Metrology: The case of EO data

IOCCG Training

22-23 Apr. 2024

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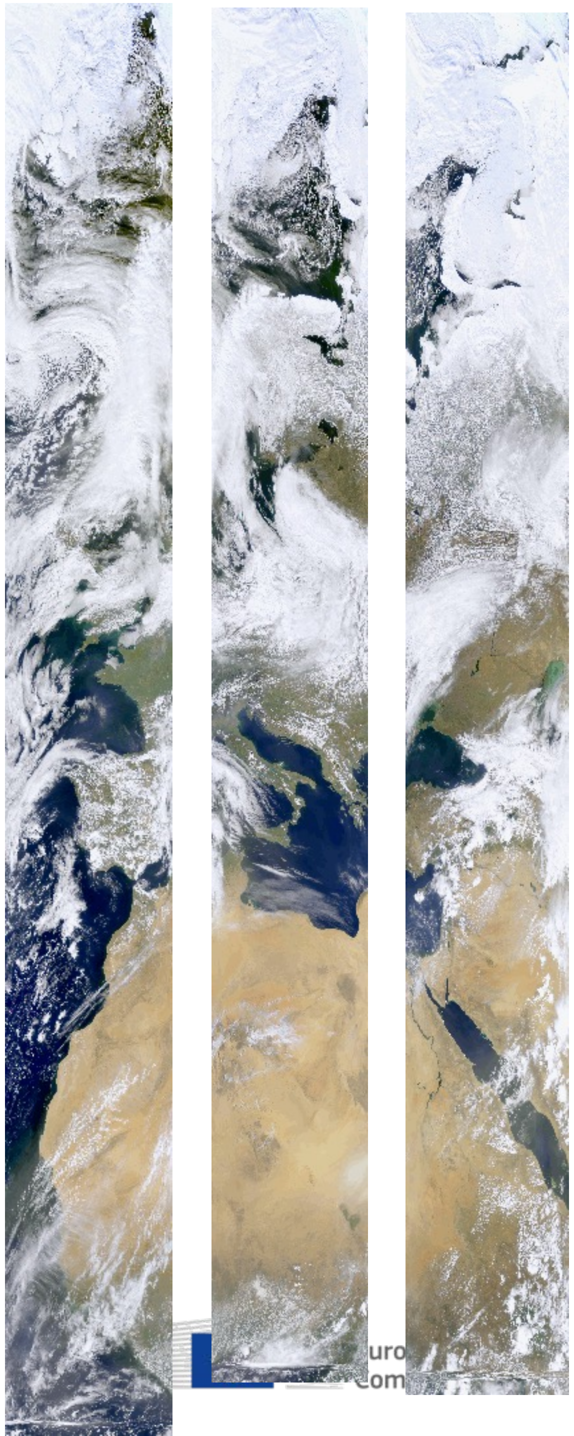
European Commission

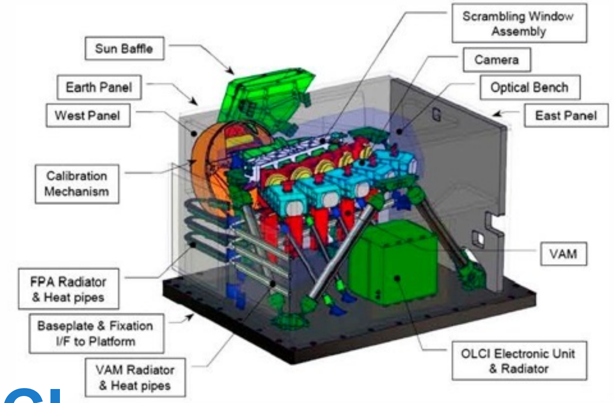
Specific challenges to EO

- Traceability chain broken at launch
- Earth observation framework (no repeatability)



Specific challenges to EO

- Traceability chain broken at launch
- Earth observation framework (no repeatability)
- Field data may be sparse and unevenly distributed
- Sensors in space are complex objects

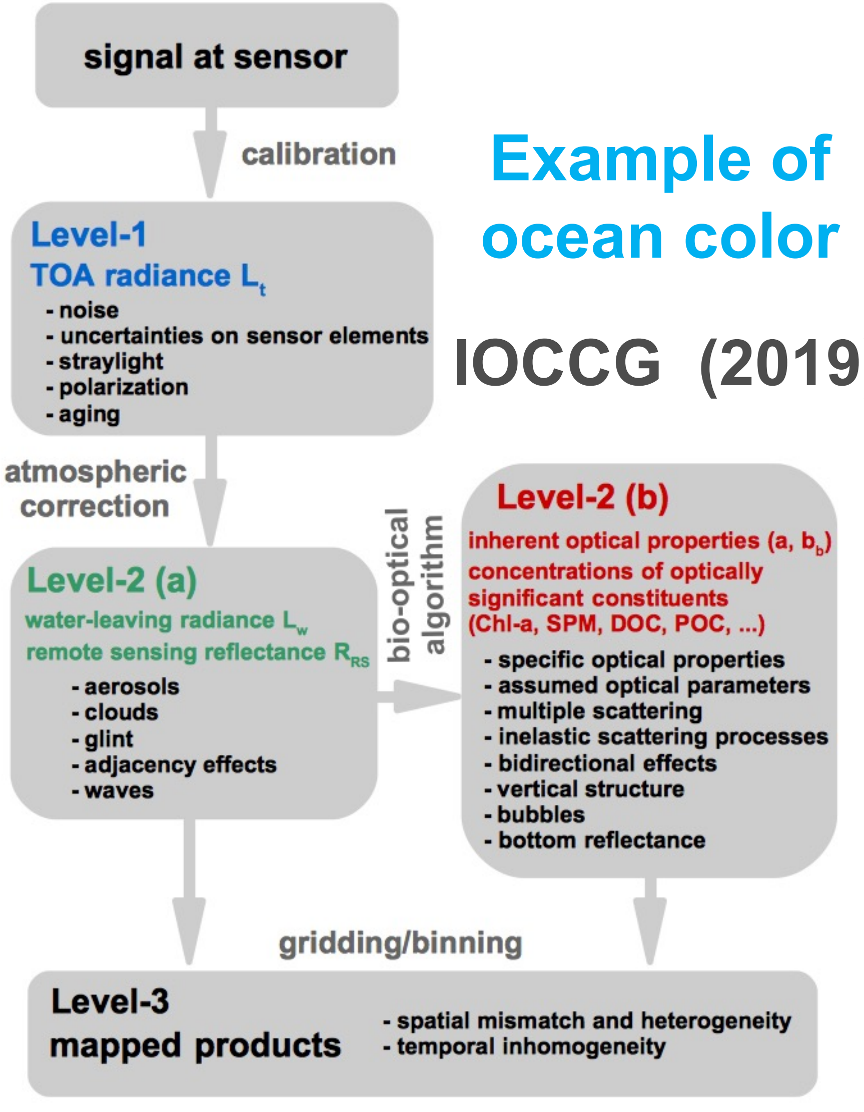


OLCI design

Donlon et al. *RSE* (2012)

Specific challenges to EO

- Traceability chain broken at launch
- Earth observation framework (no repeatability)
- Field data may be sparse and unevenly distributed
- Sensors in space are complex objects
- Massive amounts of data with poorly characterized error correlation undergoing complex processing



signal at sensor

calibration

Level-1
TOA radiance L_t
- noise
- uncertainties on sensor elements
- straylight
- polarization
- aging

atmospheric correction

Level-2 (a)
water-leaving radiance L_w
remote sensing reflectance R_{RS}
- aerosols
- clouds
- glint
- adjacency effects
- waves

bio-optical algorithm

Level-2 (b)
inherent optical properties (a, b_b)
concentrations of optically significant constituents (Chl-a, SPM, DOC, POC, ...)
- specific optical properties
- assumed optical parameters
- multiple scattering
- inelastic scattering processes
- bidirectional effects
- vertical structure
- bubbles
- bottom reflectance

gridding/binning

Level-3
mapped products
- spatial mismatch and heterogeneity
- temporal inhomogeneity

Example of ocean color

IOCCG (2019)

Propagation of Uncertainties (1)

Raw satellite data (L0)

Calibrated radiances (L1)

Climate data record (L2)

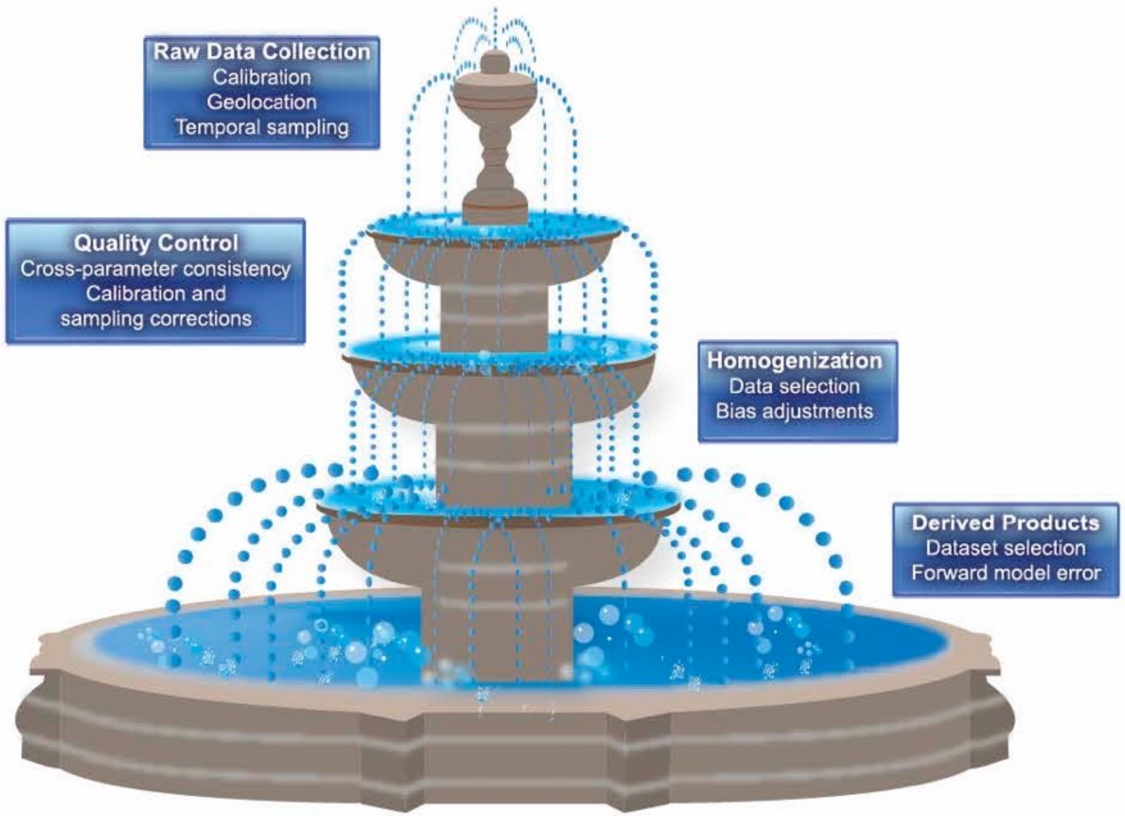
Gridded CDR (L3)

Analysed / processed (L4+)

Climate index / information

Each transformation injects new uncertainty

Uncertainty from low-level data propagates to high-level information



Matthews et al. BAMS 2013

University of Reading

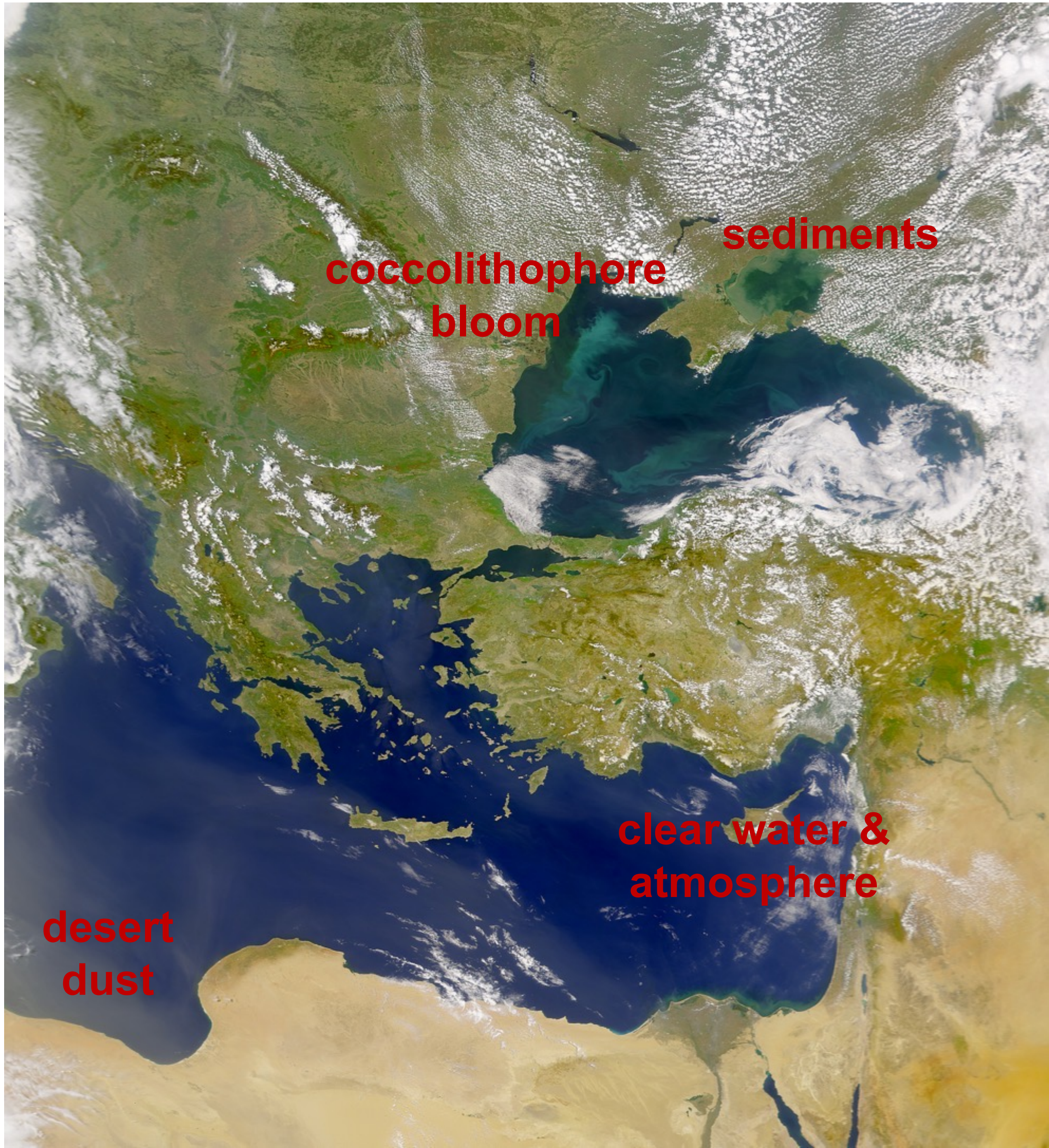
Fiduceo

European Commission

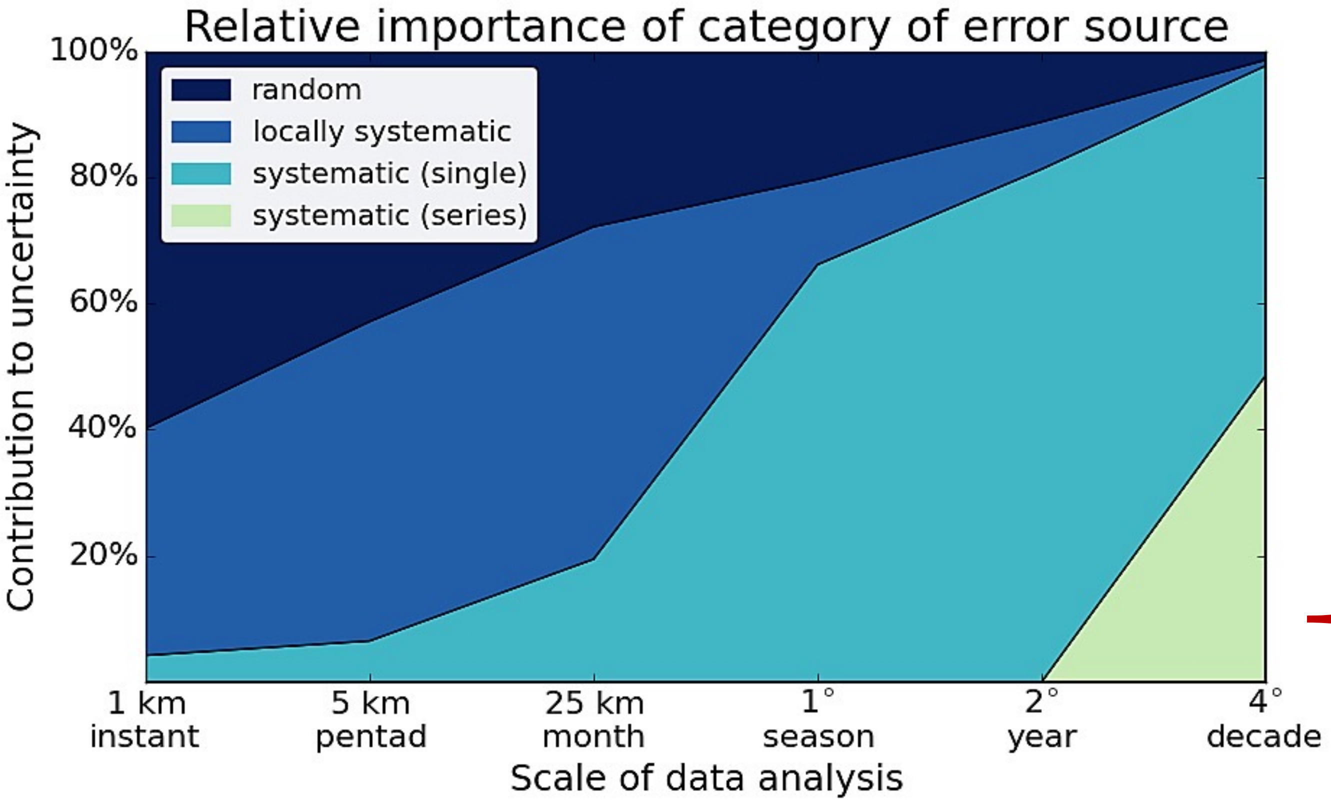
A word on errors

- Input
- Model structure / parameters
- Numerical / technical
- Editing

- Random
- Locally (time/space) systematic
- Systematic
    - Uncorrelated
    - Spectrally correlated
    - Spatially correlated
    - …

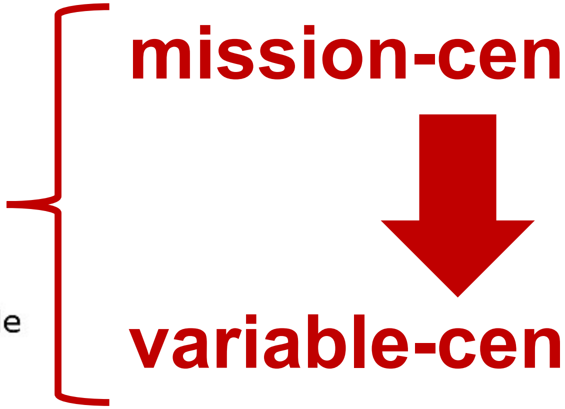


Propagation of Uncertainties (2)



Merchant et al. ESSD (2017)

- Random errors tend to be averaged out with increased compositing level
- Initially small systematic contributions might end up being highly relevant (e.g., for climate studies)



mission-centric view

variable-centric view

Requirements: depend on applications

- **McClain et al. 1992:**
Radiometric accuracy to within 5% absolute and 1% relative
Water-leaving radiance to within 5% absolute
Chlorophyll-a concentration to within 35% over the range 0.05–50 mg m^{-3}
Global primary production to within 50% absolute with a precision to within 10%,

- **Mission-specific: e.g., OLCI (Drinkwater & Rebhan 2017), PACE (Werdell et al. 2019)**

- **Requirements for Ocean Color Climate Data Records**

	Space res.	Time res.	Accuracy	Stability (dec.$^{-1}$) (2)
L_{WN} / R_{RS}	4-km	daily	5% (1)	0.5%
[Chl-a]	30-km	weekly	30%	3%

GCOS (2011)

1: for the blue and green wavelengths in open ocean

2: maximum acceptable change in systematic error per decade

Sources of Uncertainties for EO data

Setting the stage

Setting the stage (1)

Top-Of-Atmosphere Radiance, written as:

$$L_{toa}(\lambda) = L_{atm}(\lambda) + t_d(\lambda).L_w(\lambda) + t_d(\lambda).L_{wc}(\lambda) + t(\lambda).L_g(\lambda) \qquad (1)$$

L_{toa}: top-atmosphere radiance at sensor;
L_{atm}: atmospheric path radiance $=L_r + L_a$ in single scattering approximation;
L_w: water leaving radiance;
L_{wc}: radiance due to white caps (foam);
L_g: glint (specular reflection;
t_d: diffuse transmittance;
t: beam transmittance.

signal of interest

$$t(\lambda, \theta) = exp[-(\tau_r(\lambda) + \tau_a(\lambda))/\cos\theta].exp[-\tau_{O3}(\lambda)/\cos\theta] \qquad (1)$$

$$t_d(\lambda, \theta) = \underbrace{exp[-0.5C_r(\lambda, \theta)\tau_r(\lambda)/\cos\theta]}_{\text{Rayleigh}}.\underbrace{exp[-\beta_a(\lambda, \theta)\tau_a(\lambda)/\cos\theta]}_{\text{aerosols}}.\underbrace{exp[-\tau_{O3}(\lambda)/\cos\theta]}_{\text{ozone}}$$

depend on molecular and aerosol optical thickness and geometry

NB: A mathematically ill-posed problem

Setting the stage (2): Optical Properties

Preisendorfer 1961

Apparent:

- may vary with variations in illumination conditions (ambient light)
- depend on geometry of observation
- measured under existing illumination conditions (in the field)

ex: $R_{RS}(\lambda)$, $K_d(\lambda)$

Inherent:

- inherent property of the medium
- independent of illumination conditions (ambient light)
- obey additive principles
- measured under strictly-defined light conditions

ex: $a(\lambda)$, $b(\lambda)$, $c(\lambda)$, ...

Setting the stage (3)

$L_w(\lambda) = \alpha\, R_{RS}(\lambda)$ = function (IOPs) ≈ function(b_b,a) for each λ

back-scattering

pure water

particles

$$b_b(\lambda) = b_{b,w}(\lambda) + b_{b,p}(\lambda)$$

absorption

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

pure water

phyto plankton

non-pigmented particles

CDOM

!! undetermined problem !!

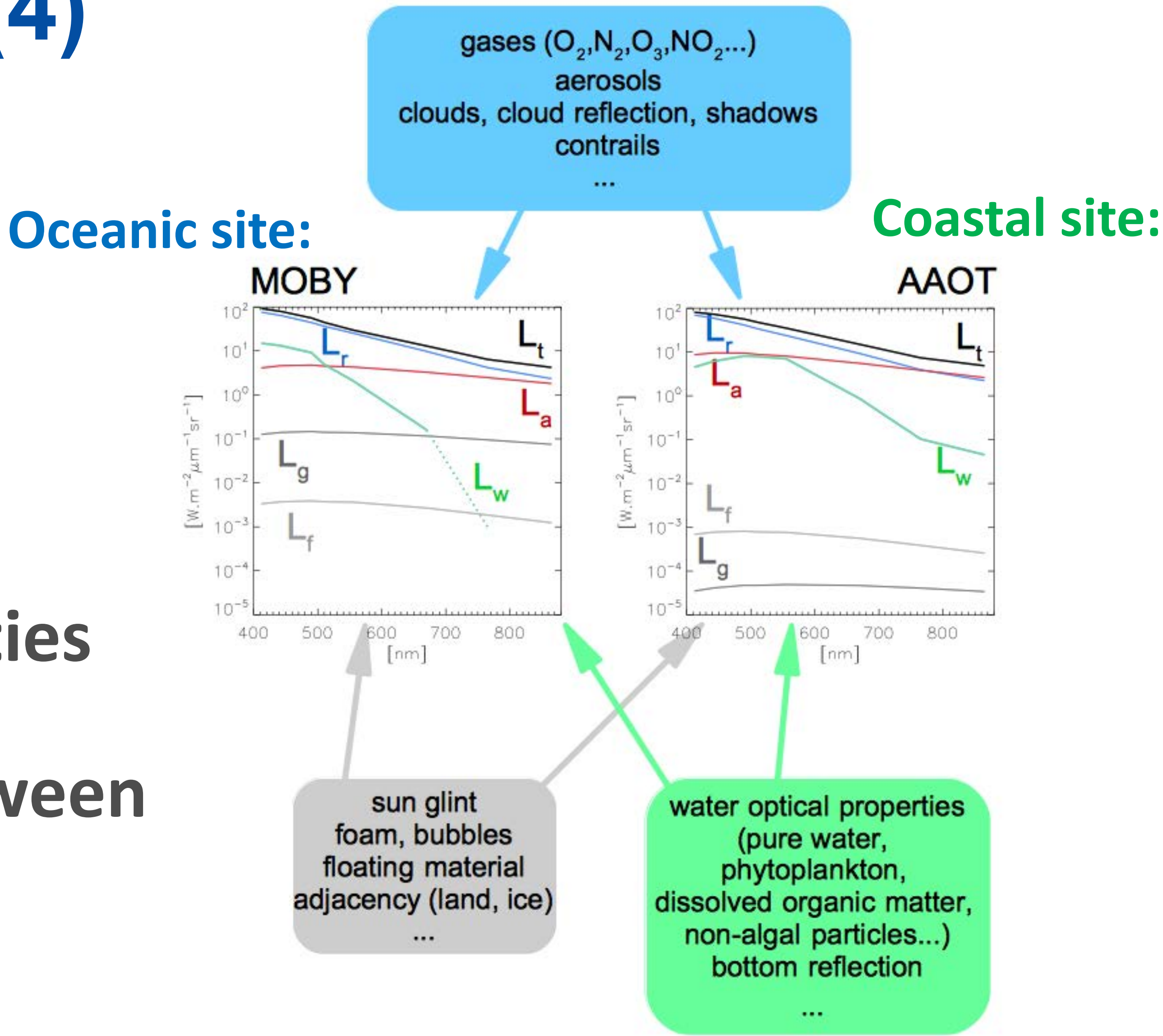
need assumptions

Setting the stage (4)

Radiance budget:
(clear-sky)

- Many factors affecting L_t and affected by uncertainties

- ~ Order of magnitude between L_t and L_w



gases (O_2,N_2,O_3,NO_2...)
aerosols
clouds, cloud reflection, shadows
contrails
...

Oceanic site:

Coastal site:

sun glint
foam, bubbles
floating material
adjacency (land, ice)
...

water optical properties
(pure water,
phytoplankton,
dissolved organic matter,
non-algal particles...)
bottom reflection
...

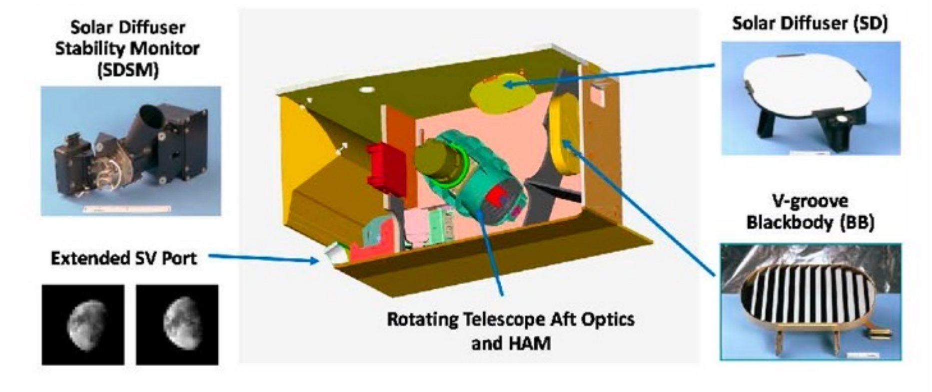
Sources of Uncertainties for EO data

from L1 to L2

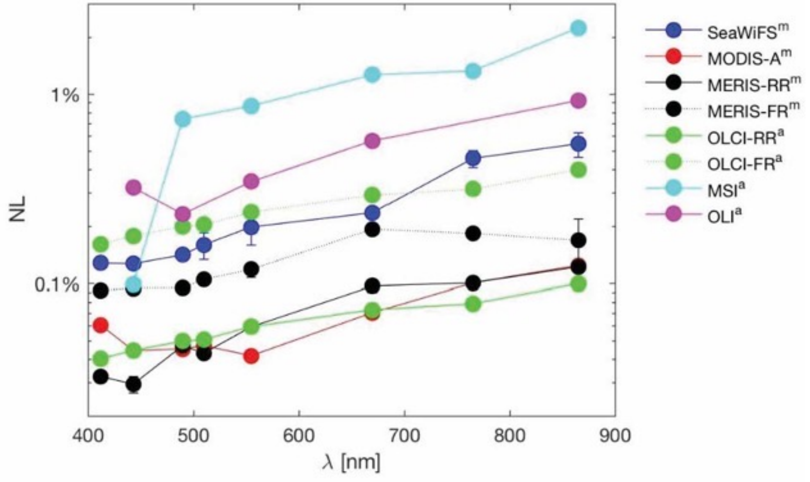
Top-Of-Atmosphere Signal

- Calibration
- Noise
- Spectral response function; out-of-band response
- Dark current
- Radiometric angular dependency (RVS)
- Sensitivity to polarized light
- Straylight
- …

VIIRS (Xiong et al. *RS* 2015)



NL=100/SNR



IOCCG (2019) (adapted from Bulgarelli & Zibordi 2018)

White Caps

Stramska & Petelski, *JGR*, 2003

White caps occur for wind speed >~ 3 m.s^{-1}.

Relationship between white cap reflectance and wind speed is variable.

Anguelova & Webster, *JGR* 2006.

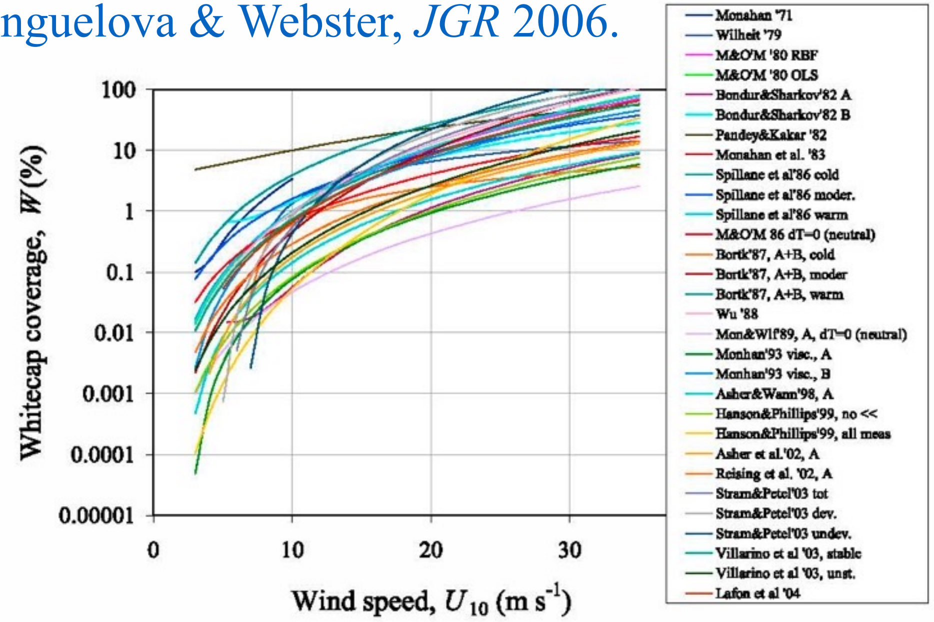


Figure 1. Various parameterizations for $W(U_{10})$ relation.

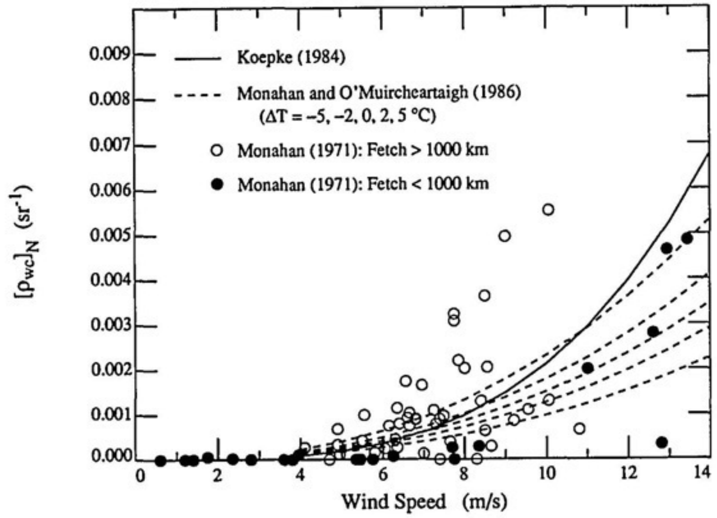


Fig. 1. $[\rho_{wc}]_N = r_{wc} f$ as a function of wind speed and atmospheric stability. For the Monahan and O'Muircheartaigh[17] relationship (dashed curves), the lower the value of $[\rho_{wc}]_N$, the greater the stability of the atmosphere. The solid curve is from Ref. 21, and the circles are from Ref. 11.

Gordon & Wang, *Appl. Opt.*, 1994.

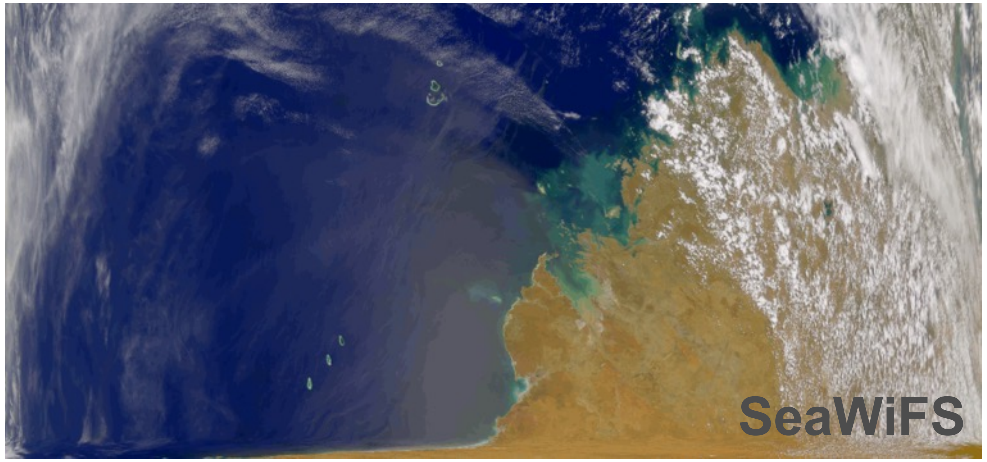
Sun Glint

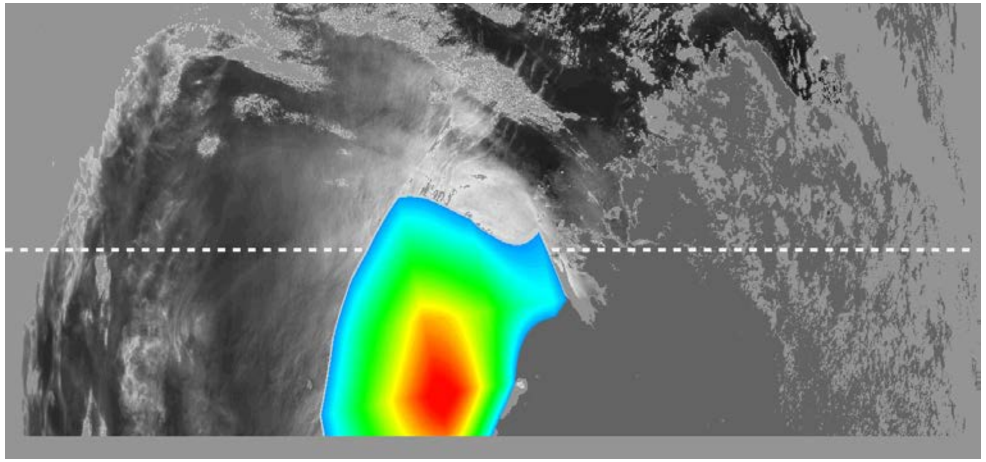
Determination of the area affected by glint and glint radiance

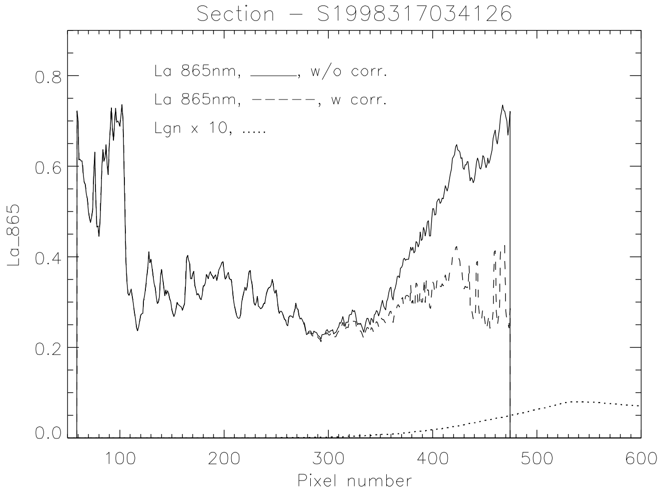
using geometric criteria

function for the orientation (slope) of wave facets (as a function of wind) + Fresnel law

Cox, C., W. Munk: Statistics of the sea surface derived from sun glitter. *J. Mar. Res.*, 13, 198-208, 1954.



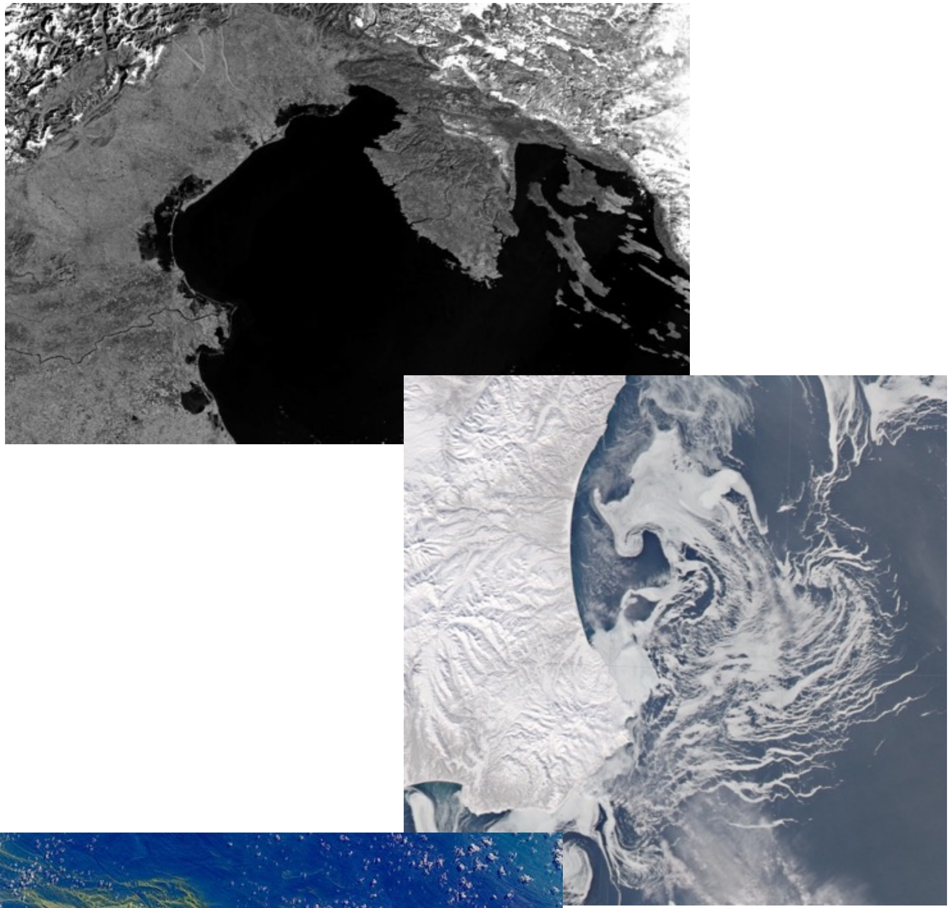




redrawn from Wang, M., S. Bailey: Correction of sun glint contamination on the SeaWiFS ocean and atmosphere products. *Appl. Opt.*, 4790-4798, 2001.

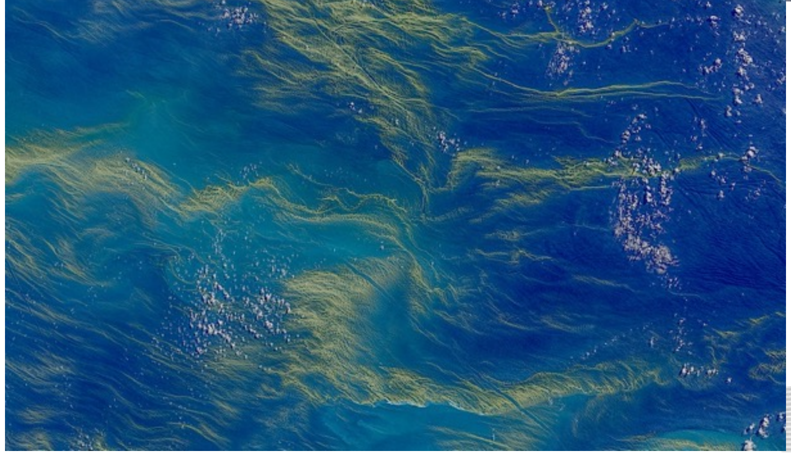
Ambiguity of Target

- Adjacency effects from land, ice, clouds, …



- Bottom effects

- Unexpected surface features (mucilage, blooms, sargassum, ships, ship wake, wind farms, …)



Aerosols: Nature (1)

solid or liquid particles suspended in air with diameters of 0.002-100 µm

Classifications:

- Primary	**/ Secondary**
(emitted directly into the atmosphere)	**(formed in the atmosphere by gas-to-particle conversion processes)**

- Natural / Anthropogenic

- Tropospheric / Stratospheric

- Geographical location of the source
- Chemical composition
- Particle size

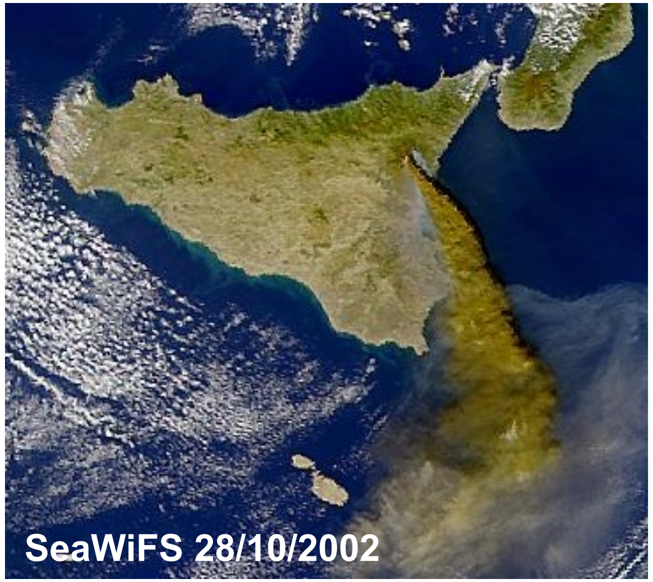
Aerosols: Nature (2)

Natural:

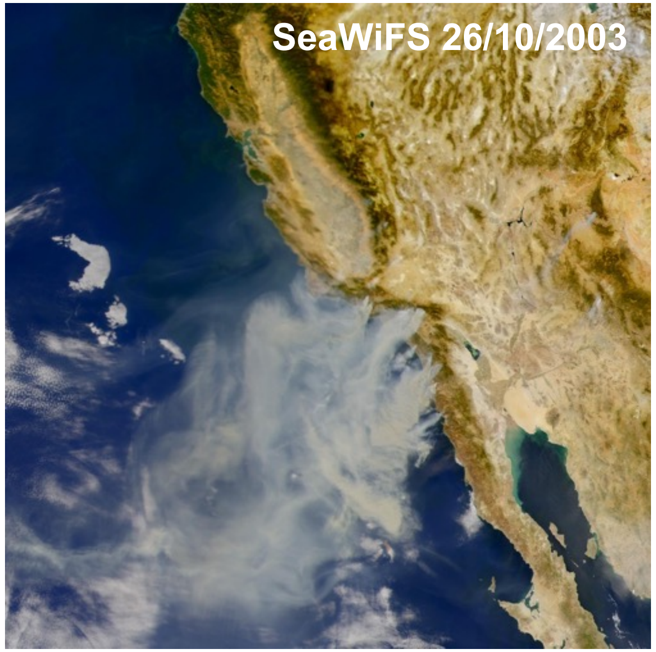
Sea salt
Soil dust
Bioaerosols (bacteria, virus, pollen, fungi, cell debris, biofilms)
Volcanic dust
Sulfate from biogenic gases / volcanic SO_2

Anthropogenic:

Industrial particulates
Dust
Soot
Biomass burning
Sulfate / Nitrate from SO_2 / NO_x
Organics


SeaWiFS 28/10/2002


SeaWiFS 05/03/1998


SeaWiFS 26/10/2003

Aerosols: Microphysical properties (1)

Aerosol samples collected during summer 1998 in Germany

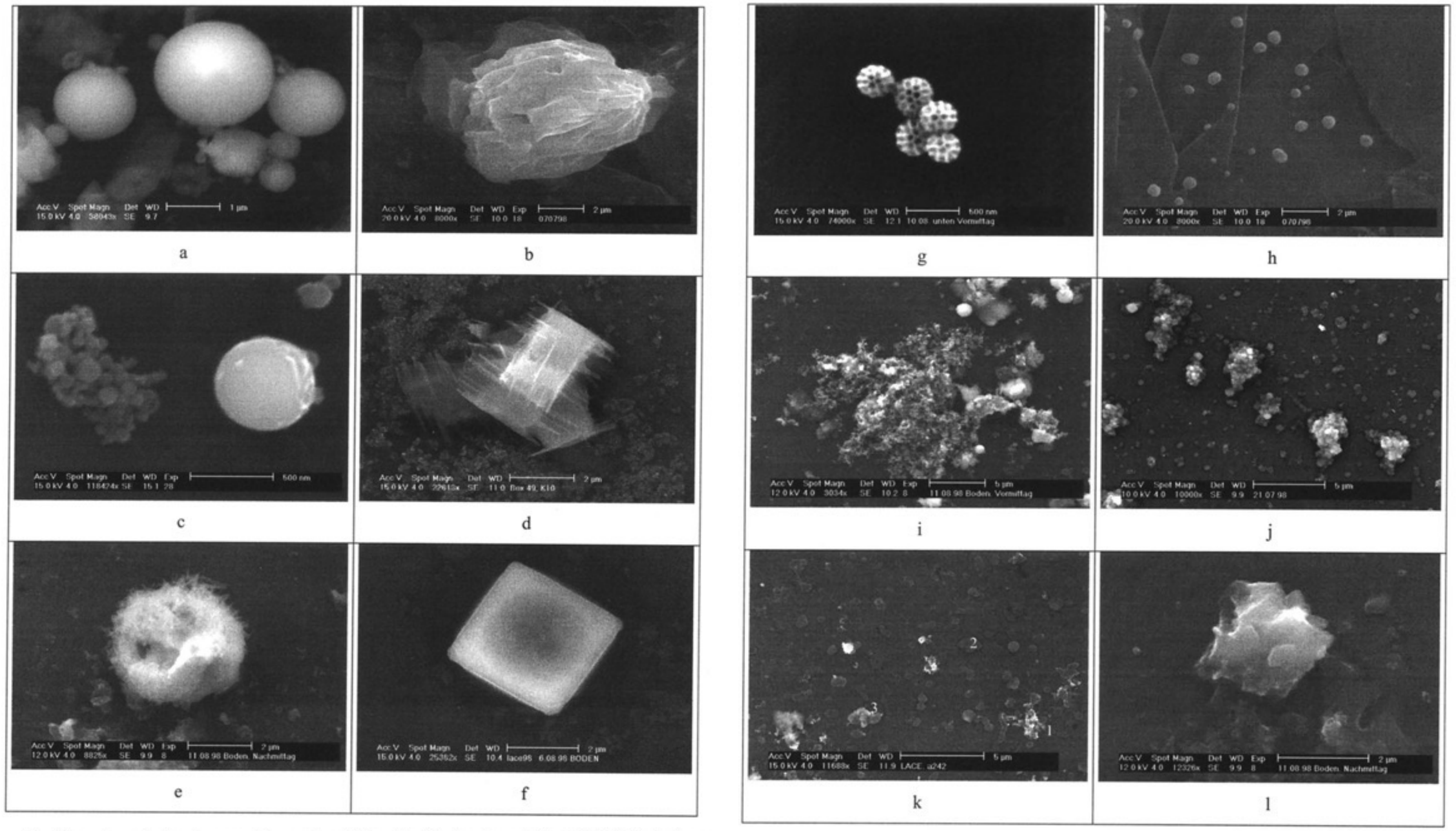
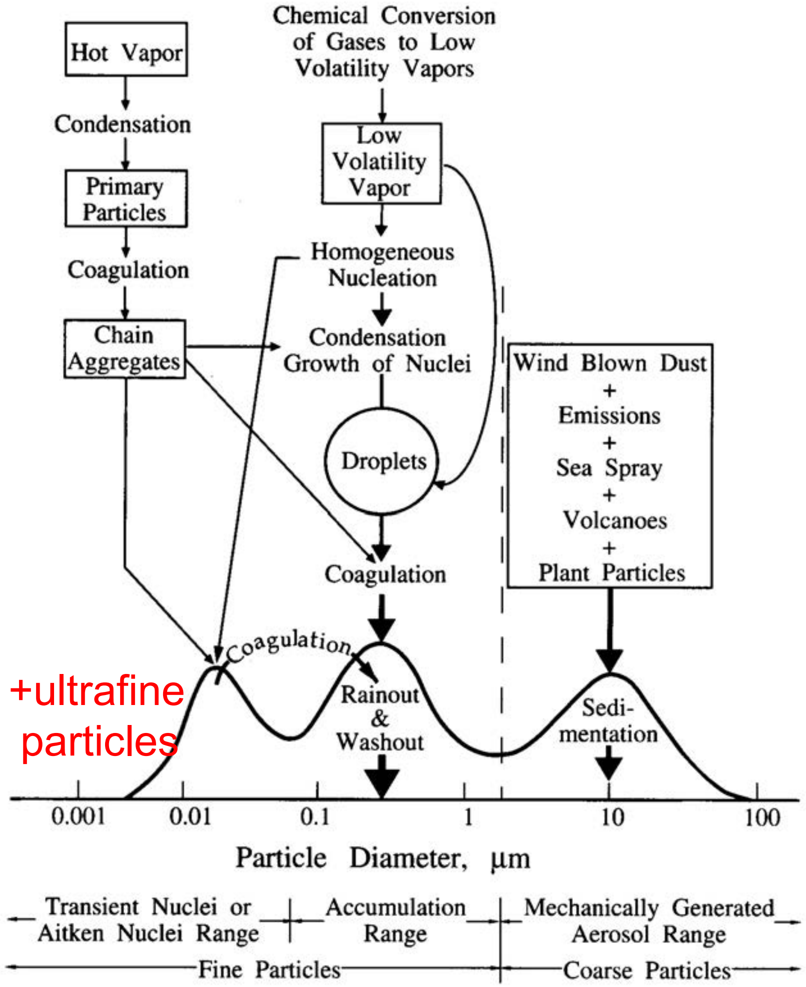


Figure 1. Secondary electron images of aerosol particles: (a) silicate spheres (fly ash); (b) silicate (presumably soil material); (c) iron oxides spheres; (d) calcium sulfate; (e) carbonate; (f) sea salt; (g) biological particle; (h) carbon/sulfate mixed particles; (i) large soot agglomerate and small silicate fly ash particles (bright spheres); (j) ammonium sulfate agglomerates; (k) soot (1), ammonium sulfate (2), and carbon/sulfate mixed particles (3); (l) carbon-rich particle (C_{rest}).

Ebert, et al., “Complex refractive index ofaerosols during LACE 98 as derived from the analysis of individual particles.” *J. Geophys. Res.*, 107, 8121, 10.1029/2000JD000195, 2002.

Aerosols: Microphysical properties (2)

Size spectrum and processes:



+ultrafine particles

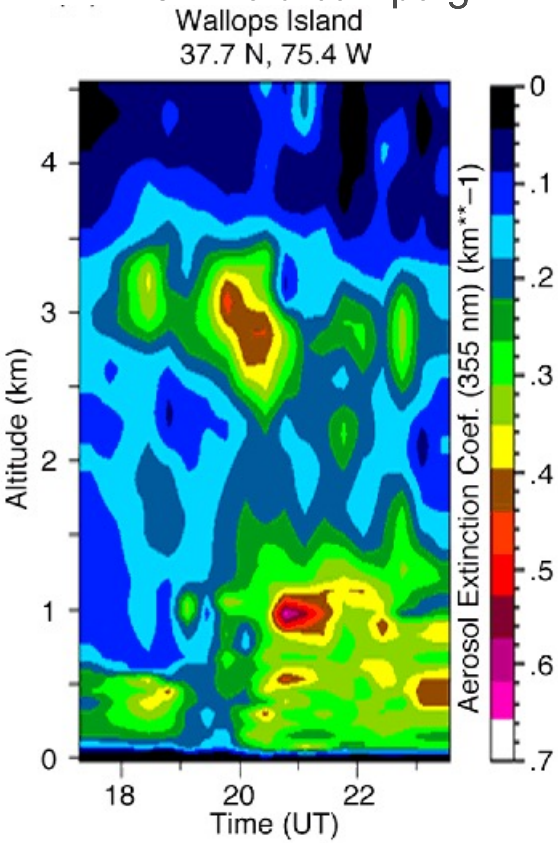
Whitney & Cantrell 1976

Once in the atmosphere, aerosols may:

- be transported to long distances
- be removed (dry deposition, wet removal)
- have their size and/or composition changed by microphysical transformation (humidity, interaction with clouds)
- be affected by chemical transformation

Aerosols: Vertical distribution

TARFOX field campaign



17/07/1996

http://geo.arc.nasa.gov

Hamonou, et al., “Characterization of the vertical structure of Saharan dust export to the Mediterranean basin.” *J. Geophys. Res.*, 104, 22257-22270, 1999.

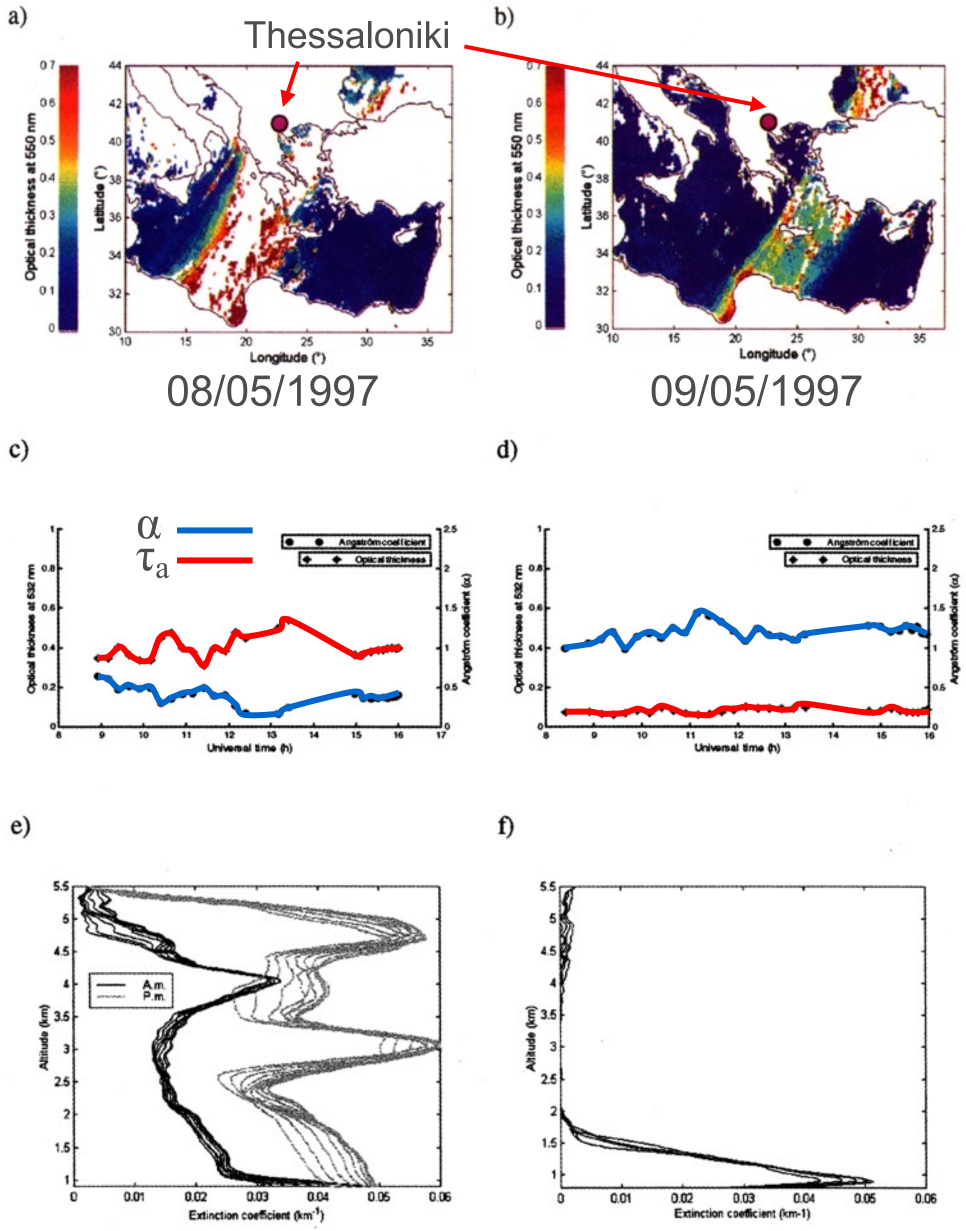


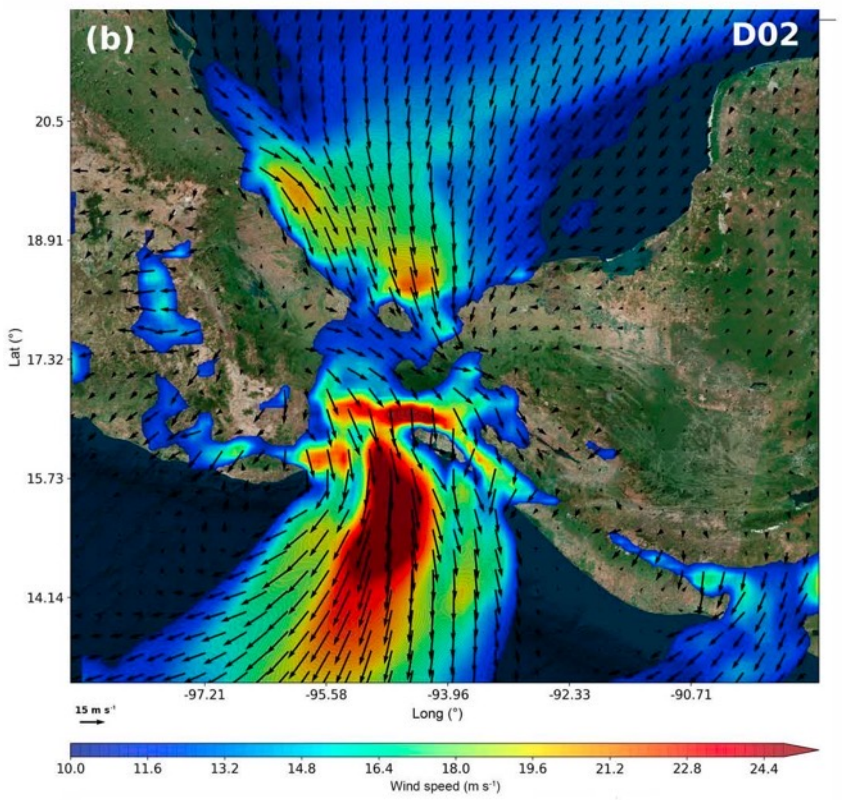
Plate 1. (a and b) Meteosat-derived dust optical thickness at 550 nm for May 8 and 9, 1997, respectively (pink circles show the measurement site location); (c and d) Sun photometer-derived optical thickness at 532 nm and Angström exponent for the same dates; (e and f) extinction coefficient profilesat 532 nm derived from lidar measurements for the same dates (A.M. profiles areperformed between 0930 and 1100 UT whereas P.M. profiles are performed between 1700 and 2000 UT).

Ancillary Atmospheric Variables

- Surface pressure
- Wind speed
- Water vapor
- Relative humidity
- Ozone concentration
- ….

Retrieval &
Space/time characteristics

Gulf of Tehuantepec



Prosper et al. *ESD* 2019

Relationship IOPs - AOPs

The relationship between AOPs (*R*, R_{RS}) and IOPs (a,b,c, β) is not straightforward and is often simplified (e.g., Zaneveld *JGR* 1995).

$$R(\theta_0) = f(\theta_0)\frac{b_b}{a} = f'(\theta_0)\frac{b_b}{b_b + a}$$

Morel & Gentili, *AO* 1991, 1993

$f \sim 0.33$

2 approaches to link AOPs to IOPs

$$r_{rs}(\lambda) = \frac{f(\lambda)}{Q(\lambda)}\frac{b_b(\lambda)}{a(\lambda)} = \frac{f'(\lambda)}{Q(\lambda)}\frac{b_b(\lambda)}{b_b(\lambda) + a(\lambda)}$$

$f/Q \sim 0.085\text{-}0.10$

often $b_b \ll a$

$$r_{rs}(\lambda) = l_1\frac{b_b(\lambda)}{b_b(\lambda) + a(\lambda)} + l_2\left(\frac{b_b(\lambda)}{b_b(\lambda) + a(\lambda)}\right)^2$$

Gordon et al., *JGR* 1988

Ex.: $l_1 \sim 0.0949$, $l_2 \sim 0.0794$

Normalization to $R_{RS} = L_{WN}/E_0$

$$L_W(\lambda,\theta,\theta_0,\phi,\tau_a,IOP,w) = \Re(\theta,w)\frac{f'(\lambda,\theta_0,\tau_a,IOP,w)}{Q(\lambda,\theta,\theta_0,\phi,\tau_a,IOP,w)}\frac{b_{b,t}(\lambda)}{b_{b,t}(\lambda)+a_t(\lambda)}E_d(0^+,\lambda,\theta_0,\tau_a) \qquad (1)$$

water leaving radiance; depends on:

- the bidirectional geometry,
- the water content,
- the atmospheric content,
- the air-sea interface

$$L_{WN}(\lambda) = \frac{L_w(\lambda)}{E_d(0^+,\lambda)}E_0(\lambda) = \frac{L_w(\lambda)}{\cos\theta_0 t_d(\theta_0,\lambda)} \qquad (2)$$

normalized water leaving radiance

$$L^{ex}_{WN}(\lambda) = L_{WN}(\lambda)\frac{\Re(0,w)}{\Re(\theta,w)}\frac{f'(\lambda,0,\tau_a,IOP,w)}{f'(\lambda,\theta_0,\tau_a,IOP,w)}\frac{Q(\lambda,\theta,\theta_0,\phi,\tau_a,IOP,w)}{Q(\lambda,0,0,0,\tau_a,IOP,w)} \qquad (3)$$

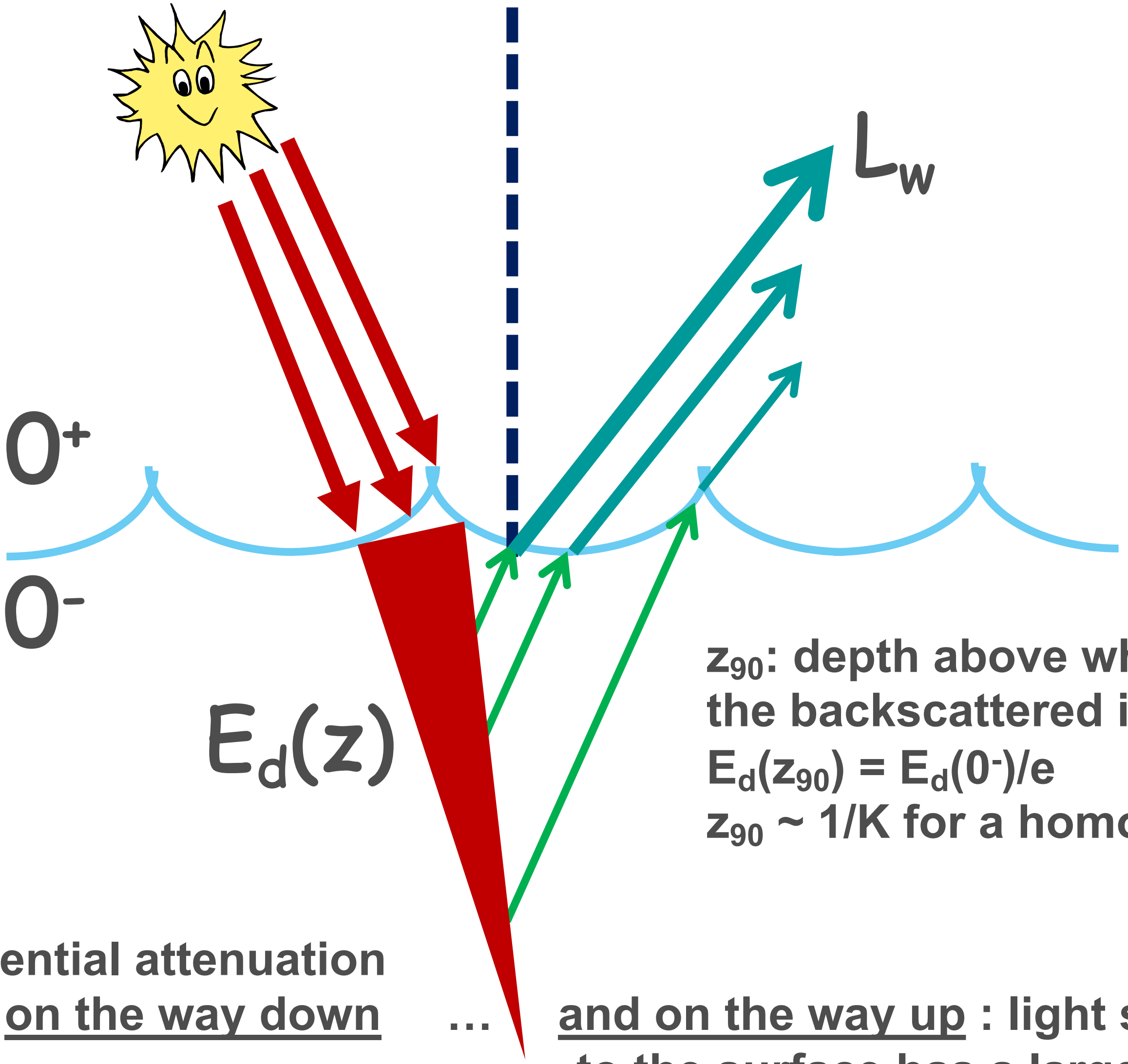
“exact” normalized water leaving radiance

Gordon & Clark, *Appl. Opt.*, 20, 4175-4180, 1981.
Morel et al., *Appl. Opt.*, 41, 6289-6306, 2002.

The “exact” L_{WN} would be the hypothetical radiance that would be measured if the Sun were at zenith, in the absence of atmosphere, and with the Earth at its mean distance from the Sun.

NB: see uncertainty tree

Vertical Distribution in Water (1)



“satellite” value:

$$\overline{C} = \frac{\int_0^{z_{90}} C(z)g(z)dz}{\int_0^{z_{90}} g(z)dz}$$

with

$$g(z) = \exp\left[-2\int_0^{z} K(z')dz'\right]$$

Gordon & McCluney, *AO* 1975,
Gordon & Clark, *AO* 1980

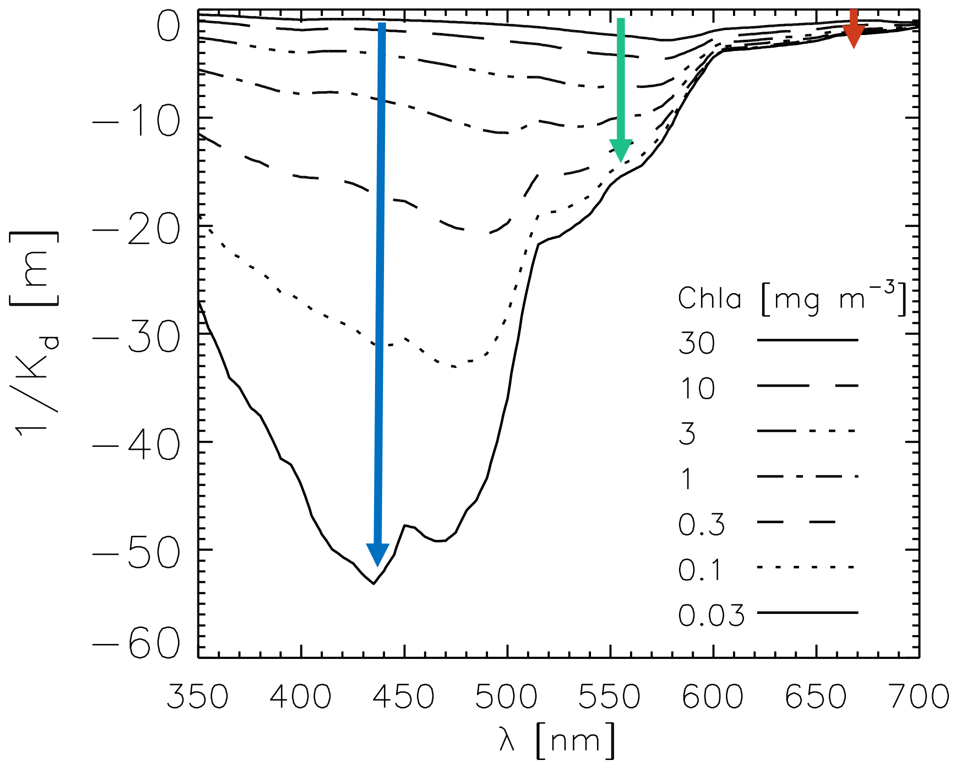
z_{90}: depth above which 90% of the backscattered irradiance originates
$E_d(z_{90}) = E_d(0^-)/e$
$z_{90} \sim 1/K$ for a homogeneous ocean

exponential attenuation
<u>on the way down</u> …

<u>and on the way up</u> : light scattered close to the surface has a larger weight on L_w.

Vertical Distribution in Water (2)

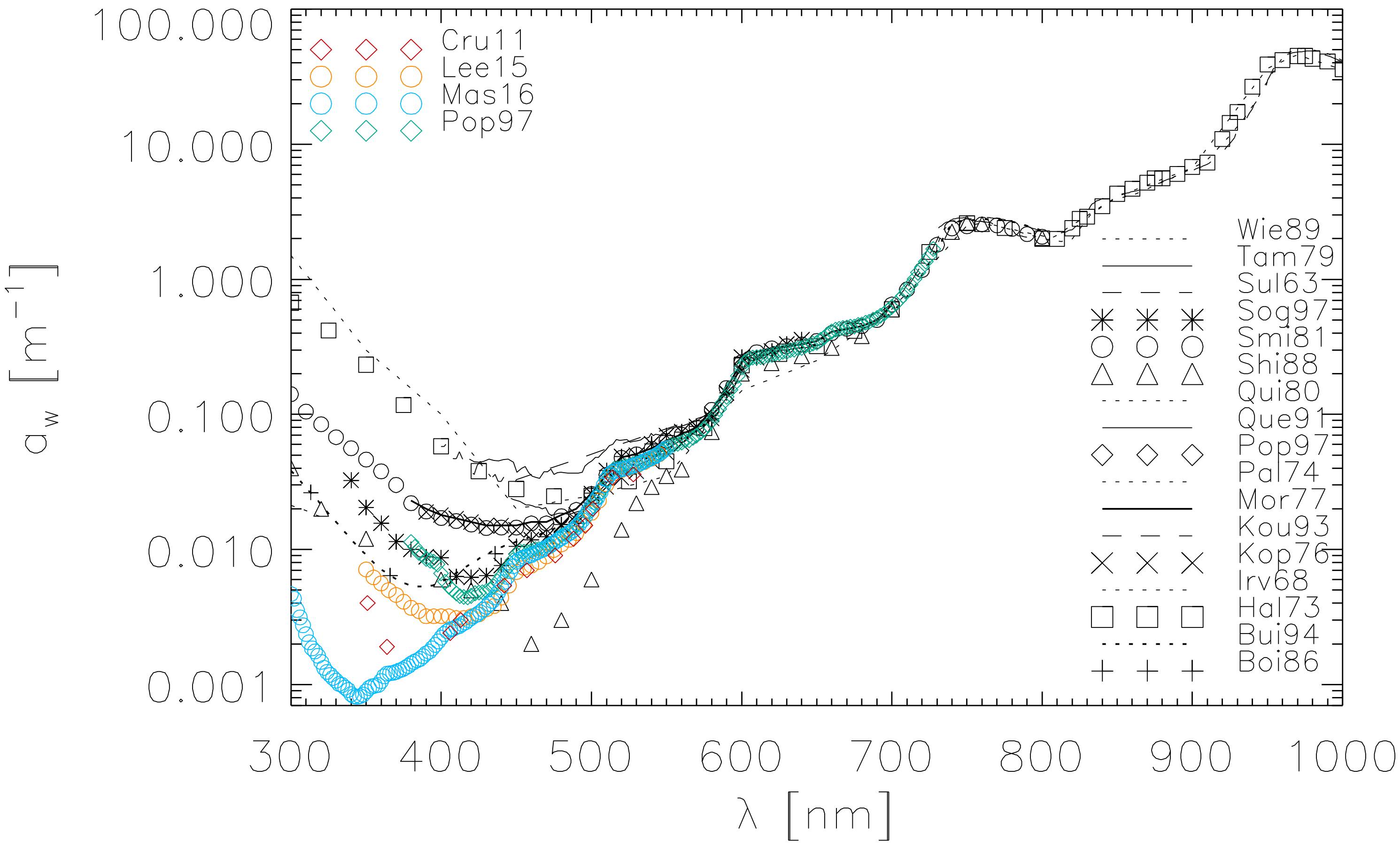
Different penetration depths across the spectrum



In multi-band algorithms, R_{RS} is not “sensitive” to the same layer

Pure Water Absorption

$a_w = f(S,T)$



Nature of particles (hydrosols) and dissolved substances

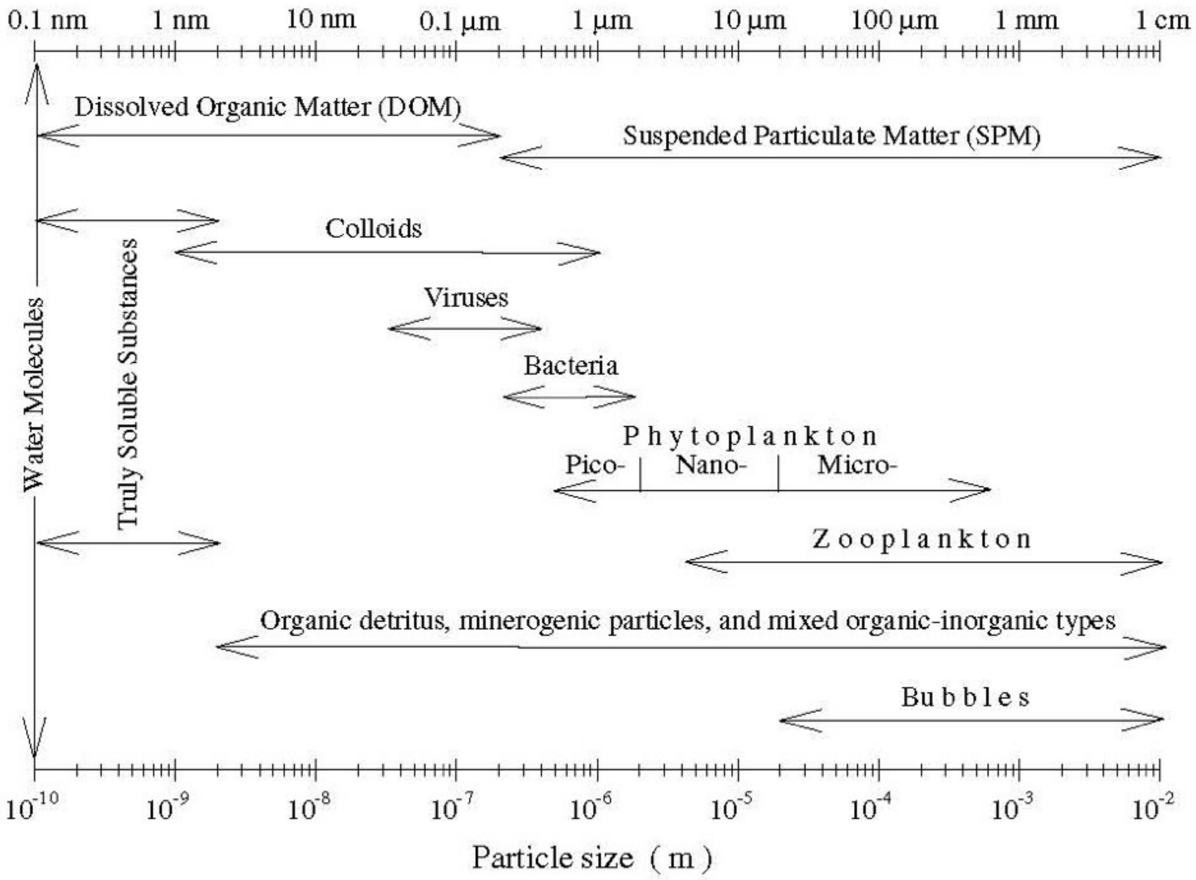


Fig. 1. Schematic diagram showing various seawater constituents in the broad size range from molecular size of the order of 10^{-10} m to large particles and bubbles of the order of 10^{-3} 10^{-2} m in size. The arrow ends generally indicate approximate rather than sharp boundaries for different constituent categories.

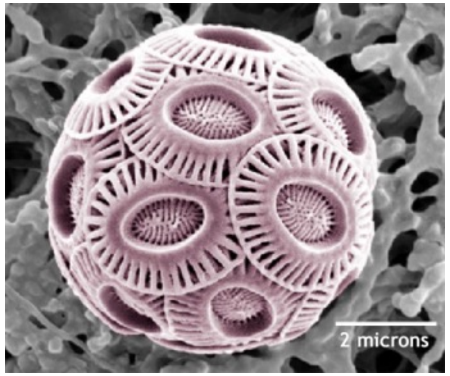
Optically significant agents:

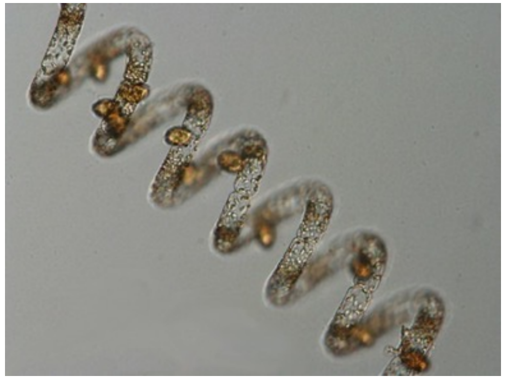
- ❖ pure water
- ❖ bubbles (+coating)
- ❖ microorganisms
- ❖ non-living organic particles
- ❖ minerogenic particles
- ❖ colloids

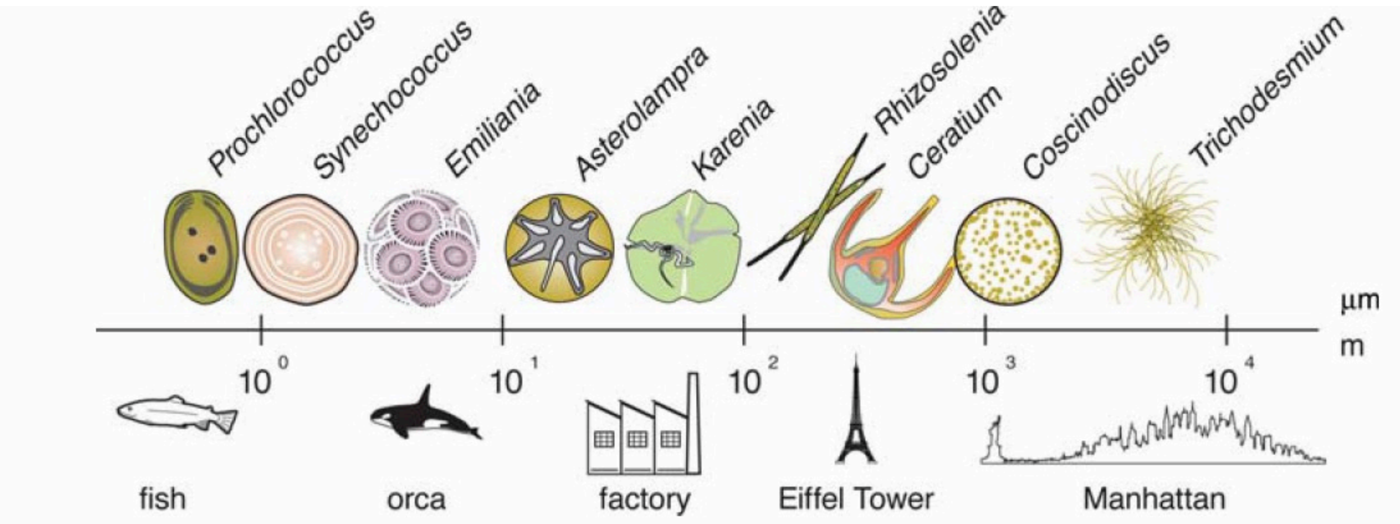
…

Stramski, et al., “The role of seawater constituents in light scattering in the ocean.” *Prog. Oceanogr.*, 61, 27-56, 2004.

Algal Cells







A comparison of the size range (maximum linear dimension) of phytoplankton relative to macroscopic objects.

Phytoplankton represents a large variability of sizes and shapes

Finkel et al., *JPR* 2010

Definition of Optical Properties

$L_w(\lambda) = \alpha\, R_{RS}(\lambda)$ = function (IOPs) ≈ function(b_b,a) <u>for each λ</u>

pure water   particles

back-scattering $b_b(\lambda) = b_{b,w}(\lambda) + b_{b,p}(\lambda)$

absorption $a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{np}(\lambda) + a_{cdom}(\lambda)$

pure water   phyto plankton   non-pigmented particles   CDOM

need for assumptions (e.g., on spectral shapes)

<u>but beware natural variability!</u>

$$a_{ph}(\lambda) = \sum_{i=1}^{N} a_{ph,i}(\lambda)$$

Absorption by different phytoplankton species

$$a_{ph}(\lambda) = a^*_{ph}(\lambda).Chl$$

$$b_{b,p}(\lambda) = b^*_{b,p}(\lambda).TSM$$

Examples of <u>specific</u> inherent optical properties (sIOP)

Natural Variability in IOPs (1)

Phytoplankton:

- ➢ combinations of pigments
- ➢ package effect
- ➢ size
- ➢ …

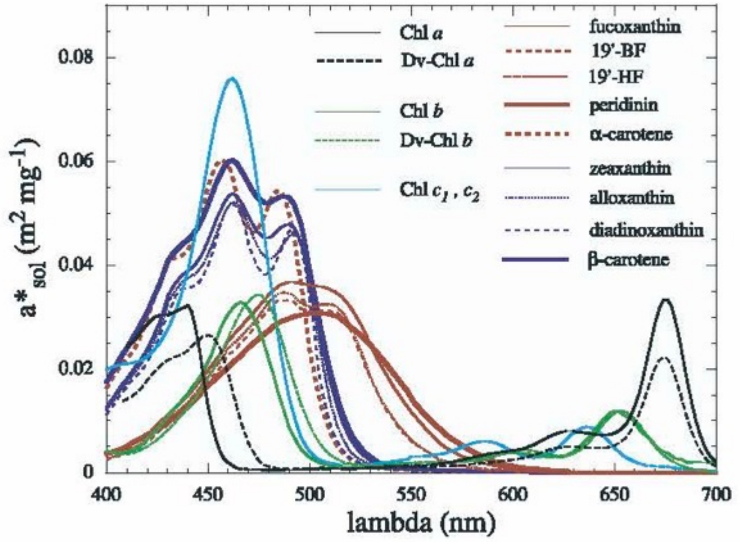
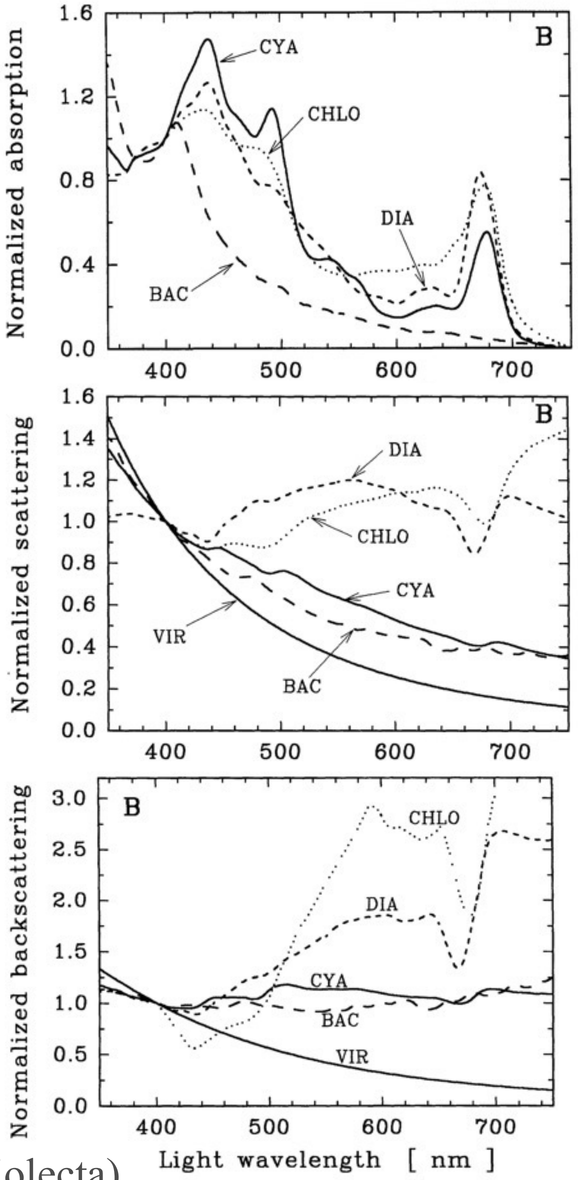


Figure 1. Assumed in vivo weight-specific absorption spectra of the main pigments, $a^*_{sol,i}(\lambda)$ (in m^2 mg^{-1}), as derived from absorption spectra of individual pigments in solvent (see text). Absorption spectra of photosynthetic and nonphotosynthetic carotenoids are shown in red and blue, respectively.

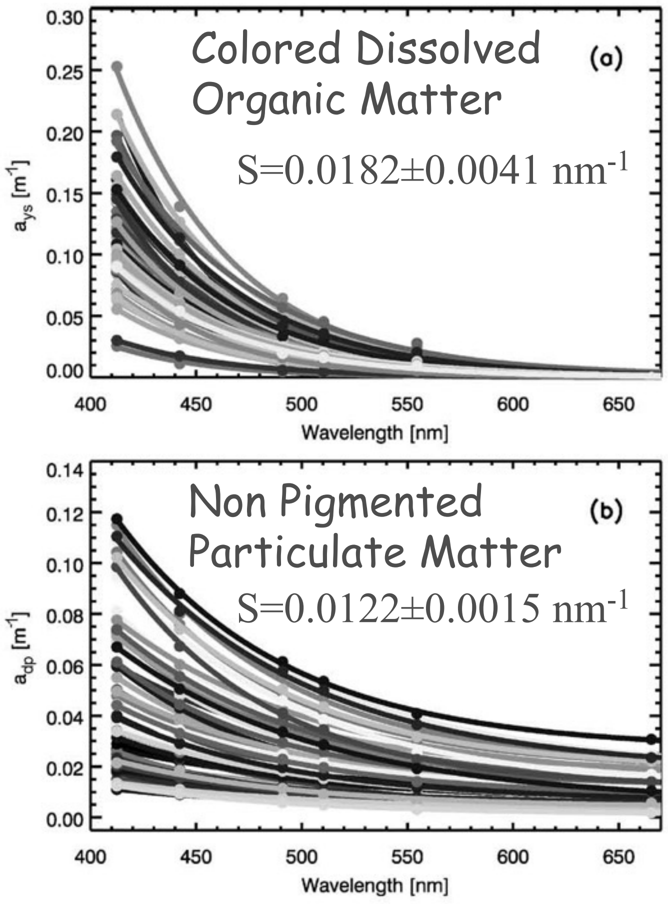
Bricaud et al. *JGR* 2004

Stramski & Mobley, *AO* 1997



BAC: heterotrophic bacteria
CHLO: chlorophyte (Dunaliella tertiolecta)
CYA: cyanobacteria (Synechococcus)
DIA: diatom (Thalassiosira pseudonana)

Natural Variability in IOPs (2)



D'Alimonte et al., *IEEE* 2004

Absorption often represented by exponential functions:

Absorption by non pigmented particles:

$$a_{np}(\lambda) = a_{np}(\lambda_0).e^{-S_{np}(\lambda-\lambda_0)}$$

Absorption by dissolved substance (CDOM):

$$a_{ds}(\lambda) = a_{ds}(\lambda_0).e^{-S_{ds}(\lambda-\lambda_0)}$$

- **large variability of S in nature, possibly associated with different types of constituents**
- **part of this variability is due to method of calculations of the slope (linear/non linear fit, spectral range)**

S_{ds}: 0.010-0.025 nm^{-1}, 0.014-0.018 nm^{-1} typical]

Natural Variability in IOPs (3)

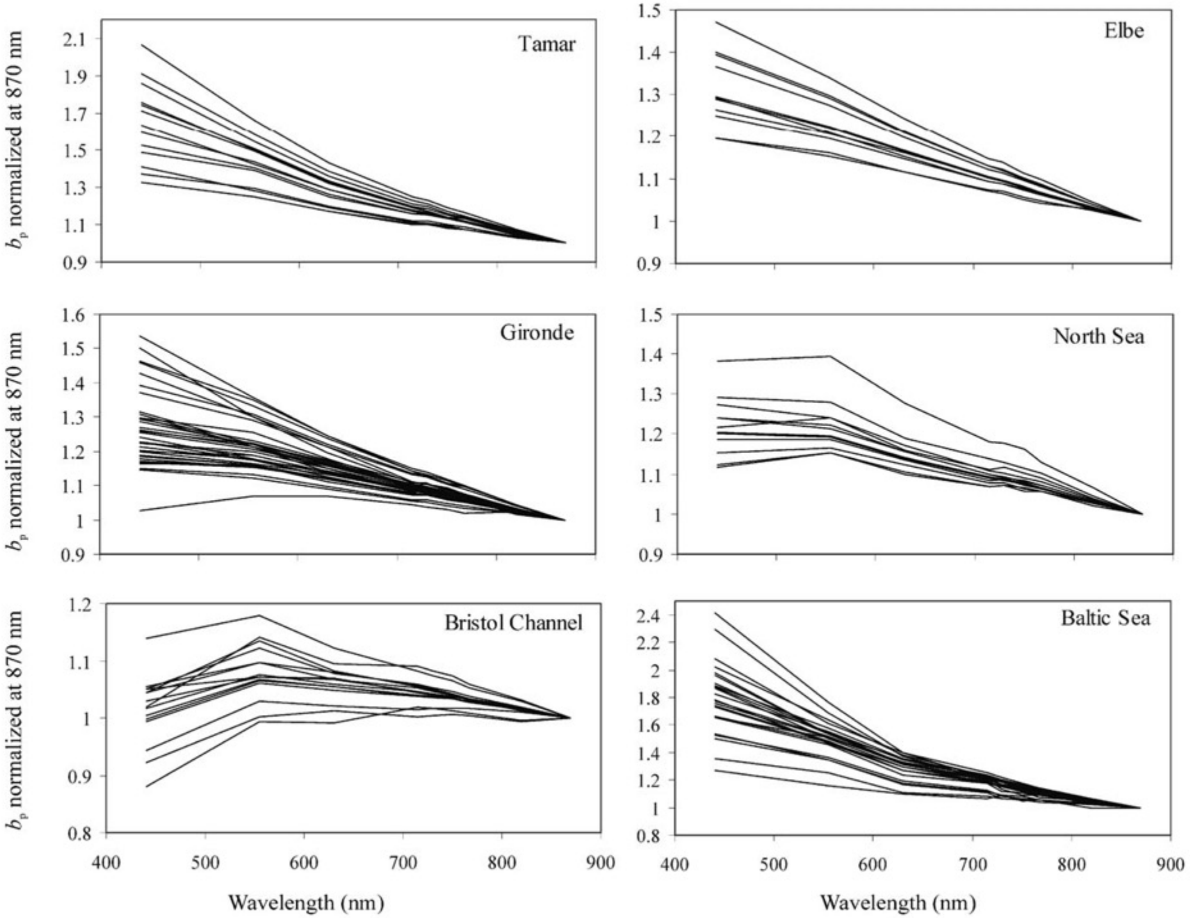


Fig. 5. Typical site-by-site measured b_p spectra (normalized at 870 nm).

Doxaran et al., *LO* 2009

Scattering by particles

scattering

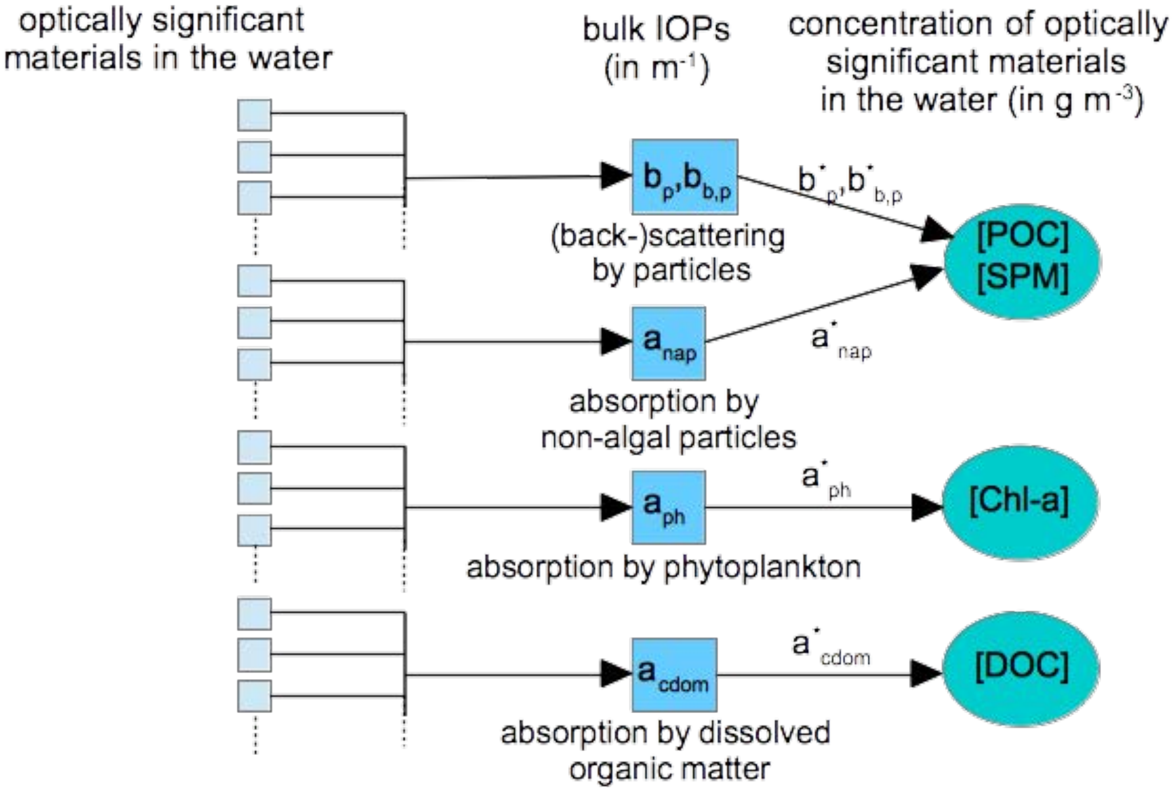
$$b_p(\lambda) = b_p(\lambda_0)\left(\frac{\lambda_0}{\lambda}\right)^{\eta_b}$$

back-scattering

$$b_{b,p}(\lambda) = b_{b,p}(\lambda_0)\left(\frac{\lambda_0}{\lambda}\right)^{\eta}$$

η ~ 0 (large) to 2 (small)

Natural Variability in sIOPs (1)



Relationships between IOPs and mass concentrations of constituents

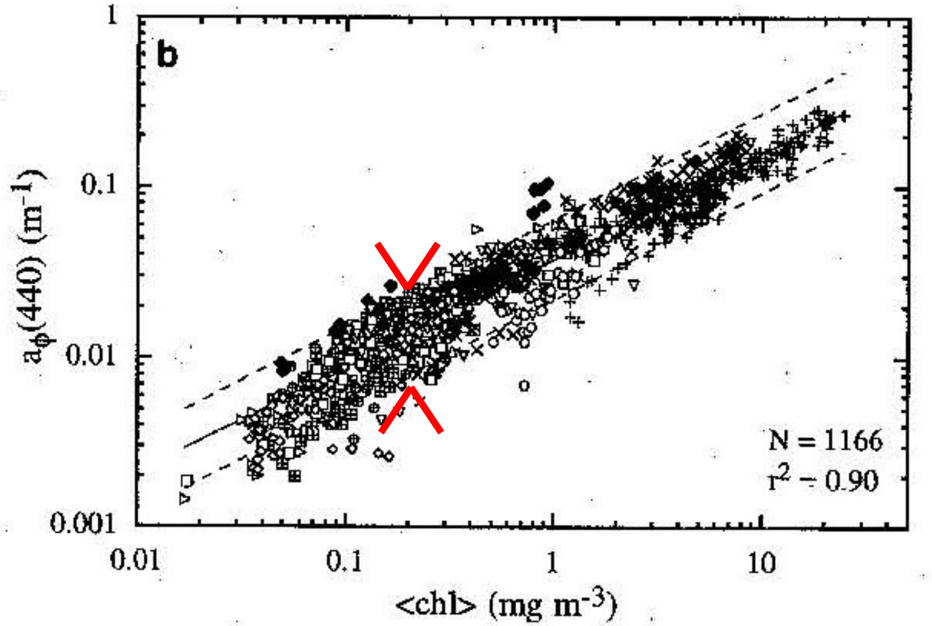
$$a_{ph}(\lambda) = a^*_{ph}(\lambda).Chl$$

$$b_{b,p}(\lambda) = b^*_{b,p}(\lambda).TSM$$

Examples of <u>specific</u> inherent optical properties (sIOP)

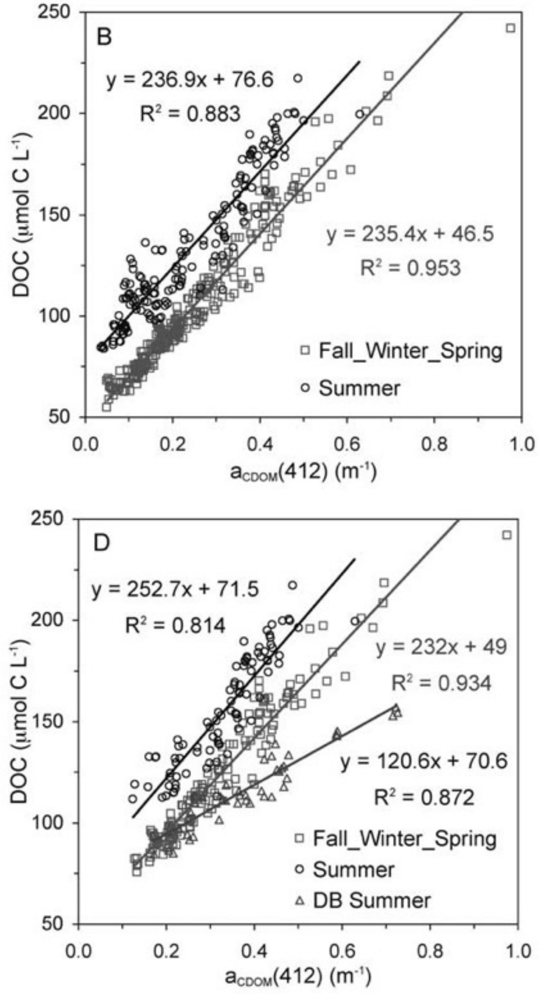
Natural Variability in sIOPs (2)

variations a_{ph} vs. Chla



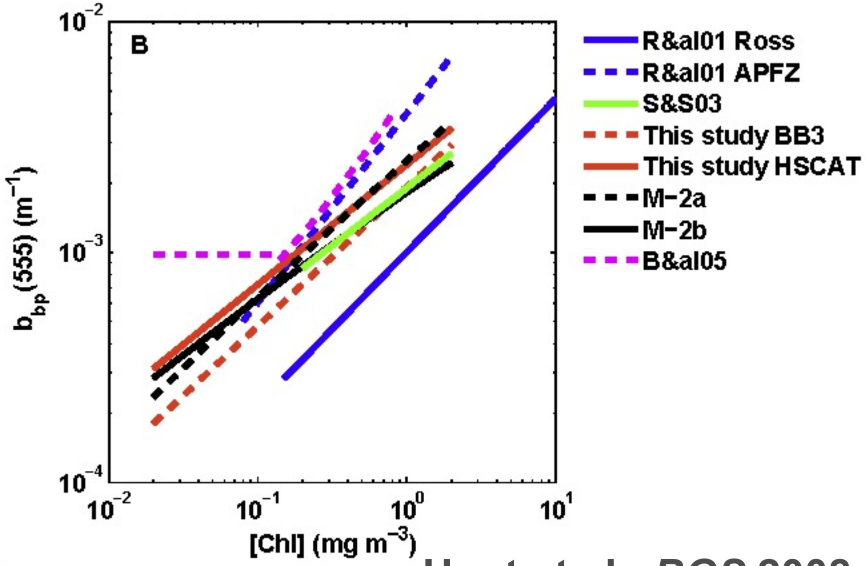
Bricaud et al. *JGR* 1998

variations a_{CDOM} vs. DOC



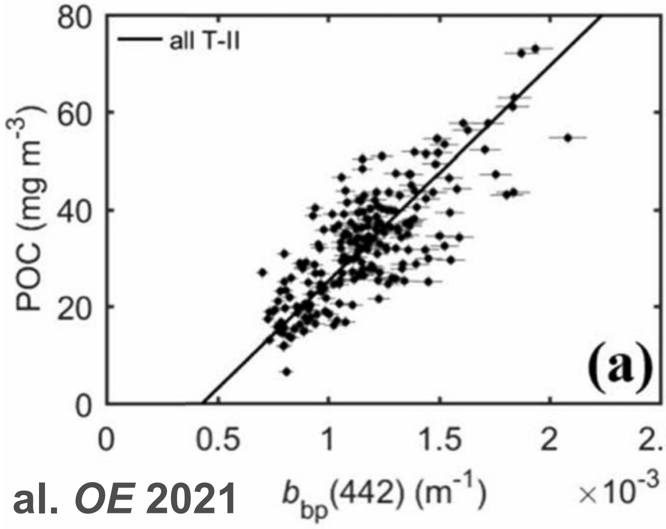
Mannino et al., *JGR* 2008
US coastal waters

variations $b_{b,p}$ vs. Chla



Huot et al., *BGS* 2008

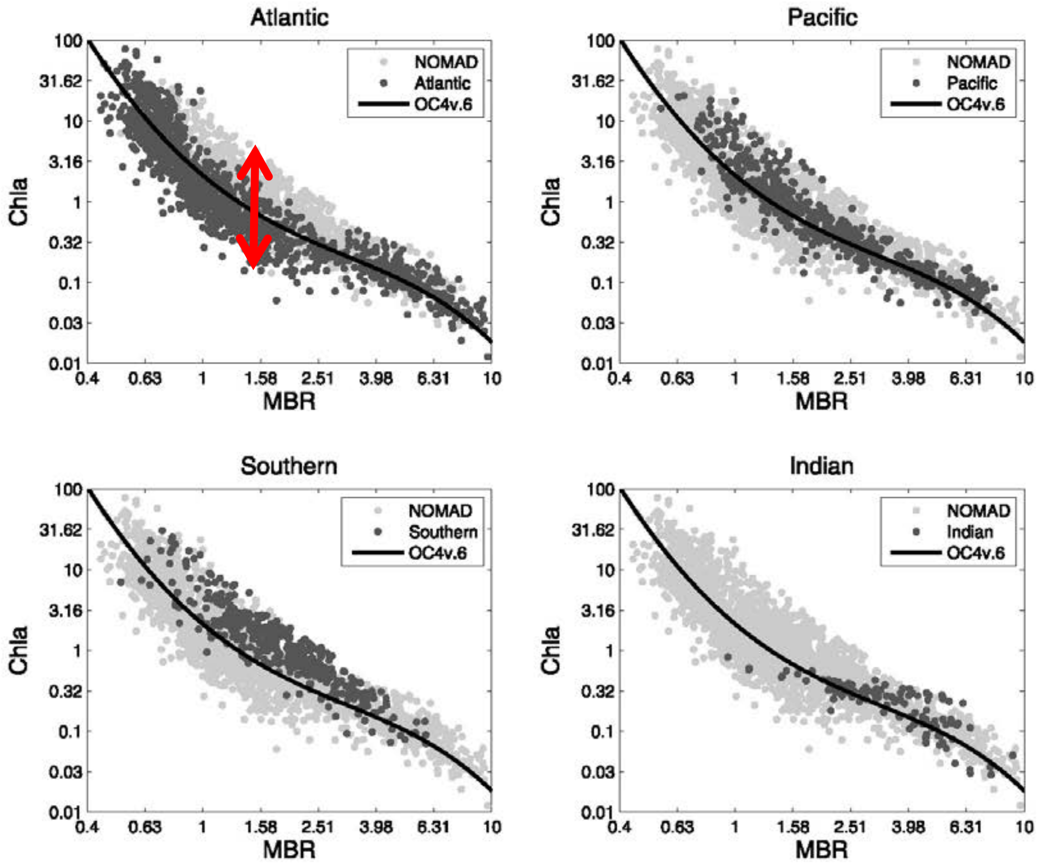
variations $b_{b,p}$ vs. POC



Qiu et al. *OE* 2021
South China Sea

Natural Variability: Implications

- Introduces model errors
- Leads to scattering around empirical relationships



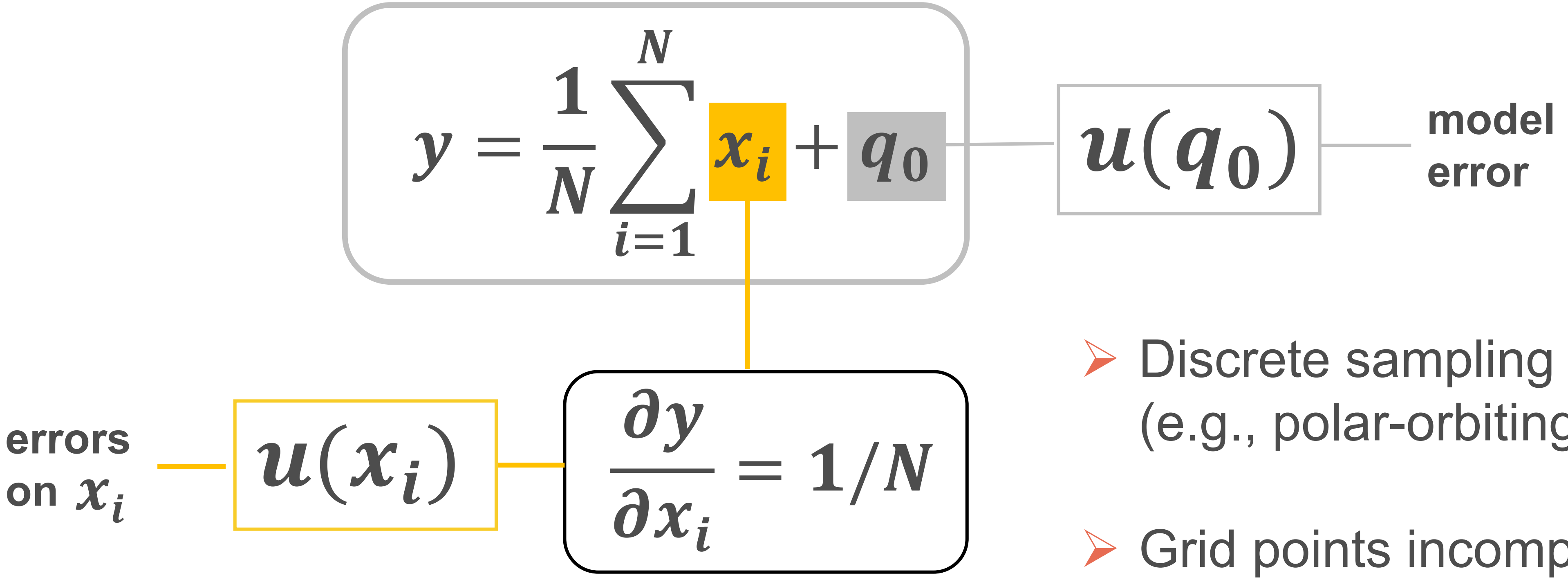
Szeto et al., *JGR* 2011

Sources of Uncertainties for EO data

from L2 to L3 - Editing

Data Editing: Case of Composites (1)

Uncertainty tree:



$$y = \frac{1}{N}\sum_{i=1}^{N} x_i + q_0$$

$u(q_0)$ model error

errors on x_i — $u(x_i)$ — $\frac{\partial y}{\partial x_i} = 1/N$

- ➢ Discrete sampling for a daily datum (e.g., polar-orbiting)
- ➢ Grid points incompletely/variably filled
- ➢ Incomplete suite of days for a time composite

Data Editing: Case of Composites (2)

Uncertainty for a time/space/mission composite (e.g., for an average):

$$y = \frac{1}{N}\sum_{i=1}^{N} x_i \quad \Longrightarrow \quad u^2(y) = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N} u(x_i)\, u(x_j) r(x_i, x_j)$$

Assuming an "average" correlation:

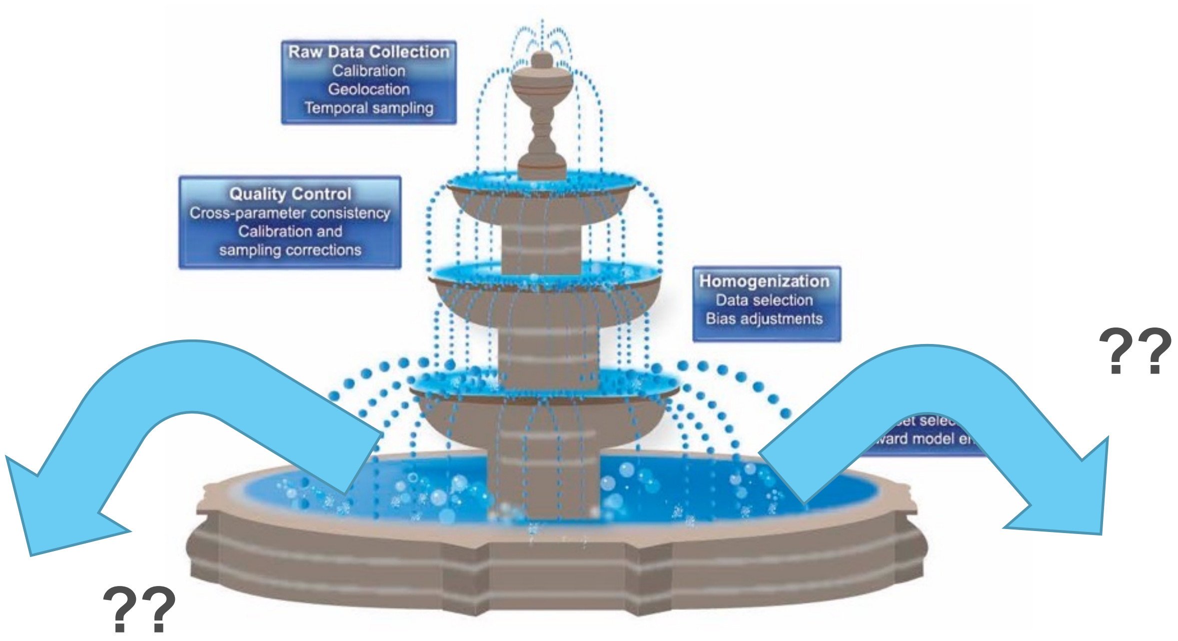
$$u^2(y) = \frac{1-\bar{r}}{N^2}\sum_{i=1}^{N} u^2(x_i) + \frac{\bar{r}}{N^2}\left(\sum_{i=1}^{N} u(x_i)\right)^2$$

$$\xrightarrow{\bar{r} = 0} \quad u(y) = \frac{1}{\sqrt{N}}\sqrt{\frac{1}{N}\sum_{i=1}^{N} u^2(x_i)}$$

$$\xrightarrow{\bar{r} = 1} \quad u(y) = \frac{1}{N}\sum_{i=1}^{N} u(x_i)$$

NB: systematic contributions are not expressed here!

Isn’t it overflowing?



Matthews et al. BAMS 2013

Some claims might be over-optimistic ….
but it works!

NSF included Ocean Color as one of the landmark achievements in biology oceanography in its review “50 Years of Ocean Discovery (1950-2000)”

The potential of Ocean Color can be fully realized if we are able to derive trustworthy uncertainty budgets