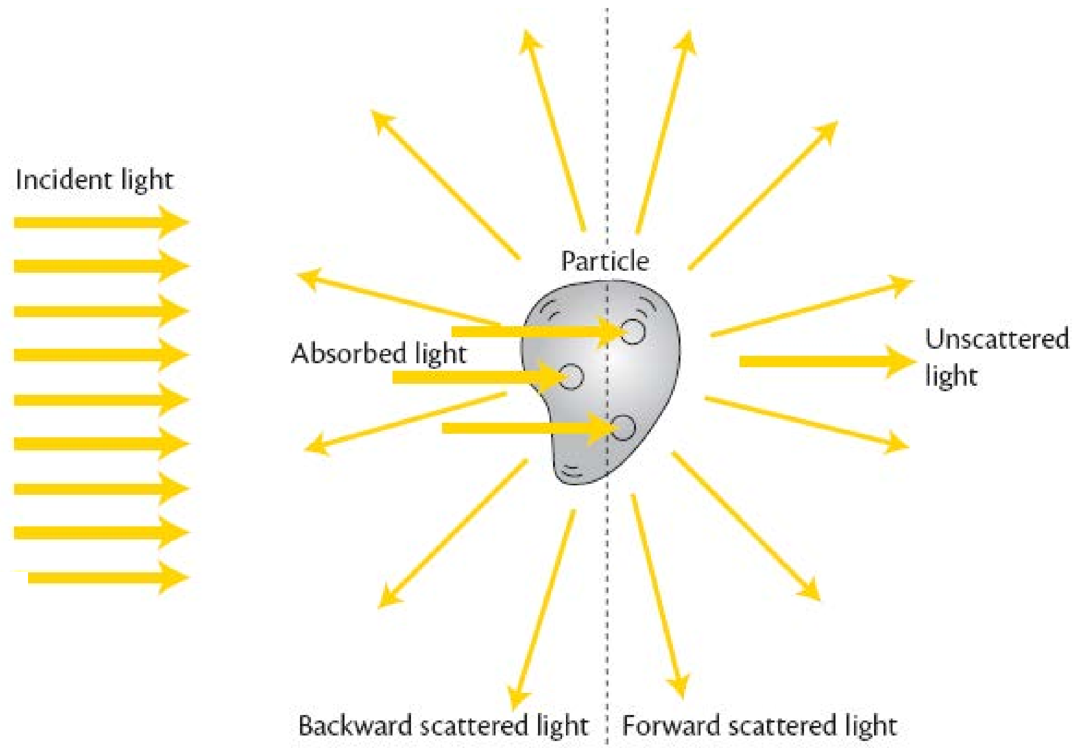
The link between particle properties (size, composition, shape, internal structure, packaging) and their IOPs.

- Mie theory provides a prediction of IOPs from size and bulk composition (→complex refractive index), for homogenous spheres
- We often are interested in the inverse problem: given IOPs, what are the properties of the particles? Modeling is a useful tool.
- How well do model predictions hold up for non-spherical, non-homogenous particles?

Scattering of light by spherical particles (Mie scattering).

The problem (Bohren and Huffman, 1983):

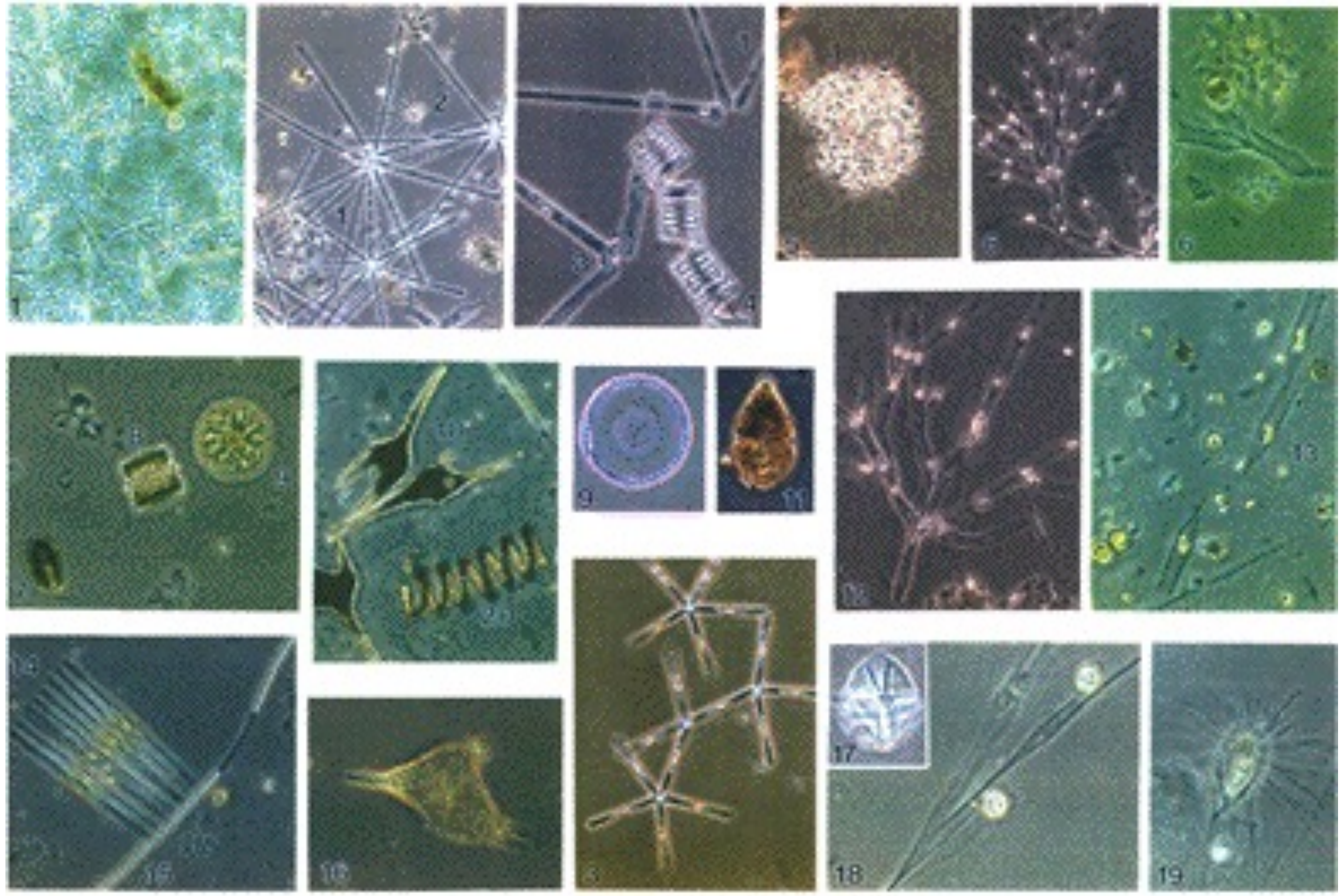
Given a particle of a specified size, shape and optical properties that is illuminated by an arbitrarily polarized monochromatic wave, determine the electromagnetic field at all points in the particles and at all points of the homogeneous medium in which it is embedded.



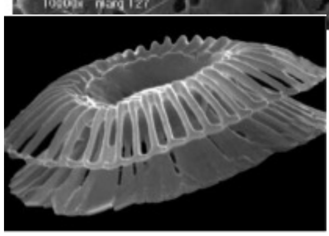
Mie theory assumes that the incident wave is a collimated plane harmonic wave impinging on a homogeneous spherical particle.

What particles scatter/absorb in the ocean?

Phytoplankton:



© 1993 Gertrud Cronberg

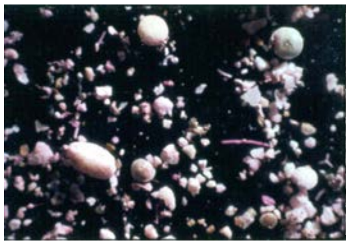


Variable in shape, size and pigment composition.

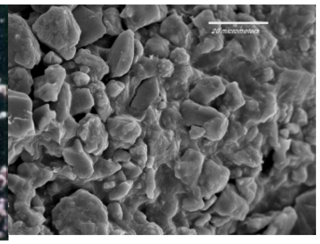
→ Variable in scattering and absorption properties

What particles scatter/absorb in the ocean?

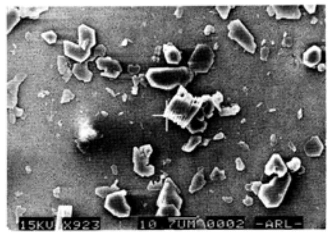
Non-algal particles: Organic and inorganic.



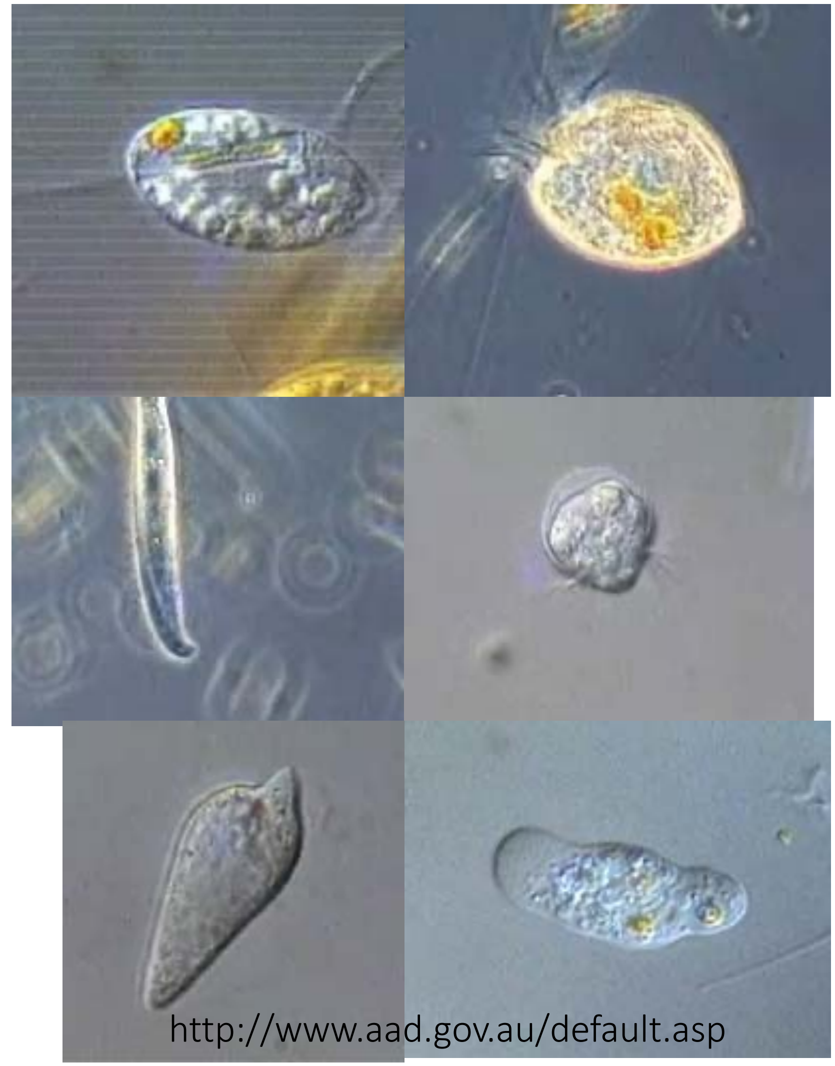
Sand



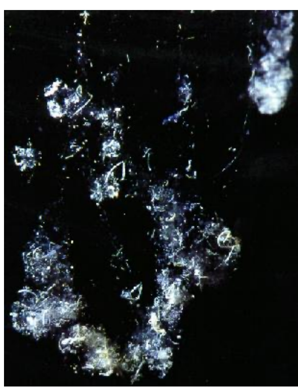
Silt

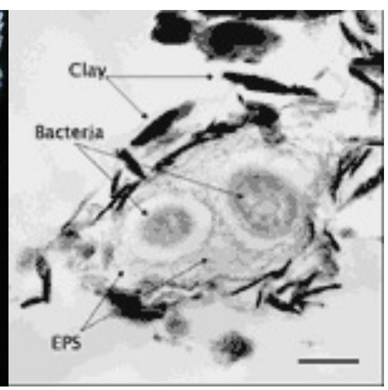


clay



Aggregates:





Variable in scattering and absorption properties

What are the particle properties of interest?

suspended sediment

size
density → sinking speeds

Shape → ecosystem structure

pigmentation

refractive index

Carbon Content

Composition

inorganic carbon $CaCO_3$

Silica

Some relevant properties

- **Size** – characteristic length scale of particle (e.g. $\propto$ Volume$^{1/3}$). What is the size of a non-spherical object?

- **Composition** – characterized by the bulk index of refraction of the particle. How does the particle change the light speed compared to ambient water?

- **Shape** – how much does it depart from a sphere? What is the surface roughness (amplitude, length scale)?

- **Internal structure** – inhomogeneities within the particle (membrane, cytoplasm, chloroplast, vacuole).

- **Porosity or "packaging"** – How "solid" the particle is. Ratio of interstitial water volume to total volume.

Why might we care about optical theory and Mie's solution?

These solutions provide a calibration to our sensors (LISST, b_b, flow-cytometers).

In addition, for a given concentration of particles of a given *size/wavelength ratio* and *index of refraction* we expect a given signal (some are shape independent).

Why might we care about optical theory and Mie's solution?

These solutions provide a calibration to our sensors (LISST, b_b, flow-cytometers).

In addition, for a given concentration of particles of a given *size/wavelength ratio* and *index of refraction* we expect a given signal (some are shape independent).

Examples (from optics class alumni!)

- Rebecca Green – used Mie theory to analyze flow-cytometer data, assigning size based on forward and side scattering of single cells.

- Giorgio Dall'Olmo – used Mie theory to analyze diel cycles in optical properties.

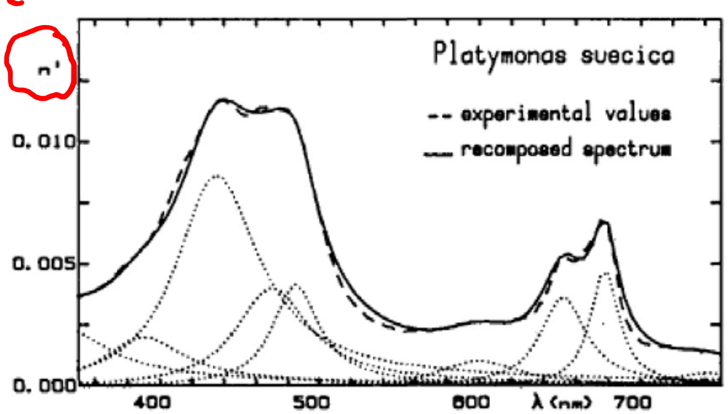
- Tiho Kostadinov – used Mie theory to look at effects of changes of population PSD on Rrs.

The inverse problem

Find the optical constants consistent with absorption measurements of a phytoplankton culture (Bricaud and Morel, 1986)

Absorption measurements:

n'

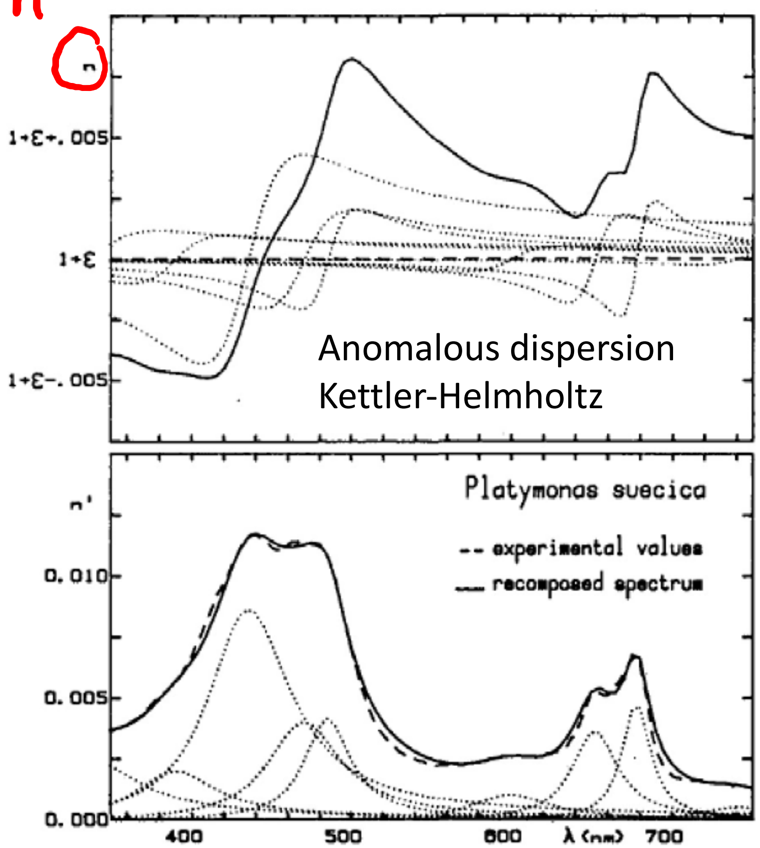


The inverse problem

Find the optical constants consistent with absorption measurements of a phytoplankton culture (Bricaud and Morel, 1986)

Absorption measurements:

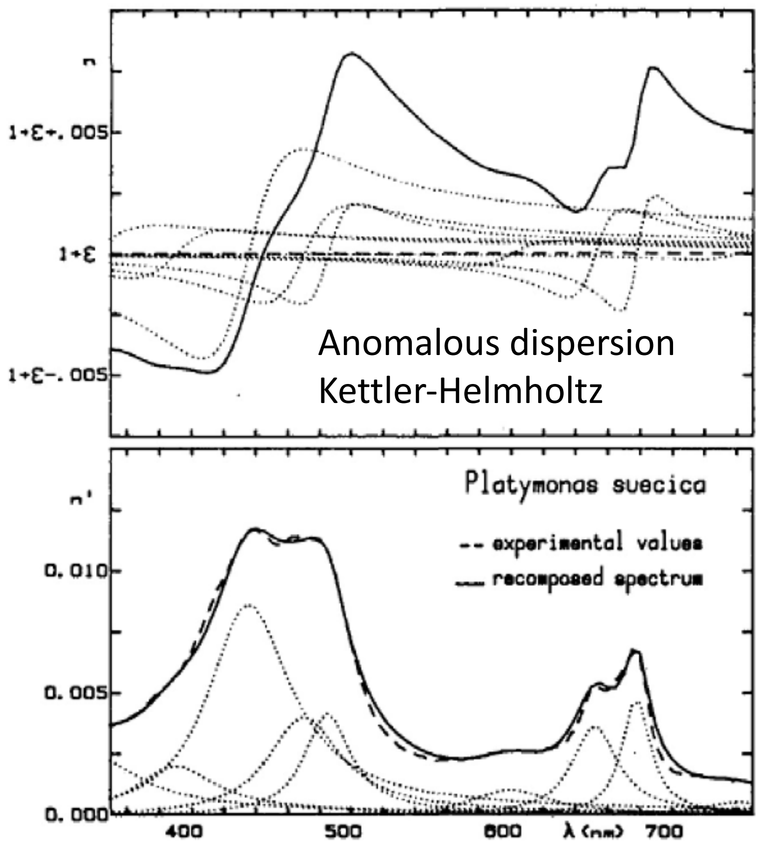
n



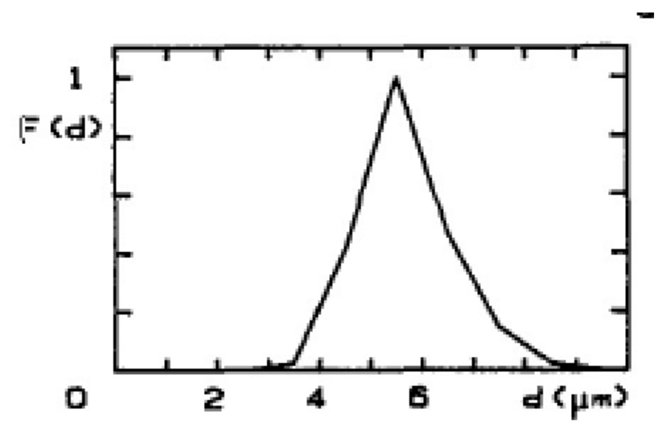
The inverse problem

Find the optical constants consistent with absorption measurements of a phytoplankton culture (Bricaud and Morel, 1986)

Absorption measurements:



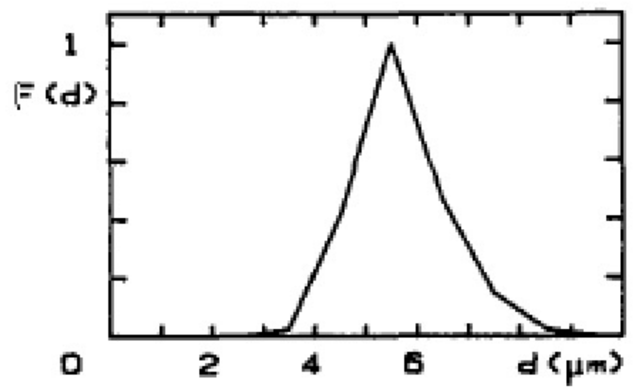
Size distribution:



The inverse problem

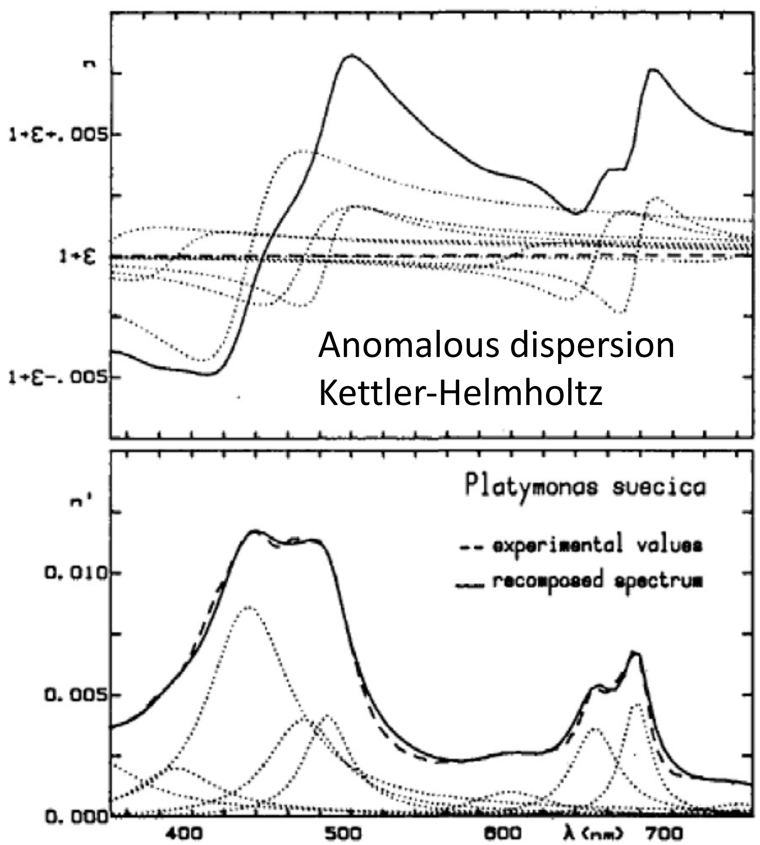
Find the optical constants consistent with absorption measurements of a phytoplankton culture (Bricaud and Morel, 1986)

Size distribution:

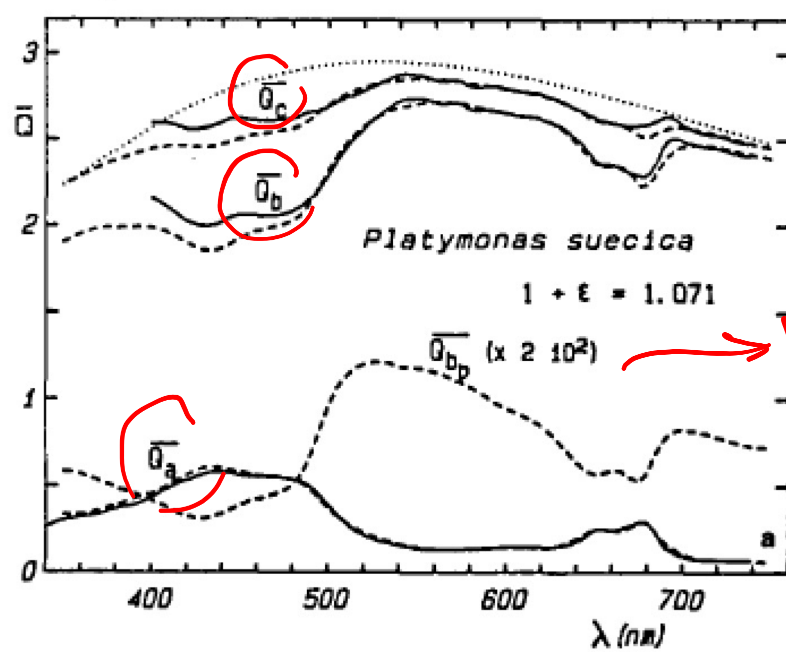


Mie

Absorption measurements:

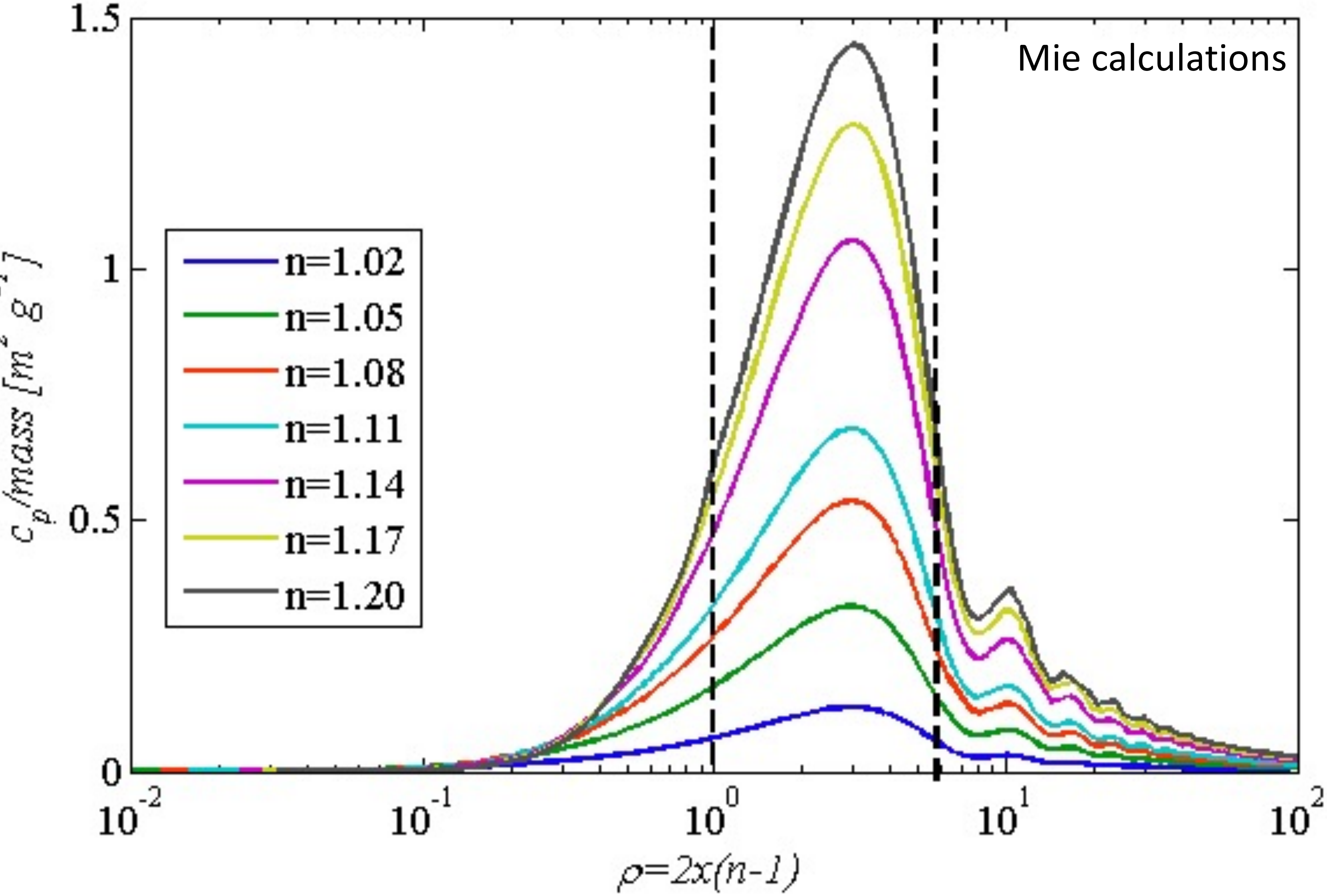


Results:



backscattering

Normalization 'simplifies' things



Size parameter x = $\pi D/\lambda$ Phase shift parameter $\rho = 2x(n-1)$

Scattering tends to have a 'similar' dependence for similar ρ (*not* similar *D!)*

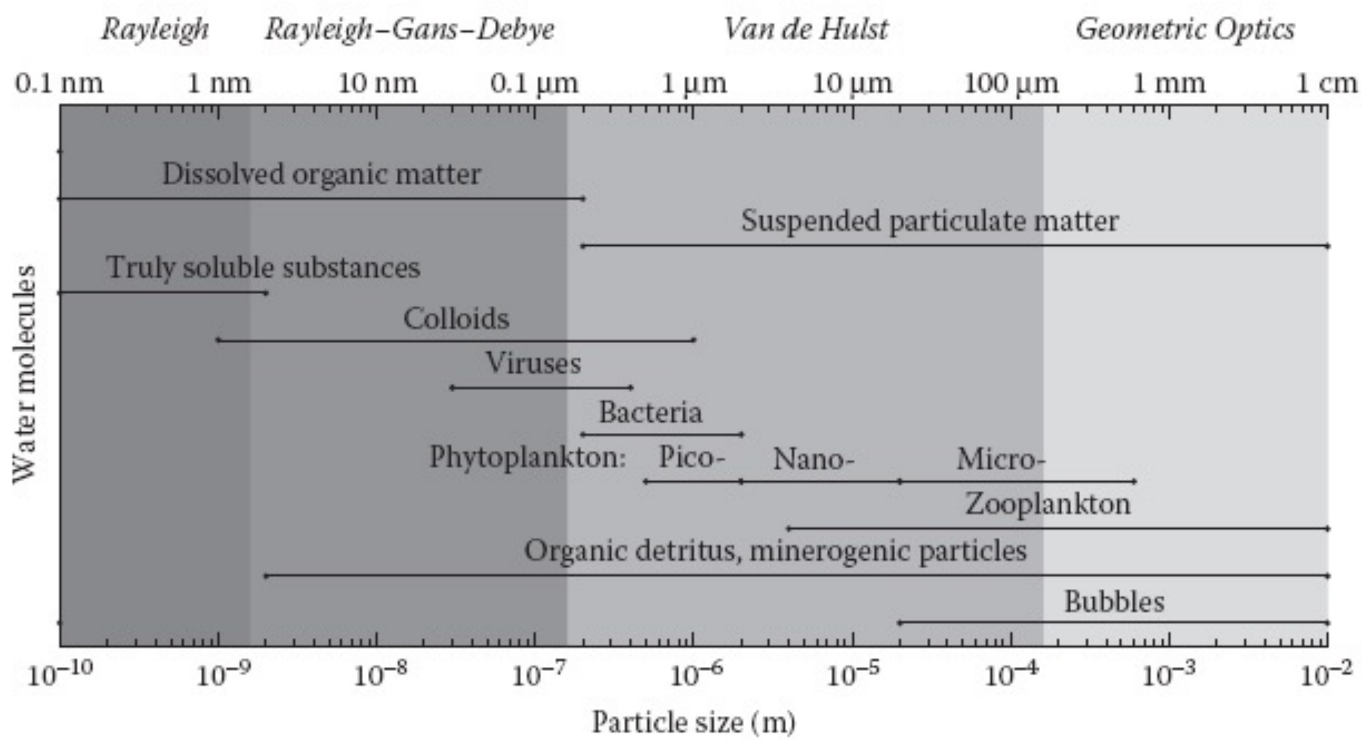
Optical regimes – primarily size-dependent

Table 1 Size ranges roughly corresponding to the size regions defined for two different refractive indices given $\lambda = 676$ nm

Size region	$n = 1.05$	$n = 1.17$	Equivalent ρ
RAY	$D \ll 0.2$ µm	$D \ll 0.2$ µm	$\rho \ll 0.1$
RGD	$D < 5$ µm	$D < 2$ µm	$\rho < 3$
VDH	$5 < D < 200$ µm	$2 < D < 65$ µm	$3 < \rho < 100$
GO	$D \gg 200$ µm	$D \gg 65$ µm	$\rho \gg 100$

How does size affect optical properties?

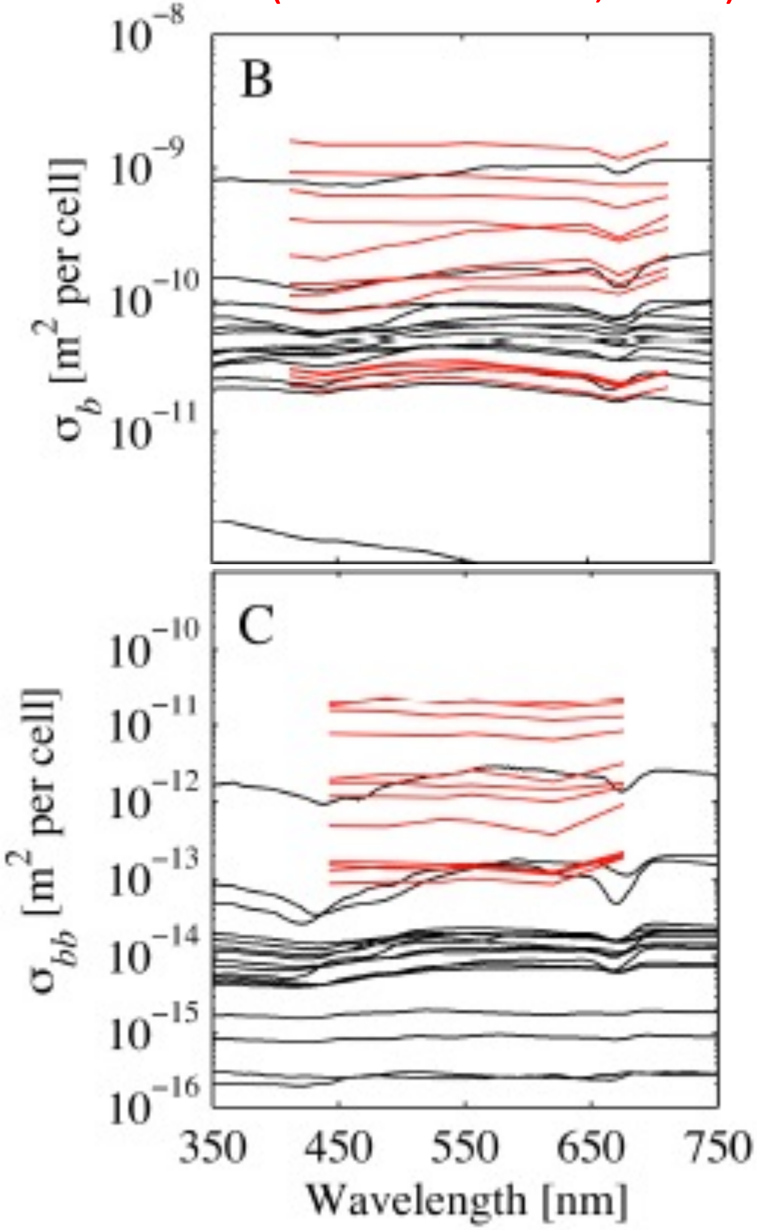
How can we use optical properties to learn about size?



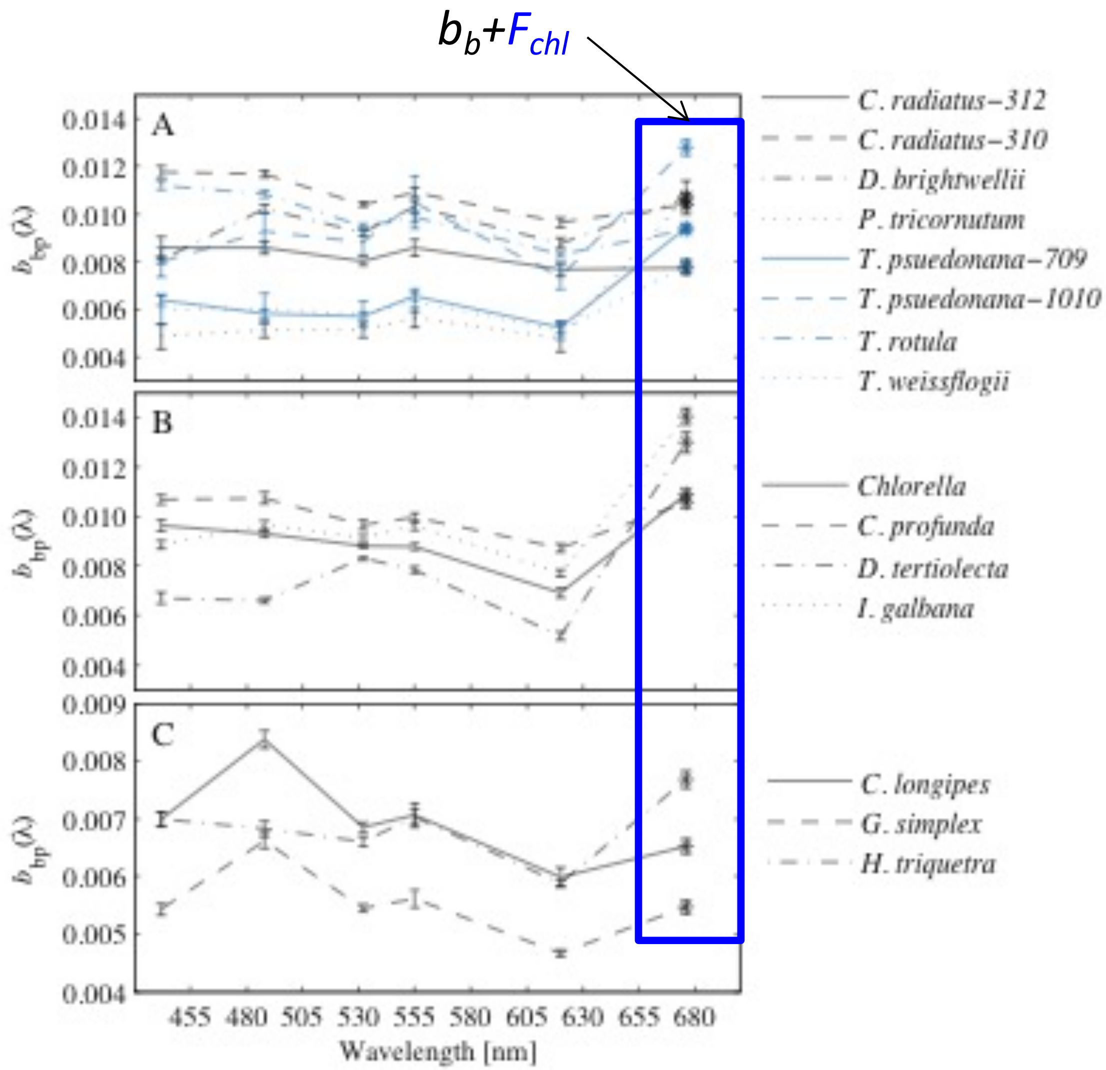
Clavano et al. 2007

Scattering and backscattering by phytoplankton

In cultures (Whitmire et al., 2010)



Comparison with Mie theory
(Stramski et al., 2001)



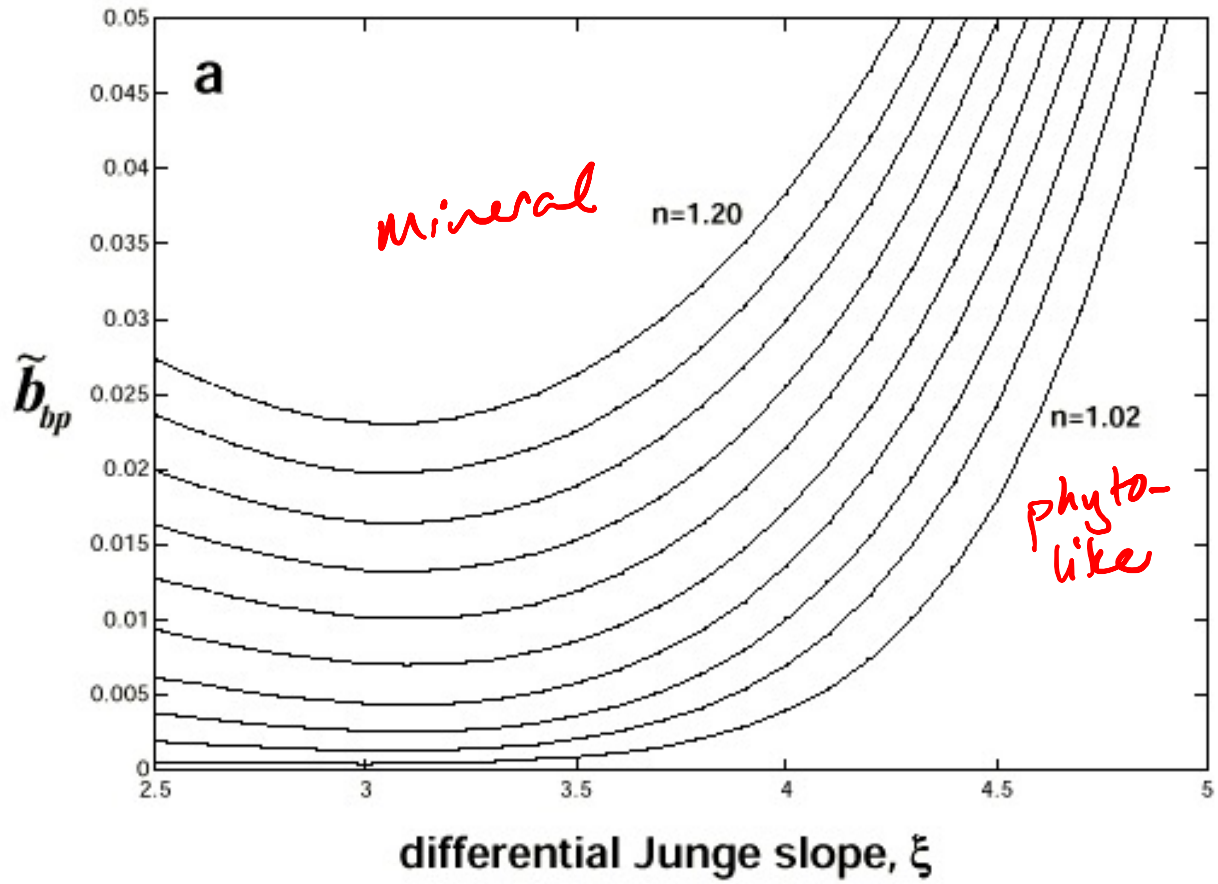
Whitmire et al., 2010

“Missing backscattering enigma”
(Stramski et al., 2004)

Backscattering ratio - sensitivity to composition and size

Backscattering ratio $\left(\tilde{b}_{bp} \equiv b_{bp}/b_p\right)$ depends on:

1. Index of refraction (*n*)
2. Slope of PSD (ξ)

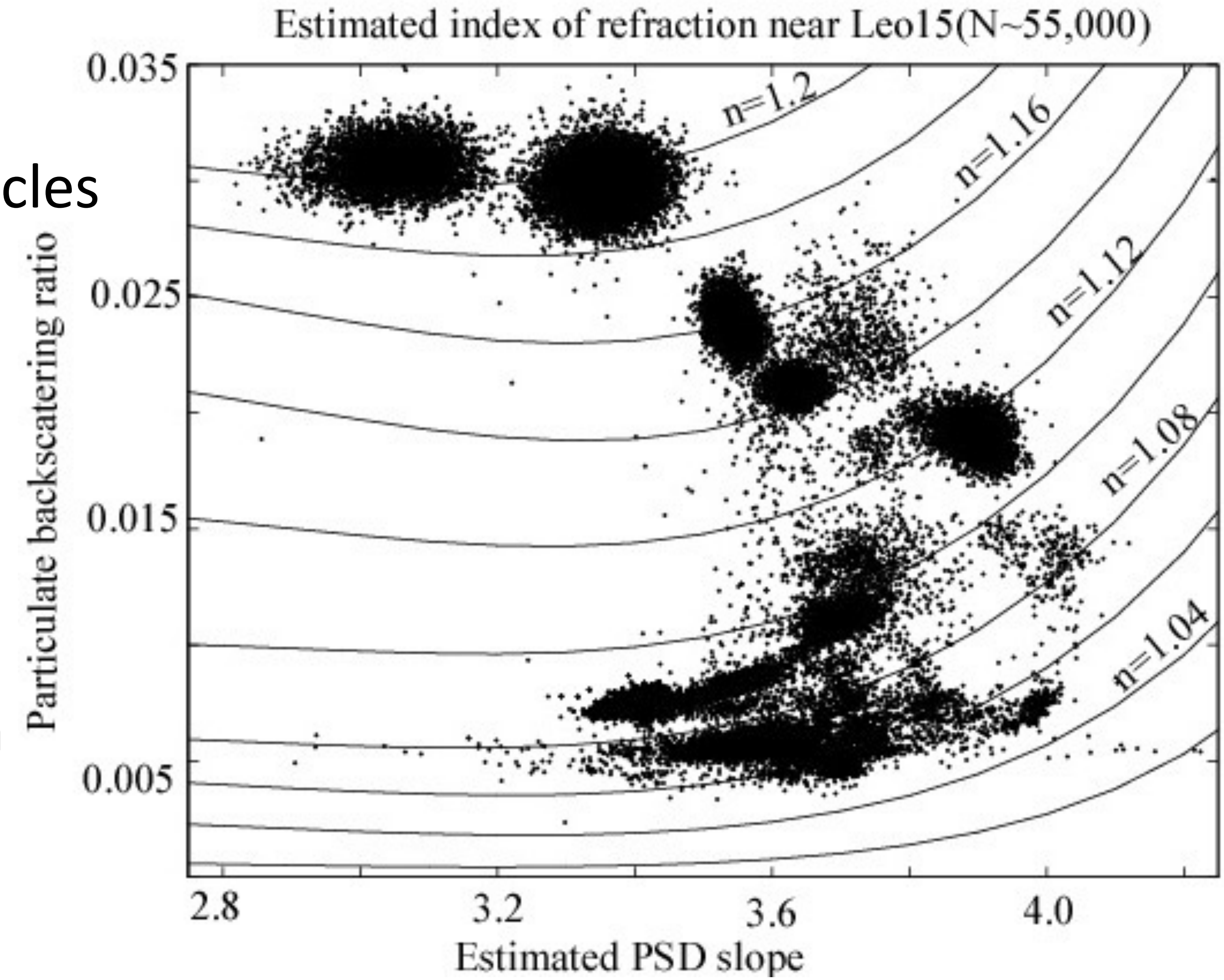


Twardowski et al., 2001

Backscattering ratio (55,000 observations from NJ shelf): consistent with theoretical prediction.

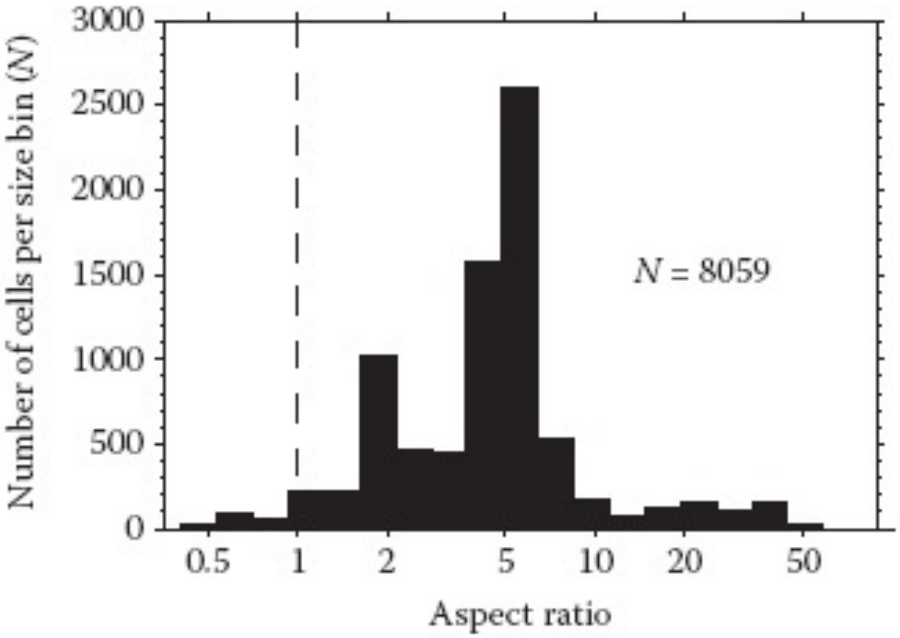
Varies from: inorganic particles

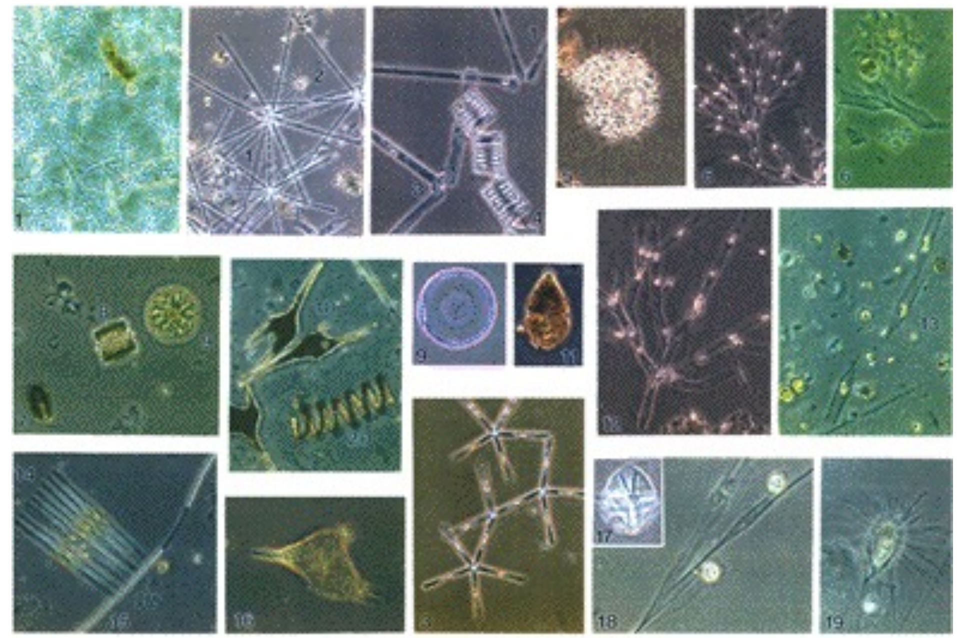
phytoplankton



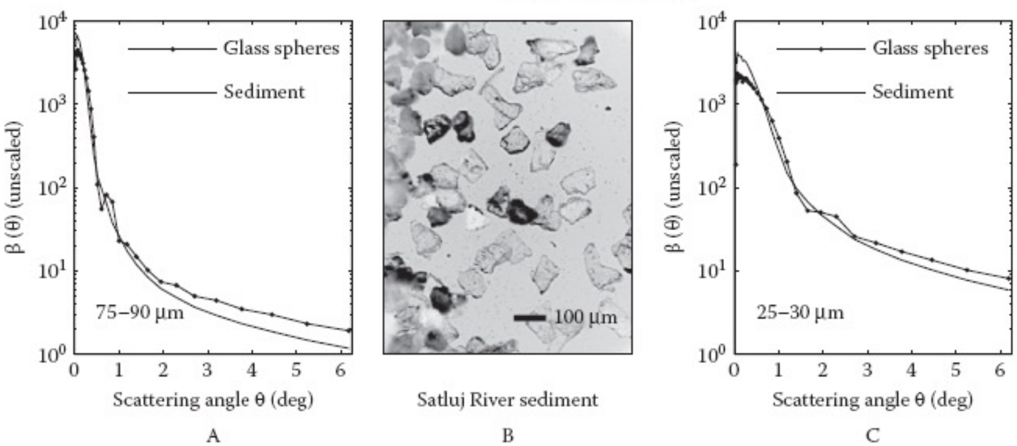
Boss et al., 2004

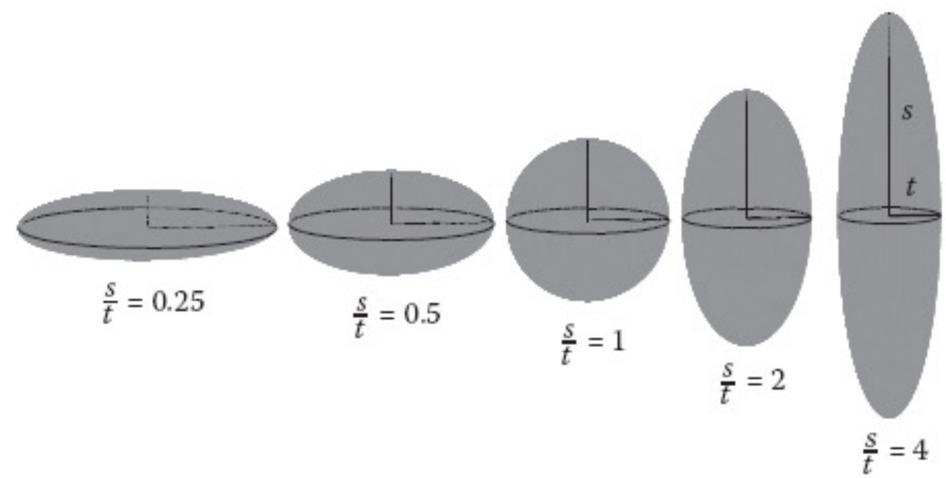
Particles are not spheres... does it matter for IOPs?





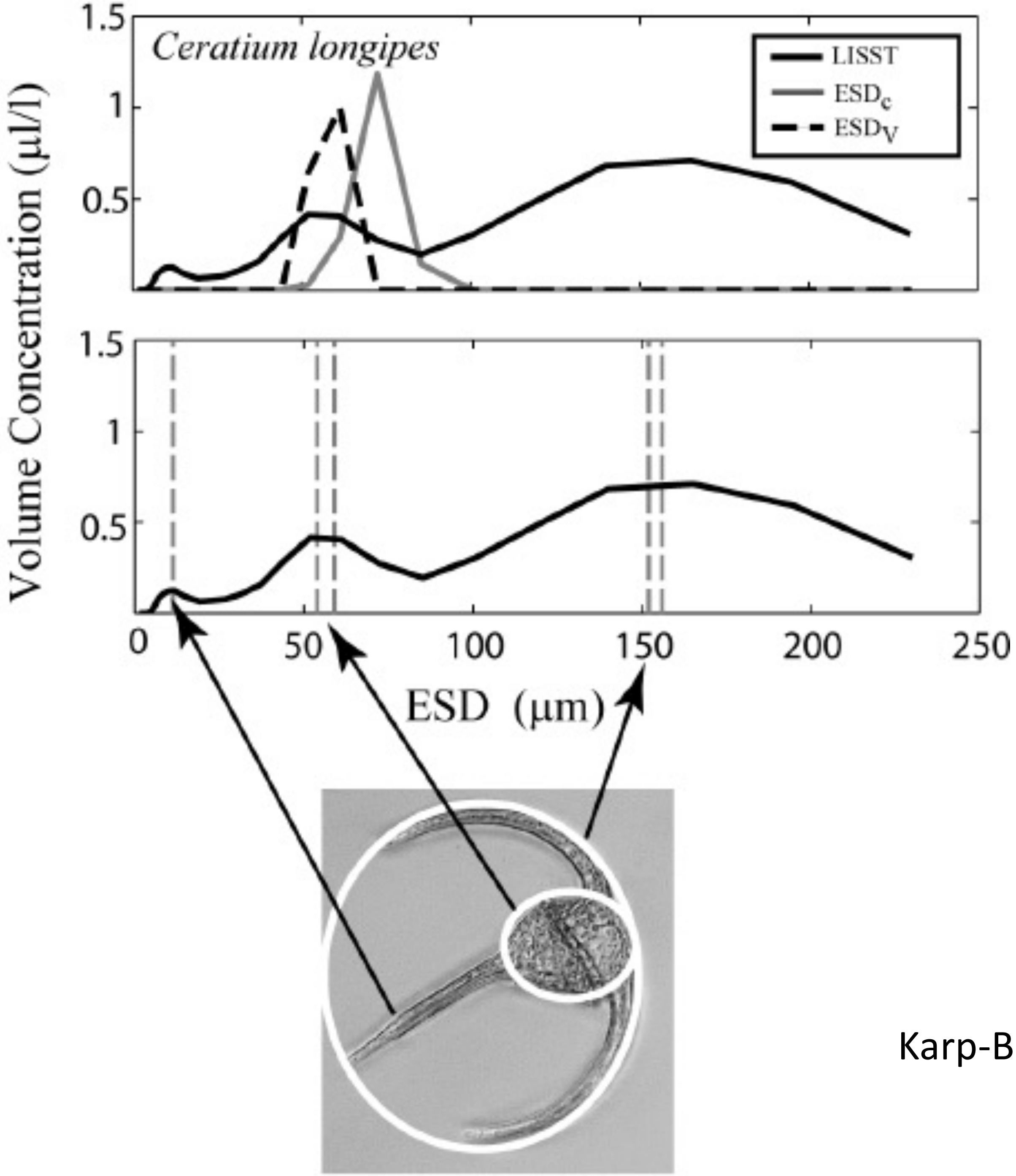
© 1993 Gertrud Cronberg





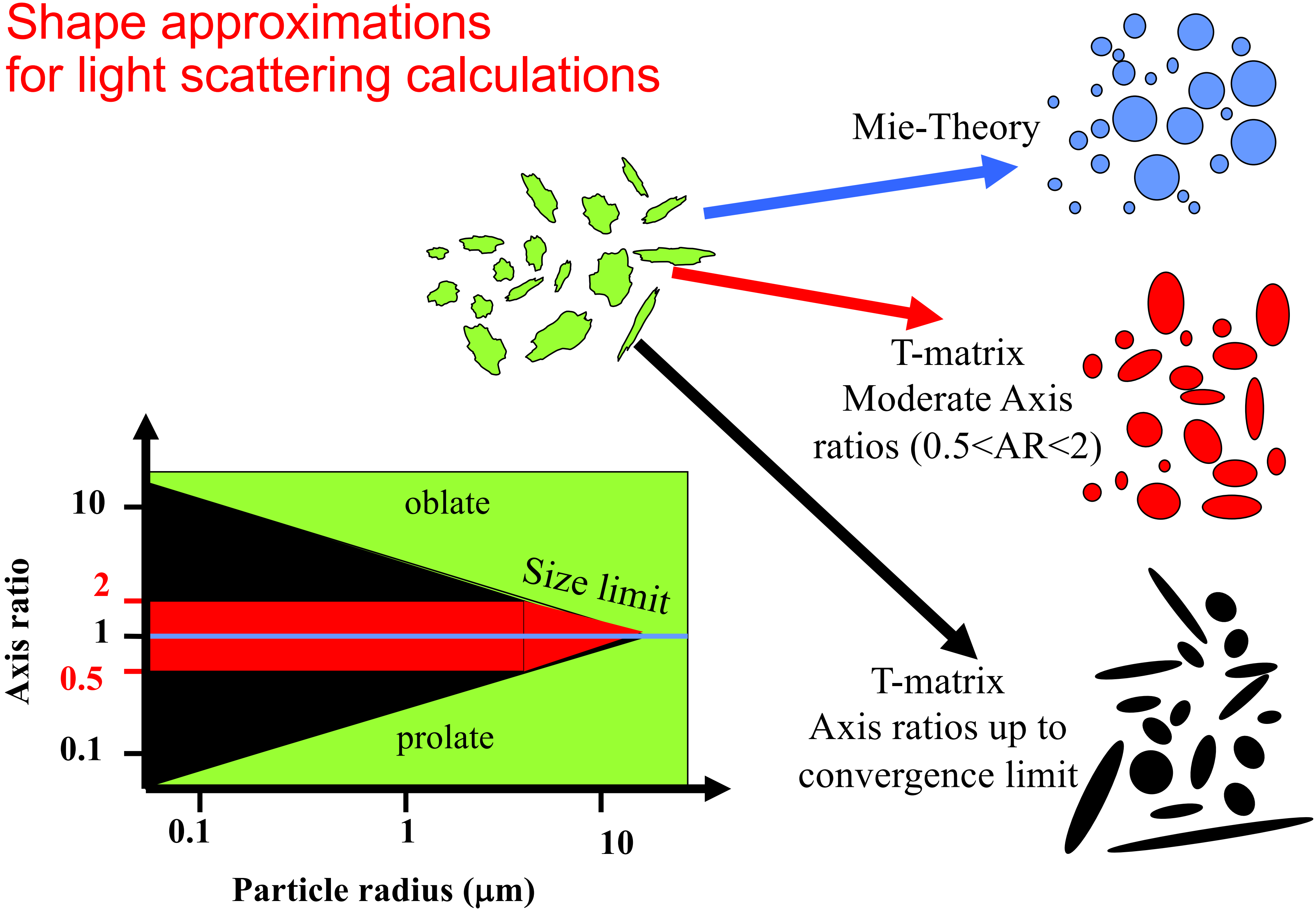
Clavano et al., 2007

Shape consideration



Karp-Boss et al., 2007

Shape approximations for light scattering calculations



Slide from Hester Volten (RIVM)

Quantifying differences due to shape:

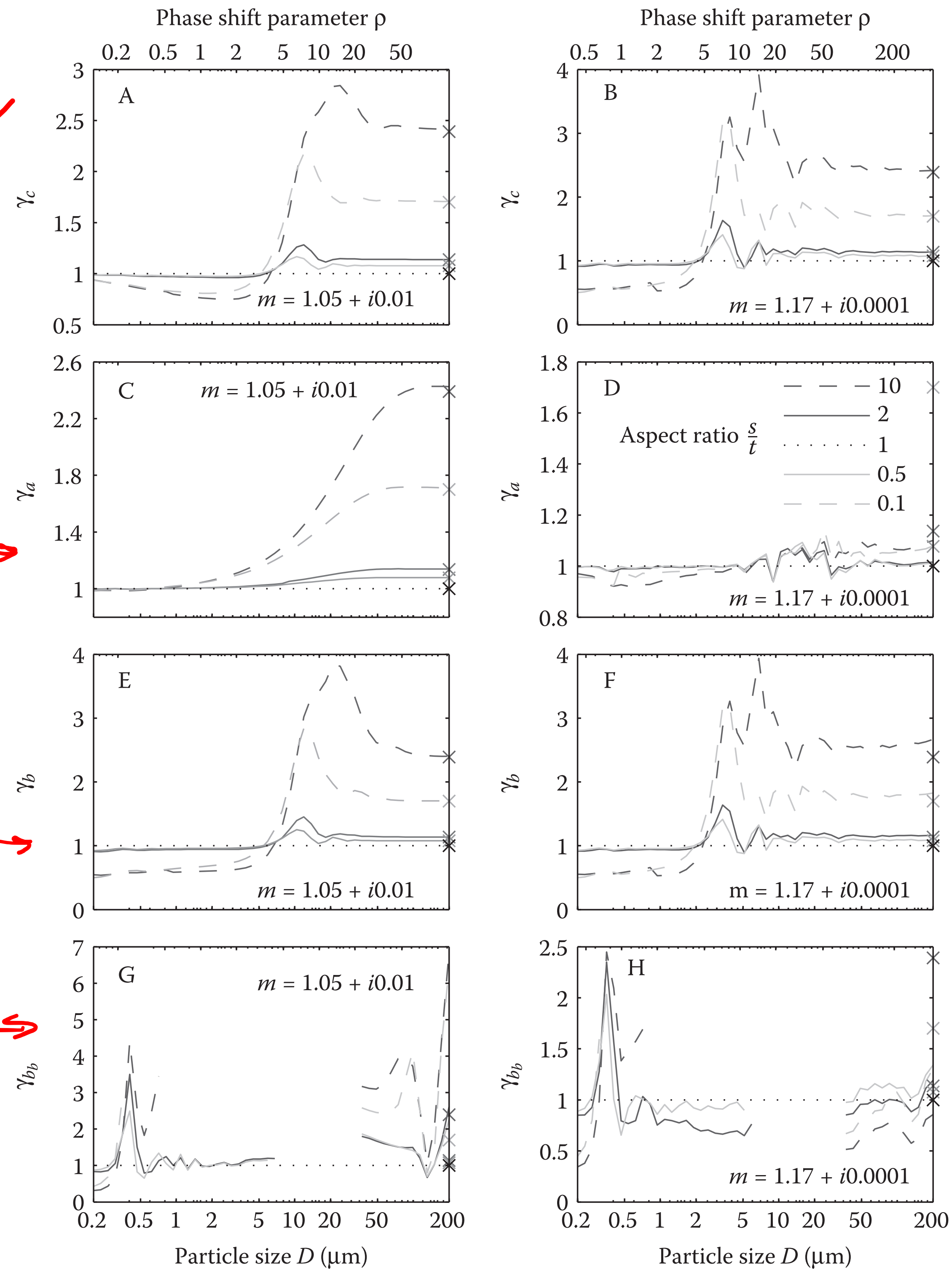
Modeled bias in optical efficiencies for non-spheres (*note: here γ is ratio of Q relative to a sphere*)

- Departure from spherical shape leads to size-dependent biases in optical efficiencies
- Non-spheres have larger cross-sections than spheres

Clavano et al., 2007

Phyto-like

Min-



Does orientation matter?

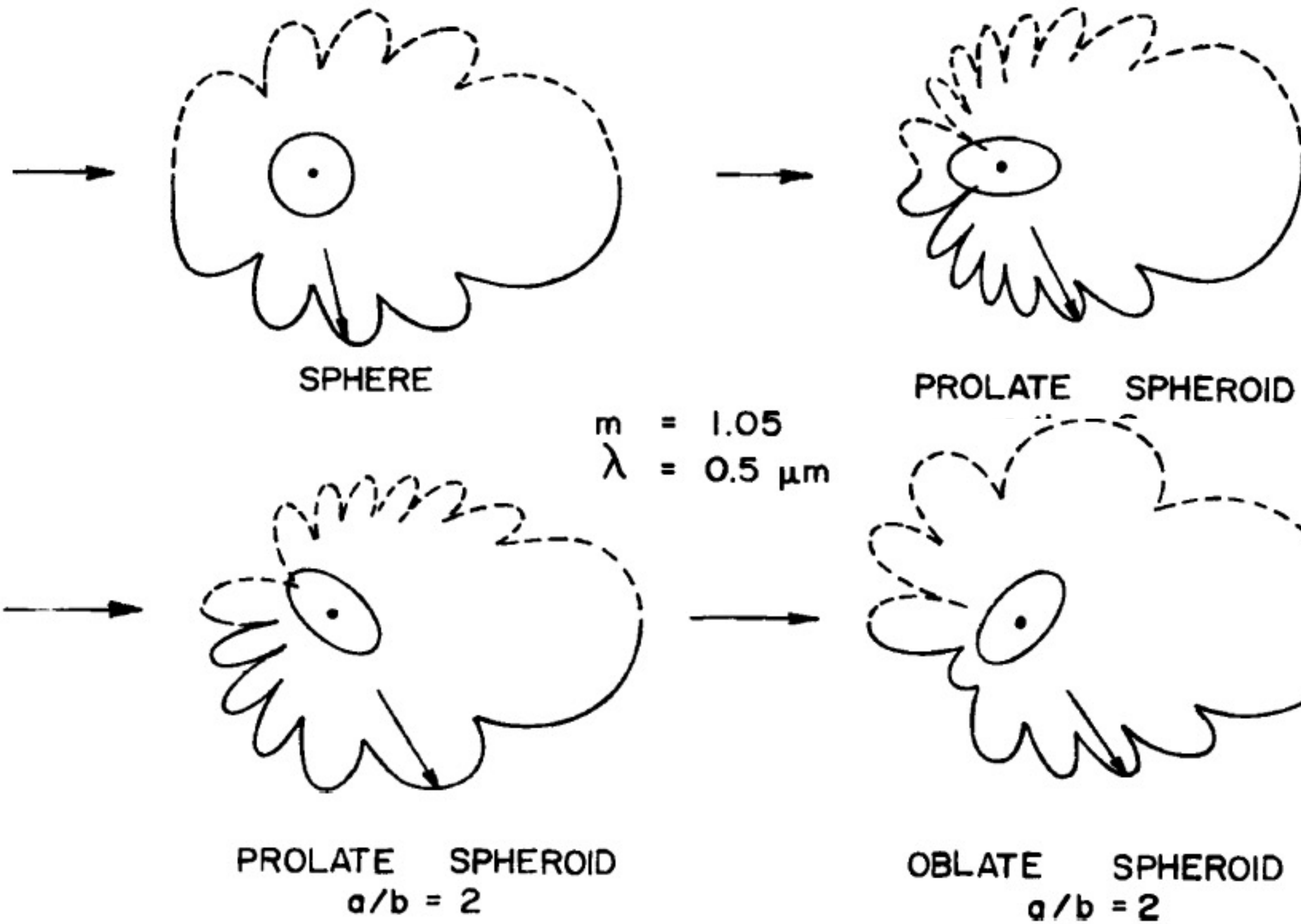
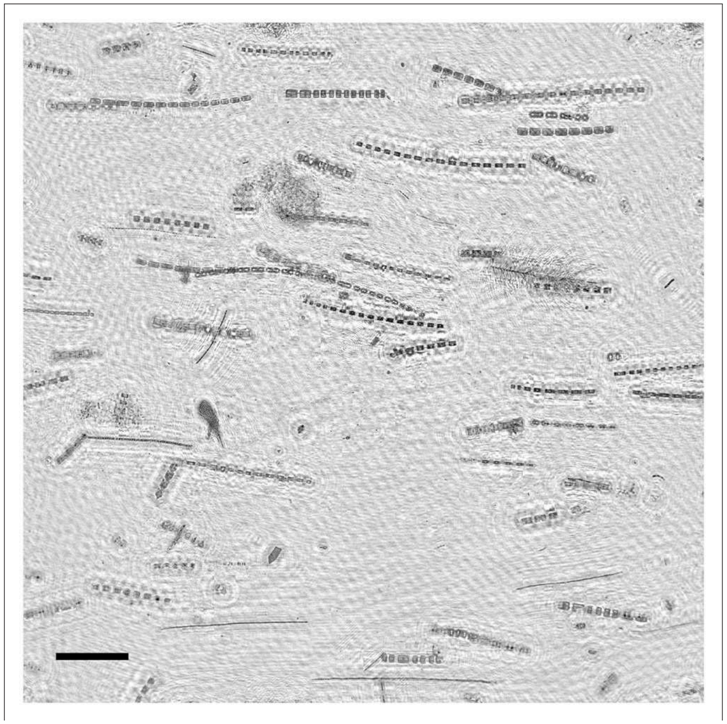
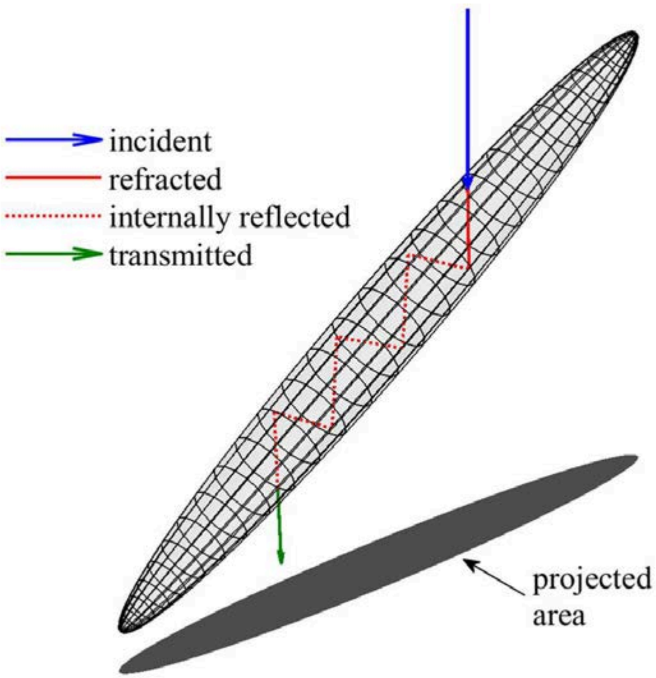


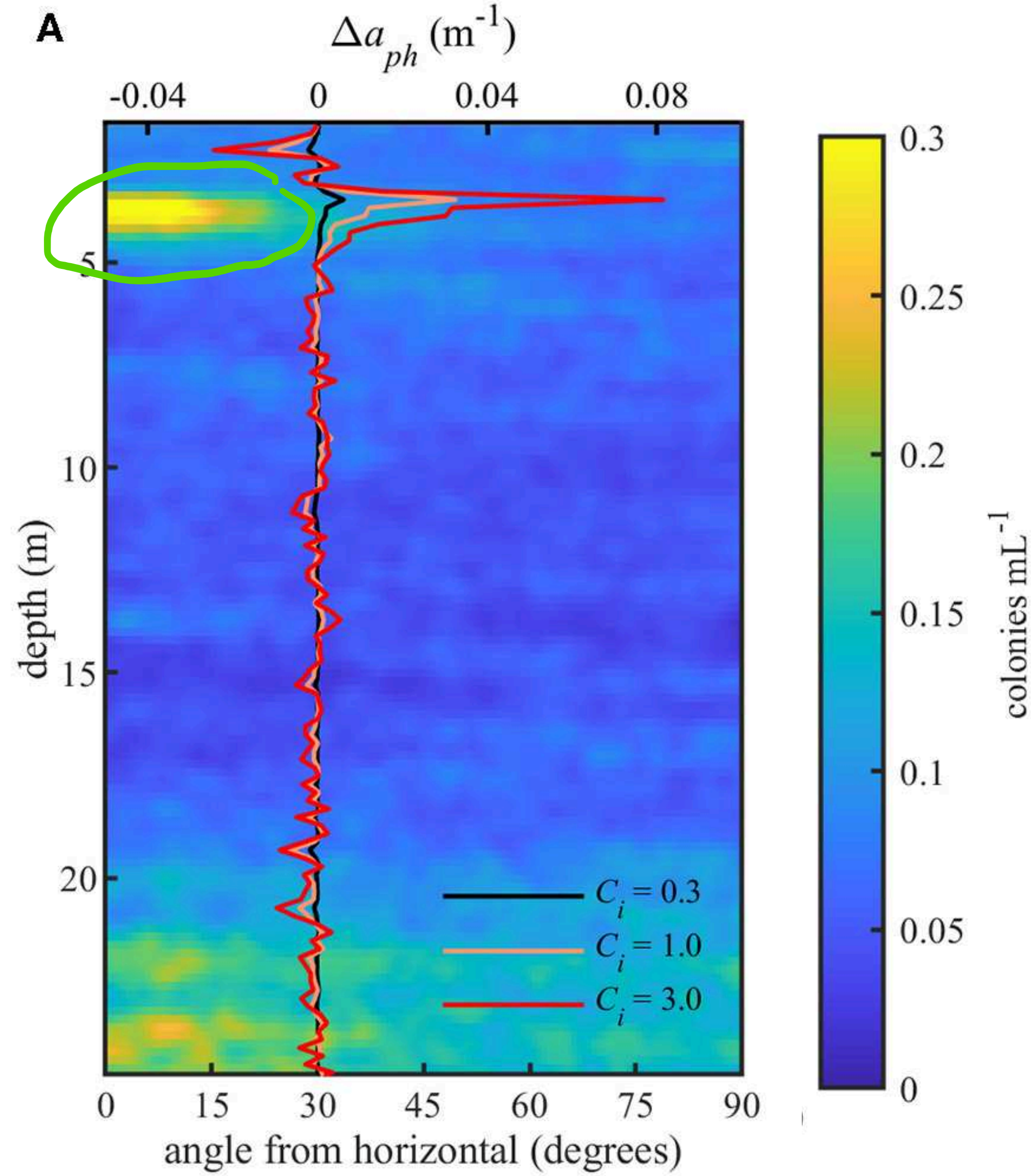
Figure 13.6 Polar scattering diagrams for equal-volume spheroids. The incident light is unpolarized. From Latimer et al. (1978).

Does orientation matter?

- In situ digital holography (more on this later today)
- *D. brightwellii* diatom colonies with preferential orientation increased a_ϕ by 4.5-24.5%.

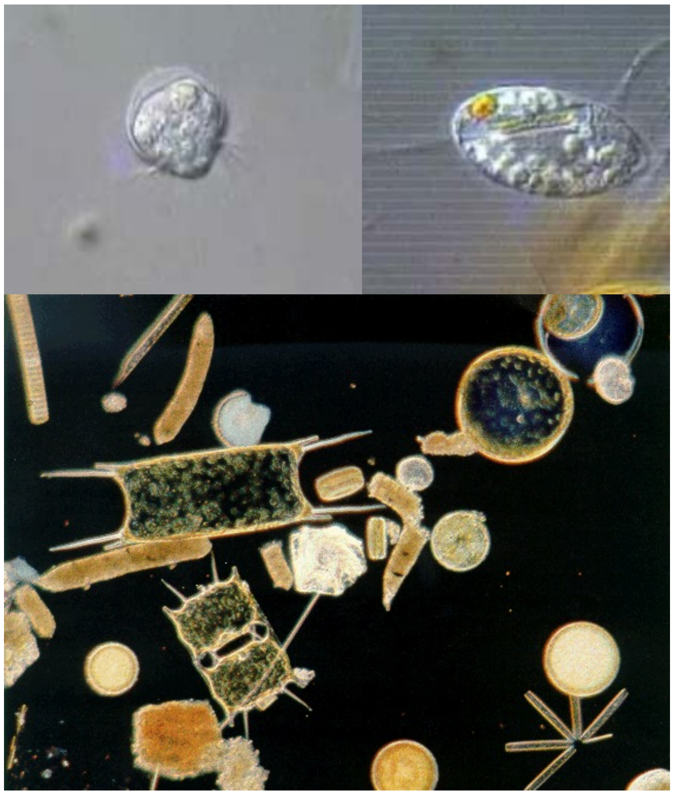


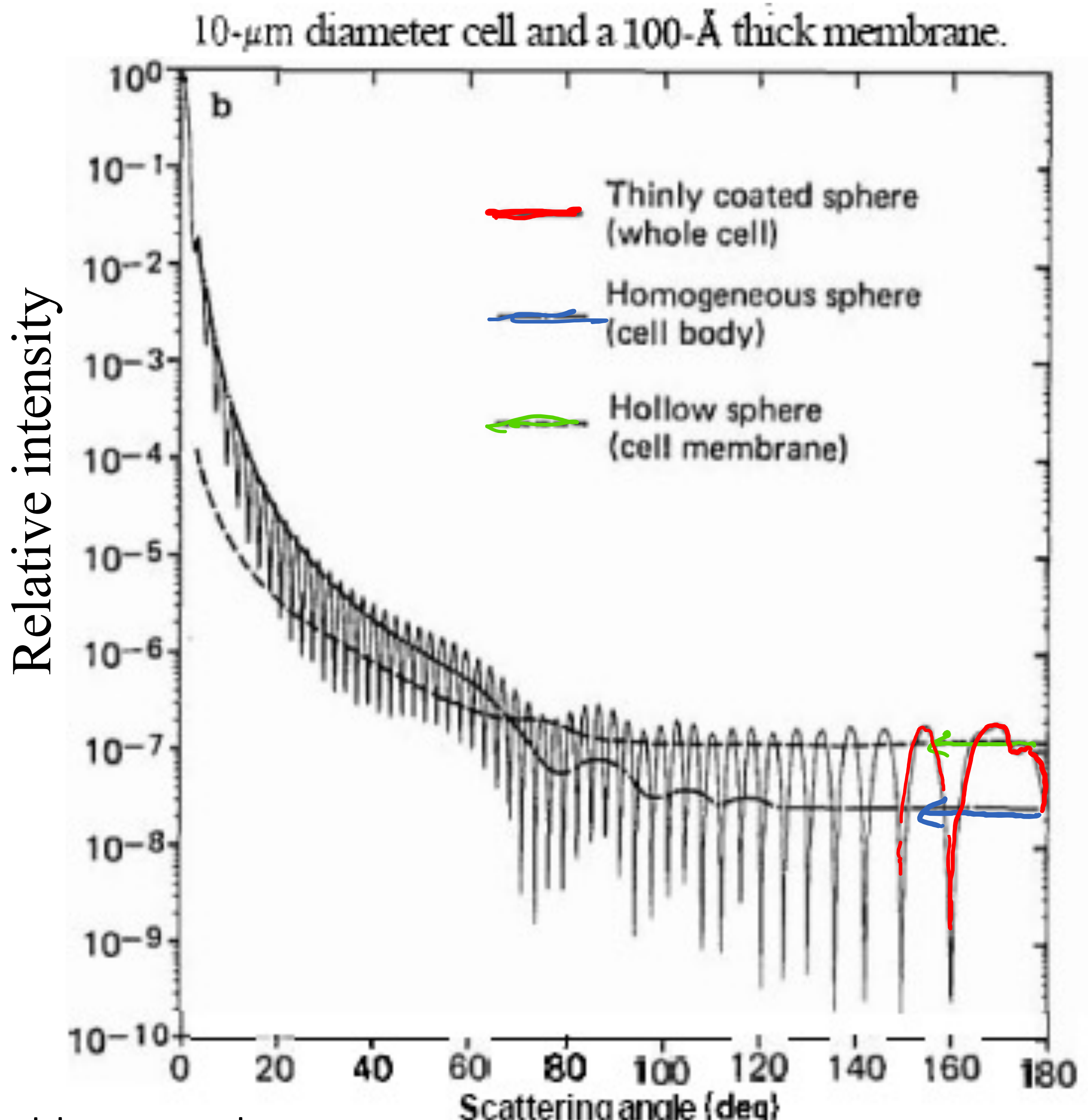




McFarland, et al. 2020

Internal structure:

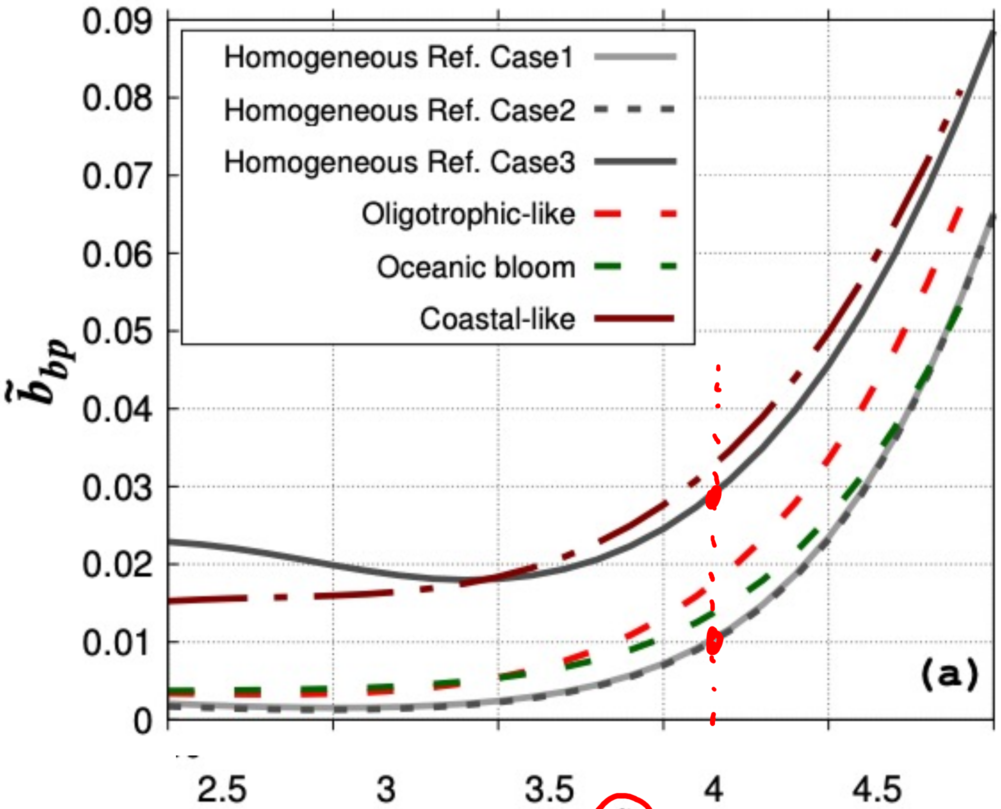




Backscattering dominated by membrane.

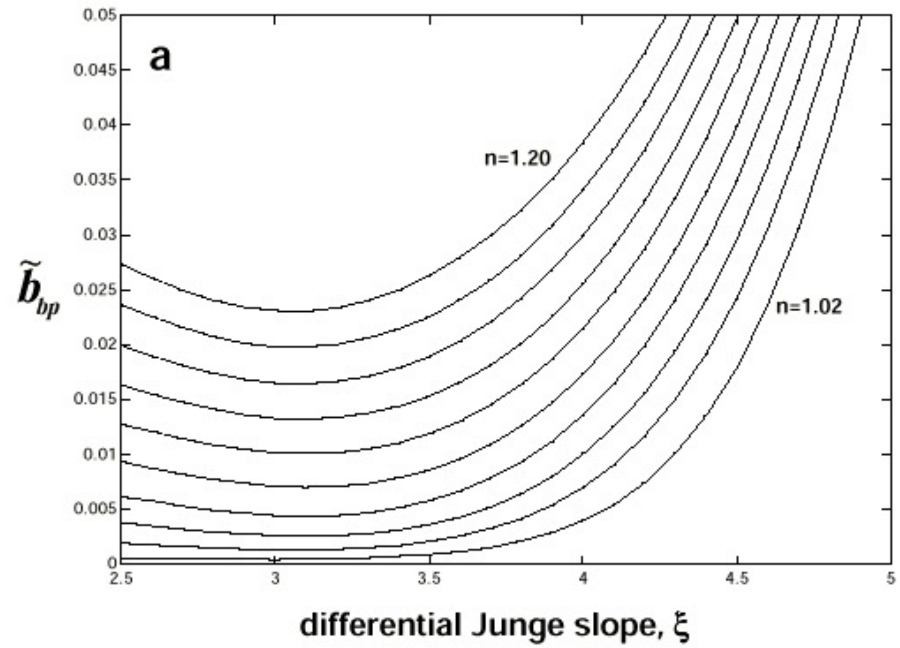
Meyer, 1979

Coated-sphere model predicts higher backscattering ratio



larger ξ smaller

Duforier-Gaurier et al., 2018



Twardowski et al., 2001

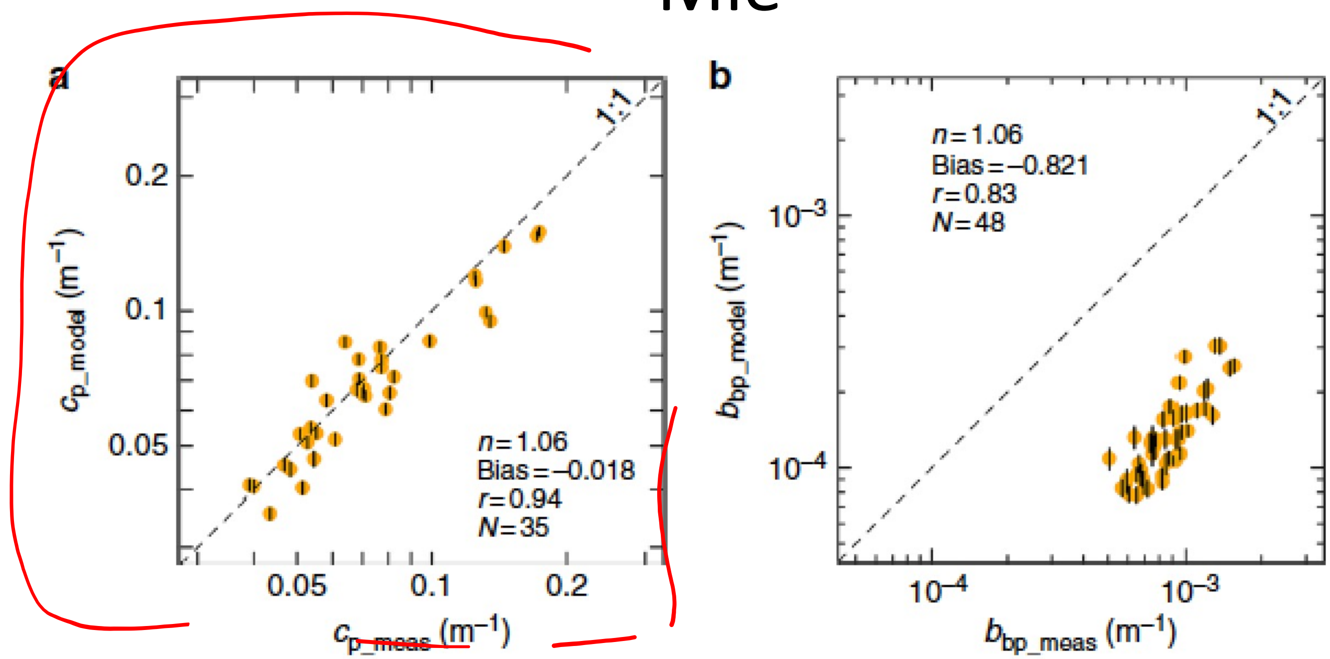
For ξ=4,

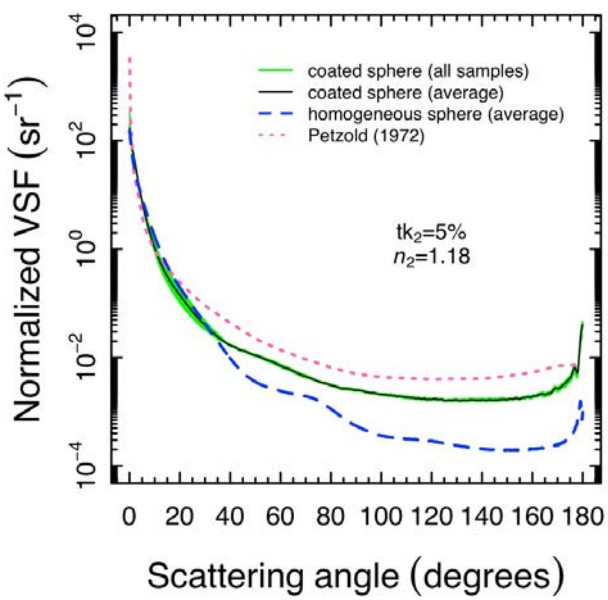
58% increase for phytoplankton

12% increase for inorganic

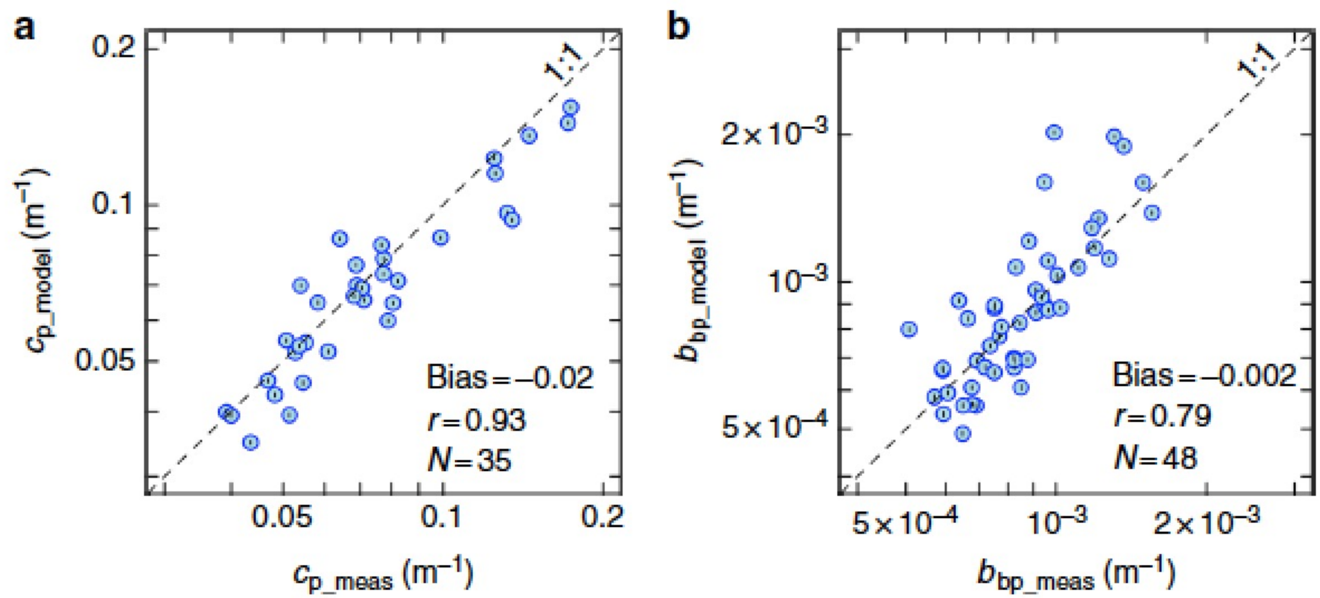
We get better agreement with observation if we account for internal structure:

Mie





Coated spheres (inside=1.06, shell=1.13) :



Organelli et al., 2018

Backscattering by Nonspherical Particles: A Review of Methods and Suggested New Approaches

CRAIG F. BOHREN

Department of Meteorology, Pennsylvania State University, University Park

SHERMILA BRITO SINGHAM[1]

Life Sciences Division, Los Alamos National Laboratory, Los Alamos, New Mexico

When criticized for using Mie theory where its applicability is dubious, modelers sometimes respond that although they know that Mie theory is inadequate, it is the only game in town. Better to do wrong calculations than to do none at all. Modelers have to model.

We suggest an alternative to modeling. It is called not modeling—not modeling, that is, until adequate methods are at hand.

Backscattering of light from disklike particles: is fine-scale structure or gross morphology more important?

Howard R. Gordon

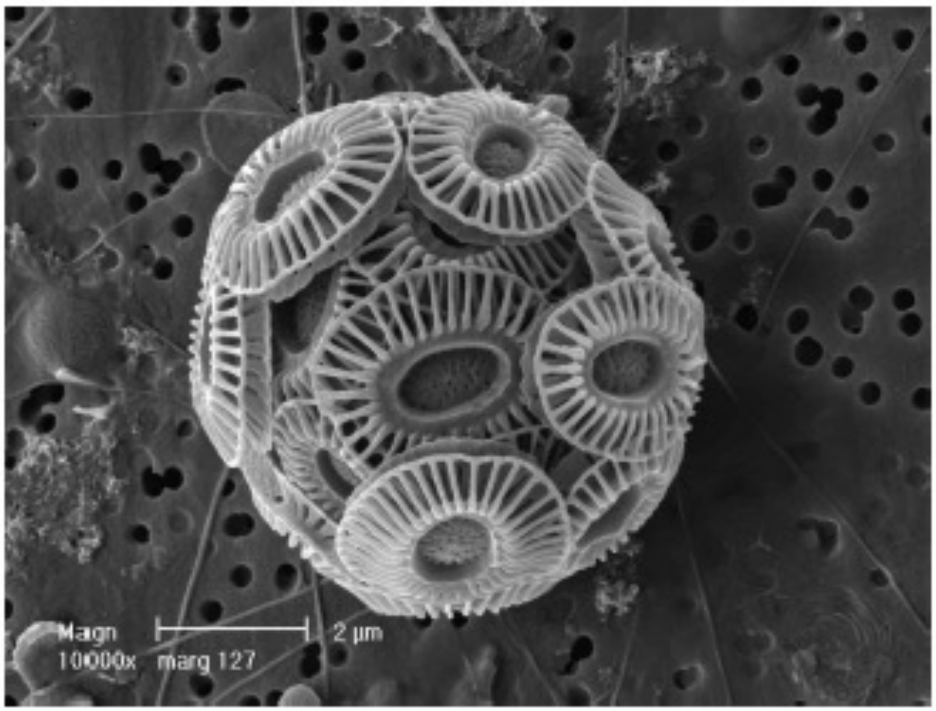
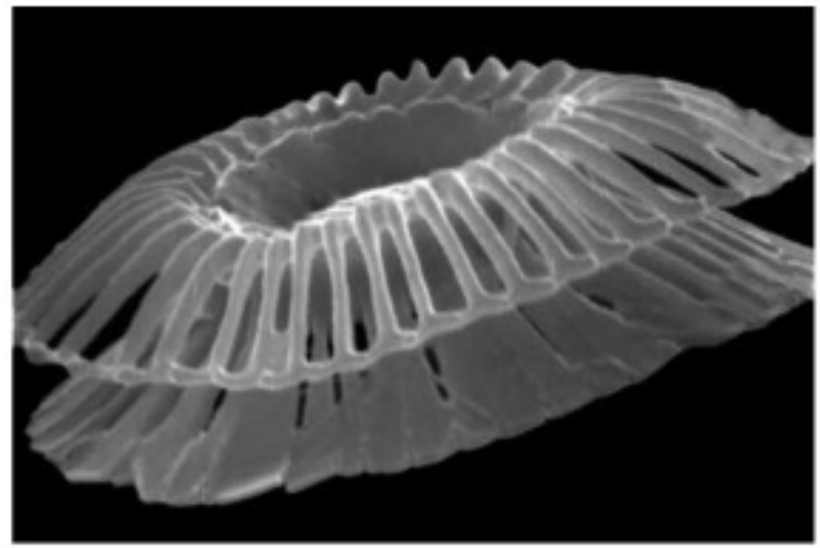
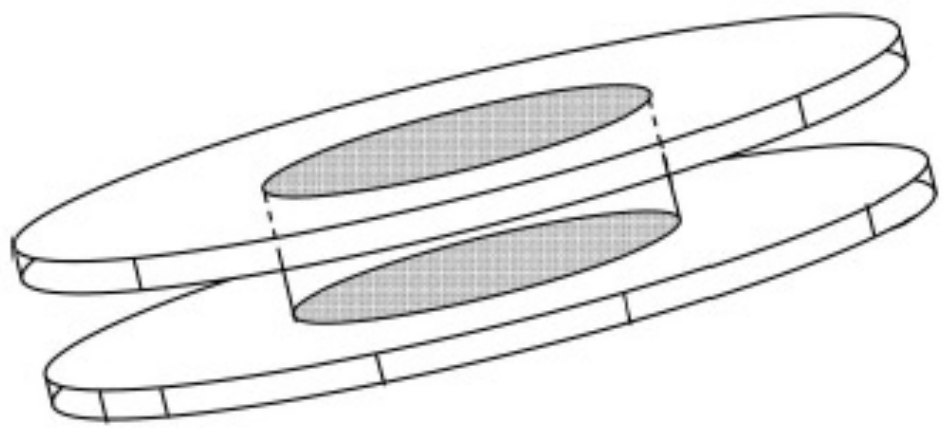
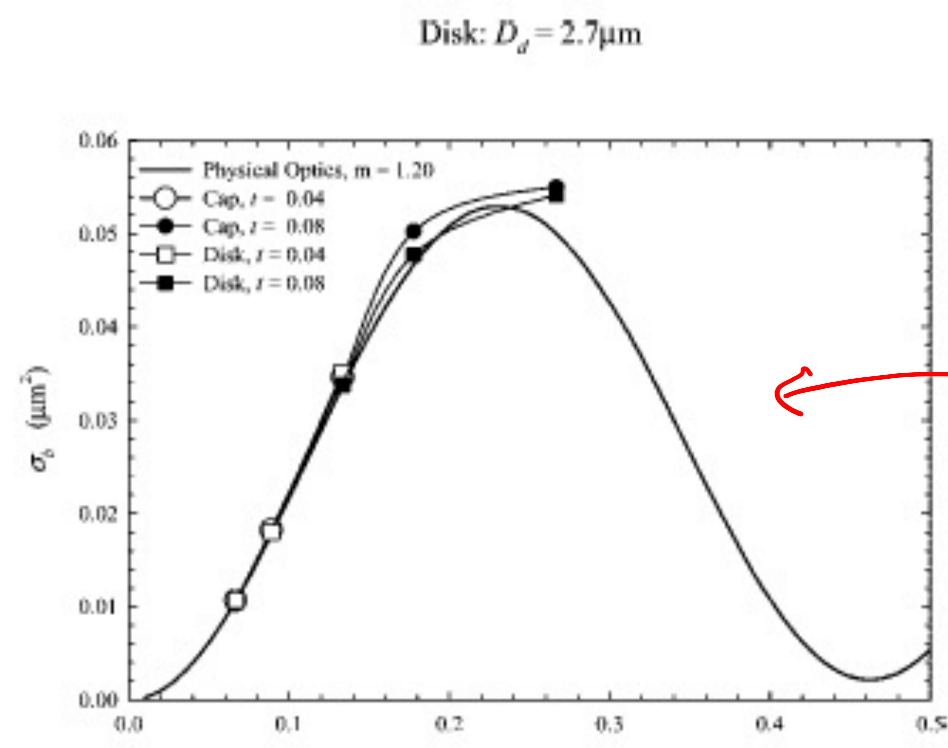
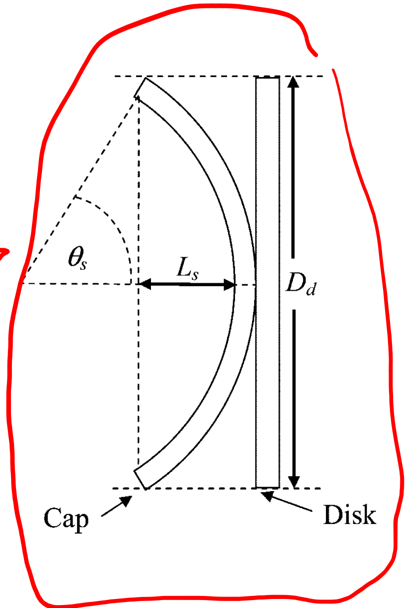


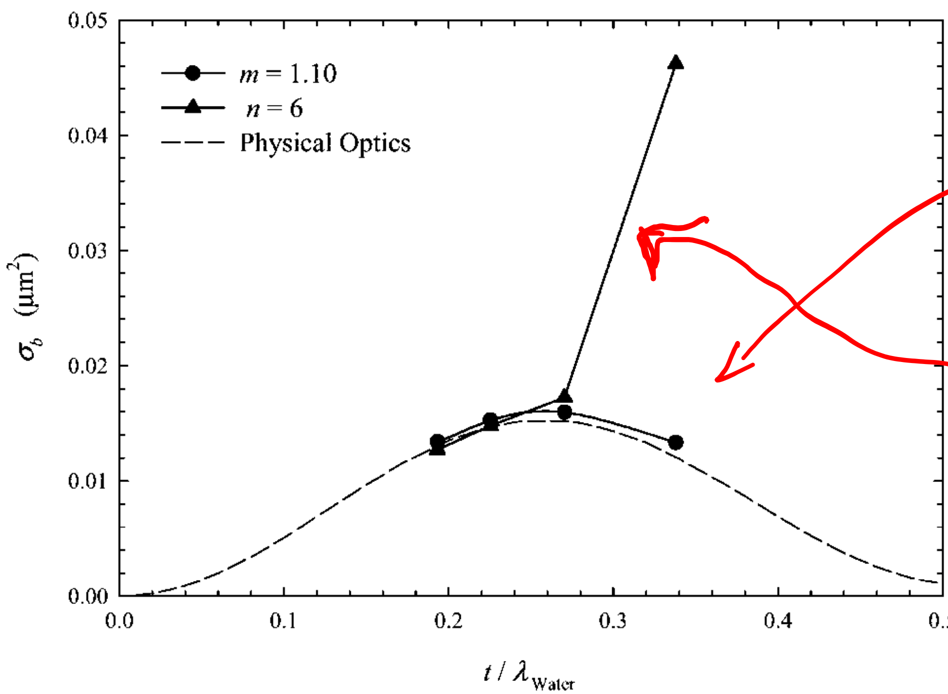
Fig. 1. Scanning electron micrograph image of a single cell of *E. Huxleyi* (the spherically shaped object) resting on a filter pad. The individual disklike structures covering the cell are the coccoliths (Fig. 2.). The pore size of the filter (small holes in the background) is 0.2 μm. The horizontal white bar in the lower left has a length of 2 μm. (Photo courtesy of Jeremy Young, The Natural History Museum, London.)

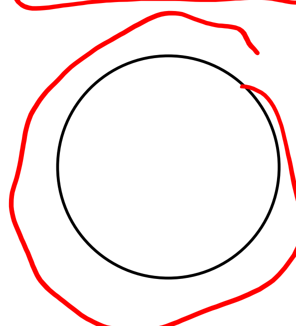


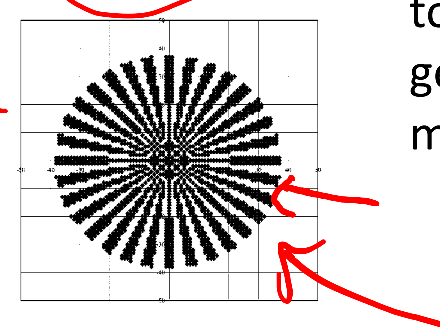












Gordon, 2006:

Take-home:
Gross morphology is the major control on backscattering (for coccolith-like particles)

Fine structures with sizes > 0.25λ *did* cause backscattering to depart from a geometric optics model.

Aggregation (packing) in the marine environment

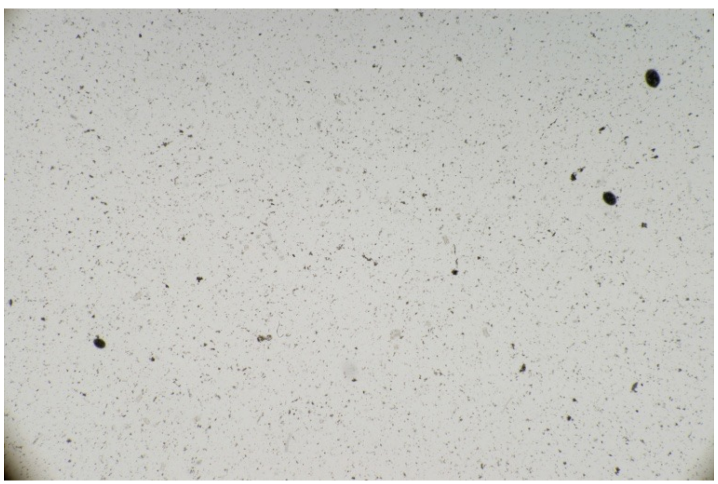
The rate of aggregation depends on [concentration]^2

Mechanisms for encounter: Brownian motion, differential settling, turbulent shear, and biological processes

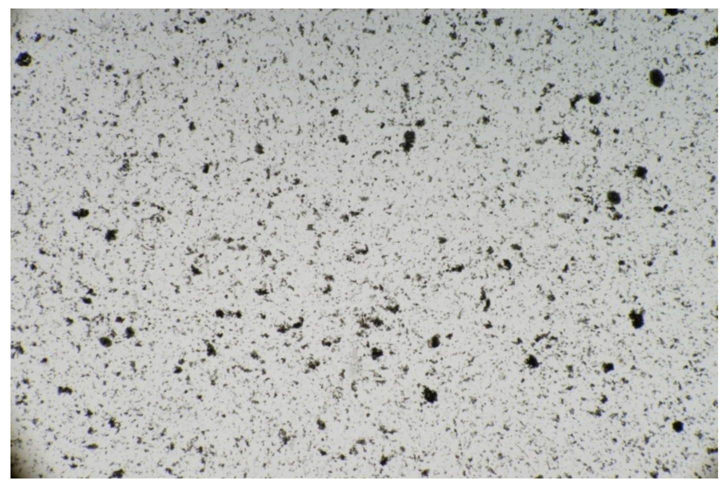
Aggregates sink faster than their component particles.

Aggregates break when shear is too high

Camera pictures at 1 meter above bottom, at a 12m deep site within 1day:

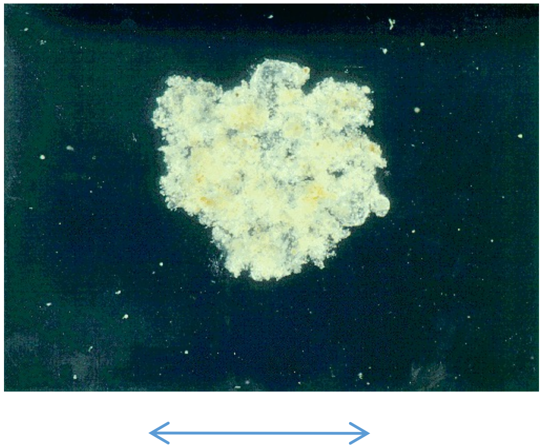


Dominated by <100um particles



Dominated by >1000um particles

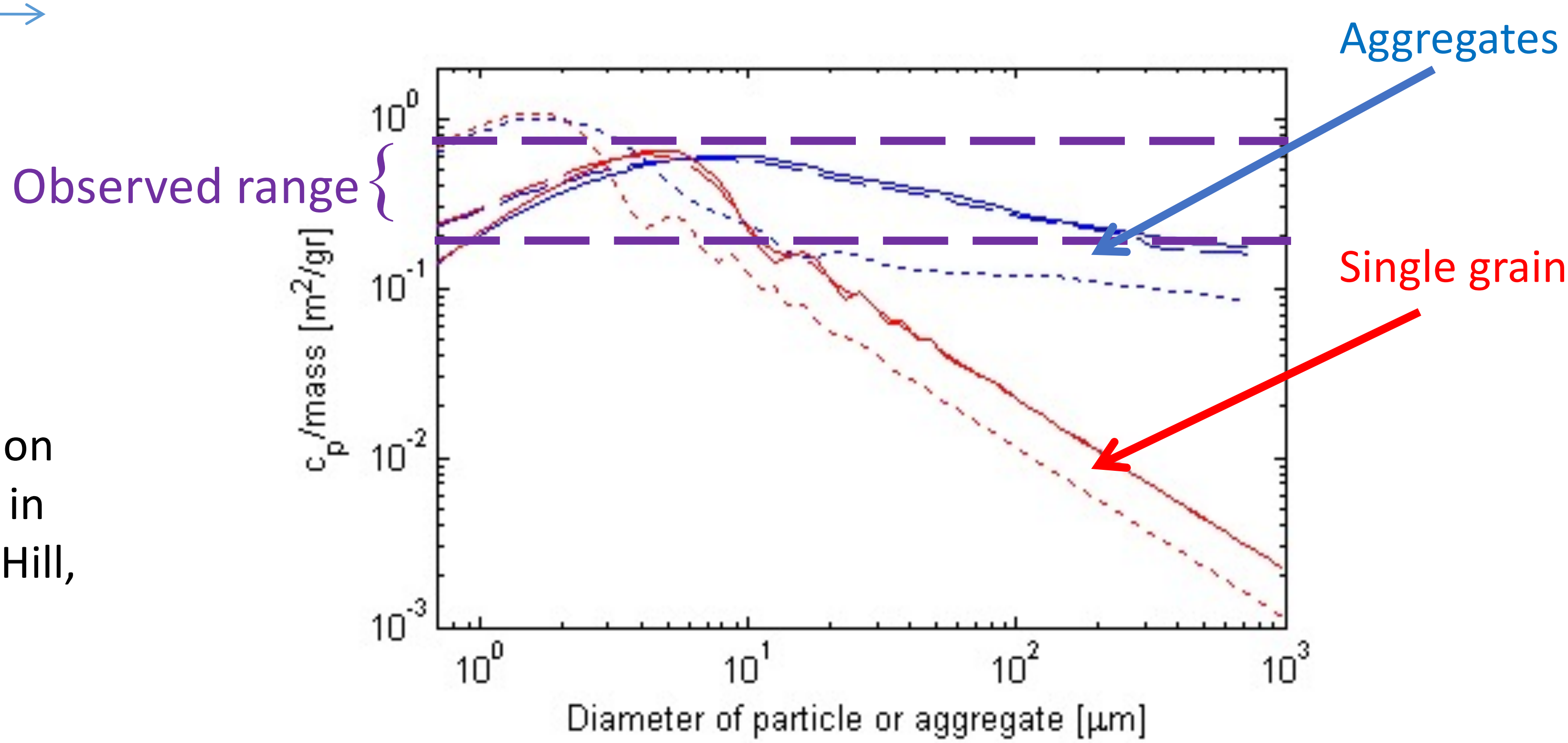
Aggregation (packaging) and IOPs



4mm

For marine aggregates, size and solid fraction are related: the bigger the aggregate, the greater its fluid fraction, like a stretched-out cotton ball.

Theoretical calculations

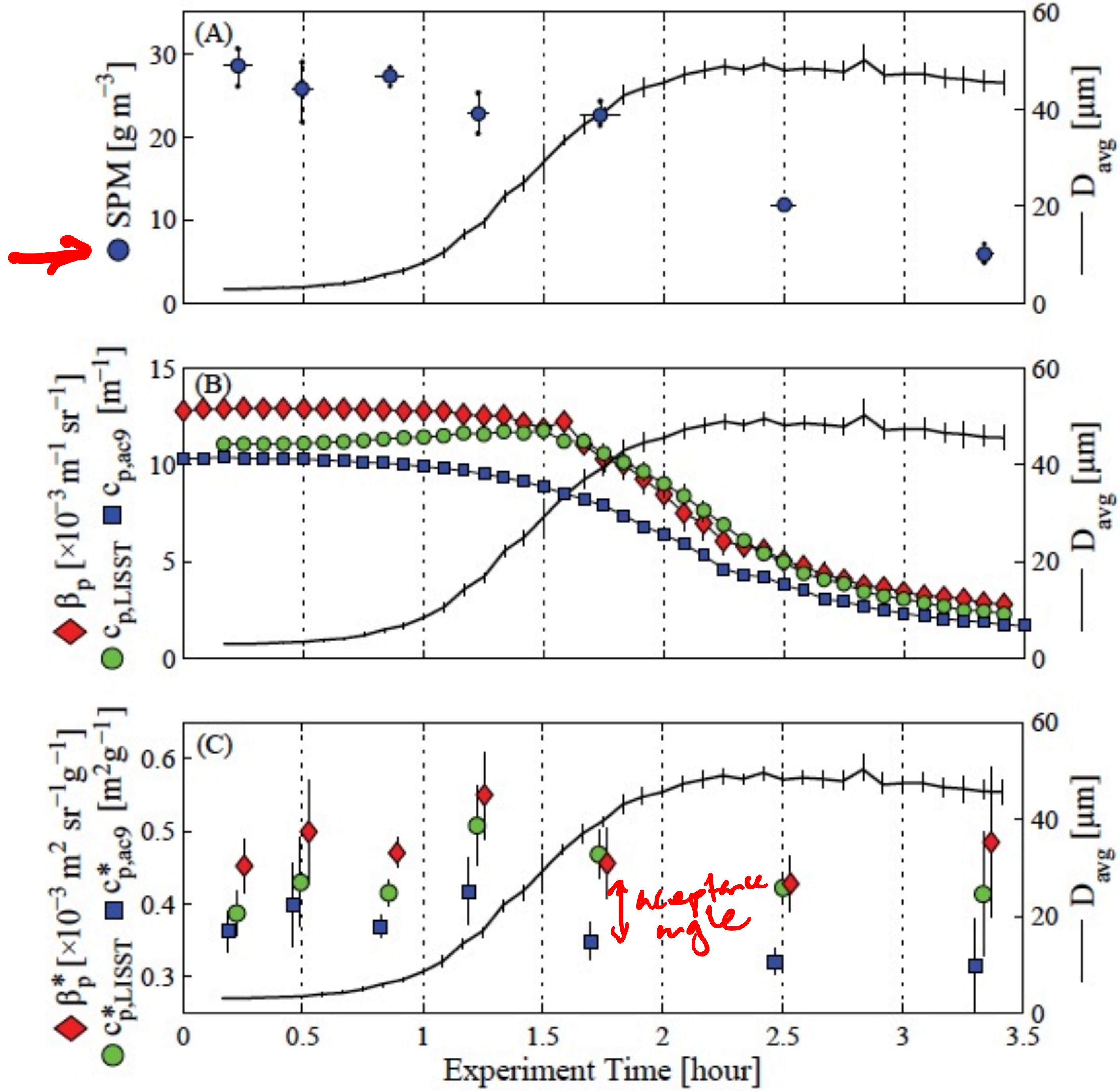


Water fraction modeled as in Khelifa and Hill, 2006

Boss et al., 2009, OE

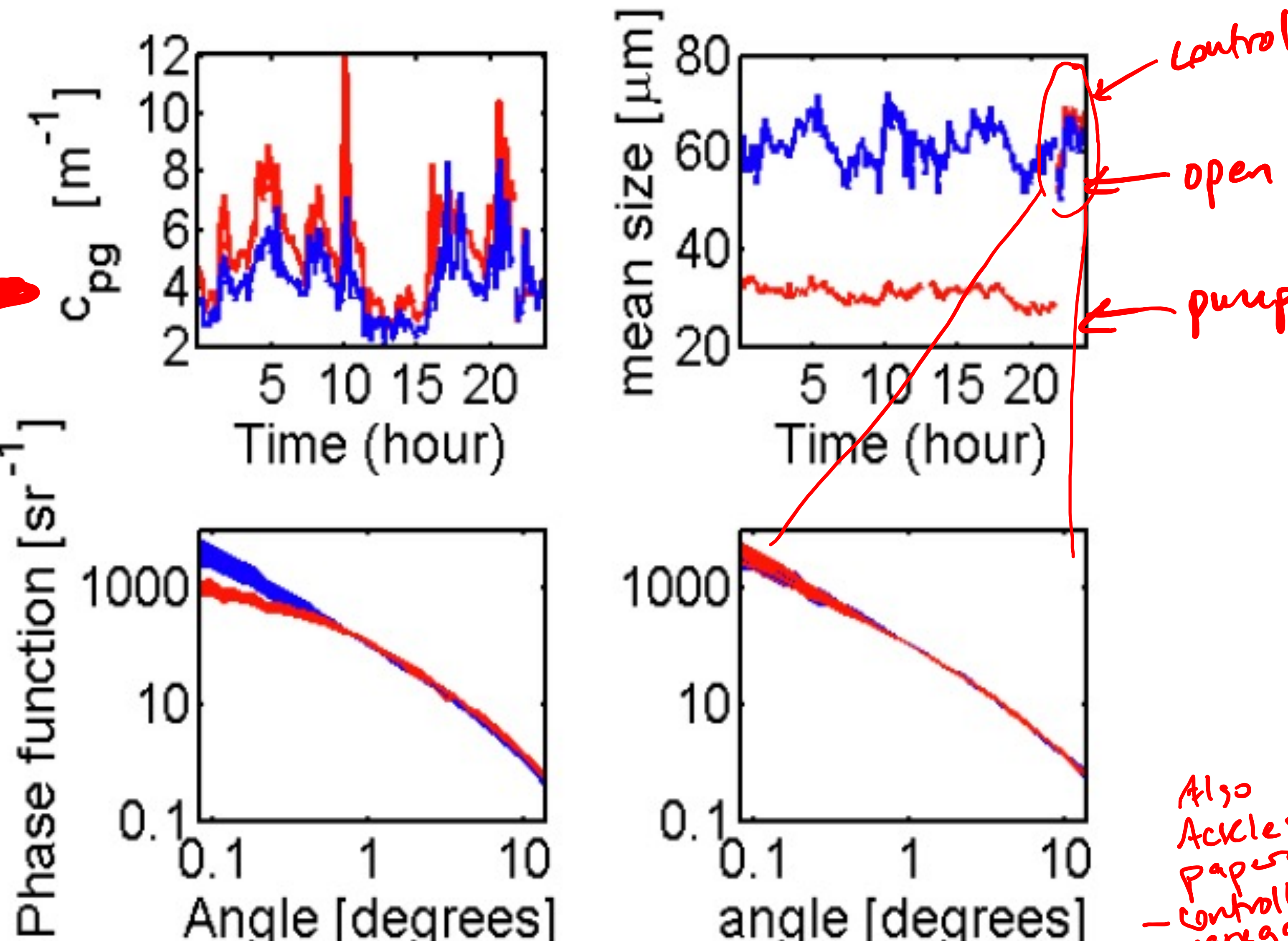
Aggregation approximately 'conserves' *area* not *volume*

Effect of aggregation on the mass-specific attenuation - lab experiment



Slade et al., 2011

How do we test that aggregation is important in-situ?



Also Ackleson papers
– controlled aggregate breakage

Boss et al., 2009, OE

Small effect on c_p large effect on β

Cetinić, Opt. Express, 2016 (pump effects)

→It is important that we consider aggregation when dealing with particle suspensions.

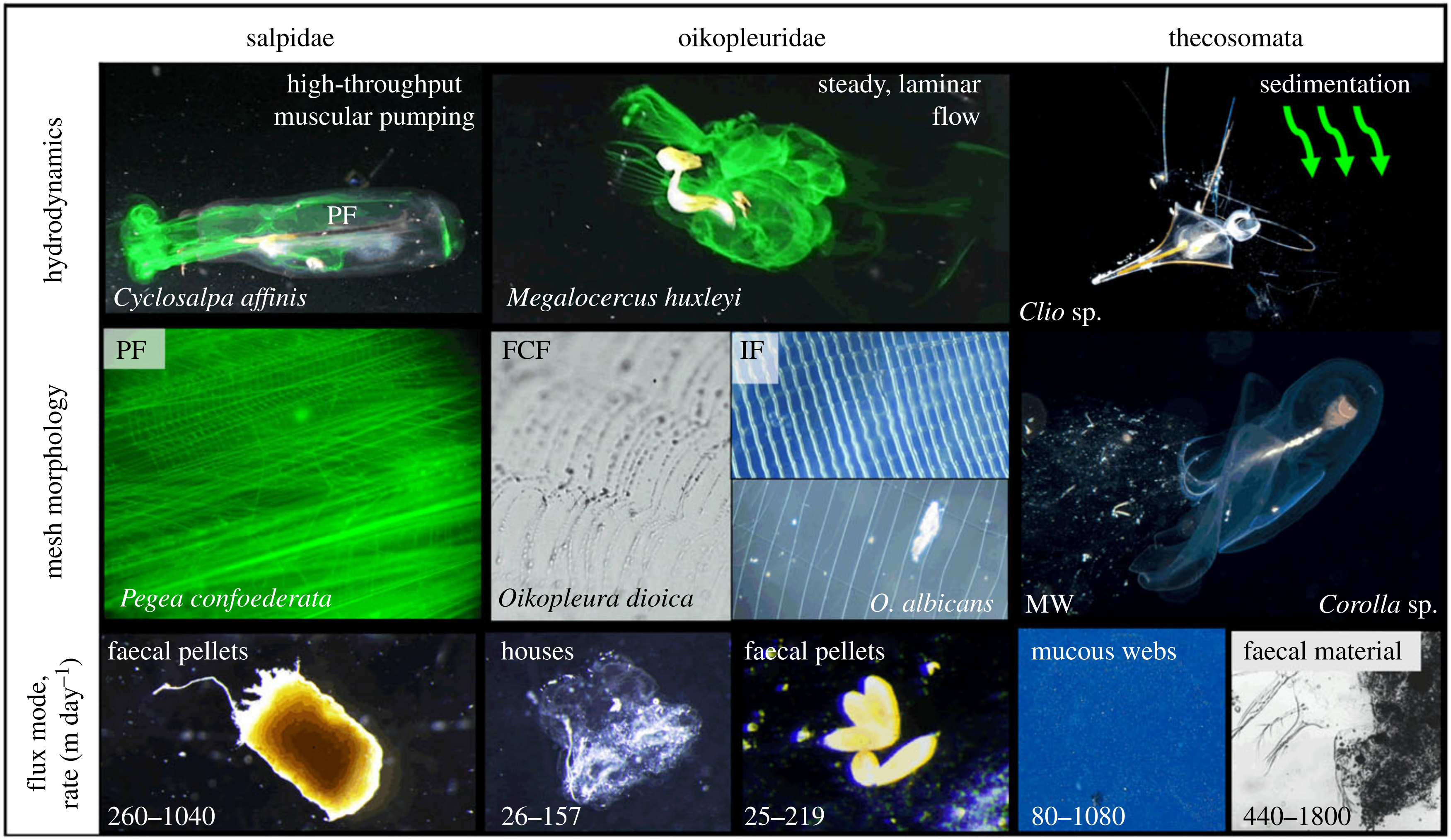
For aggregates we cannot simply assume:

$$OP \neq \int_{D_{\min}}^{D_{\max}} C_{OP,Mie}(D)N(D)dD$$

Such suspensions occur in open ocean as well as coastal areas

Aggregation is essential for *predicting* the under-water light field as settling velocity, $w_s \propto \Delta\rho \times D^2$ and w_s increases with *D*.

"Biological aggregation" processes...?



3
rspb.royalsocietypublishing.org *Proc. R. Soc. B* **285**: 20180056

Figure 2. Hydrodynamics, mesh morphologies, and flux of mucous-mesh grazers. PF: pharyngeal filter; FCF: food-concentrating filter; IF: inlet filter prior- (top) and post-inflation of the house (bottom); MW: mucous web. Photographs courtesy of: Linda Ianniello for *Clio* sp. and *Corolla* sp., S. Bush for Peraclidae mucous web, © 2008 MBARI, Ron Gilmer for *Cavolinia uncinata* faecal material [10]. Salpidae flux rates based on the faecal pellets of *Pegea confoederata* [24]; Oikopleuridae flux rates based on *Oikopleura dioica* faecal pellets [25] and houses [26]; Thecosomata flux rates based on the mucous webs of *Limacinia retroversa* [27] and faecal material of *Corolla spectabilis* [9]. (Online version in colour.)

Conley et al., 2018

Summary:

There is still a lot of work to do in ocean optics:

1. Account for diversity in shape.
2. Account for diversity in internal structure.
3. Account for diversity in packaging.

Both theoretical and observational (VSF, polarization) advances are needed.