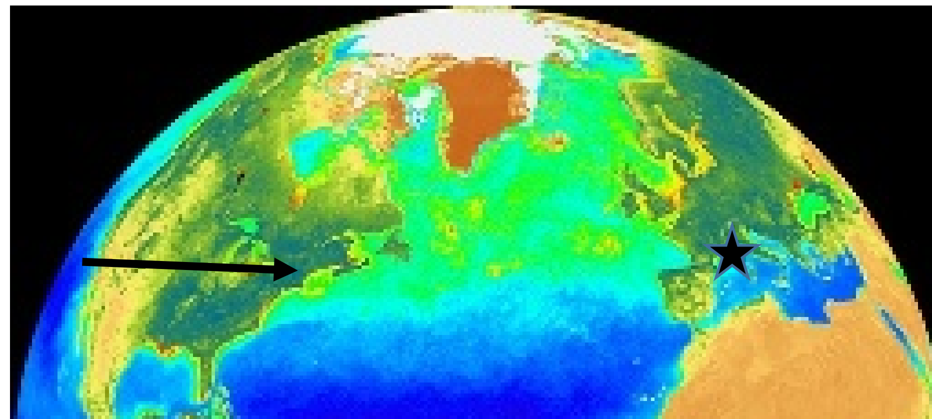
Introduction to IOPs and their measurement (fundamentals)

Collin Roesler

19 July 2022

Intro to me

- Where do I come from (geographically)?



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    - *Episode 1 "Sharks" with Dr. Eugenia Clark*

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      and... sponds to climate forcing
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    - ...me... Labs prep for PhD w...
  - ...og... of Washington (...
    - Inverse modeling of absorption and remote sensing reflectan...
    - Career-spanning relationship with Ocean Optics Course
  - Post doc, Oregon State University (Ron Zaneveld)
    - Testing and caracterizing new IOP instrumentation

Satellite Color Observations of the Phytoplankton Distribution in the Eastern Equatorial Pacific During the 1982-1983. El Niño

GENE FELDMAN, DENNIS CLARK, AND , DAVID HALPERN Authors Info & Affiliations

SCIENCE • 30 Nov 1984 • Vol 226, Issue 4678 • pp. 1069-1071 • DOI: 10.1126/science.226.4678.1069

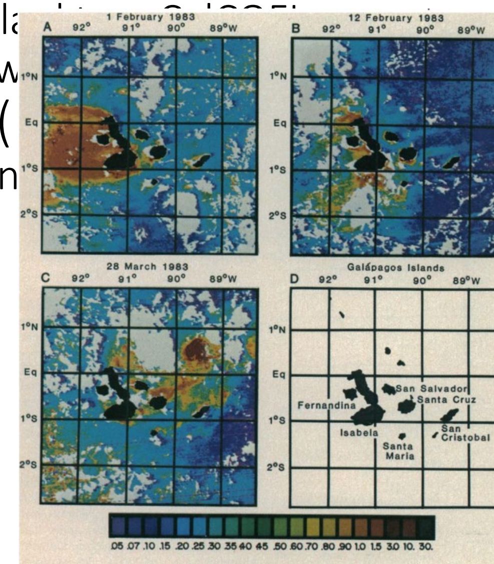

Fig. 2. Color-encoded maps of phytoplankton pigment concentrations acquired on overpasses of the Galápagos Islands (D) derived from Nimbus-7 Coastal Zone Color Scanner imagery on (A) 1 February 1983, orbit 21581; (B) 12 February 1983, orbit 21733; and (C) 28 March 1983, orbit 22341. In this presentation, the major islands are black and the clouds white.

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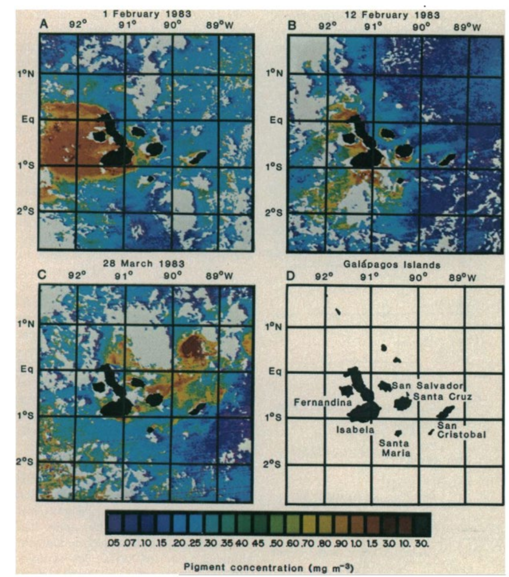

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    - College course on climate coincided with this paper → life-long interest in understanding how ocean ecosystems responds to climate forcing
  - M.S. Physical Oceanography, Oregon State University (Dudley Chelton)
    - Time series analysis, large data sets, climate forcing on zooplankton, CalCOFI
    - 2nd summer optics course, Friday Harbor Labs prep for PhD with CZCS
  - Ph.D. Biological Oceanography, Univ of Washington (Mary Jane Perry)
    - Inverse modeling of absorption and remote sensing reflectance
    - *Career-spanning relationship with Ocean Optics Course*
  - Post doc, Oregon State University (Ron Zaneveld)
    - Testing and characterizing new IOP instrumentation
  - Positions at:
    - University of Connecticut
    - Bigelow Laboratory for Ocean Science
    - University of Maine
    - Bowdoin College Dept of Earth and Oceanographic Science

Perry MJ. 2020. *Annu. Rev. Mar. Sci.* 12:1–22

Intro to me

- Where do I come from (geographically)?
- How did I get here (scientifically)?
- What about outside of science?






What are we covering in this lecture?

- After delving into *the interaction of light and matter*, and *optics of marine particles*, this lecture will place that theory in the context of what is required for accurate measurement of the inherent optical properties (i.e., what we want from a sensor). Then reality set in and places physical constraints on those specification (i.e., what we settle for). Examples of commonly implemented measurement strategies for *in situ* measurement of absorption and attenuation, as well as discrete benchtop measurement of particulate absorption will be explored.
- Focus on two commercially-available technologies as models for measuring IOPs

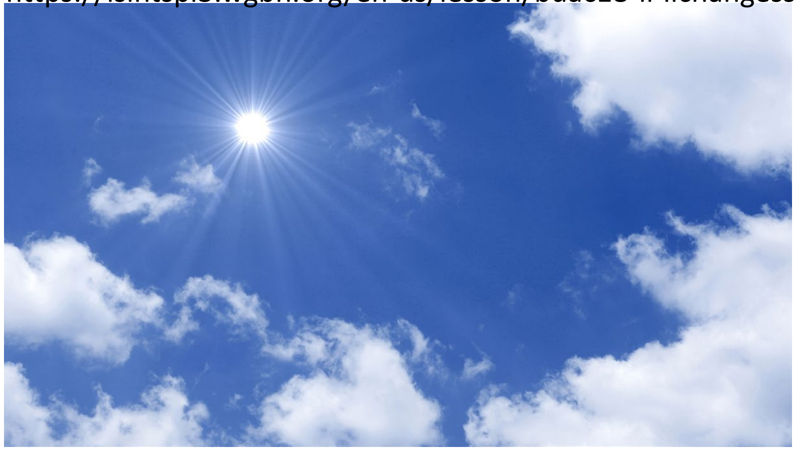
So far…

- Enjoyed a few hours of:
  - optical theory
  - Playing with light
- We hope that you have been able to find:
  - some topics that are within your comfort zone
  - some topics that are outside your comfort zone
  - Some topics that spark your curiosity
  - Some lingering questions
- Let’s spend the next hour
  - putting theory to practice
  - Building optical intuition

Compare the light fields: top of the atmosphere, Earth's surface, below ocean surface

http://www.space.com/12934-brightness-sun.html

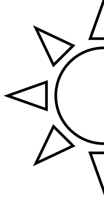
https://lsintspl3.wgbh.org/en-us/lesson/buac18-il-ilchangessky/1



- Similarities

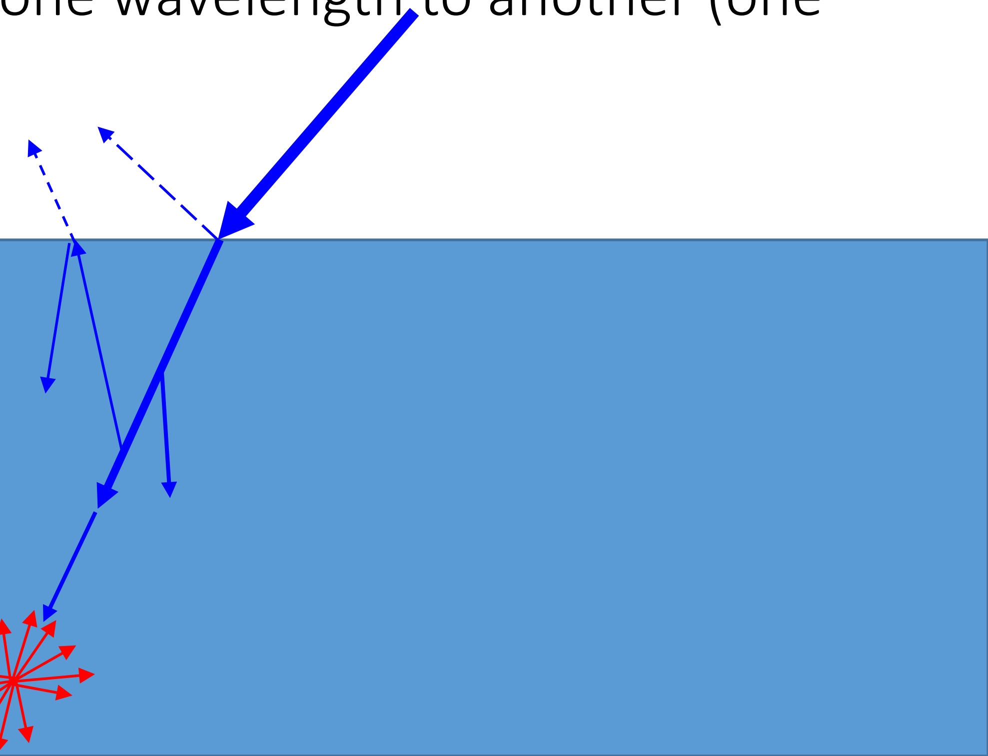
- Differences

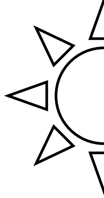
https://www.shutterstock.com/nb/video/clip-1014907747-sun-underwater-sky-scenery



As light penetrates the ocean surface and propagates to depth, what processes affect the light transfer?

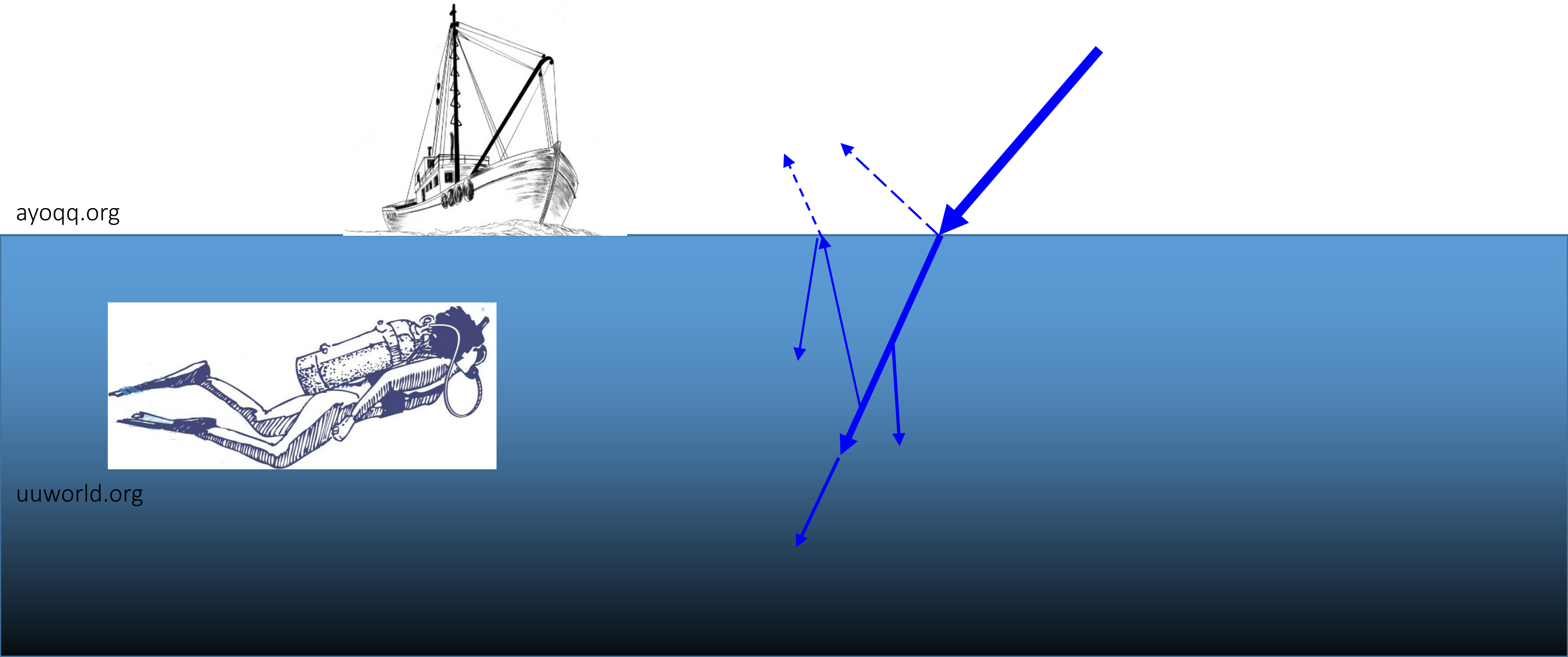
- Absorption – removes light
- Scattering – redirects light
- Re-emission – converts from one wavelength to another (one direction to another)
- A portion leaves the surface

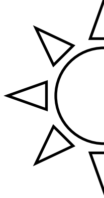




Case study 1:
Consider an ocean that has no scattering but does have absorption

- What changes?
- What do the sailors see from a boat (reflectance)?
- What does the diver see (transmission)?





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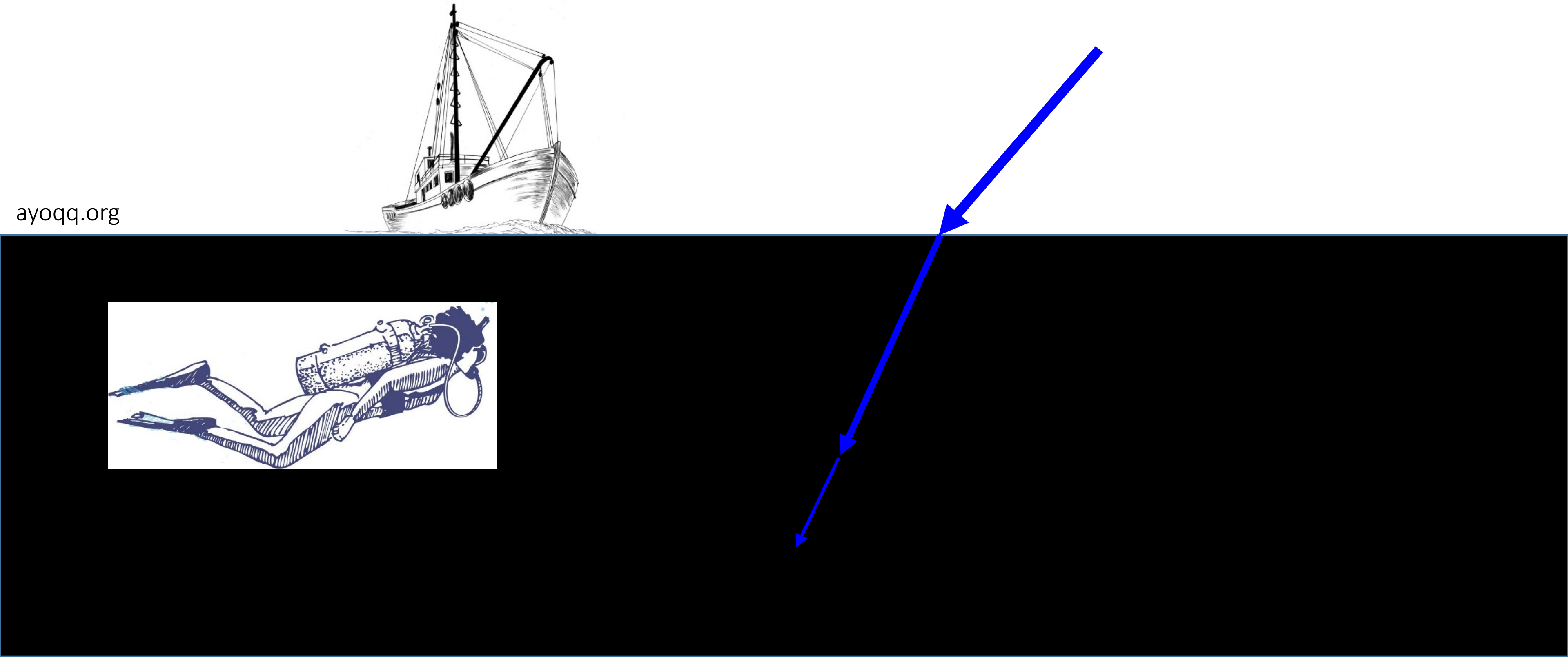
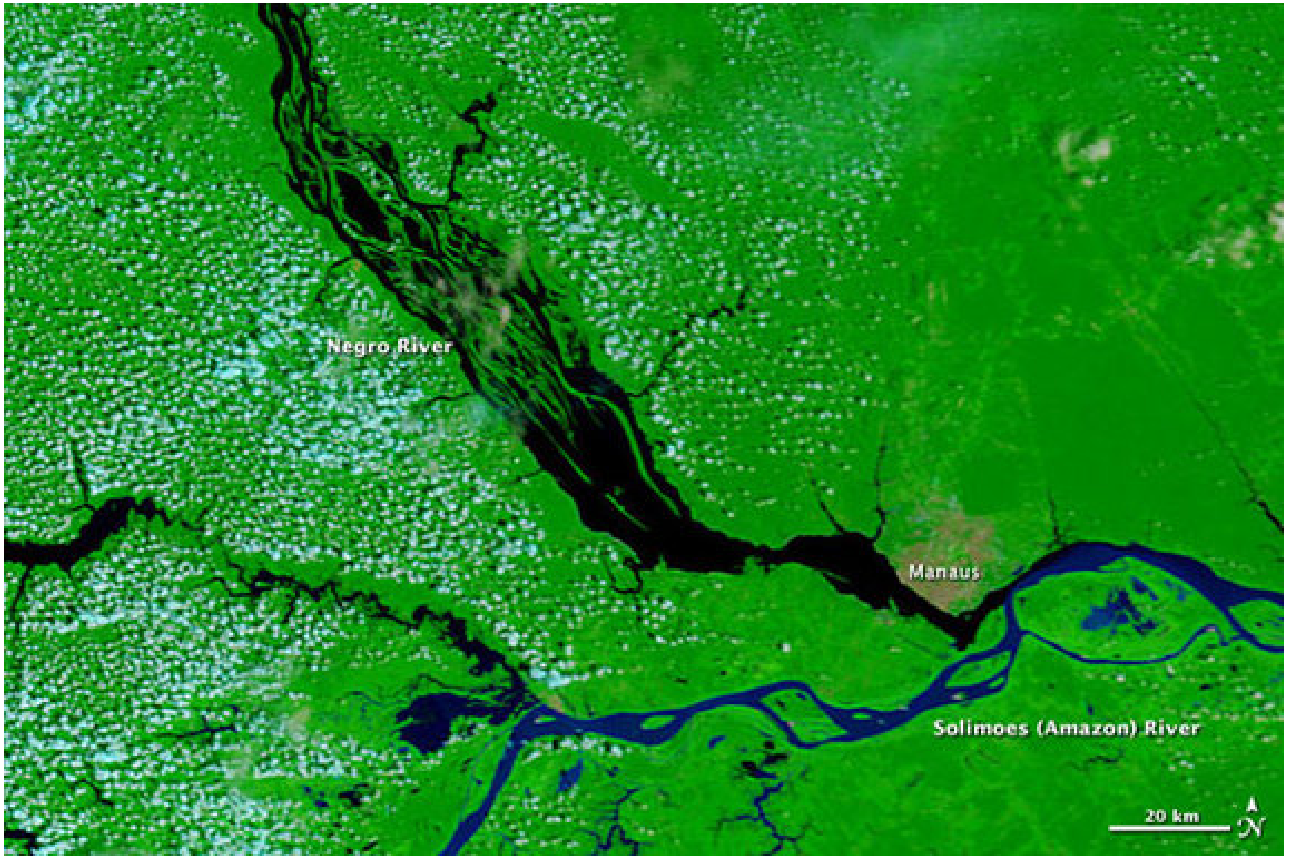


Case study 1:
Consider an ocean that has no scattering but does have absorption

- Is there a natural analog?



The Rio Negro in 2010
Credit: MODIS Rapid Response Team
NASA GSFC

Case study 1:
Consider an ocean that has no scattering but does have absorption

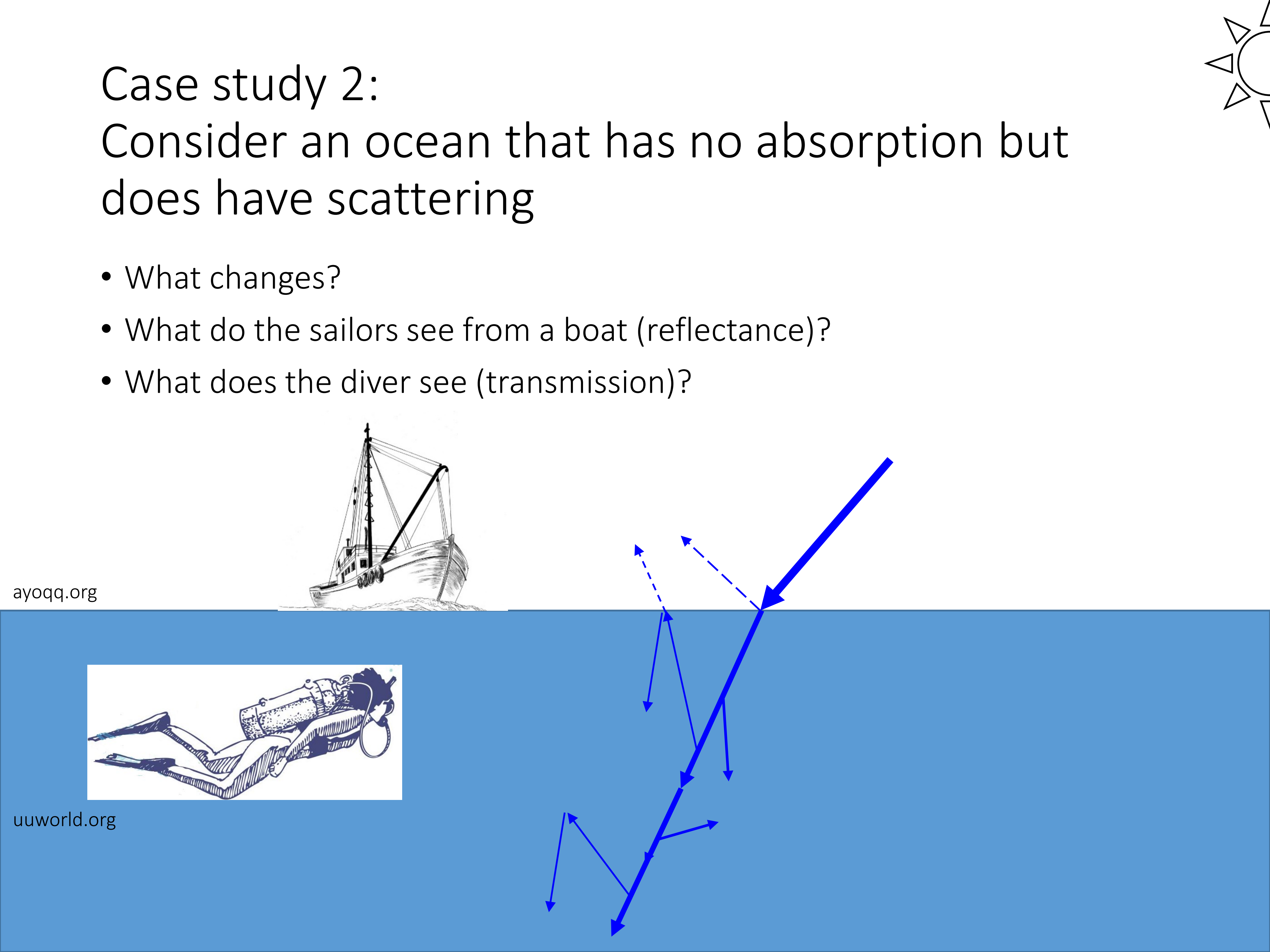
http://2.bp.blogspot.com/-4NPGeVA5zVs/T-iCGJp3GlI/AAAAAAAAEaI/3cTvA31bth4/s1600/encontro-do-negro-e-solimoes.jpg

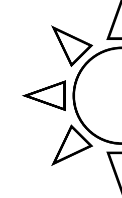
Case study 1:
Consider an ocean that has no scattering but does have absorption

http://www.mongabay.com/images/pictures/brazilrio_negro_beach_close.html

Case study 2:
Consider an ocean that has no absorption but does have scattering

- What changes?
- What do the sailors see from a boat (reflectance)?
- What does the diver see (transmission)?





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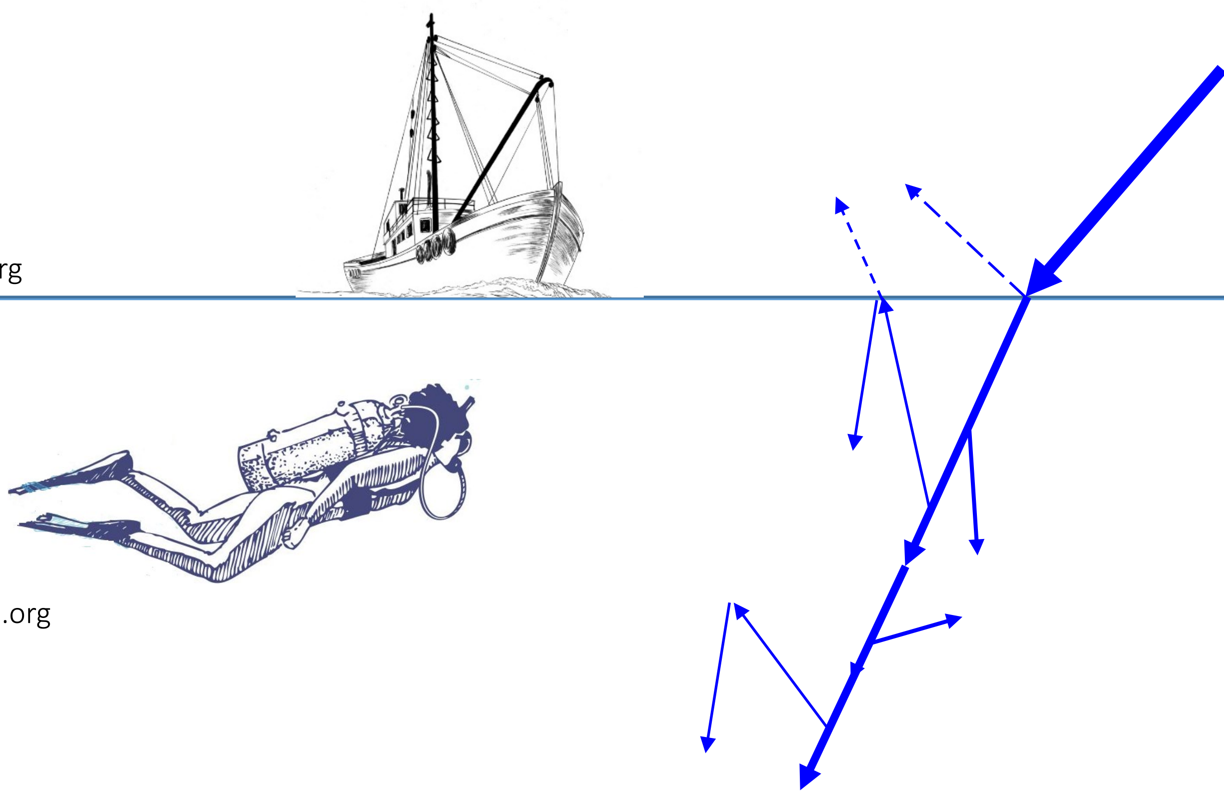

ayoqq.org

uuworld.org

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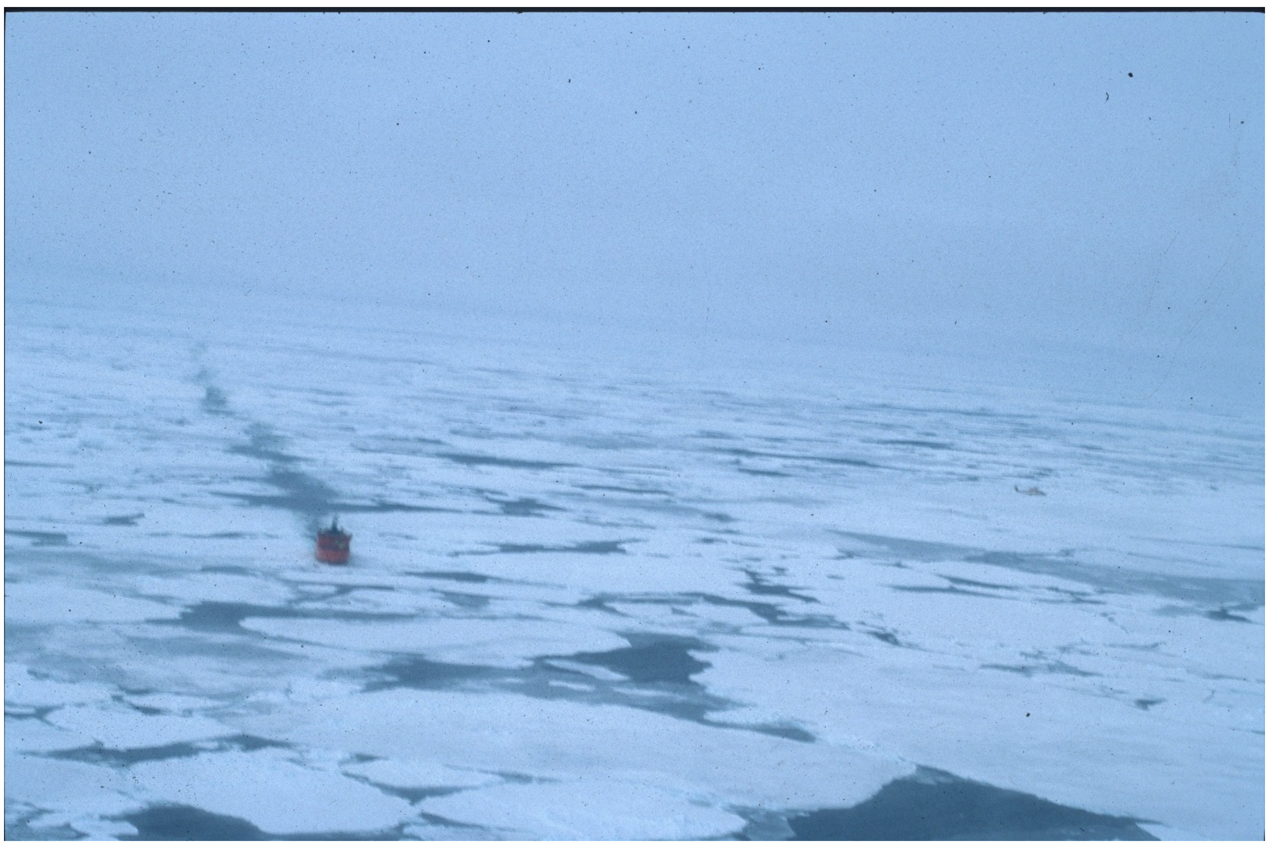

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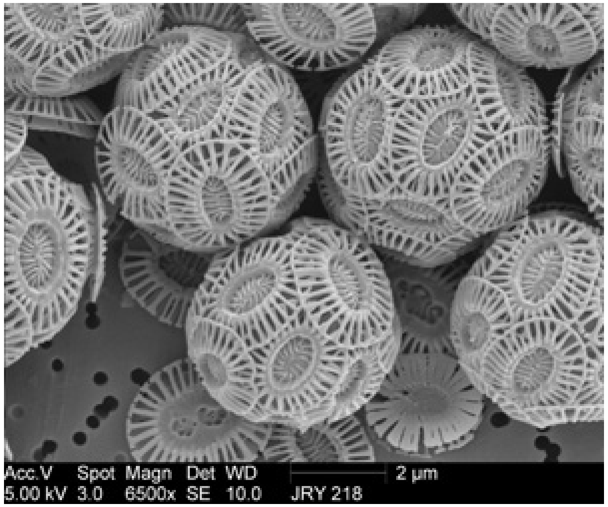
http://www.co2.ulg.ac.be/peace/objects/218-01.JPG



- Is there a natural analog?

https://www.blurb.fr/b/11031810-ultra-fine-art-of-coccolithophores

https://www.bigelow.org/enews/English%20Channel%20Bloom.jpg

https://themarinedetective.com/2018/07/29/why-is-our-cold-ocean-suddenly-tropical-blue/

Case study 2:
Consider an ocean that has no absorption but does have scattering

- Is there a natural analog?

https://www.escapecampervans.com/blog/guide-to-iconic-lakes-in-banff/

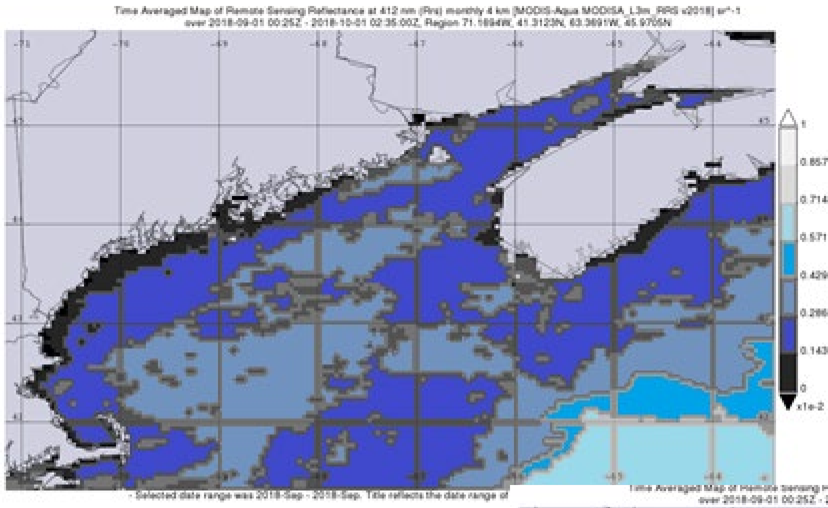
http://www.alamy.com Image ID: CX4R4C

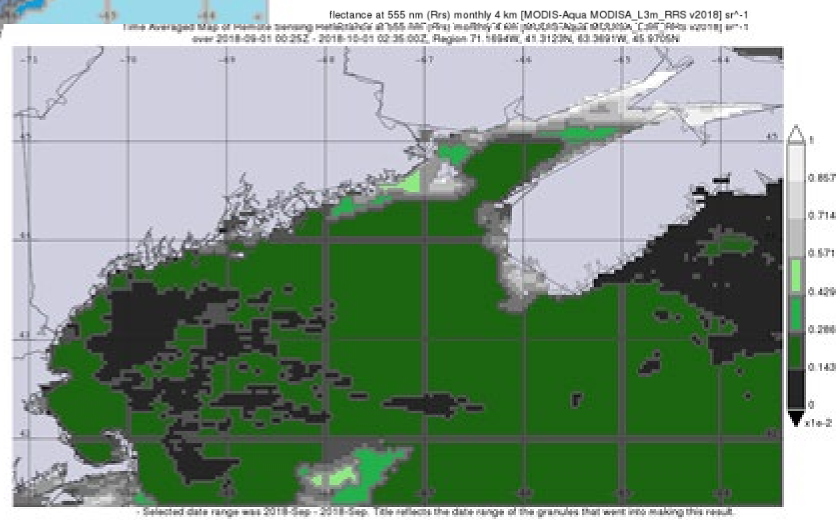
While these examples have generally considered the whole visible spectrum, it is important to realize that within narrow wavebands, the ocean may behave as a pure absorber or pure scatterer and thus appear nearly “black” or “white” in that waveband

- Pure absorber in near infrared (water absorption)
- Approaches pure scatterer in the uv/blue (clear water)

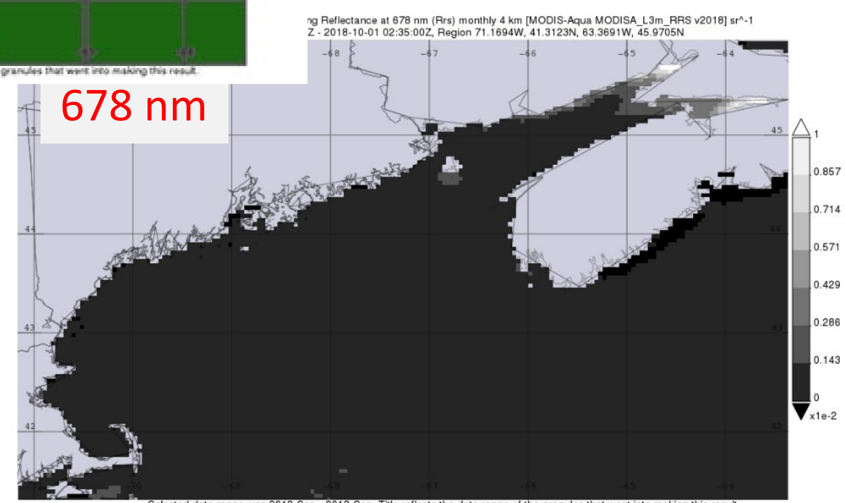
MODIS-AQUA reflectance images

Gulf of Maine September 2018





678 nm



https://giovanni.gsfc.nasa.gov/giovanni

Before *measuring* IOPs it is helpful to review measurement *theory*

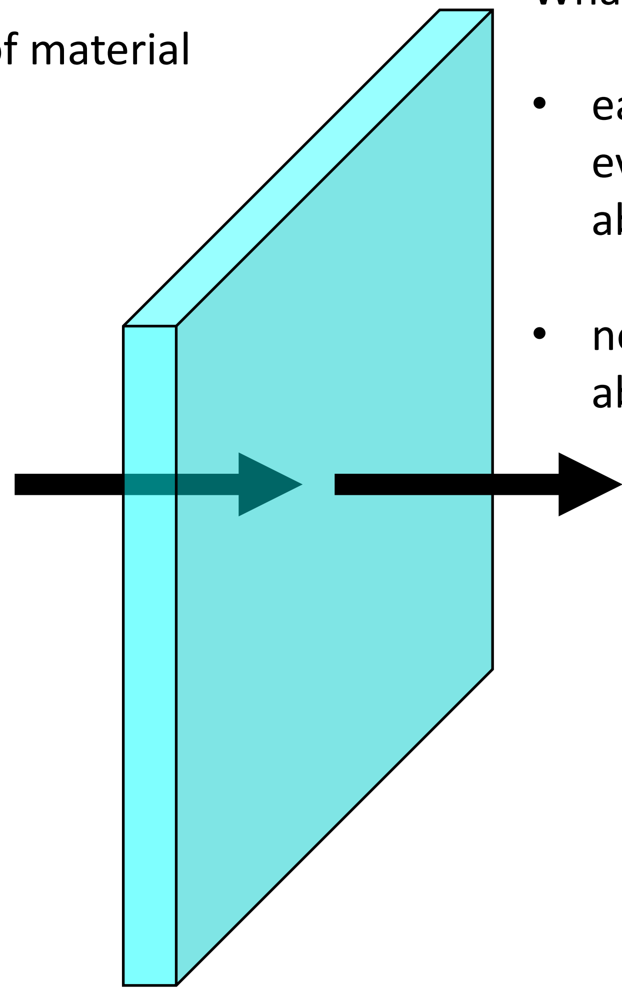
Consider a *thin* slab of material

What is *thin*?

- each photon has probability for one optical event (transmitted or scattered or absorbed, not scattered then absorbed)
- no event is shaded (e.g., one layer of absorbing molecules)

Φ_o

Incident Radiant Power (W/m^2)

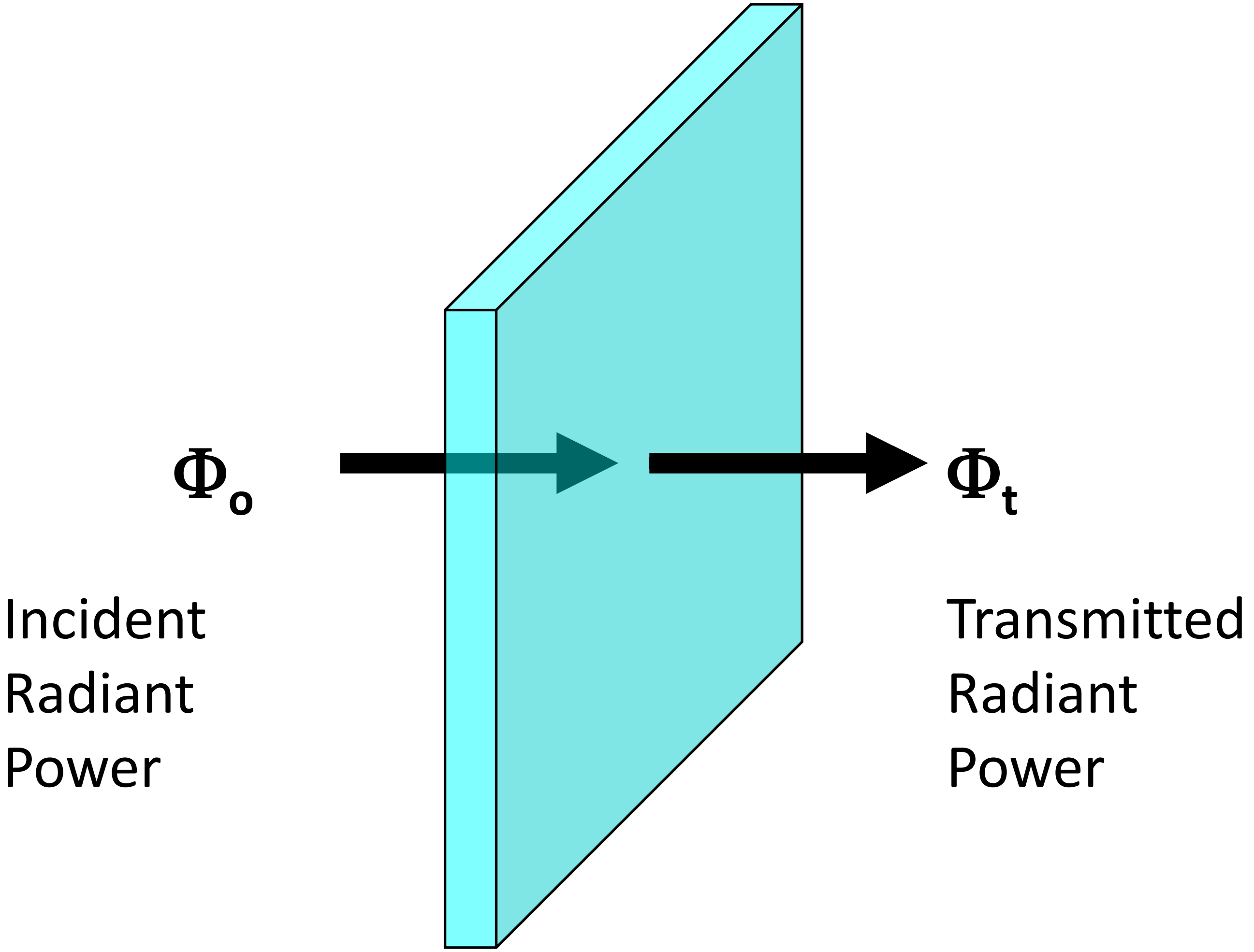


Φ_t

Transmitted Radiant Power (W/m^2)

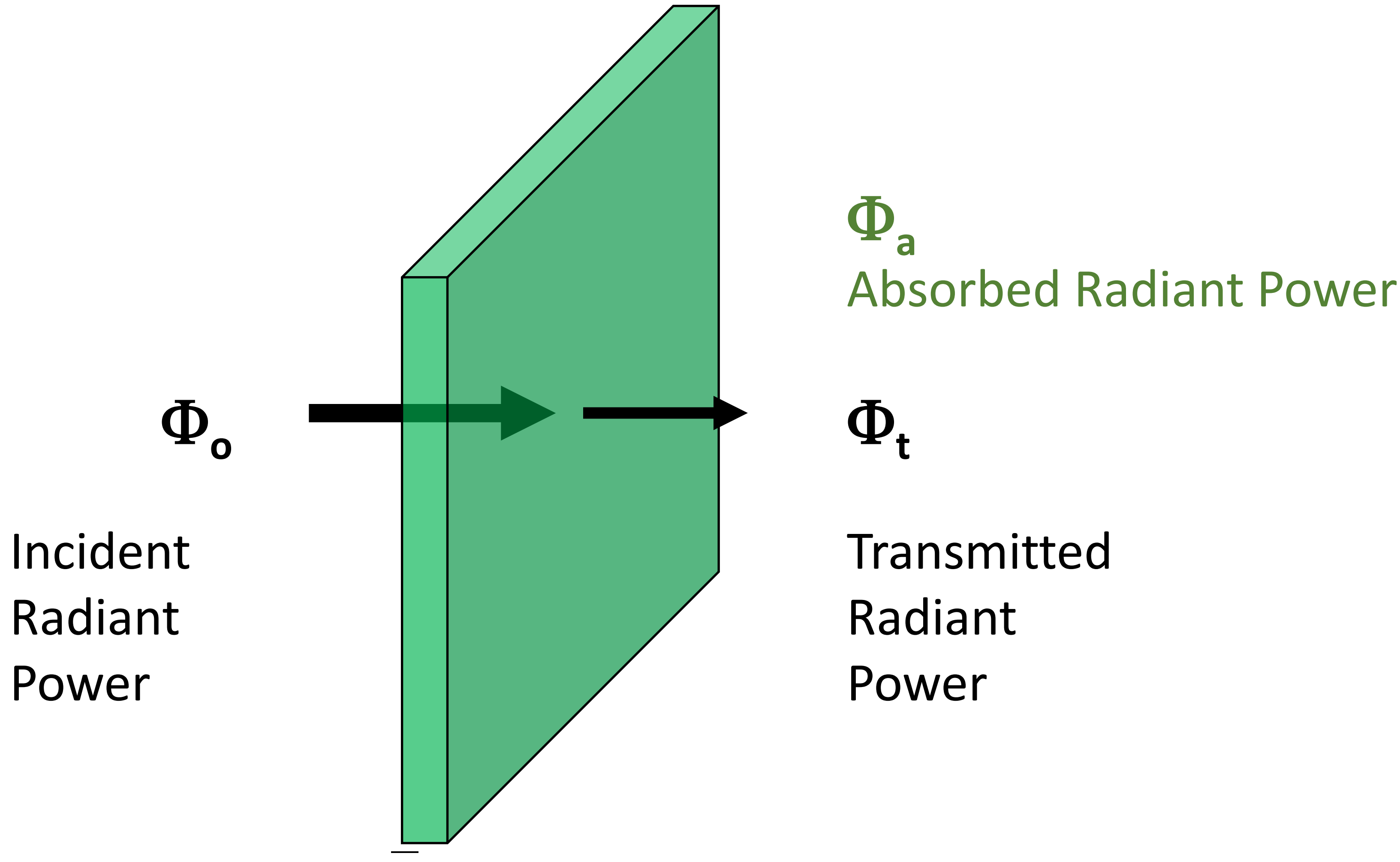
$\Phi_o = \Phi_t$ No attenuation

IOP *Theory*

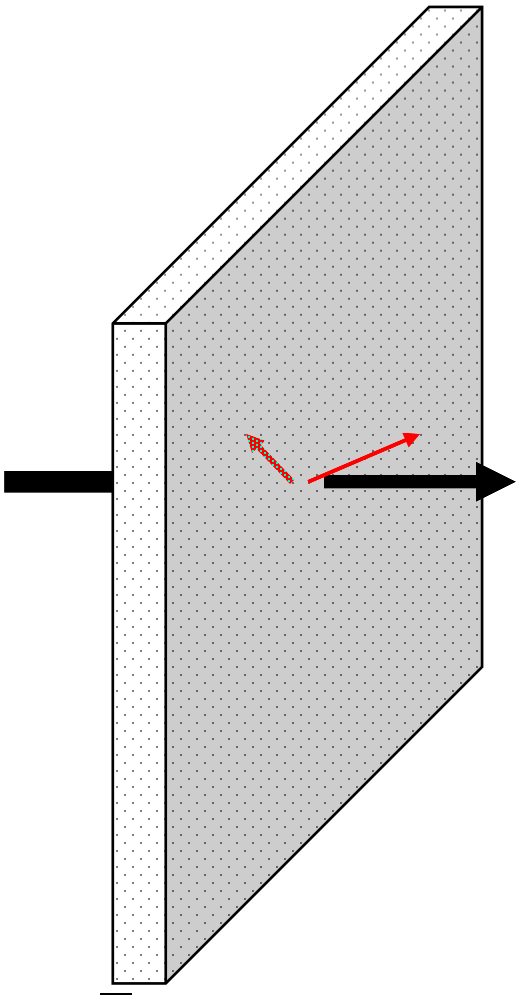


If $\Phi_t < \Phi_o$ there is attenuation

Consider loss due solely to absorption



Consider loss due solely to scattering



Φ_b
Scattered Radiant Power

Φ_o

Incident
Radiant
Power

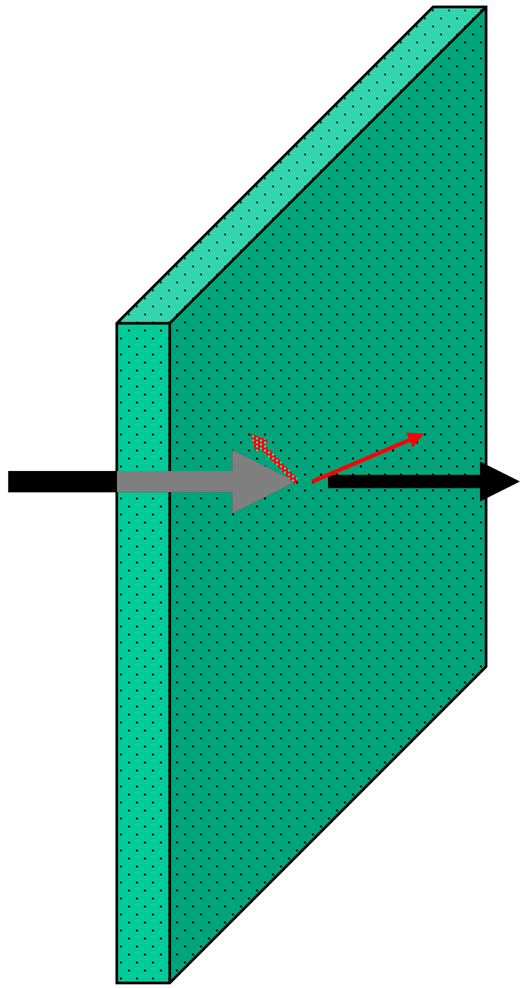
Φ_t

Transmitted
Radiant
Power

Consider loss due to *beam* attenuation (absorption + scattering)

Φ_o

Incident Radiant Power



Φ_a Absorbed Radiant Power

Φ_b Scattered Radiant Power

Φ_t

Transmitted Radiant Power

Conservation of Radiant Power

$$\Phi_o = \Phi_t + \Phi_a + \Phi_b$$

Derivation of Absorption

Absorptance

$\boldsymbol{A}$ = fraction of incident radiant power absorbed

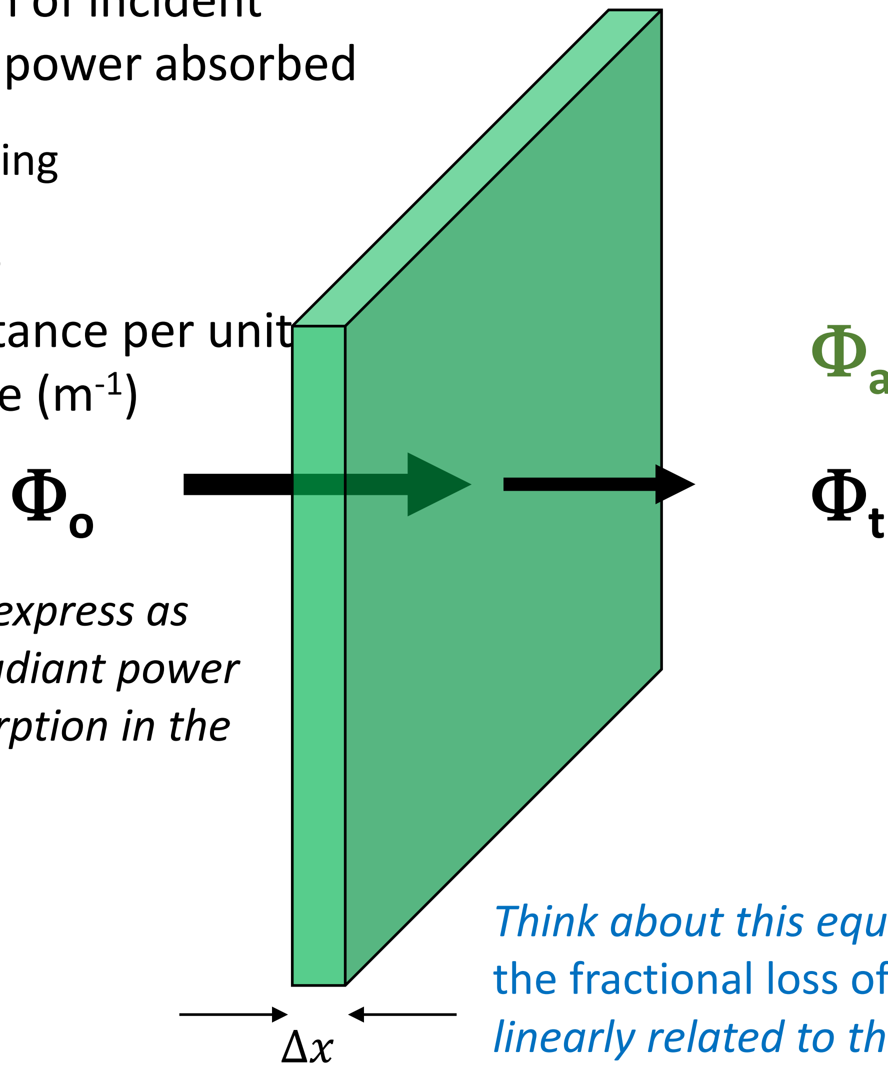
$$\boldsymbol{A} = \frac{\Phi_a}{\Phi_o} = \frac{\Phi_o - \Phi_t}{\Phi_o}$$

If no scattering

Absorption

a = absorptance per unit distance (m^{-1})

$$\mathrm{a} = \frac{\boldsymbol{A}}{\Delta x}$$



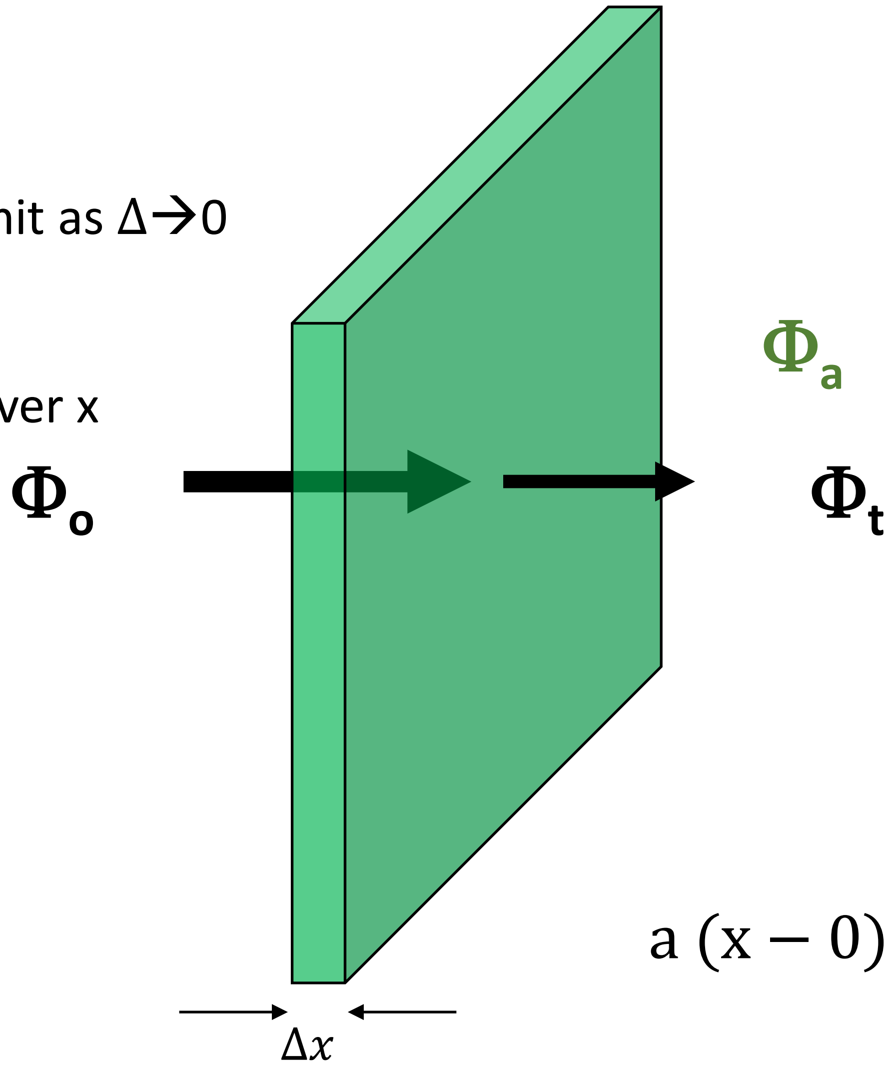
Rearrange, express as fractional radiant power loss to absorption in the layer

$$\mathrm{a}\Delta x = \frac{-\Delta\Phi}{\Phi}$$

$$\frac{-\Delta\Phi}{\Delta x} = \Phi\,\mathrm{a}$$

Think about this equation:
the fractional loss of radiant power over the layer is *linearly related to the radiant power → "Lambert 1760"*

Derivation of Absorption



$$a\Delta x = \frac{-\Delta\Phi}{\Phi}$$

Take the limit as Δ→0

$$a\Delta x = \lim_{\Delta x \to 0} \frac{-\Delta\Phi}{\Phi}$$

Integrate over x

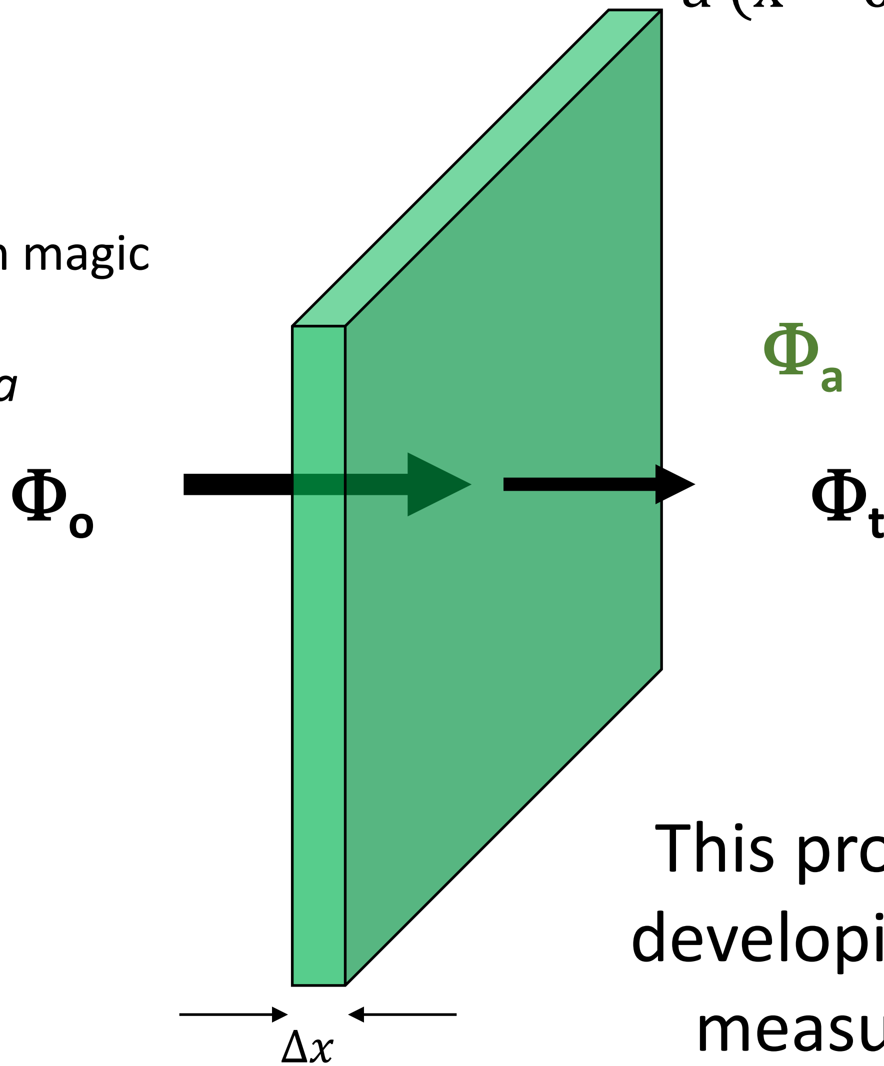
$$\int_0^x a\, dx = -\int_0^x \frac{d\Phi}{\Phi}$$

Evaluate

$$a\, x\, |_0^x = -\ln\Phi\, |_0^x$$

$$a\,(x - 0) = -(\ln\Phi(x) - \ln\Phi(0))$$

Derivation of Absorption



$$a\,(x - 0) = -(\ln\Phi(x) - \ln\Phi(0))$$

Evaluate

$$a\,x = -(\ln\Phi_t - \ln\Phi_0)$$

Logarithm magic

$$a\,x = -(\ln\frac{\Phi_t}{\Phi_0})$$

Solve for *a*

$$a\,(m^{-1}) = \frac{-1}{x}(\ln\frac{\Phi_t}{\Phi_0})$$

Absorption coefficient (m^{-1})

a = loss of radiant power per unit distance

This provides a guide towards developing sensors and making measurements (practicum)

Absorption through particles

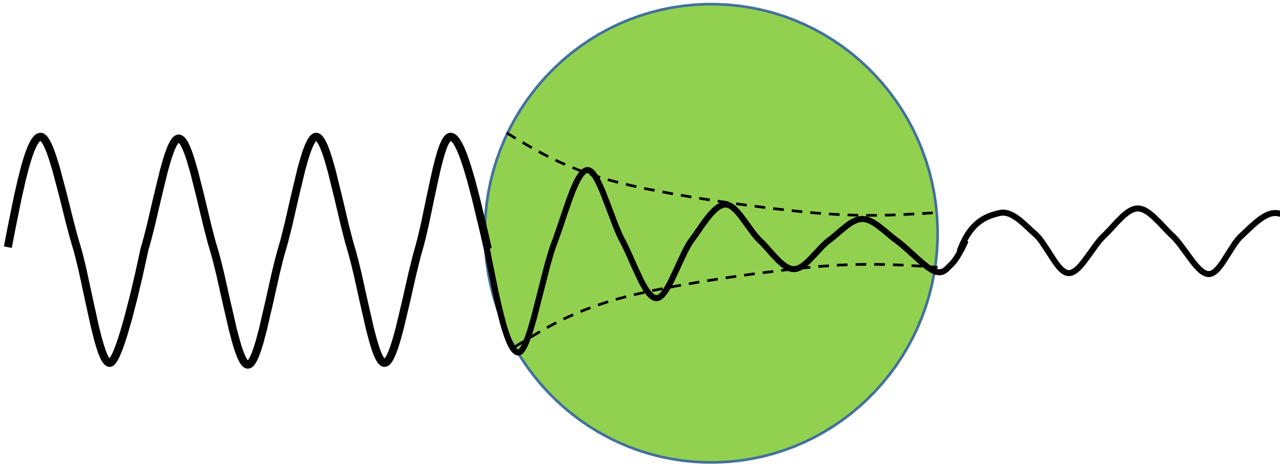
$$a\ (m^{-1}) = \frac{-1}{x}(\ln\frac{\Phi_t}{\Phi_0})$$

$$\ln\frac{\Phi_t}{\Phi_0} = -\,ax$$

$$\frac{\Phi_t}{\Phi_0} = e^{-ax}$$

$$\Phi(x) = \Phi_0\ e^{-ax}$$

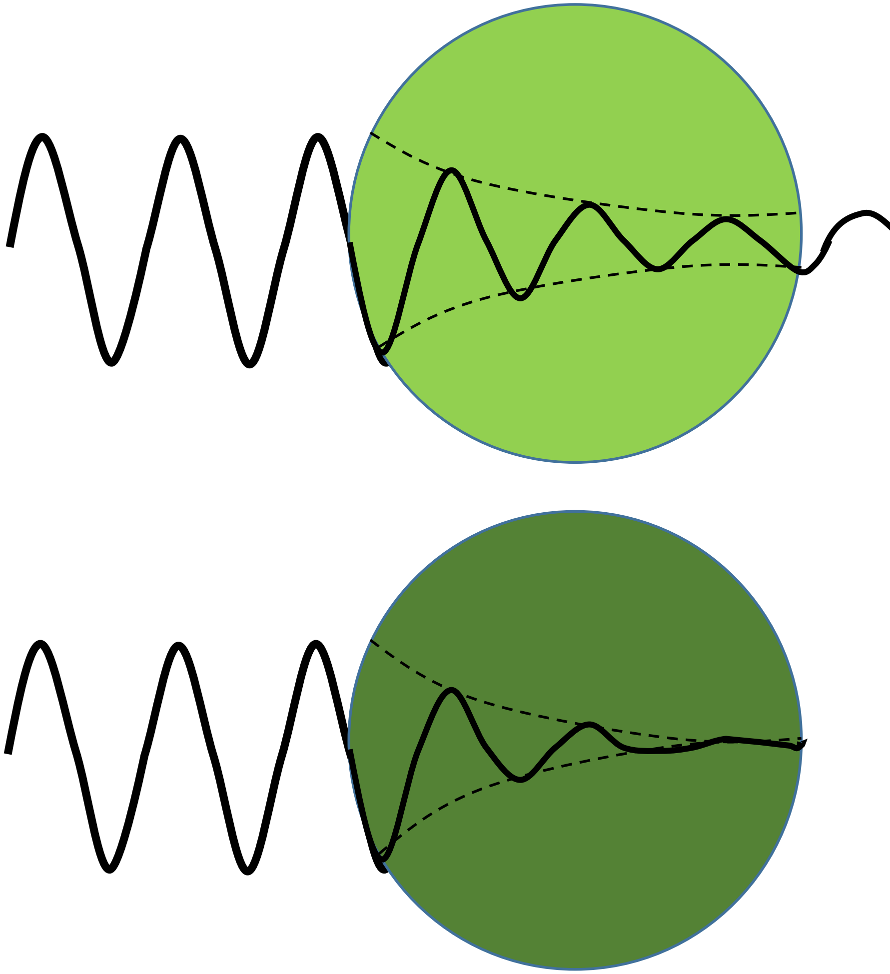
- As the EM wave passes through the absorbing matter
- Amplitude decreases exponentially



- Wavelength does not change

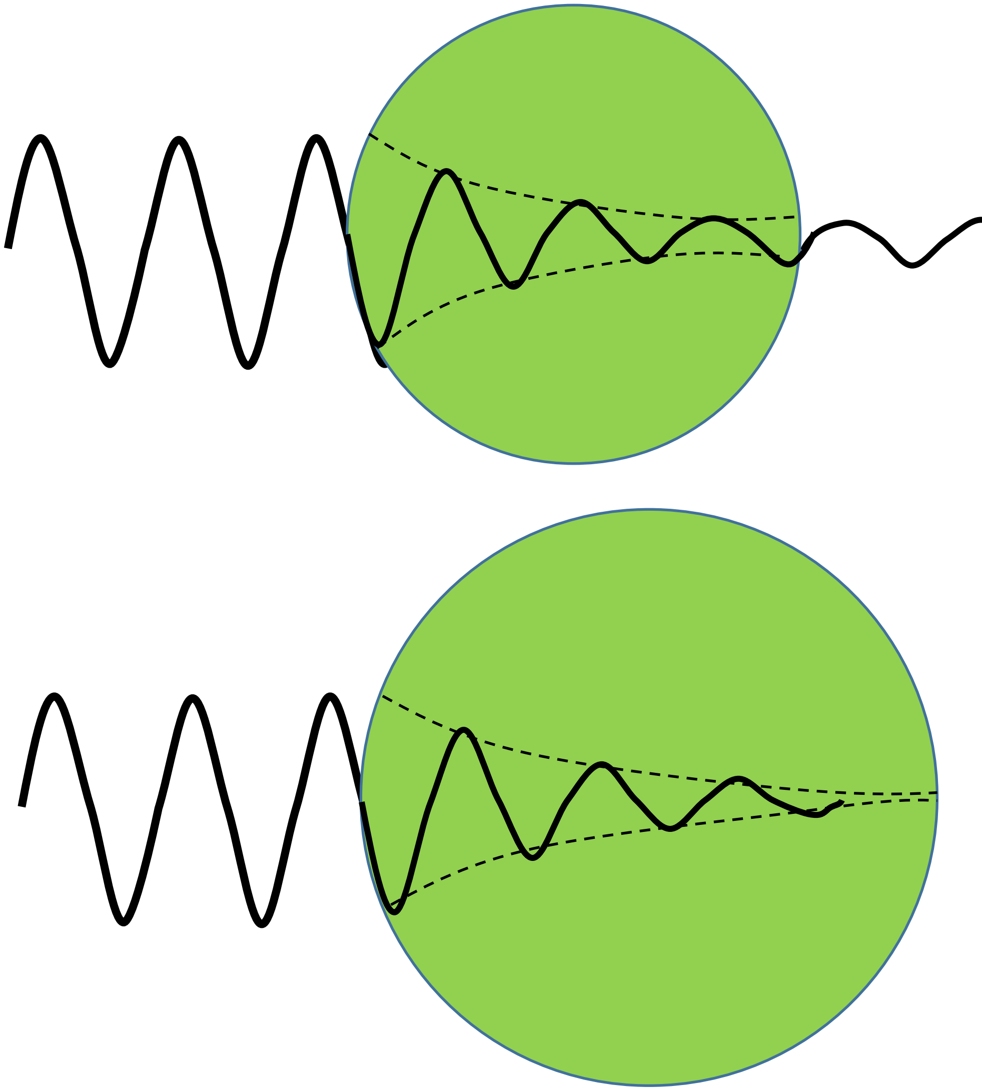
Absorption through particles

- As the **absorption coefficient** increases, less light passes through the particle



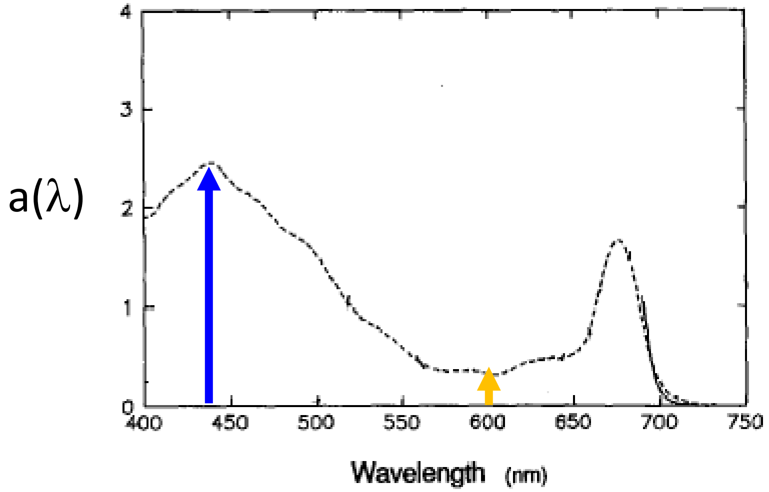
Absorption through particles

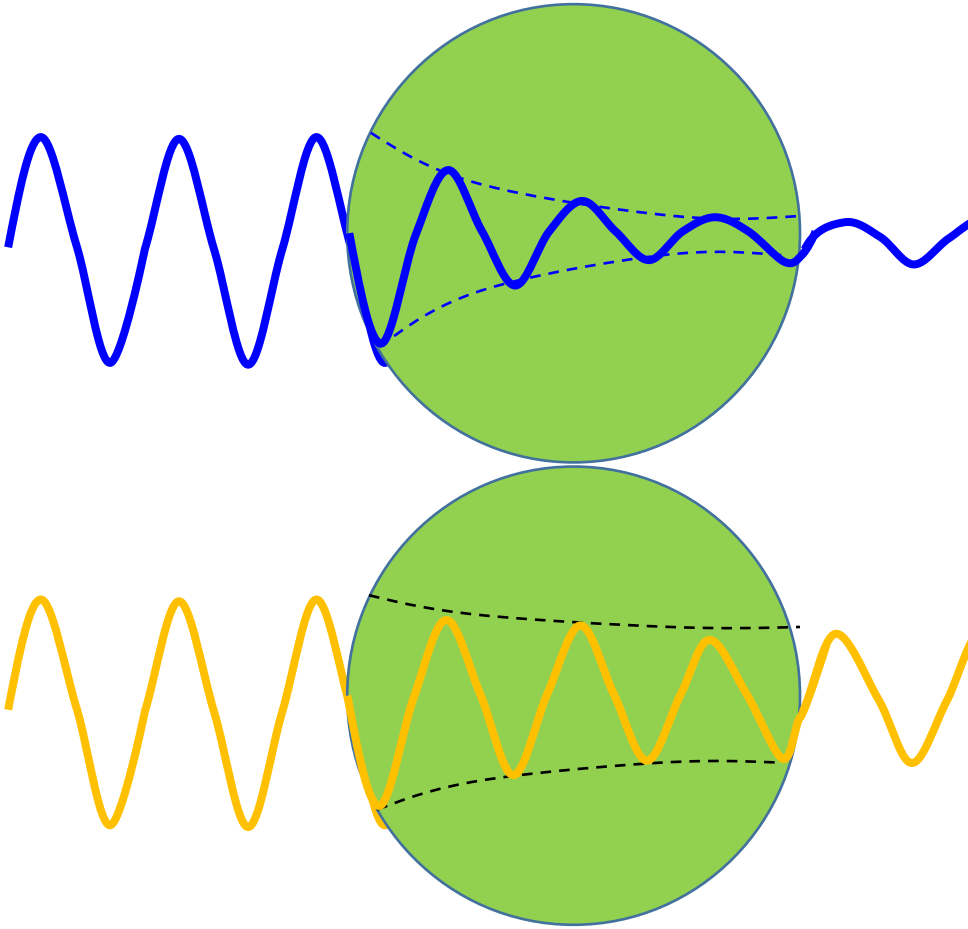
- As the **pathlength** through the particle increases, the less light passes through the particle



Absorption through particles

- Each wavelength of the absorption spectrum is attenuated differently through the particle (e.g., phytoplankton cell)



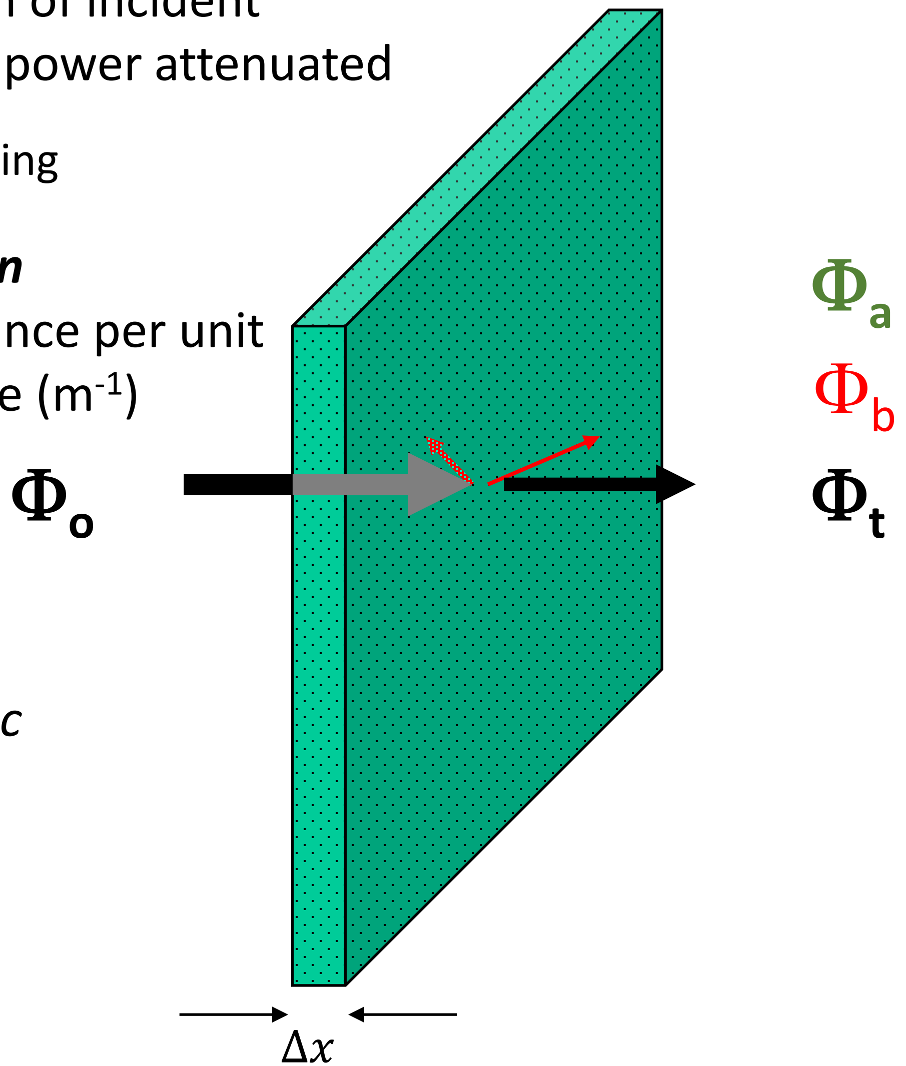


Derivation of beam Attenuation

Attenuance
C = fraction of incident radiant power attenuated

If no scattering

Attenuation
c = attenuance per unit distance (m^{-1})



Solve for *c*

$$\boldsymbol{C} = \frac{\Phi_{a+b}}{\Phi_o} = \frac{\Phi_o - \Phi_t}{\Phi_o}$$

$$\mathrm{c} = \frac{\boldsymbol{C}}{\Delta x}$$

$$\mathrm{c}\Delta x = \frac{-\Delta\Phi}{\Phi}$$

...fill in steps...

$$\mathrm{c}\ (m^{-1}) = \frac{-1}{x}(\ln\frac{\Phi_t}{\Phi_0})$$

Attenuation coefficient (m^{-1})
c = loss of radiant power per unit distance

Let’s build an attenuation meter

- What components do we need?
  - Light source
  - Sample volume
  - Detector
- Sketch the configuration, keeping in mind theory, what constraints do we need to put on the components?
  - Light source
  - Sample volume
  - Detector
- What technological challenges can you identify?

Let’s build a scattering meter

- What components do we need?
  - Light source
  - Sample volume
  - Detector
- Sketch the configuration, keeping in mind theory, what constraints do we need to put on the components?
  - Light source
  - Sample volume
  - Detector
- What technological challenges can you identify?

Let’s build an absorption meter

- What components do we need?
  - Light source
  - Sample volume
  - Detector
- Sketch the configuration, keeping in mind theory, what constraints do we need to put on the components?
  - Light source
  - Sample volume
  - Detector
- What technological challenges can you identify?

In situ observations of IOPs
Commercially-available WETLabs ac sensors

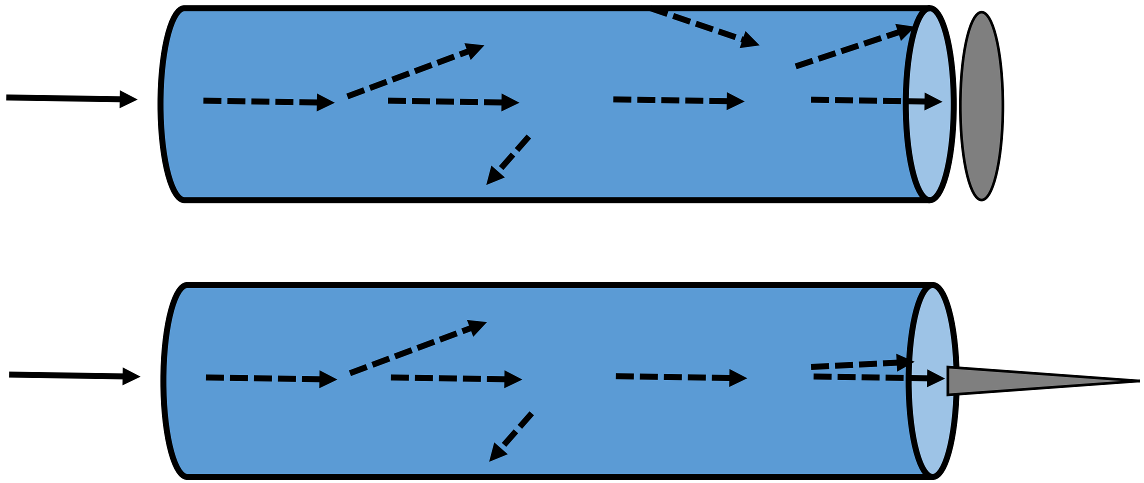
- **Quantitative** measurements of absorption and attenuation
- Scattering derived by difference

Bio-optical Sensors - Absorption

- Measurement Reality – Sensors
  - Reflecting tube absorption meters

a - Maximize scattered light collection
absorption

c – minimize scattered light collection
beam attenuation



b = c – a **scattering**

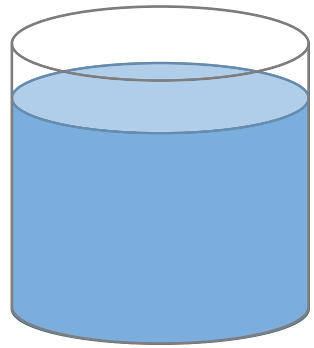
Some scattered light not collected by absorption tube, leads to overestimation of absorption →correction

Some scattered light collected by attenuation tube, leads to underestimation of attenuation → report detection angle

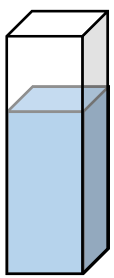
In situ observations of IOPs
Commercially-available WETLabs ac sensors

- Requires
- **pure water** calibration
- Corrections
  - Temperature and salinity of samples relative to pure water calibration
  - Non-ideal configurations for absorption and attenuation
- Strategies for robust measurements

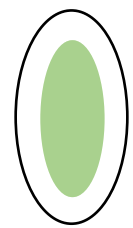
Discrete sample analyses in a spectrophotometer



Dr Sasha Kramer, 2018
EXPORTS North Pacific



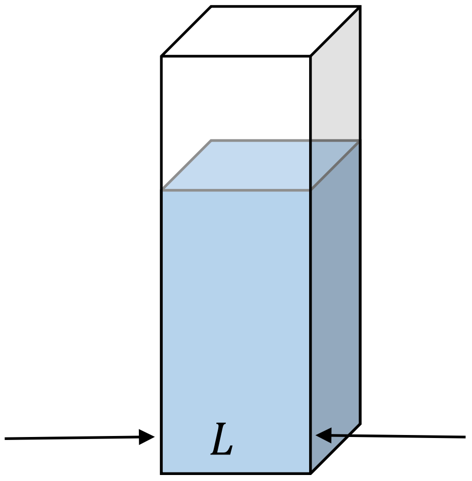
← Filtration →



- Separates particles from *dissolved*
- Concentrates particles from dilute medium

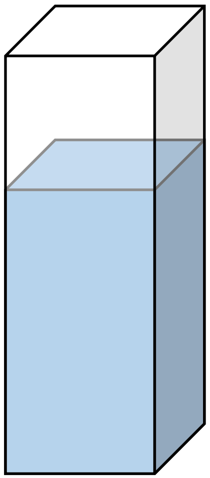
Measuring absorption - solutions

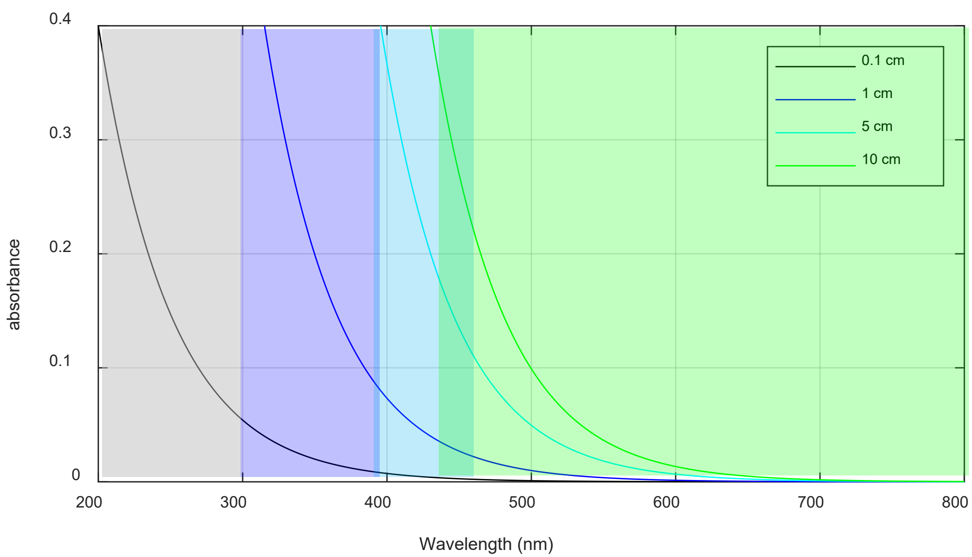
- Spectrophotometers output *absorbance, A,* rather than *absorptance,* $\boldsymbol{A}$
  - $\boldsymbol{A} = \frac{\Phi_a}{\Phi_o}$
  - $A = log_{10}\left(\frac{\Phi_0}{\Phi_t}\right) = -log_{10}\left(\frac{\Phi_t}{\Phi_o}\right) = -log_{10}(1 - \boldsymbol{A})$
  - Absorbance sometimes called *optical density*
- Reference material (Baseline correction)
  - $A_{sample} - A_{ref}$
  - $= -\left(log_{10}\left(\frac{\Phi_t}{\Phi_o}\right)_{\boldsymbol{sample}} - log_{10}\left(\frac{\Phi_t}{\Phi_o}\right)_{\boldsymbol{ref}}\right)$
  - $= -\,log_{10}\left(\frac{\Phi_{t,sample}}{\Phi_{t,ref}}\right)$
- $a = \ln(10) \times \frac{A}{L} = 2.303 \times \frac{A}{L(m)}$

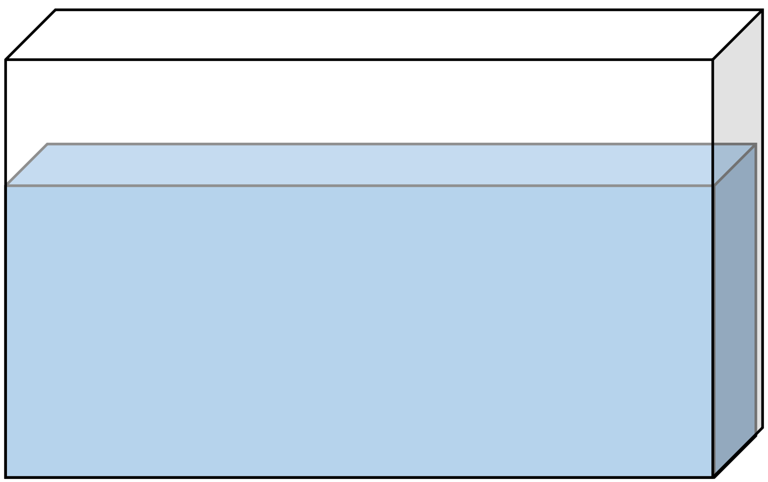


Measuring absorption

- Sample is not an infinitesimally thin layer
- absorbance, $A = -log_{10}\left(\frac{\Phi_t}{\Phi_o}\right)$
- Recommendation
  - $0.1 < A < 0.4$
  - $80\% < T < 40\%$
- Adjust the pathlength to maintain correct A range
- May require two different pathlengths along the spectrum



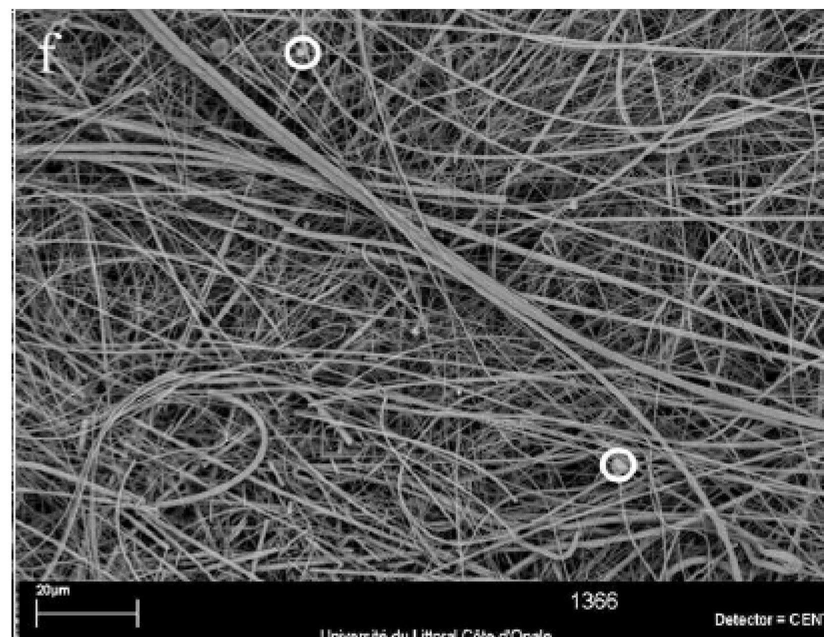




Measuring Absorption – Particles on Filters

- Filters create challenges for measuring absorption
- How many can you think of?

- Separates particles from *dissolved*
- Concentrates particles from dilute medium onto a glass fiber filters →

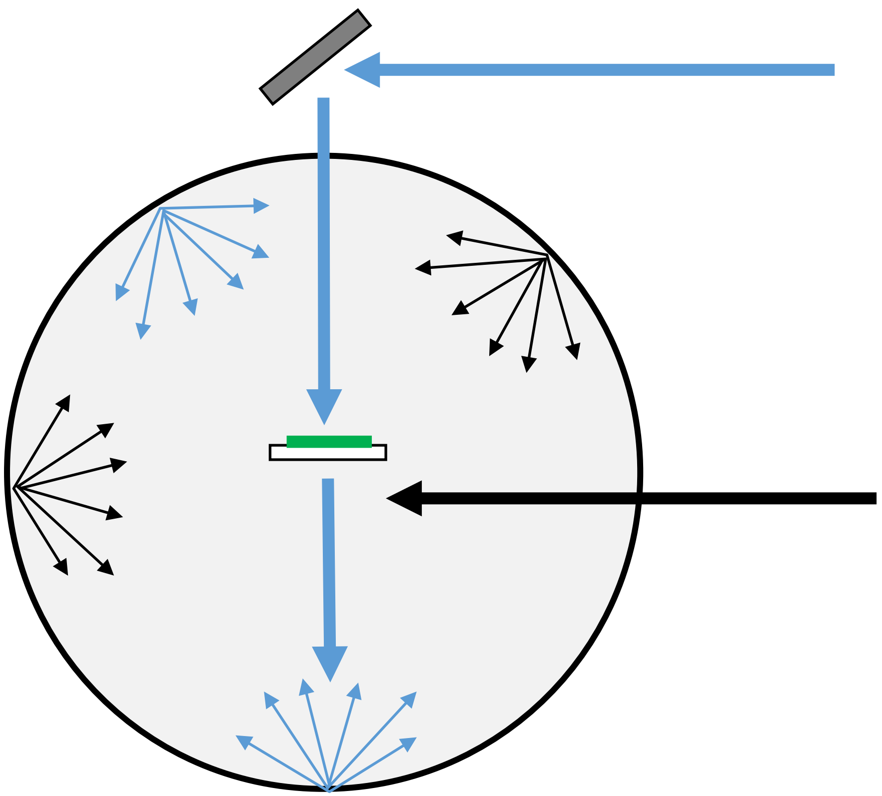


Neukermans et al 2012 Limnol Oceanogr

Sketch the configuration for measuring absorption by particles on a filter pad

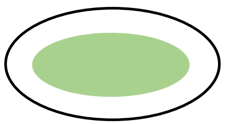
Measure in Spectrophotometer with Center-mounted Integrating Sphere

- Sample Beam
  - Passes through sample filter first → sample absorption
  - Multiply scatters off reflective sphere
  - Pass through sample multiple times → pathlength amplification
- Reference Beam
  - Multiply scatters off reflective sphere
  - Pass through sample multiple times → pathlength amplification
- Sample Beam – Reference Beam = single pass through filter
- From which you can calculate *a*

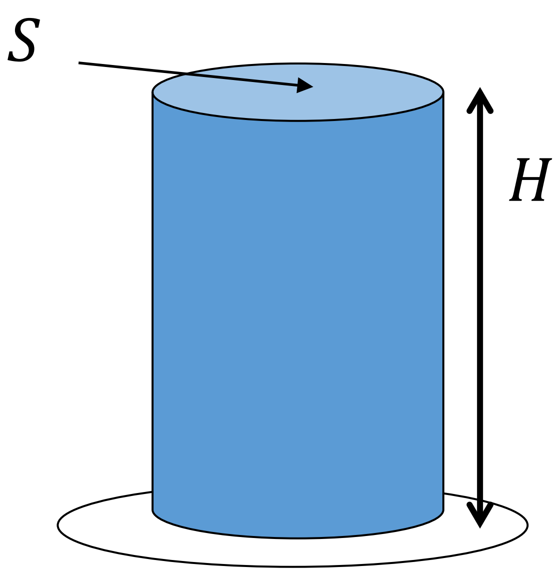


Compute absorption

- $a = 2.303 \times \frac{A}{L(m)}$



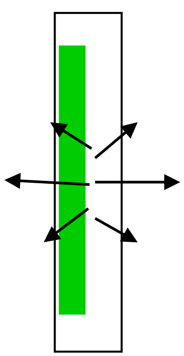
- What is the pathlength, L?
- Convert the volume filtered into a cylinder of water of area, S, and height, H
- The pathlength is $H = \frac{V_{filt}}{\pi\, r_{eff}{}^2}$

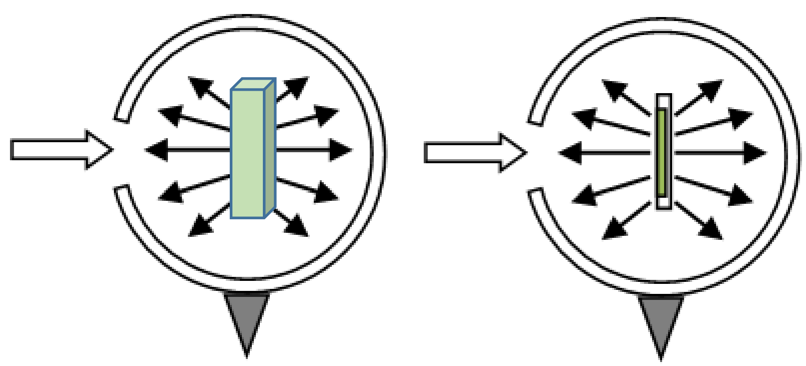


- $a = 2.303 \times 100 \left(\frac{cm}{m}\right) \times \frac{A}{\left(\frac{V_{filt}(ml)}{\pi\, r_{\mathrm{eff}}{}^2 (cm^2)}\right)}$

Filter pad

- Optical properties of the filter pad subtracted in baseline
- Creates highly scattering environment around the particles
  - multiple scattering increases probability of absorption,
  - Overestimates absorption
  - Pathlength Amplification Correction – derive from paired suspension and filter pad measurements





Theoretical (Roesler 1998) and empirical (Stramski et al 2015) show factor of 2

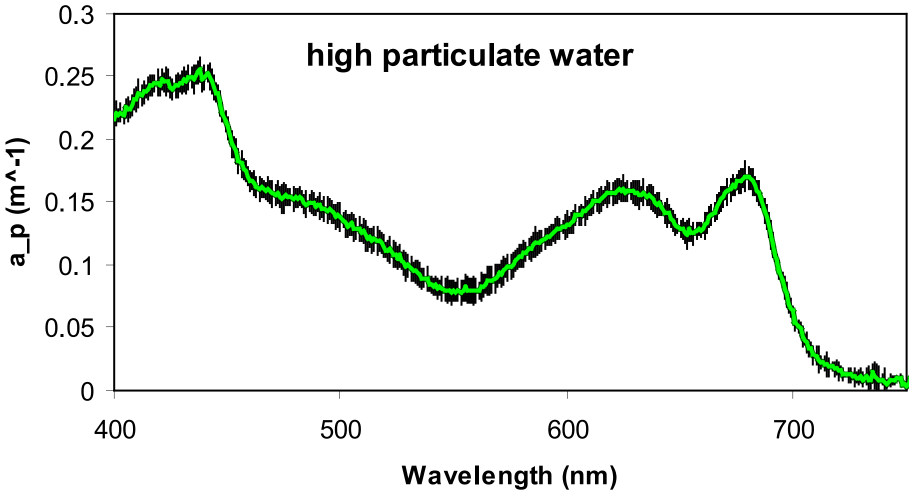
Compute absorption

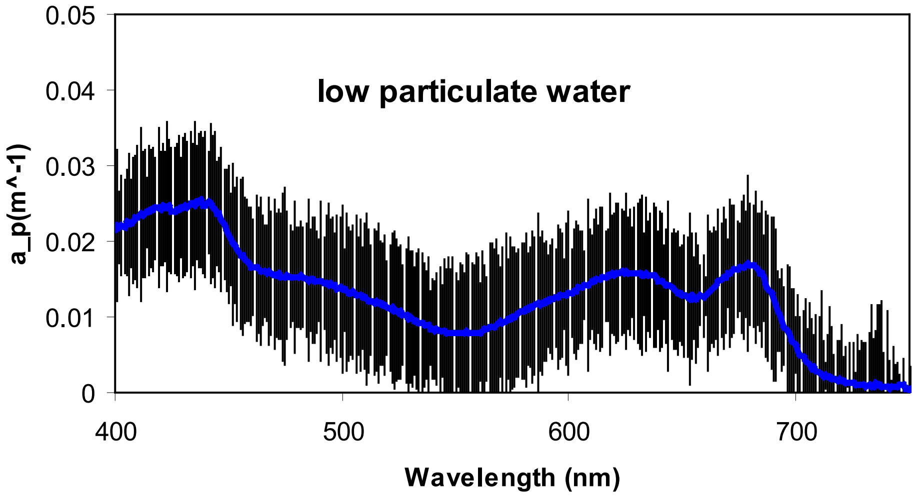
- *Measure* baseline corrected sample
- $A_{sample\_Bcorr}(\lambda) = A_{sample\_on\_pad}(\lambda)$ - $A_{Baseline\_blankpad}(\lambda)$
- *Apply pathlength amplification correction (Stramski et al. 2015)*
- $A_{sample_{BcorrAcorr}}(\lambda) = 0.323 \times A_{sample\_Bcorr}(\lambda)^{1.0867}$
- *Compute spectral absorption coefficient*
- $a_{part}(\lambda) = 2.303 \times 100\left(\frac{cm}{m}\right) \times \frac{A_{sample_{BcorrAcorr}}(\lambda)}{\left(\frac{V_{filt}(ml)}{\pi\, r_{\mathrm{eff}}{}^{2}(cm^{2})}\right)}$

Absorption - *uncertainty calculation*

- Run 3-5 blank pads relative to your baseline
- Compute the standard deviation of the blank scans, $\sigma_{A\_bl}(\lambda)$
- substitute $\sigma_{A\_bl}(\lambda)$ for A in the absorption equation to compute $\sigma_a(\lambda)$
- note that the uncertainty will be different for each sample:
- V is different for every sample
- *A* is different for each sample, so the signal:noise will be different
- $\sigma_a(\lambda) = 2.303 \times 100 \left(\frac{cm}{m}\right) \times \frac{\sigma_{bl}(\lambda)}{\left(\frac{V_{filt}(ml)}{\pi\, r_{\mathrm{eff}}^{2}(cm^2)}\right)}$

Uncertainty example 1: impact of sample optical density

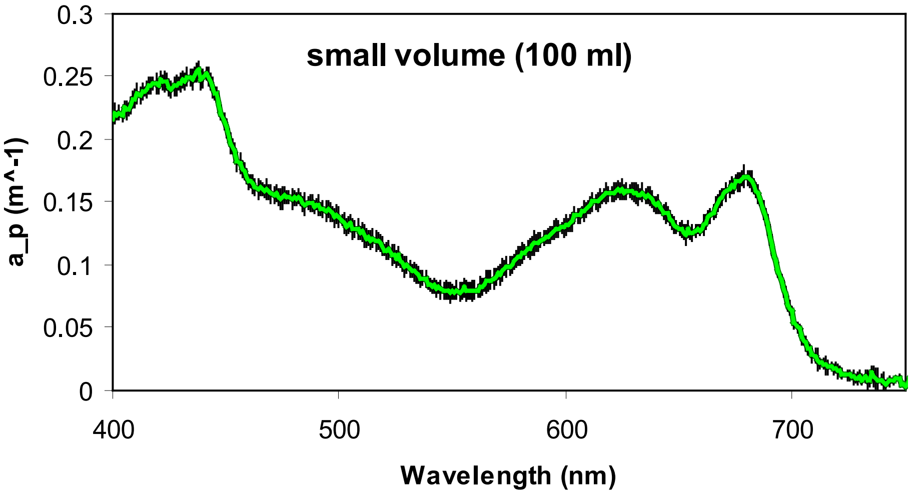


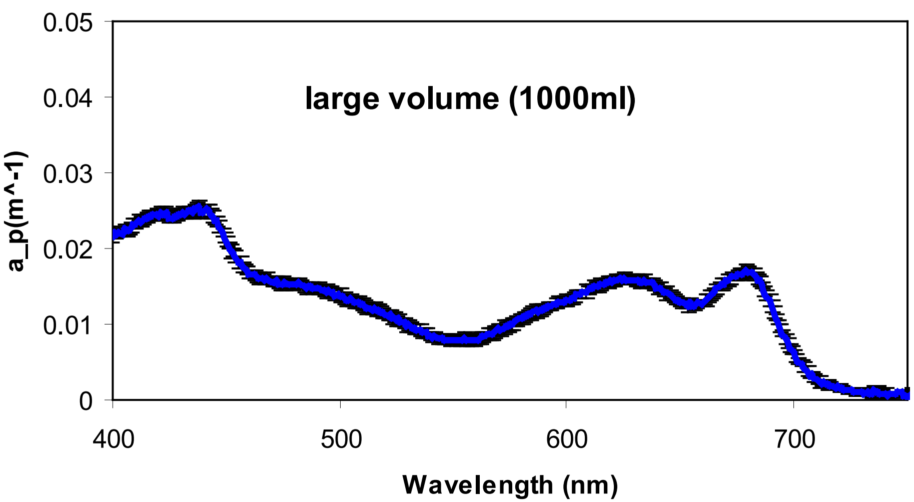


- Same volume filtered for each sample (100ml)
- $A_{\text{sample1}} \sim 10 * A_{\text{sample2}}$ (approx 0.1 vs 0.01)
- $A_{\text{filter blanks}} \sim A_{\text{sample2}}$ for low particulate waters

Roesler et al 2019 IOCCG Protocols

Uncertainty example 2: impact of volume filtered





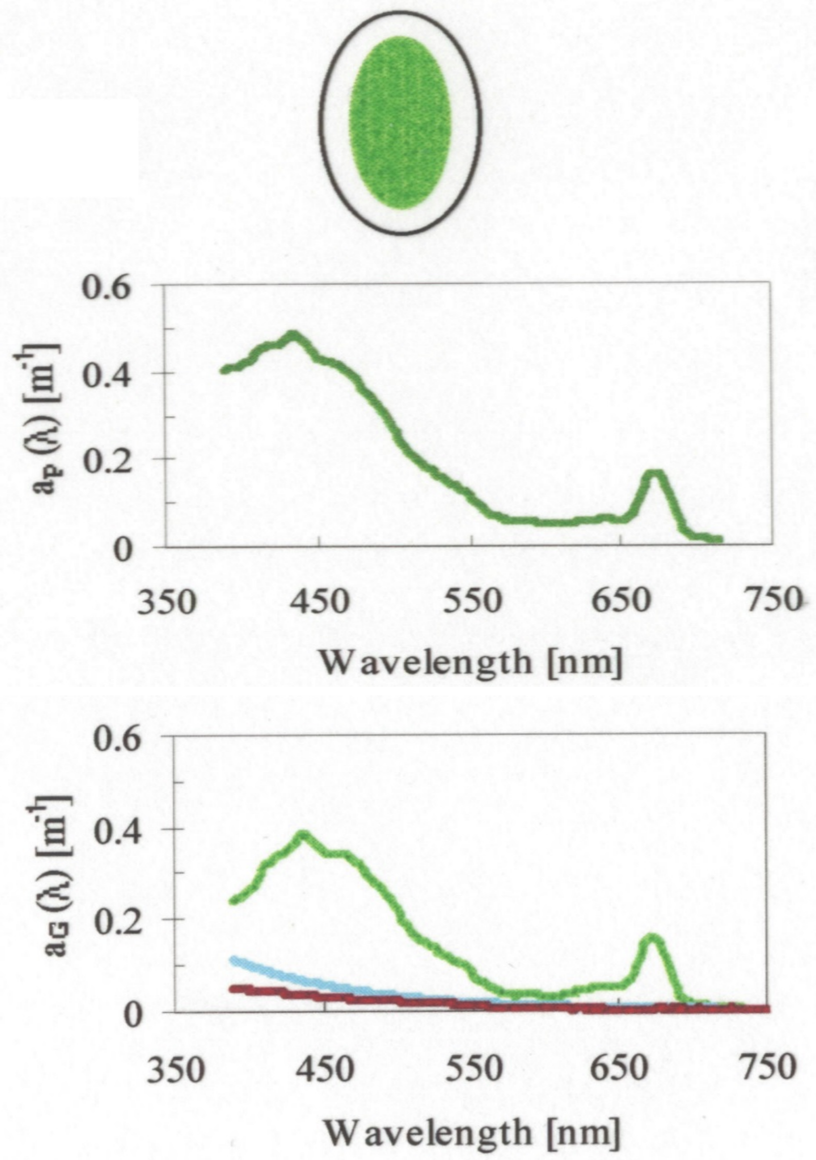
- Different V filtered for each sample (100ml vs 1000ml)
- $OD_{sample1}=OD_{sample2}$ (~0.1)
- $\sigma_{ODfilter\ blank}$~10%OD_{sample}

Better to **filter more volume** and obtain **higher OD_{sample}** relative to blanks

Roesler et al 2019 IOCCG Protocols

Partitioning of particulate absorption

- First scan is total particles, a_p
- Extract with methanol and scan again, a_{nap}
- $a_{phyt} = a_p - a_{nap}$
- Other issues
  - Phytoplankton "parts"
  - Detrital pigments
  - Phycobilipigments
  - Inorganics



Kishino et al 1985; IOCCG Protocols

Summary Filter pad technique

- Filter sample, want high loading to overcome the variability in the blank filter pad absorption itself, but not *muddy (0.1 to 0.4 absorbance (OD))*
- Reference?
- Extraction to separate particulates, nap
- Computation
  - Geometric pathlength
  - Pathlength amplification (optical pathlength)
  - Absorption calculation, a_p and a_{nap}
  - Phytoplankton calculation, $a_{phyt} = a_p - a_{nap}$

Conclusion

- We understand very well what we need to do to measure IOPs
- The practical aspect of instrument design can fail us or at least lead to numerous “correction factors” or “acceptable” uncertainties