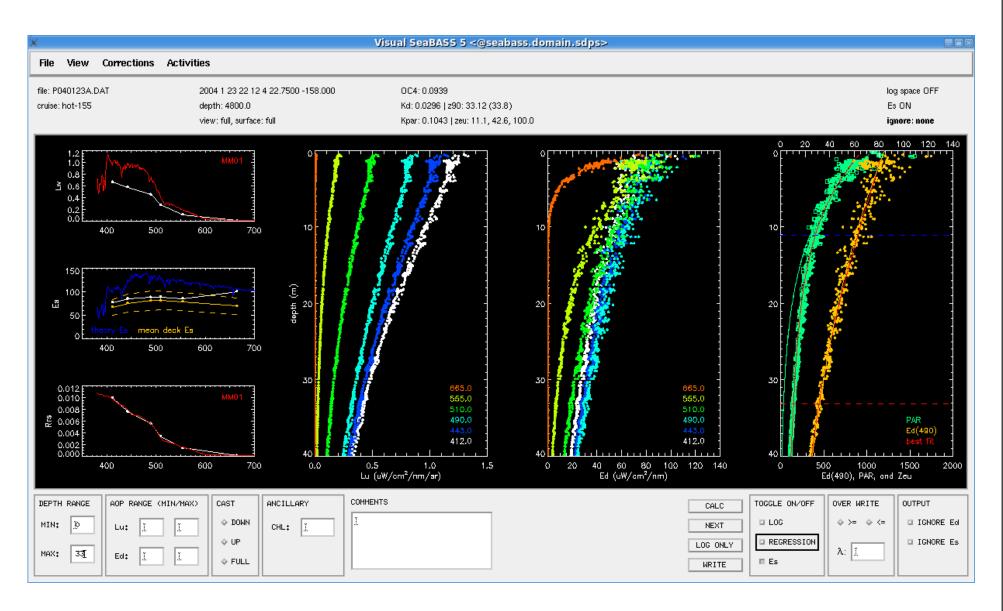
in situ, SeaWiFS, & MODIS-Aqua spectral shapes compared at MOBY site



Stumpf & Werdell 2010

AOP data analysis

$$L_u(z)$$
, $E_d(z) \rightarrow L_w$, E_s



inversion models

several flavors of a "semi-analytical" inversion algorithm ...

$$R_{rs} \approx func\left(\frac{b_b}{a+b_b}\right)$$

 $R_{rs} \approx func \left(\frac{b_b}{a + b_b} \right)$ satellite provides $R_{rs}(\lambda)$ a(λ) and $b_b(\lambda)$ are desired products

Spectral Optimization:

- define shape functions for (e.g.) $b_{bp}(\lambda)$, $a_{dq}(\lambda)$, $a_{ph}(\lambda)$
- solution via L-M, matrix inversion, etc.
- ex: RP95, HL96, GSM

Bulk Inversion:

- no predefined shapes
- piece-wise solution: $b_{bp}(\lambda)$, then $a(\lambda)$, via empirical $K_d(\lambda)$ via RTE
- ex: LS00

Spectral Deconvolution:

- partially define shape functions for $b_{bp}(\lambda), a_{dq}(\lambda)$
- piece-wise solution: $b_{bp}(\lambda)$, then $a(\lambda)$, then $a_{dq}(\lambda) + a_{ph}(\lambda)$
- ex: QAA, PML, NIWA