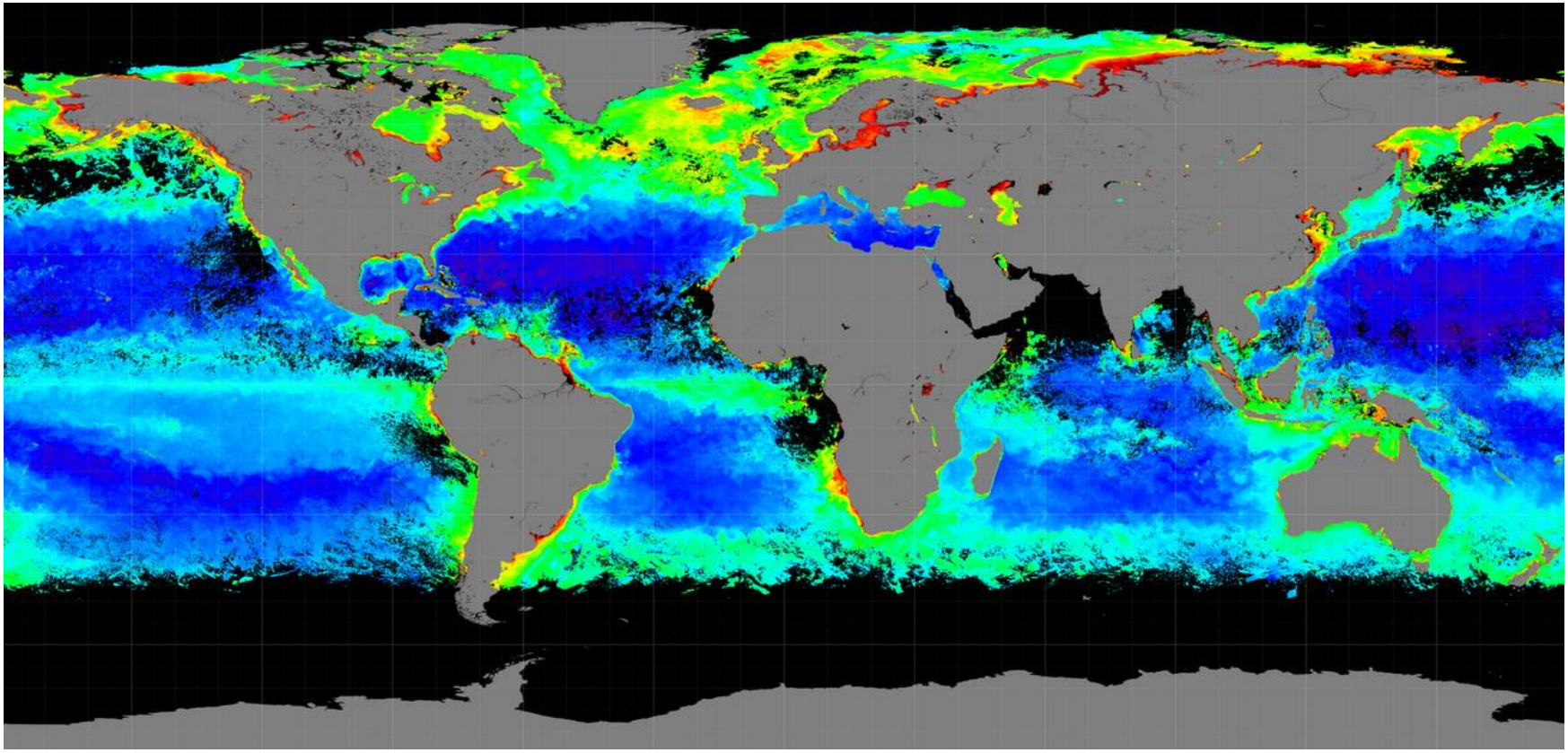
Inherent Optical Properties (IOPs)

Lecture 2: Inversion

Chl distribution of the global oceans



(OBPG)

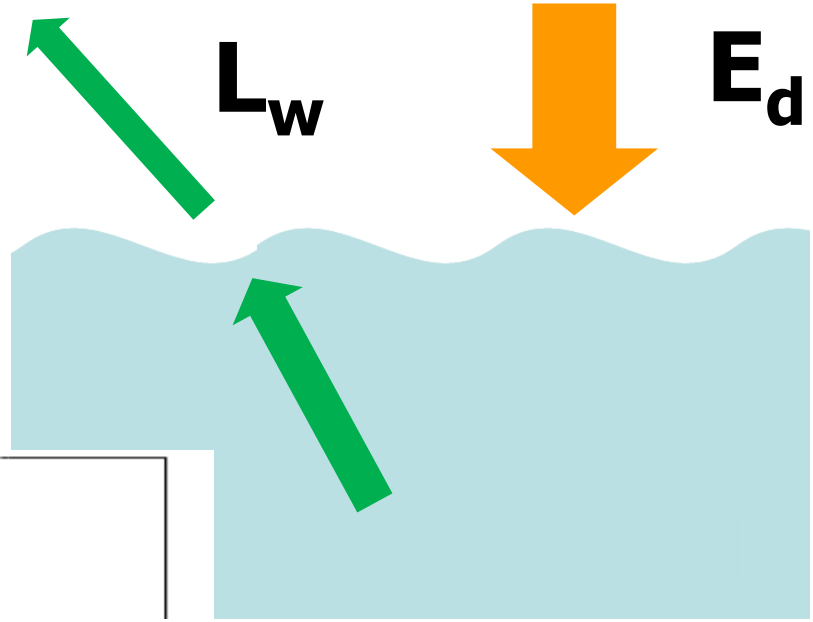
$$[Chl] = f_1\left(R_{rs}(\lambda_i)/R_{rs}(\lambda_j)\right)$$

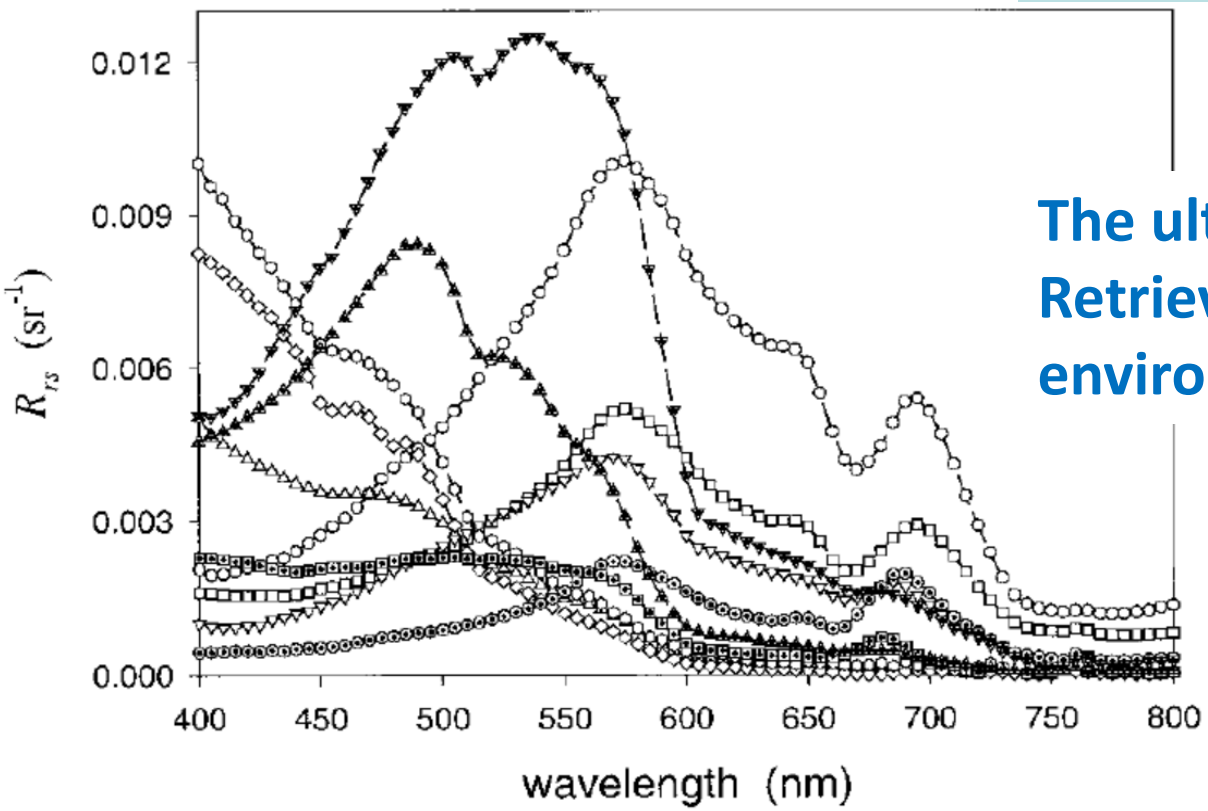
$$R_{rs}(\lambda_i)/R_{rs}(\lambda_j) = f_2\left(\frac{b_{bw}(\lambda_i)+b_{bp}(\lambda_i)}{b_{bw}(\lambda_j)+b_{bp}(\lambda_j)}\frac{a_w(\lambda_j)+a_{ph}(\lambda_j)+a_{dg}(\lambda_j)}{a_w(\lambda_i)+a_{ph}(\lambda_i)+a_{dg}(\lambda_i)}\right)$$

[Chl] is actually an IOP product

Remote-sensing reflectance (sr^{-1}):

$$R_{rs}(\lambda) = \frac{L_w(\lambda, 0^+)}{E_d(\lambda, 0^+)}$$





The ultimate objective of RS: Retrieval useful/important environmental information

How?

algorithm!

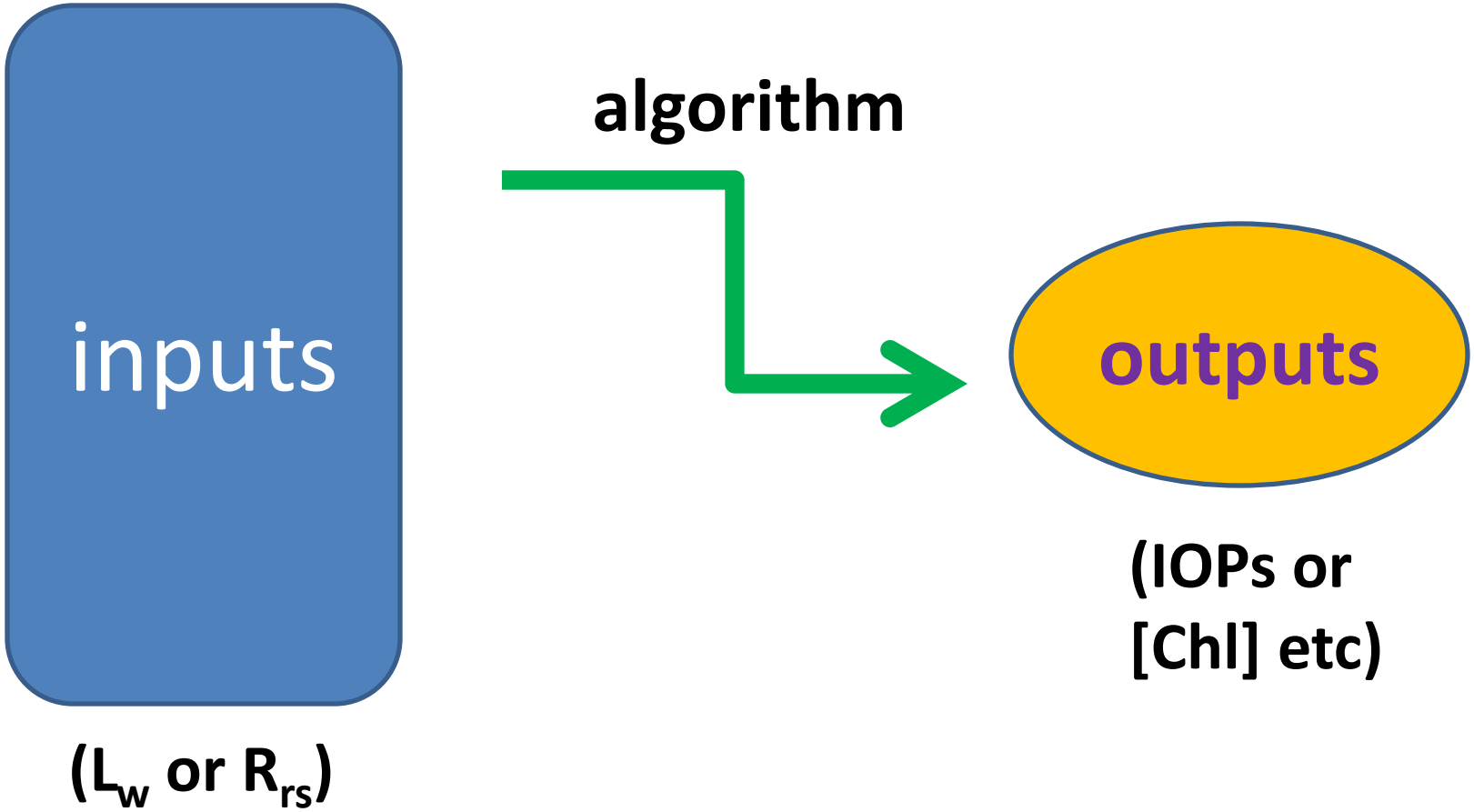
Empirical
(explicit or implicit)

No need: Bio-optical models

Semi-analytical
(algebraic or optimization)

Yes: Bio-optical models

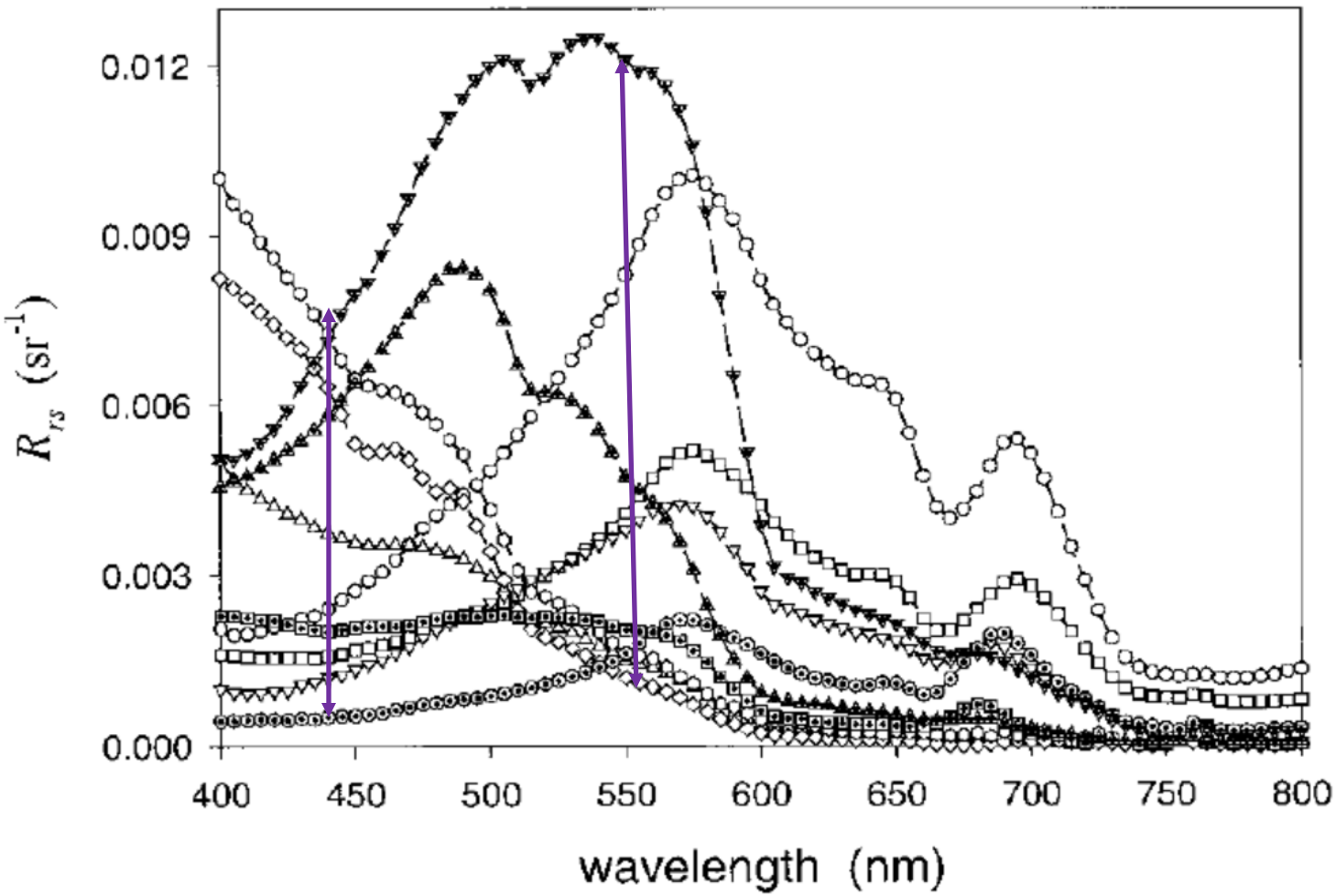
- **Bottom Up Strategy (BUS)**
- **Top Down Strategy (TDS)**


inputs
algorithm
outputs
(IOPs or
[Chl] etc)
(L_w or R_{rs})

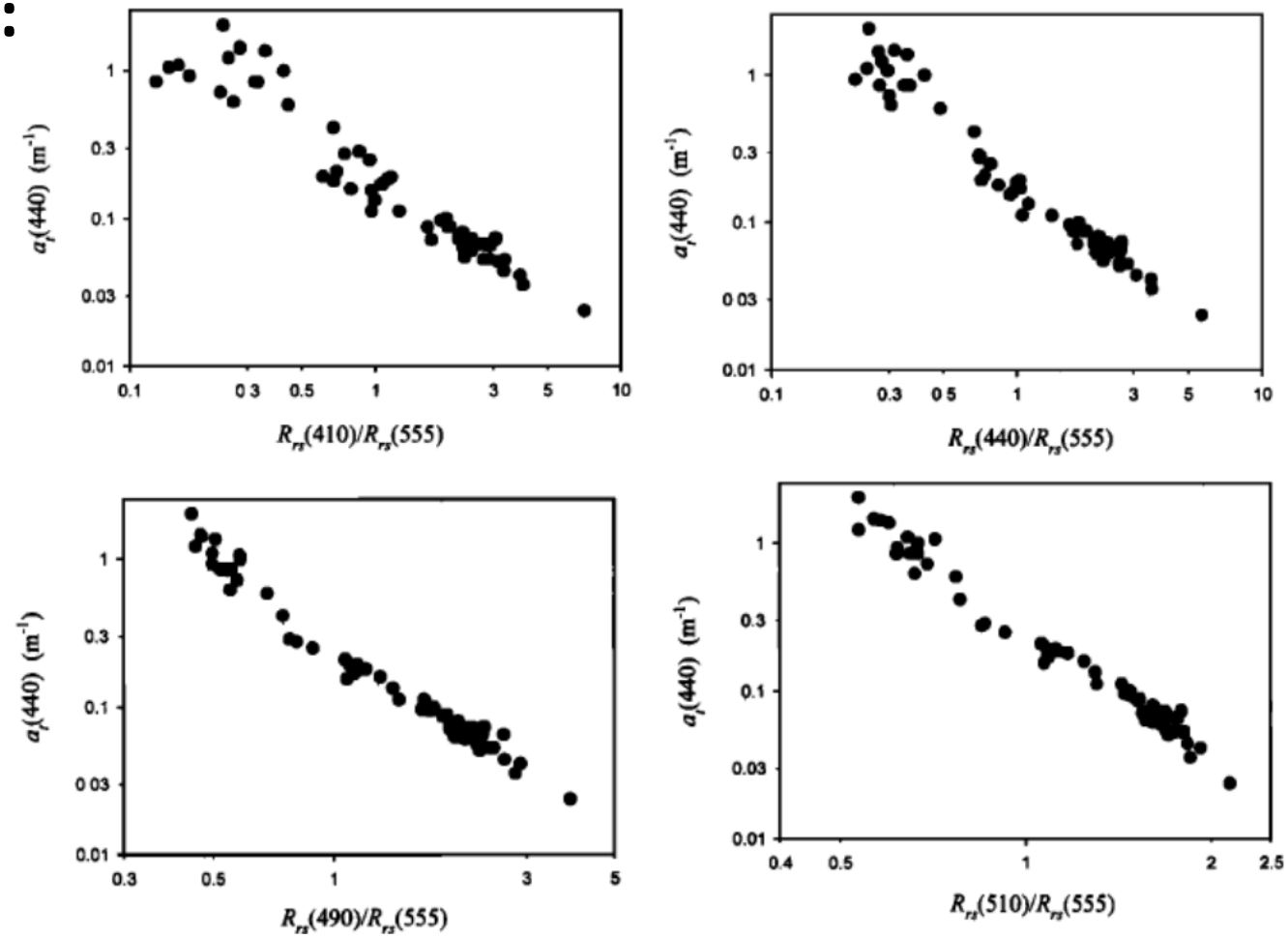
Chl based on band ratio

Algorithm	Type	Result Equation(s)	Band Ratio (R), Coefficients (a)
Global processing (GPs)	power	$C_{13} = 10^{(a0+a1*R1)}$ $C_{23} = 10^{(a2+a3*R2)}$ $[C + P] = C_{13}$; if C_{13} and $C_{23} > 1.5\ \mu g\ L^{-1}$ then $[C + P] = C_{23}$	$R1 = \log(Lwn443/Lwn550)$ $R2 = \log(Lwn520/Lwn550)$ $a = [0.053,\ 1.705,\ 0.522,\ 2.440]$
Clark three-band (C3b)	power	$[C + P] = 10^{(a0+a1*R)}$	$R = \log((Lwn443 + Lwn520)/Lwn550)$ $a = [0.745,\ -2.252]$
Aiken-C	hyperbolic + power	$C_{21} = \exp(a0 + a1*\ln(R))$ $C_{23} = (R + a2)/(a3 + a4*R)$ $C = C_{21}$; if $C < 2.0\ \mu g\ L^{-1}$ then $C = C_{23}$	$R = Lwn490/Lwn555$ $a = [0.464,\ -1.989,\ -5.29,\ 0.719,\ -4.23]$
Aiken-P	hyperbolic + power	$C_{22} = \exp(a0 + a1*\ln(R))$ $C_{24} = (R + a2)/(a3 + a4*R)$ $[C + P] = C_{22}$; if $[C + P] < 2.0\ \mu g\ L^{-1}$ then $[C + P] = C_{24}$	$R = Lwn490/Lwn555$ $a = [0.696,\ -2.085,\ -5.29,\ 0.592,\ -3.48]$
OCTS-C	power	$C = 10^{(a0+a1*R)}$	$R = \log((Lwn520 + Lwn565)/Lwn490)$ $a = [\ 0.55006,\ 3.497]$
OCTS-P	multiple regression	$[C + P] = 10^{(a0+a1*R1+a2*R2)}$	$R1 = \log(Lwn443/Lwn520)$ $R2 = \log(Lwn490/Lwn520)$ $a = [0.19535,\ -2.079,\ -3.497]$
POLDER	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs443/Rrs565)$ $a = [0.438,\ -2.114,\ 0.916,\ -0.851]$
CalCOFI two-band linear	power	$C = 10^{(a0+a1*R)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.444,\ -2.431]$
CalCOFI two-band cubic	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.450,\ -2.860,\ 0.996,\ -0.3674]$
CalCOFI three-band	multiple regression	$C = \exp(a0 + a1*R1 + a2*R2)$	$R1 = \ln(Rrs490/Rrs555)$ $R2 = \ln(Rrs510/Rrs555)$ $a = [1.025,\ -1.622,\ 1.238]$
CalCOFI four-band	multiple regression	$C = \exp(a0 + a1*R1 + a2*R2)$	$R1 = \ln(Rrs443/Rrs555)$ $R2 = \ln(Rrs412/Rrs510)$ $a = [0.753,\ -2.583,\ 1.389]$
Morel-1	power	$C = 10^{(a0+a1*R)}$	$R = \log(Rrs443/Rrs555)$ $a = [0.2492,\ -1.768]$
Morel-2	power	$C = \exp(a0 + a1*R)$	$R = \ln(Rrs490/Rrs555)$ $a = [1.077835,\ -2.542605]$
Morel-3	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs443/Rrs555)$ $a = [0.20766,\ -1.82878,\ 0.75885,\ -0.73979]$
Morel-4	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs490/Rrs555)$ $a = [1.03117,\ -2.40134,\ 0.3219897,\ -0.291066]$

(O'Reilly et al 1998)


0.012
0.009
0.006
0.003
0.000
R_{rs} (sr^{-1})
400
450
500
550
600
650
700
750
800
wavelength (nm)

Empirical:



$$a_t(440) = 10^{-0.674-0.531\rho_{25}-0.745\rho_{25}^2-1.469\rho_{35}+2.375\rho_{35}^2}, \qquad (14)$$

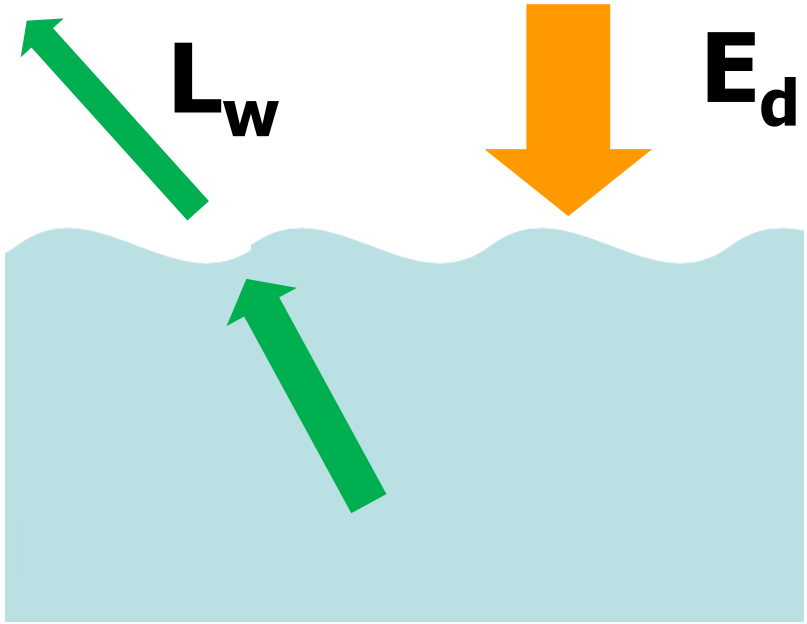
$$a_\phi(440) = 10^{-0.919+1.037\rho_{25}-0.407\rho_{25}^2-3.531\rho_{35}+1.579\rho_{35}^2}, \qquad (20)$$

(Lee et al 1998)

Physics-based algorithms (mechanistic)

Remote-sensing reflectance (sr^{-1}):

$$R_{rs}(\lambda) = \frac{L_w(\lambda, 0^+)}{E_d(\lambda, 0^+)}$$



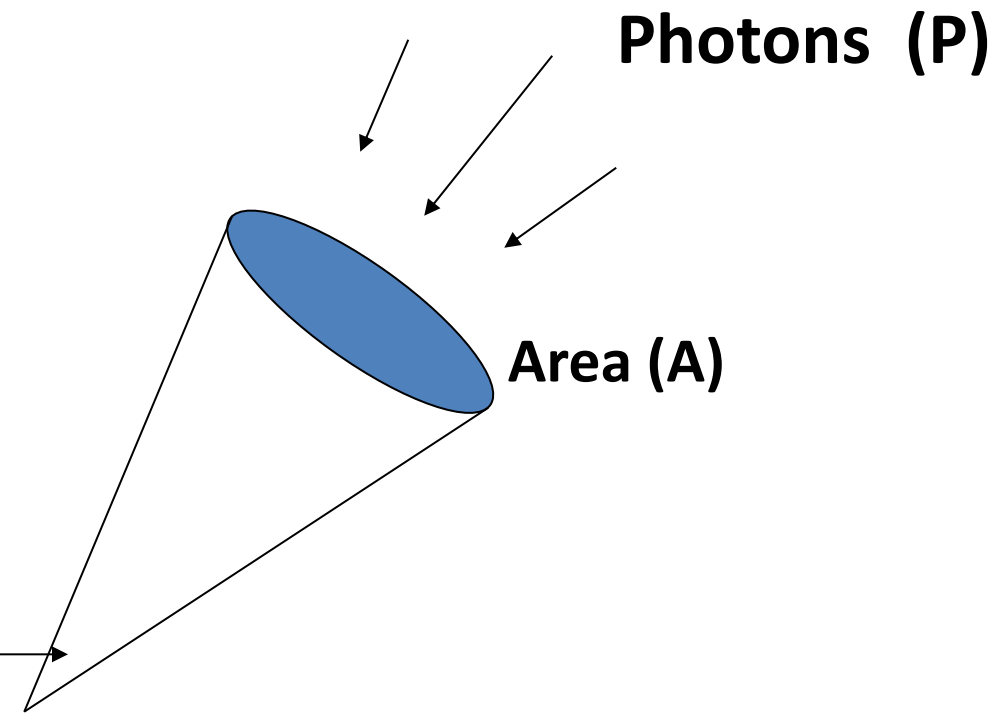
How is R_{rs} related to water's optical (biogeochemical) properties?

Basic radiometric quantity:

L: Radiance, W m^{-2} sr^{-1}

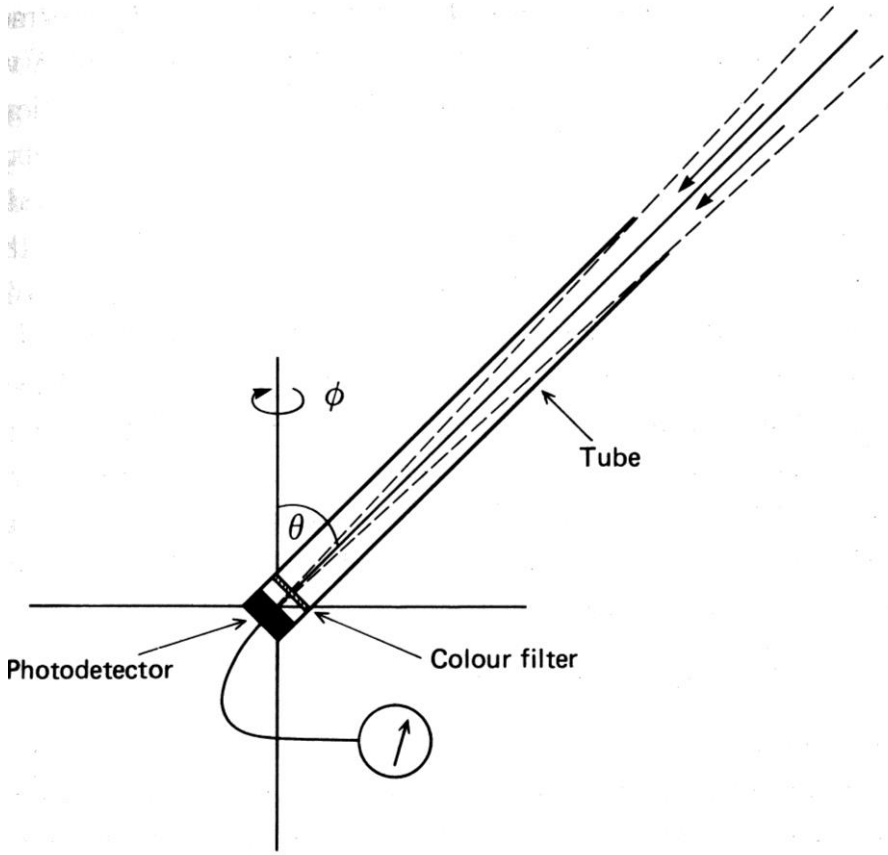
Light at a "narrow" specific direction

$$L = \frac{P}{A\, d\Omega}$$



L is a function of direction

Radiance sensor

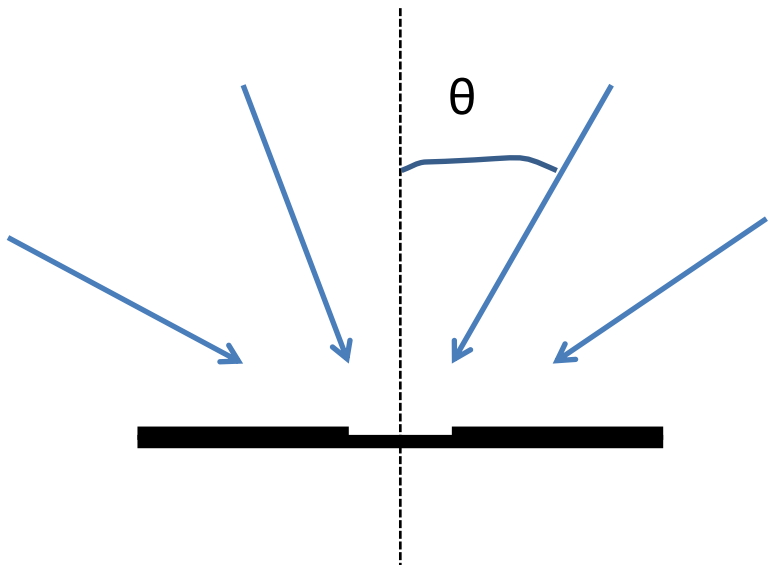


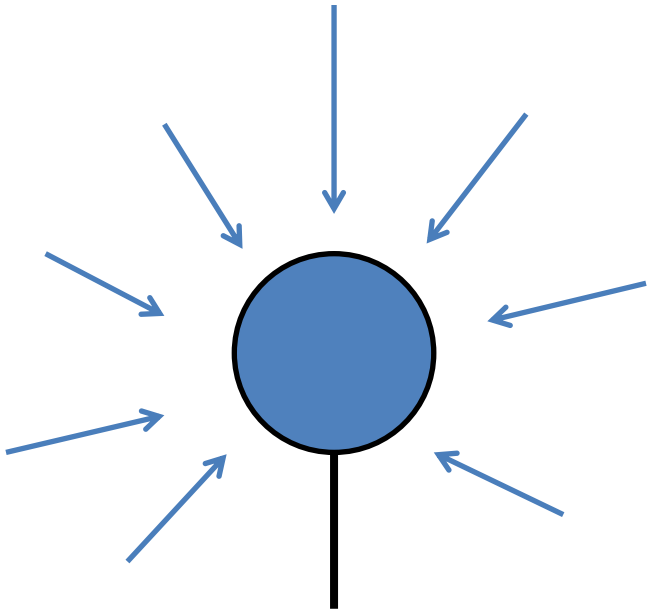
(Satlantic, inc.)

(Kirk 1994)

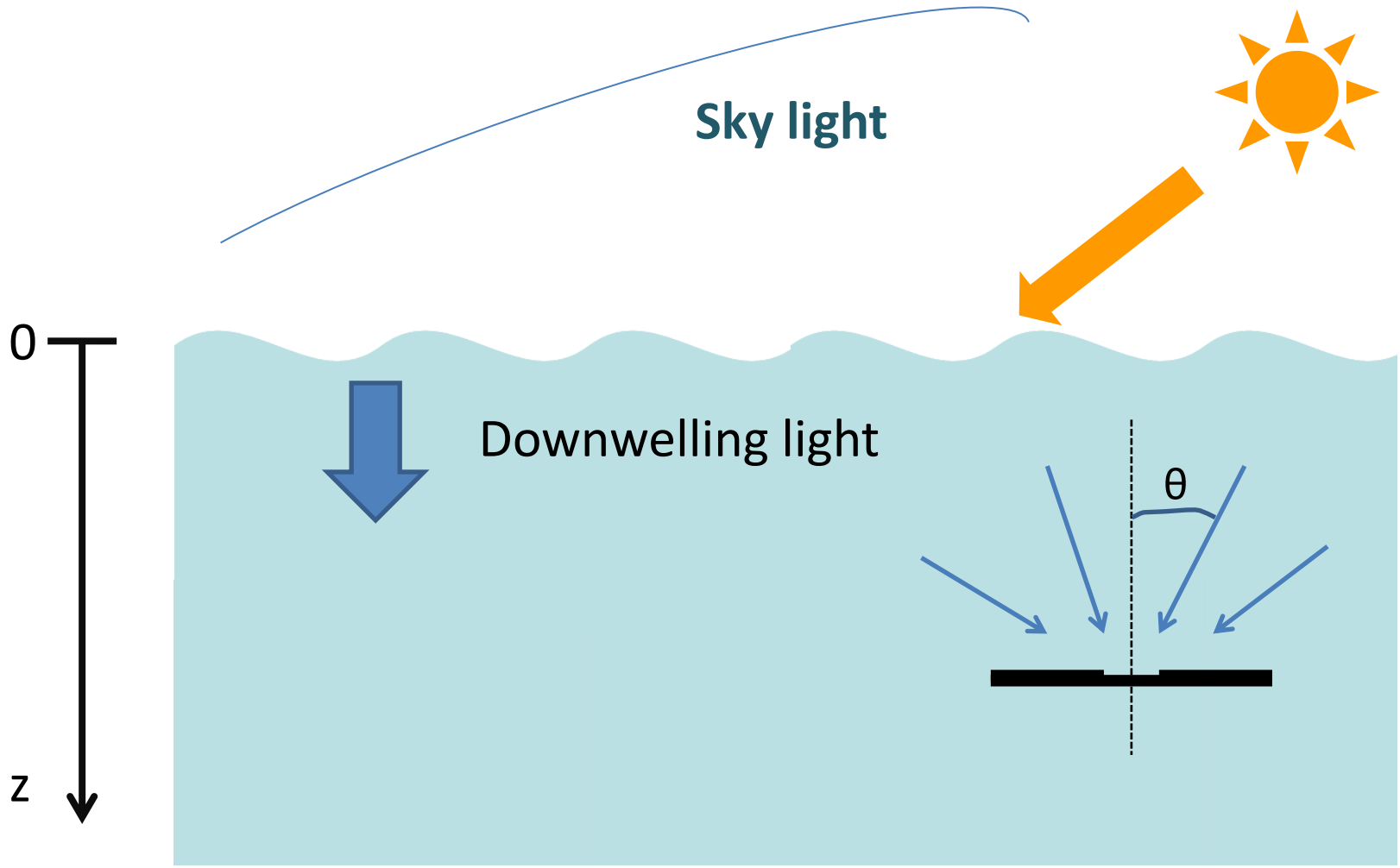
E: Irradiance, W m^{-2}

Light of a "broad" range of directions





E_d: downwelling irradiance, W m^{-2}



Irradiance sensor

(Satlantic, inc.)

diffuser

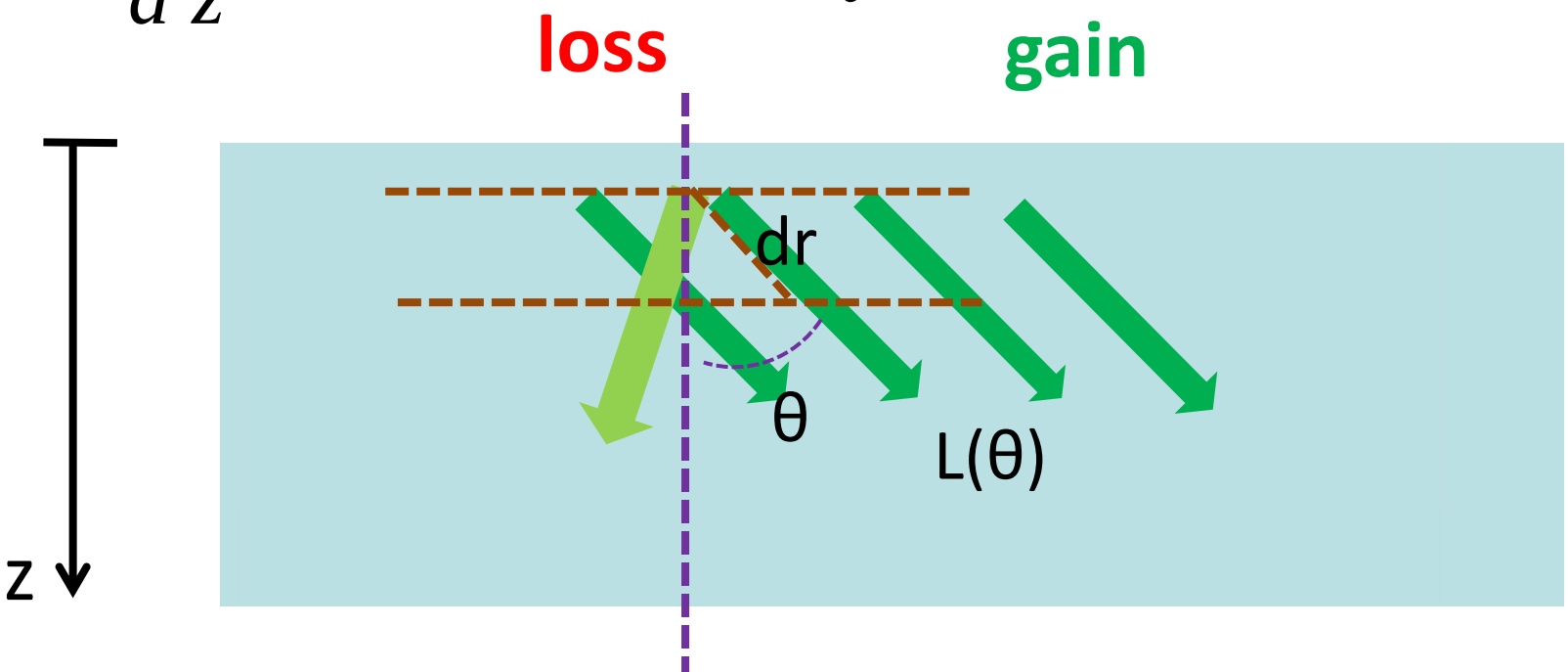
Physics-based algorithms (mechanistic)

How is R_{rs} related to water's optical (biogeochemical) properties?

Radiative Transfer Equation:

$$\frac{d\,L(\Omega)}{d\,l} = -cL(\Omega) + \int L(\Omega')\beta(\Omega',\Omega)\,d\omega$$

$$\frac{d\,L_u(\pi,z)}{d\,z} = -cL_u(\pi,z) + \int L(\Omega')\beta(\Omega',\Omega)\,d\omega$$



Exact solution: $$r_{rs}(\lambda,\Omega') = L_u(0^-,\Omega') \Big/ E_d(0^-)$$

$$r_{rs}(\lambda,\Omega') \equiv \frac{D_d(\lambda,\theta_S')}{c(\lambda)+k_L(\lambda,\Omega')-f_L(\lambda,\Omega')b_f(\lambda)} \frac{\int_0^{2\pi}\int_0^{\pi/2}\beta(\Omega',\Omega)\,L(\lambda,\Omega')\sin(\theta')\,d\theta'\,d\varphi'}{E_{od}(0^-,\lambda,\theta_S')}$$

(Zaneveld 1995)

Albert and Mobley (2003) :

$$r_{rs}(\lambda,\Omega') = q(\Omega',w)\sum_{i=1}^{4} p_i \left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^i$$

Lee et al (2004)

$$r_{rs}(\lambda,\Omega') = g_w(\Omega')\frac{b_{bw}(\lambda)}{a(\lambda)+b_b(\lambda)} + g_p(\lambda,\Omega')\frac{b_{bp}(\lambda)}{a(\lambda)+b_b(\lambda)}$$

Park and Ruddick (2005)

$$r_{rs}(\lambda,\Omega') = \sum_{i=1}^{4} g_i(\Omega',\nu_b)\left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^i$$

Van Der Woerd and Pasterkamp (2008)

$$\ln[r_{rs}(\lambda,\Omega')] = \sum_{i=1}^{4}\sum_{j=1}^{4} P_{ij}(\Omega')[\ln(a(\lambda))]^i[\ln(b(\lambda))]^j$$

Morel et al (1993, 1996, 2002):

$$r_{rs}(\lambda,\Omega') = g(\lambda, Chl, \Omega')\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}$$

Gordon et al (1988):

$$r_{rs}(\lambda,\pi) = \sum_{i=1}^{2} g_i \left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^i;$$

$$g_1 = 0.0949,\ g_2 = 0.0794$$

$r_{rs} \rightarrow R_{rs}$?

$$R_{rs} = \frac{L_w}{E_d(0^+)}$$

$$E_d(0^-) = t_E E_d(0^+) + \gamma E_u(0^-)$$

$$L_w = \frac{t_L}{n_w^{\ 2}} L_u(0^-)$$

$$R_{rs} = \frac{t_E t_L}{n_w^{\ 2}} \frac{r_{rs}}{1 - \gamma R} = \frac{0.52\, r_{rs}}{1 - 1.7\, r_{rs}}$$

Solve Rrs for IOPs or in-water constituents?

Two basic strategies:

1. Bottom-up strategy (BUS):

Assume we know the spectral shapes of the optically active components

2. Top-down strategy (TDS):

Only need the spectral shape information when it is necessary

What are we facing in RS algorithms?

$$R_{rs}(\lambda) = F(a(\lambda), b_b(\lambda))$$

$$\Downarrow$$

$$R_{rs}(\lambda) = F(a_w(\lambda), a_{ph}(\lambda), a_{dg}(\lambda), b_{bw}(\lambda), b_{bp}(\lambda))$$

$$\Downarrow$$

$$\begin{cases} R_{rs}(\lambda_1) = F(a_w(\lambda_1), \boxed{a_{ph}(\lambda_1), a_{dg}(\lambda_1),} b_{bw}(\lambda_1), \boxed{b_{bp}(\lambda_1)}) \\ R_{rs}(\lambda_2) = F(a_w(\lambda_2), a_{ph}(\lambda_2), a_{dg}(\lambda_2), b_{bw}(\lambda_2), b_{bp}(\lambda_2)) \\ \vdots \\ R_{rs}(\lambda_n) = F(a_w(\lambda_n), a_{ph}(\lambda_n), a_{dg}(\lambda_n), b_{bw}(\lambda_n), b_{bp}(\lambda_n)) \end{cases}$$

# of unknowns > # of equations!

An ill formulated math problem!

Have to increase # of equations or decrease # of unknowns!

1. Bottom-up strategy (BUS):

Build-up an Rrs spectrum block-by-block:

$$a(\lambda) = a_w(\lambda) + \sum a_{xi}(\lambda) \qquad b_b(\lambda) = b_{bw}(\lambda) + \sum b_{bxi}(\lambda)$$

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{dg}(\lambda)$$

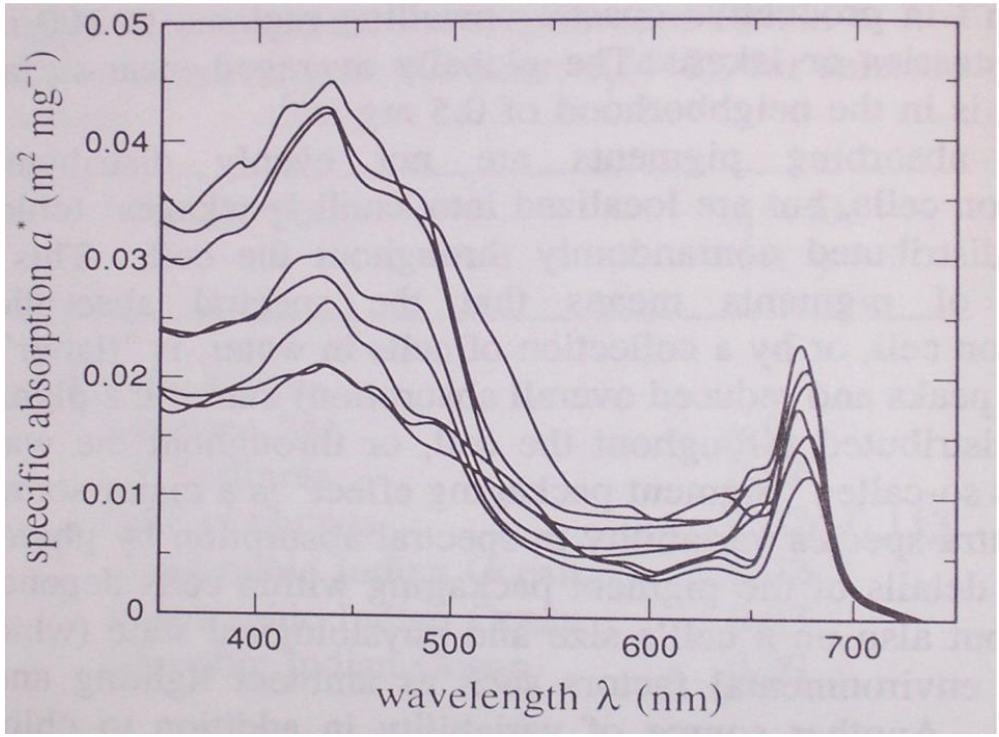
$$a(\lambda) = a_w(\lambda) + M_1 \left\langle a_{ph}(\lambda) \right\rangle + M_2 \left\langle a_{dg}(\lambda) \right\rangle$$

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda)$$

$$b_b(\lambda) = b_{bw}(\lambda) + M_3 \left\langle b_{bm}(\lambda) \right\rangle + M_4 \left\langle b_{bo}(\lambda) \right\rangle$$

$$R_{rs}(\lambda) = G \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

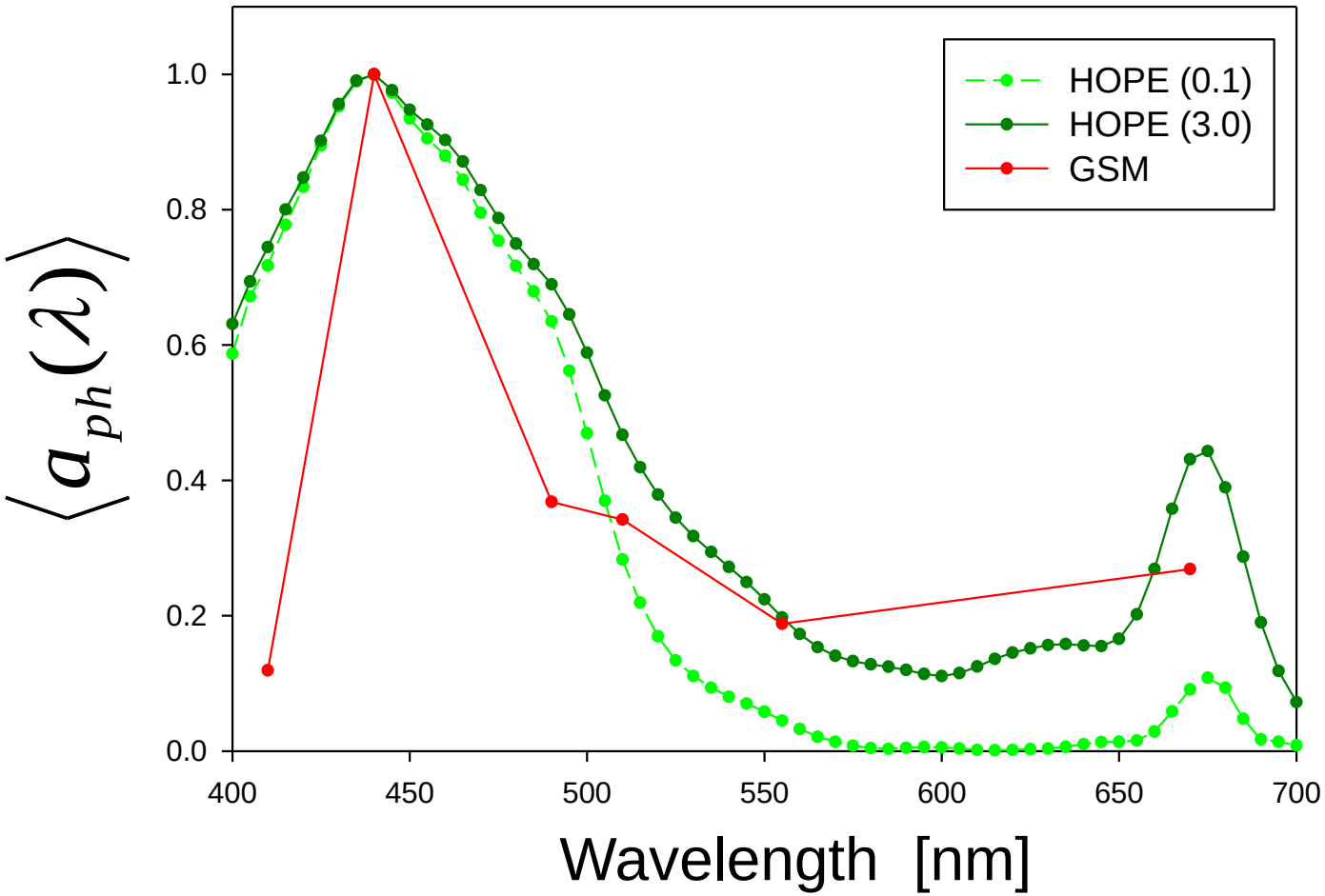
Bio-optical models (forward model)



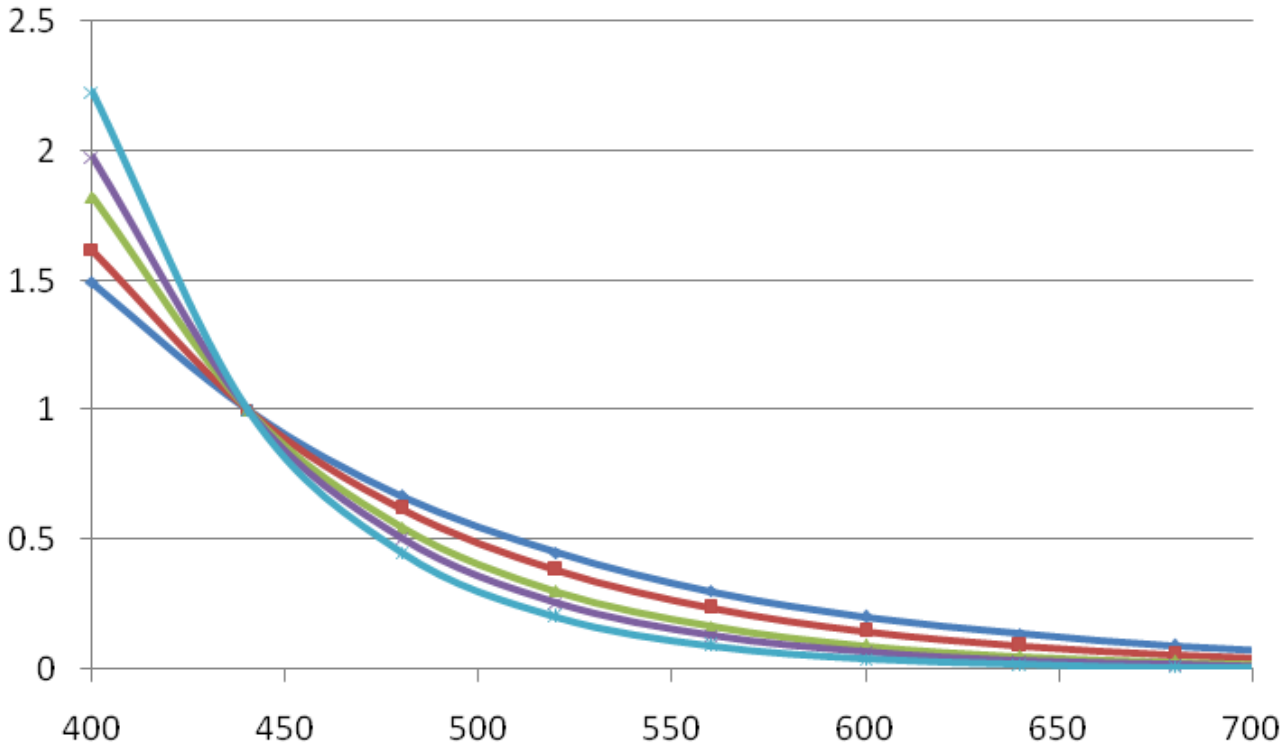
One variable: $$a_{ph}(\lambda) = P\left\langle a_{ph}(\lambda)\right\rangle$$

Two variables: $$a_{ph}(\lambda) = P_1\left\langle a_{ph1}(\lambda)\right\rangle + P_2\left\langle a_{ph2}(\lambda)\right\rangle$$

Examples of $\langle a_{ph}(\lambda) \rangle$ spectra



Absorption components: a_{dg} spectrum shapes



$$\left\langle a_{dg}(\lambda)\right\rangle = e^{-S(\lambda-440)}$$

S: 0.01 – 0.02 nm^{-1}

(*Bricaud et al* 1981)

$$\left\langle b_{bp}(\lambda)\right\rangle = \left(\frac{440}{\lambda}\right)^{\eta}$$

$$\begin{cases} R_{rs}(\lambda_1) = F(a_w(\lambda_1), b_{bw}(\lambda_1), P, G, X) \\ R_{rs}(\lambda_2) = F(a_w(\lambda_2), b_{bw}(\lambda_2), P, G, X) \\ \vdots \\ R_{rs}(\lambda_n) = F(a_w(\lambda_n), b_{bw}(\lambda_n), P, G, X) \end{cases}$$

3-variables model to describe an Rrs spectrum

$$R_{rs}(\lambda) = G \frac{b_{bw}(\lambda) + M_3 \langle b_{bm}(\lambda) \rangle + M_4 \langle b_{bo}(\lambda) \rangle}{a_w(\lambda) + M_1 \langle a_{ph}(\lambda) \rangle + M_2 \langle a_{dg}(\lambda) \rangle + b_{bw}(\lambda) + M_3 \langle b_{bm}(\lambda) \rangle + M_4 \langle b_{bo}(\lambda) \rangle}$$

$M_{1\text{-}4}$ (or $M_{1\text{-}3}$) are wavelength independent variables!

Then they could be derived by comparing the modeled Rrs spectrum with the measured Rrs spectrum.

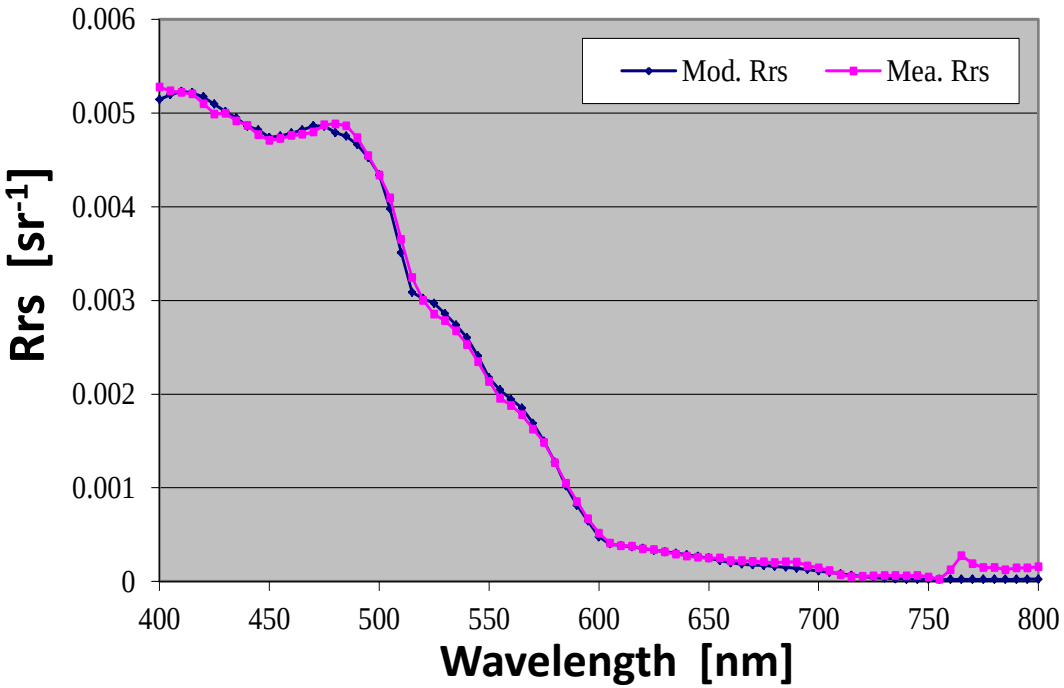
Spectral ranges used for solutions (e.g. examples of BUS):

The **blue-green** domain: e.g., Hoge and Lyon (1996), Carder et al (1999)
The **red-infrared** domain: e.g., Binding et al (2012)
The **entire spectrum** (**spectral optimization**): e.g., Bukata et al (1995), Lee et al (1994,1996,1999), Maritorena et al (2002), Boss and Roesler (2006), Brando et al (2012)

Look-Up-Tables (LUT): e.g., Carder et al (1991); Mobley et al (2005)

Spectral Optimization

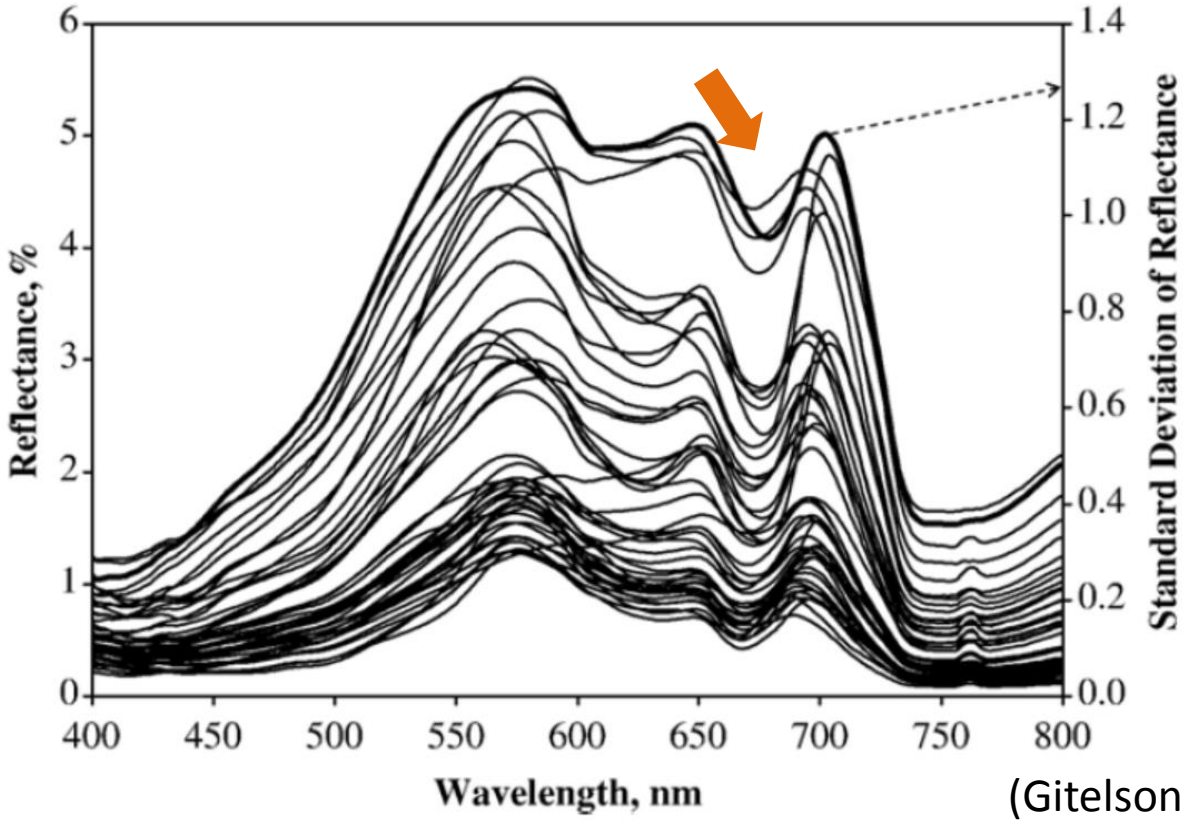
Matching between measured and modeled R_{rs}



Quantitative measure of the closure (**error function**):

$$\delta_{R_{rs}} = \frac{\sqrt{\Lambda_{\lambda 1}^{\lambda 2}\left(\tilde{R}_{rs}(\lambda) - R_{rs}(\lambda)\right)^2}}{\Lambda_{\lambda 1}^{\lambda 2} R_{rs}(\lambda)} = \sqrt{n}\,\frac{\sqrt{\sum_{\lambda 1}^{\lambda 2}\left(\tilde{R}_{rs}(\lambda) - R_{rs}(\lambda)\right)^2}}{\sum_{\lambda 1}^{\lambda 2} R_{rs}(\lambda)}$$

Algorithms using information in the red-infrared bands



(Gitelson et al 2007)

Two bands

$$Chl = f\left(\frac{Rrs(75x)}{Rrs(67x)}\right)$$

Three bands

$$Chl = f\left(\frac{Rrs(75x)}{Rrs(67x)} - \frac{Rrs(75x)}{Rrs(70x)}\right)$$

Two-, three-, four-band ratios in the red-infrared domain:

$$R_{rs}(\lambda) = G\frac{b_{bw}(\lambda) + M_3\langle b_{bm}(\lambda)\rangle + M_4\langle b_{bo}(\lambda)\rangle}{a_w(\lambda) + M_1\langle a_{ph}(\lambda)\rangle + M_2\langle a_{dg}(\lambda)\rangle + b_{bw}(\lambda) + M_3\langle b_{bm}(\lambda)\rangle + M_4\langle b_{bo}(\lambda)\rangle}$$

$$R_{rs}(\lambda) \approx G\frac{M_3\langle b_{bp}(\lambda)\rangle}{a_w(\lambda) + M_1\langle a_{ph}(\lambda)\rangle}$$

$$\frac{R_{rs}(\lambda_{red1})}{R_{rs}(\lambda_{red2})} = \frac{\langle b_{bp}(\lambda_{red1})\rangle}{\langle b_{bp}(\lambda_{red2})\rangle}\frac{a_w(\lambda_{red2}) + M_1\langle a_{ph}(\lambda_{red2})\rangle}{a_w(\lambda_{red1}) + M_1\langle a_{ph}(\lambda_{red1})\rangle}$$

Proper contrast of Rrs at λ_1 and λ_2 then leads to M_1.

2. Top-down strategy (TDS):

$$R_{rs} = G\frac{b_b}{a + b_b}$$

$$\boldsymbol{R_{rs} \rightarrow b_b \& a \rightarrow a_x}$$

Clarity (Secchi depth, light depth, TSM/SPM, etc)

Remote sensing measures the *total* effect:

Water clarity (or turbidity) is also a measure of total effect.

Examples of TDS:

Loisel & Stramski (2000), QAA (Lee et al, 2002); Smyth et al (2006); Doran et al (2007).

The Quasi-Analytical Algorithm (QAA)

Forward modeling:

$(a, b_b, \text{etc}) \Rightarrow \text{Rrs}$

$$R_{rs} \approx 0.05 \frac{b_b}{a + b_b}$$

QAA:

$(a, b_b) \Leftarrow \text{Rrs}$

The data flow of QAA:

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

$$\eta$$

$$a(\lambda_0) = a_w(\lambda_0) + \delta a(\lambda_0)$$

$$b_{bp}(\lambda_0) = F_2\left(r_{rs}(\lambda_0), a(\lambda_0), b_{bw}(\lambda_0)\right)$$

$$b_{bp}(\lambda) = b_{bp}(\lambda_0)\left(\frac{\lambda_0}{\lambda}\right)^{\eta}$$

$$a(\lambda) = F_3\left(r_{rs}(\lambda), b_{bp}(\lambda), b_{bw}(\lambda)\right)$$

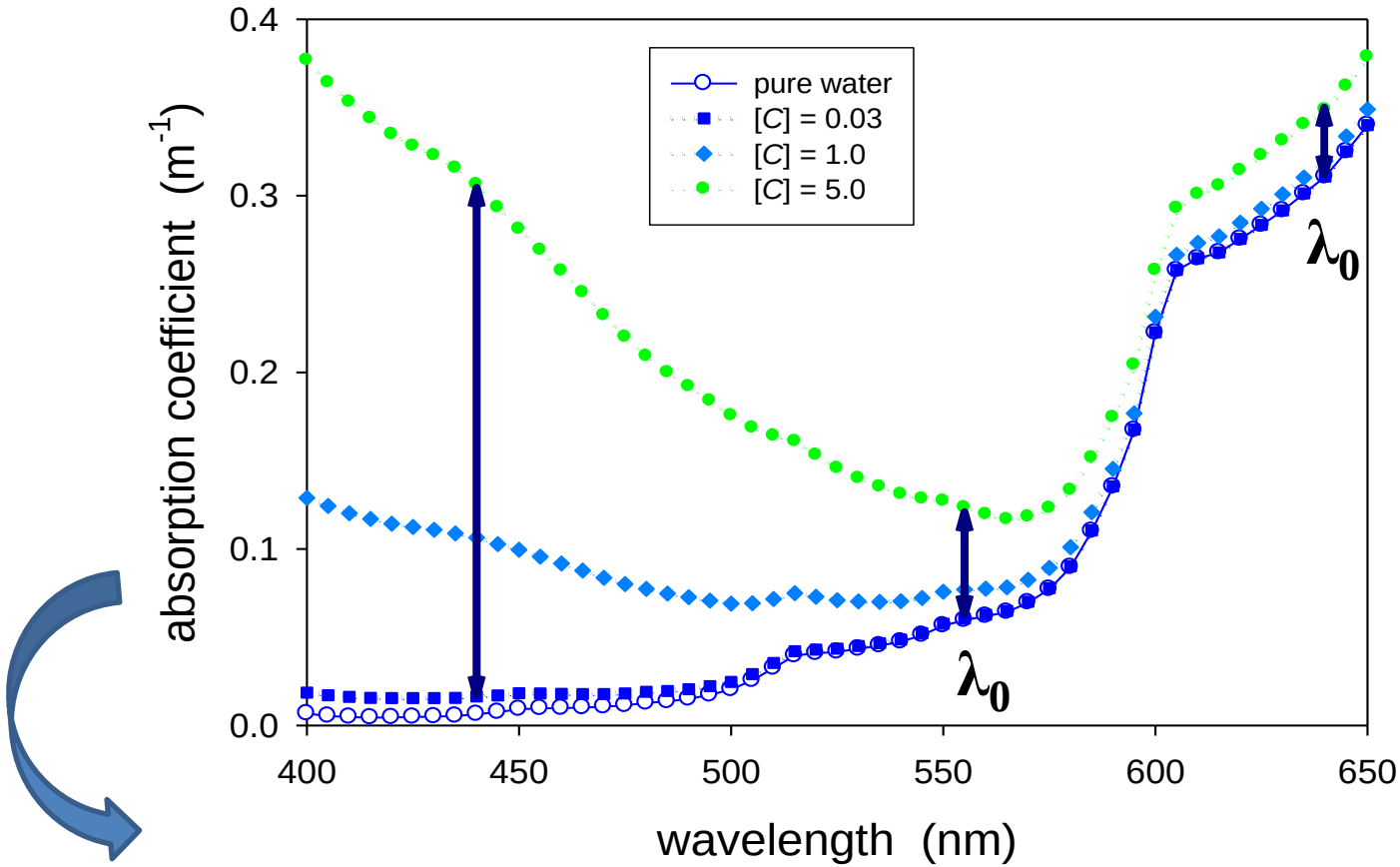
$$\begin{cases} a(411) = a_w(411) + \zeta\, a_{ph}(443) + \xi\, a_{dg}(443) \\ a(443) = a_w(443) + a_{ph}(443) + a_{dg}(443) \end{cases}$$

$$\zeta = \frac{a_{ph}(411)}{a_{ph}(443)}$$

$$\xi = \frac{a_{dg}(411)}{a_{dg}(443)}$$

(Lee et al 2002)

Logic behind QAA (and its updated versions):



For a reference wavelength, λ_0, variation of $a(\lambda_0)$ is limited.

Known $a(\lambda_0)$, enables calculation of $b_b(\lambda_0)$ from $R_{rs}(\lambda_0)$; propagate $b_b(\lambda_0)$ to $b_b(\lambda)$, then enables calculation of $a(\lambda)$ from $R_{rs}(\lambda)$.

No need of spectral model of $a_x(\lambda)$ in this process!

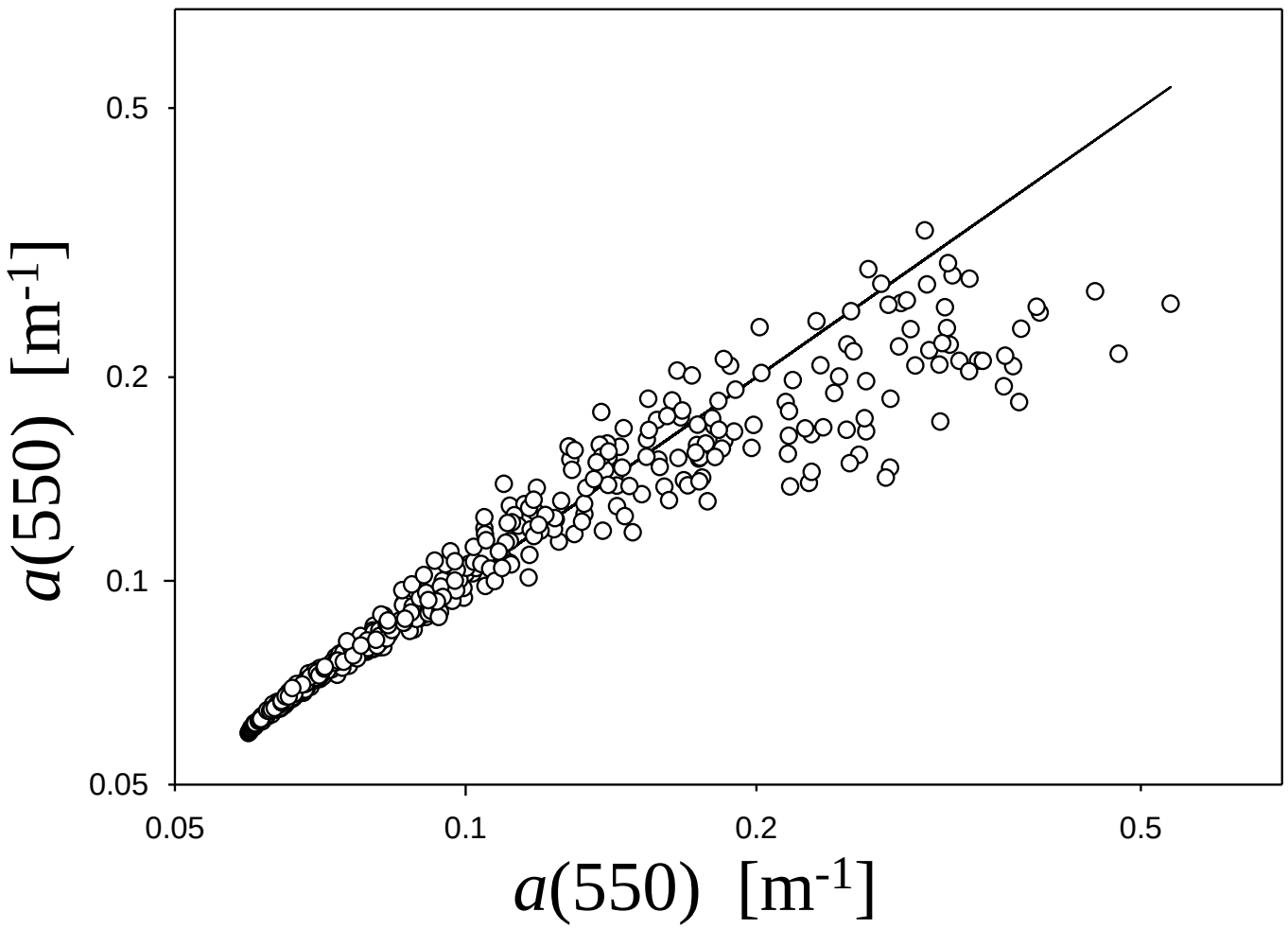
When 550 nm as the reference wavelength (λ_0)

$$a(550) = a_w(550) + 10^{-1.146 - 1.366\chi - 0.469\chi^2}$$

$$\chi = \log\left(\frac{r_{rs}(443) + r_{rs}(490)}{r_{rs}(\lambda_0) + 5\dfrac{r_{rs}(667)}{r_{rs}(490)} r_{rs}(667)} \right)$$

$a_w(550) = 0.0565$

Empirical!


0.5
0.2
0.1
0.05
0.05
0.1
0.2
0.5
a(550) [m-1]
a(550) [m-1]

Invert Rrs:

$R_{rs} \Rightarrow r_{rs} \Rightarrow \{a \& b_b\}$

$r_{rs}(\lambda) = R_{rs}(\lambda)/(0.52 + 1.7\, R_{rs}(\lambda))$

$$r_{rs} = g_0\left(\frac{b_b}{a+b_b}\right) + g_1\left(\frac{b_b}{a+b_b}\right)^2$$

g_0=0.089,g_1=0.125

$$u(\lambda) = \frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)} = \frac{-g_0 + \sqrt{(g_0)^2 + 4\, g_1 * r_{rs}(\lambda)}}{2g_1}$$

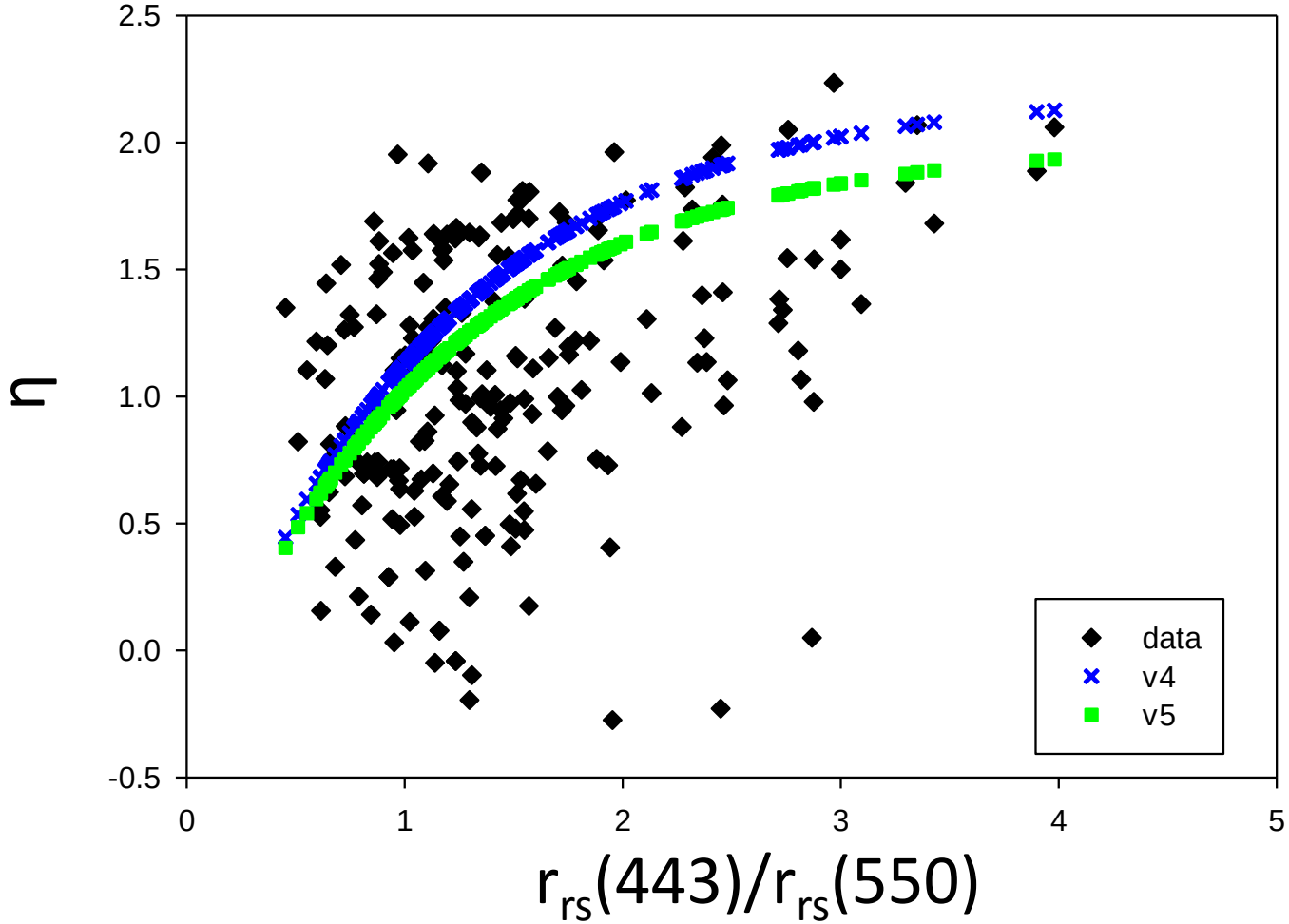
$$a(550) = a_w(550) + 10^{-1.146-1.366\chi-0.469\chi^2}$$

$$b_{bp}(550) = \frac{u(550)\,a(550)}{1-u(550)} - b_{bw}(550)$$

$$b_{bp}(\lambda) = b_{bp}(550)\left(\frac{550}{\lambda}\right)^{\eta}$$

Empirical:

$$\eta = 2.0\left(1 - 1.2\ \exp\left(-0.9\frac{r_{rs}(443)}{r_{rs}(55x)}\right)\right)$$



$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda)$$

$$a(\lambda) = \frac{(1 - u(\lambda))\, b_b(\lambda)}{u(\lambda)}$$

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{dg}(\lambda)$$

$$\Downarrow$$

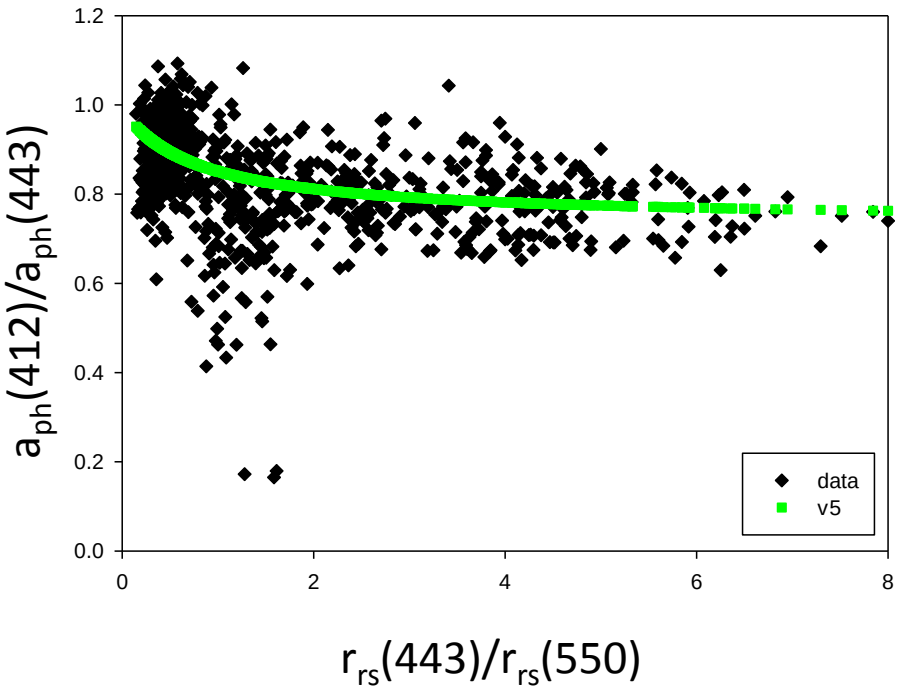
$$\begin{cases} a(410) = a_w(410) + a_{ph}(410) + a_{dg}(410), \\ a(440) = a_w(440) + a_{ph}(440) + a_{dg}(440). \end{cases}$$

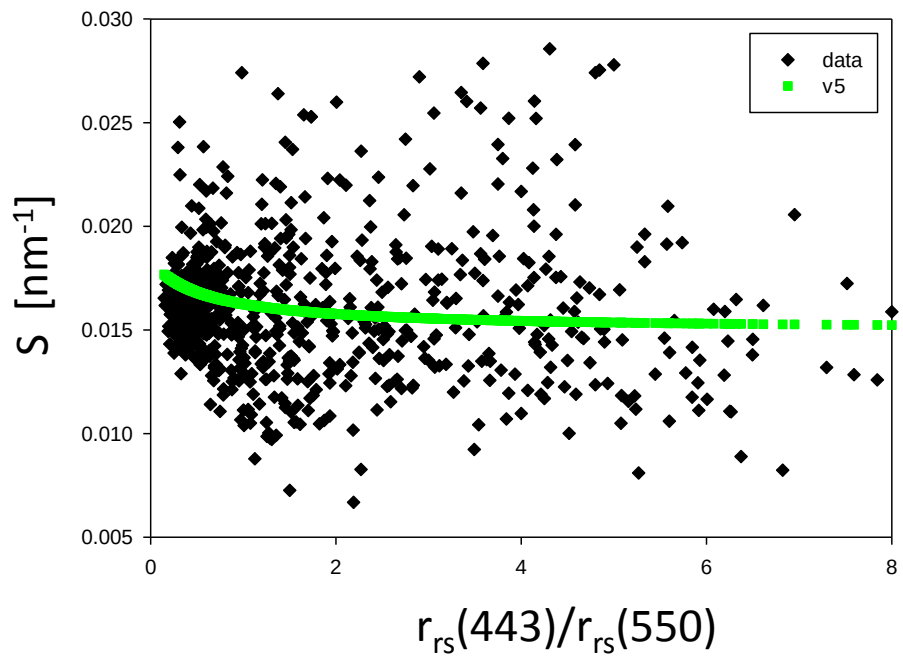
$$\zeta = \frac{a_{ph}(410)}{a_{ph}(440)} \qquad \Downarrow \qquad \xi = \frac{a_{dg}(410)}{a_{dg}(440)}$$

$$\begin{cases} a(410) = a_w(410) + \zeta\, a_{ph}(440) + \xi\, a_{dg}(440), \\ a(440) = a_w(440) + a_{ph}(440) + a_{dg}(440). \end{cases}$$

$$\begin{cases} a(410) = a_w(410) + \zeta\, a_{ph}(440) + \xi\, a_{dg}(440), \\ a(440) = a_w(440) + a_{ph}(440) + a_{dg}(440). \end{cases}$$

$$\begin{cases} a_g(440) = \dfrac{\left(a(410) - \zeta\, a(440)\right) - \left(a_w(410) - \zeta\, a_w(440)\right)}{\xi - \zeta}, \\ a_{ph}(440) = a(440) - a_w(440) - a_{dg}(440). \end{cases}$$





$$\zeta = 0.74 + \frac{0.2}{0.8 + r_{rs}(443)/r_{rs}(550)}$$

$$\xi = e^{S(443-411)},$$

$$S = 0.015 + \frac{0.002}{0.6 + r_{rs}(443)/r_{rs}(550)}$$

Empirical!

Key Points:

1. Various inversion algorithms for IOPs have been developed; but more/better ones are also expected.

2. BUS derives every component first, then (simultaneously) derives the total optical property.

Assume the spectral shapes of the optically active components are well characterized!
BUS relies more on forward bio-optical model

3. TDS derives total first, then decompose to separate components.

TDS relies more on Rrs measurement