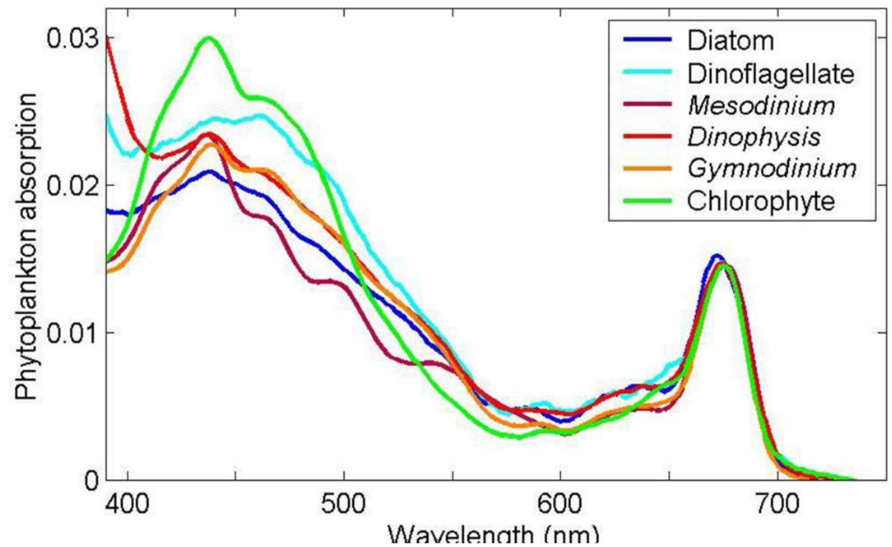
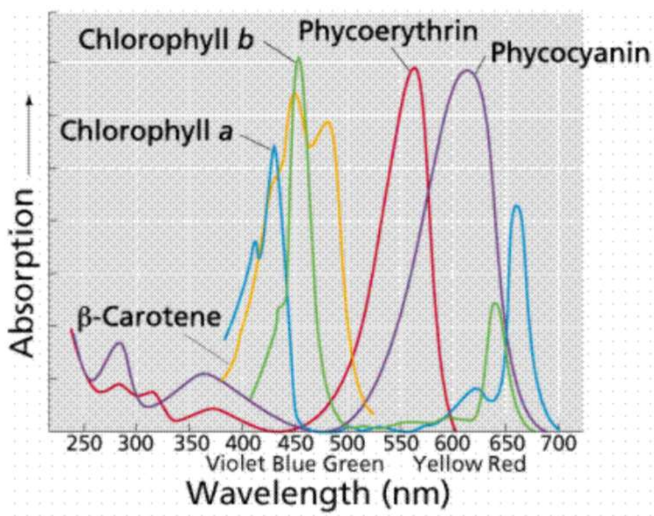
On your own go through these models

- Example 1: inversion to multiple phytoplankton absorption spectra (e.g., diatom, dino,… absorption eigenvectors)
- Example 2: inversion to pigments (e.g., fucoxanthin, peridinin,… absorption eigenvectors)
- Example 3: reformulate reflectance equation to retrieve other IOPs (e.g., beam c coefficient and spectral slope, backscattering ratio, spectral variations in backscattering spectrum)
- Example 4: linear matrix inversion allows for uncertainty quantification in the regression

Example 1: Phytoplankton come in all colors due to taxon-specific pigments that have distinct absorption spectra





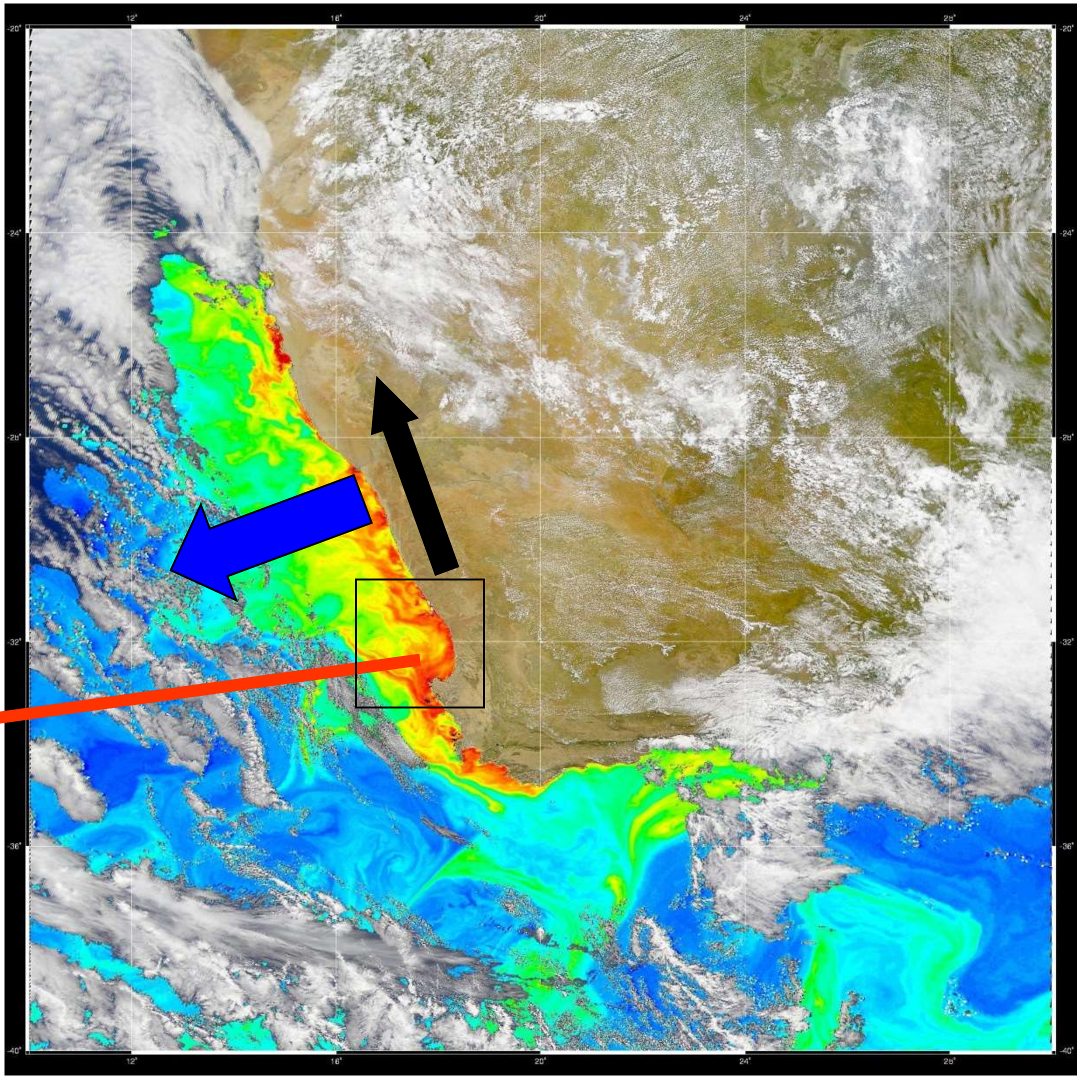
- Why limit inversion to single eigenvector?

Invert for Phytoplankton Functional Types
ex. Benguela Upwelling System

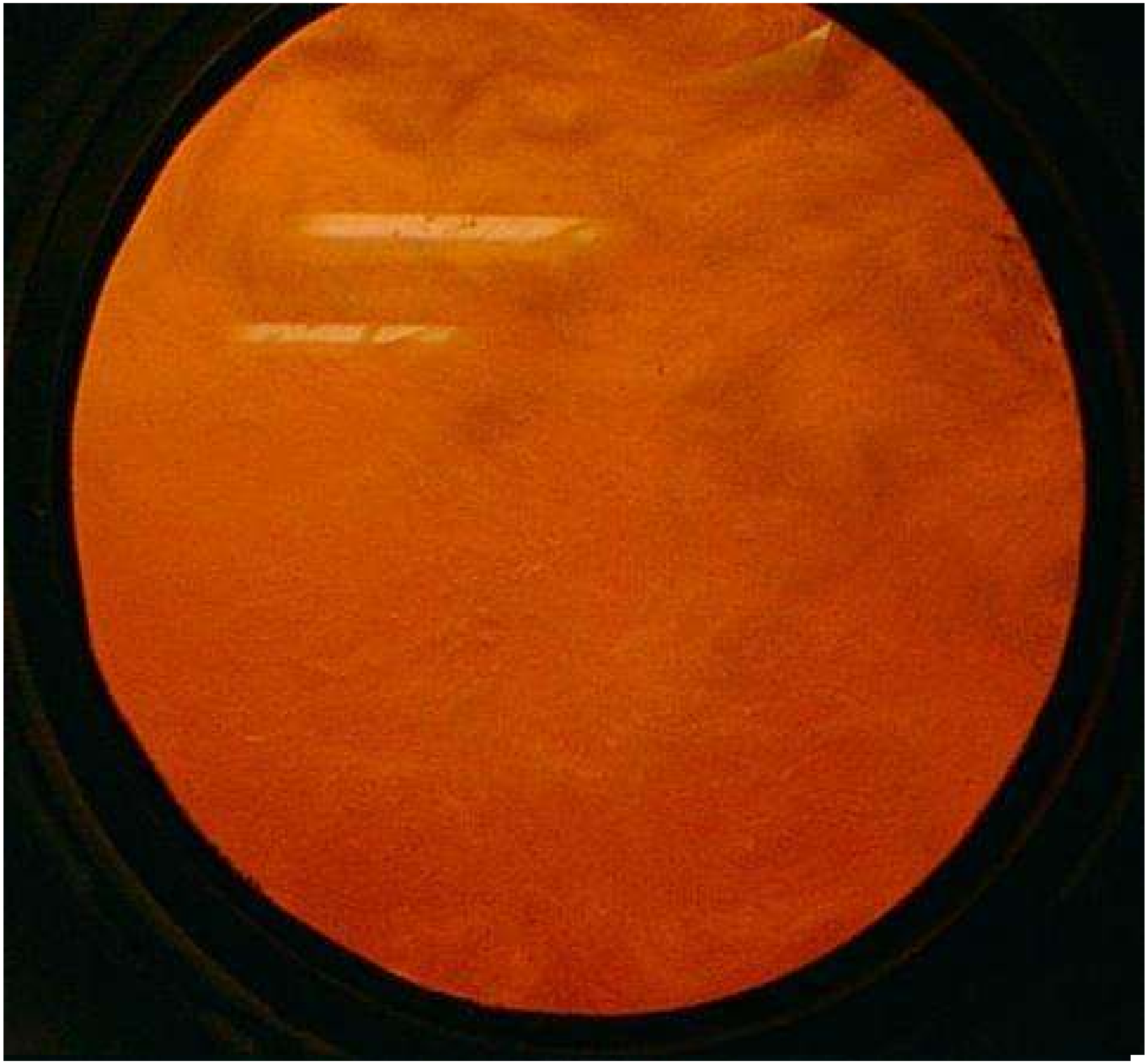
alongshore winds

offshore transport

upwelled deep nutrients
fuel expansive blooms
with variable species



The variations in water color are extreme



Day to day variations in water color

Our primary tool was a small radiometric buoy (HTSRB):

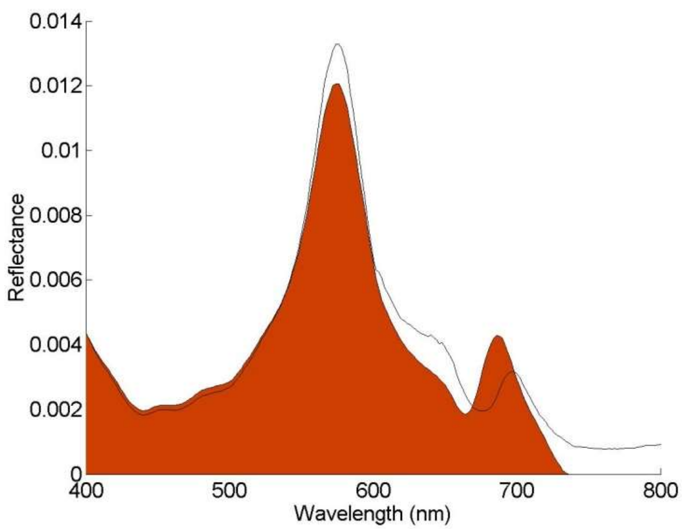
incident solar irradiance spectrum

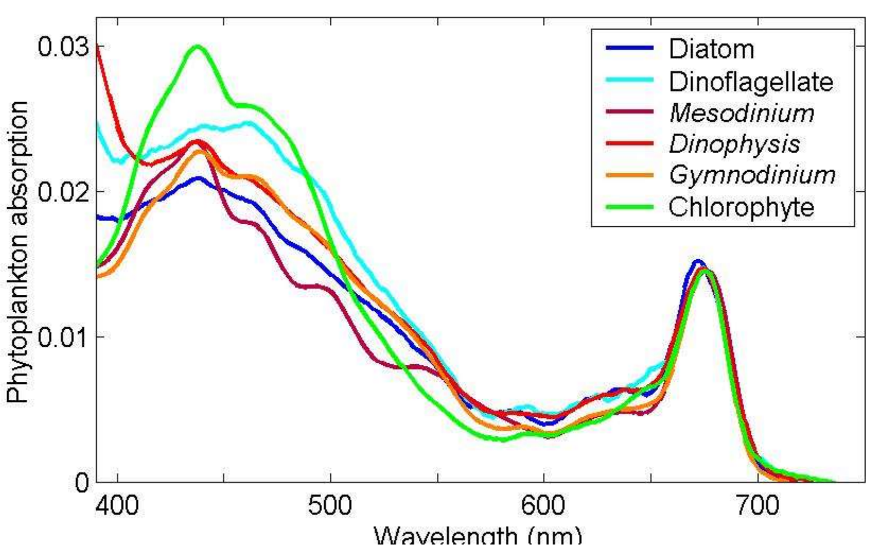
upwelled radiance spectrum

→ Lu(0-)/Ed(0+)

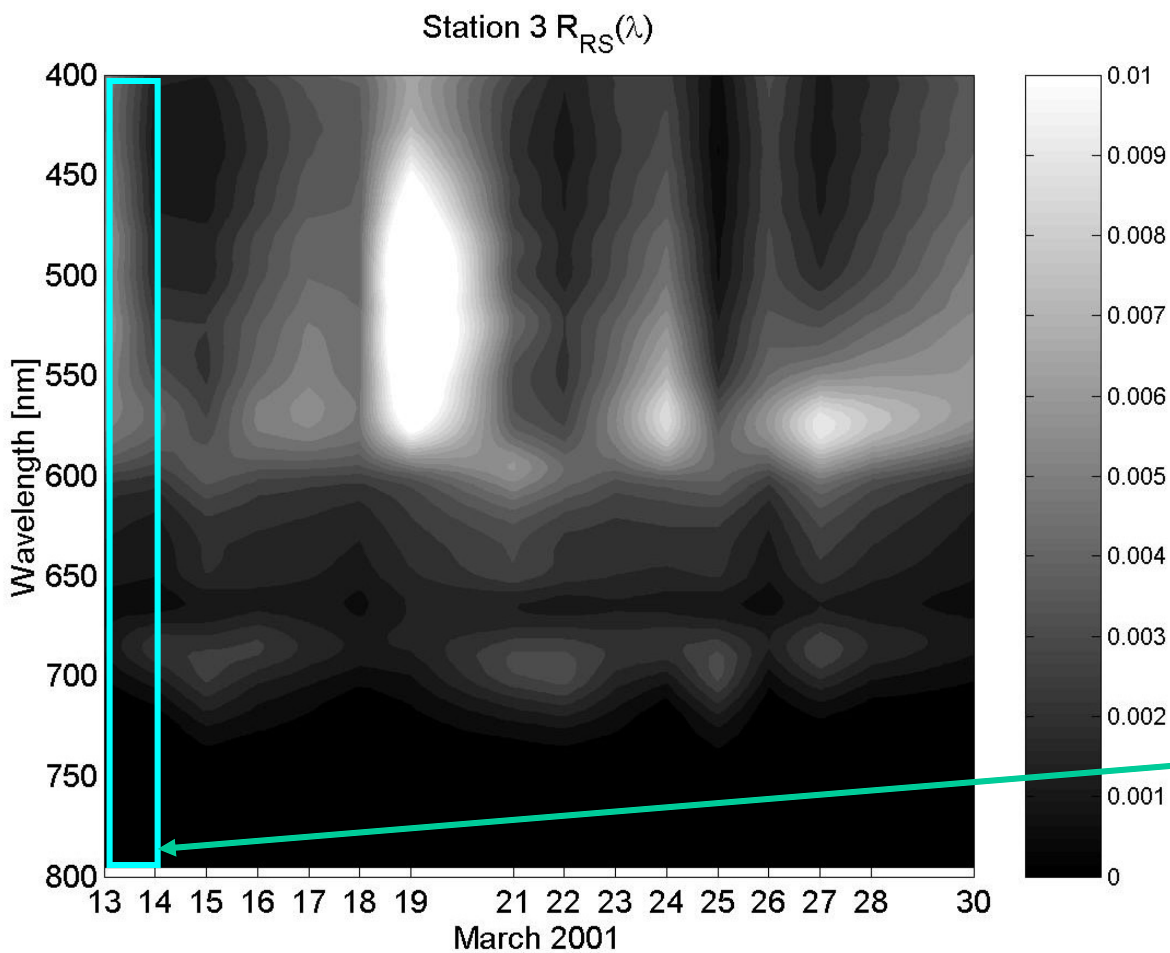
Inversion Modeling for Phytoplankton Functional Types: South African Red Tide (Roesler et al 2004)

- Time series measured daily reflectance spectra (ex below left)
- Multiple phytoplankton eigenvectors, PFTs, (below right, lab)
- Inversion to estimate PFT contributions
- Compare with PFT determined microscopically



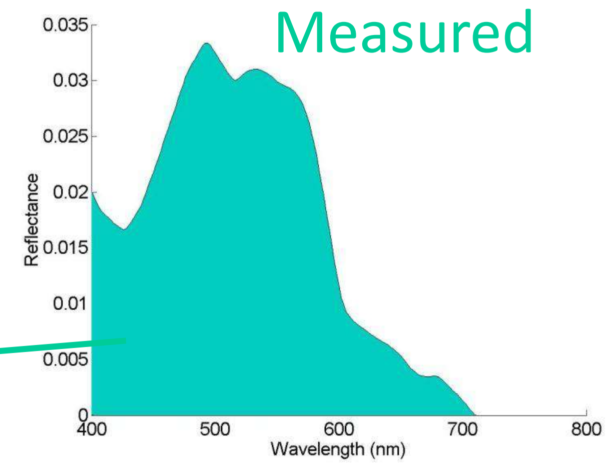


Examples from South African Time Series

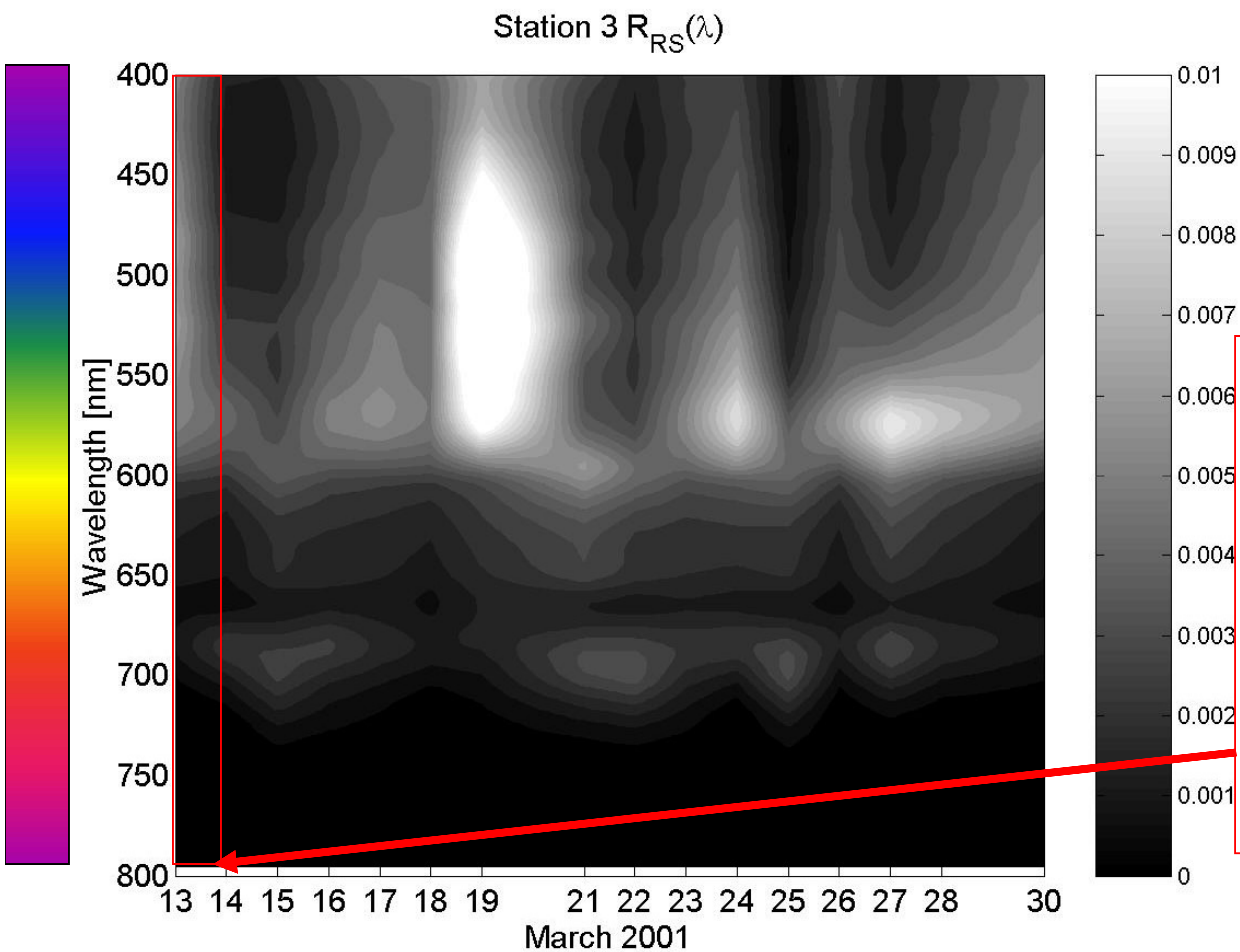


Wavelength (Y)
Time (X)
Brightness (Z)
(Fluorescence)

Modeled
Measured

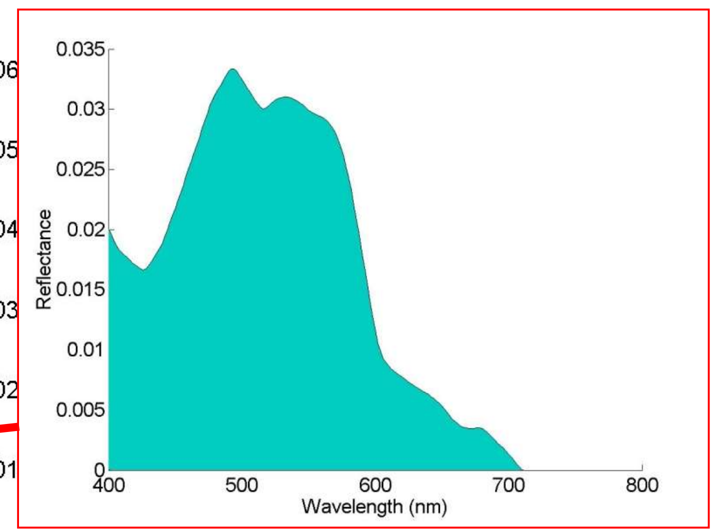


Examples from South African Time Series



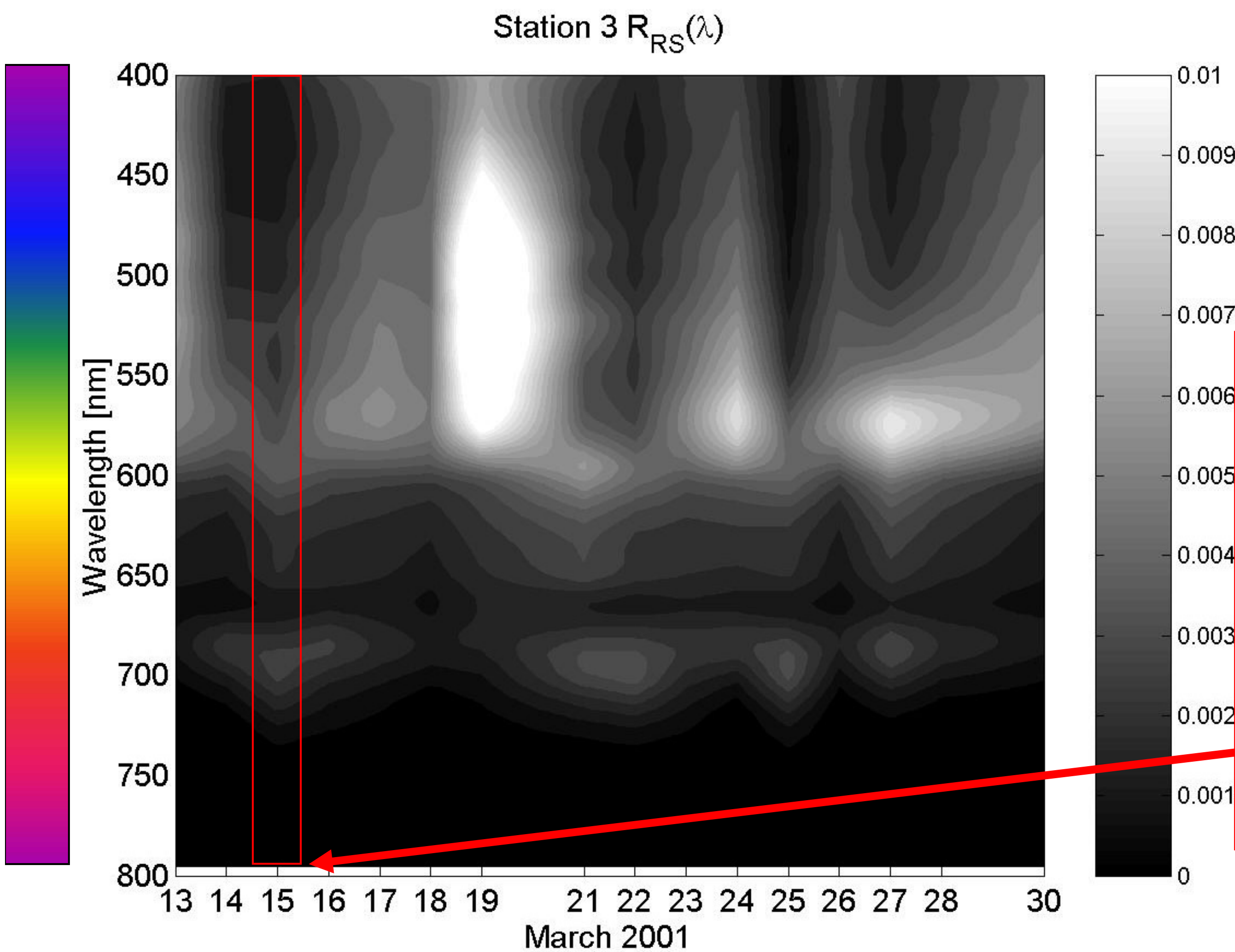
Measured

Modeled (line)



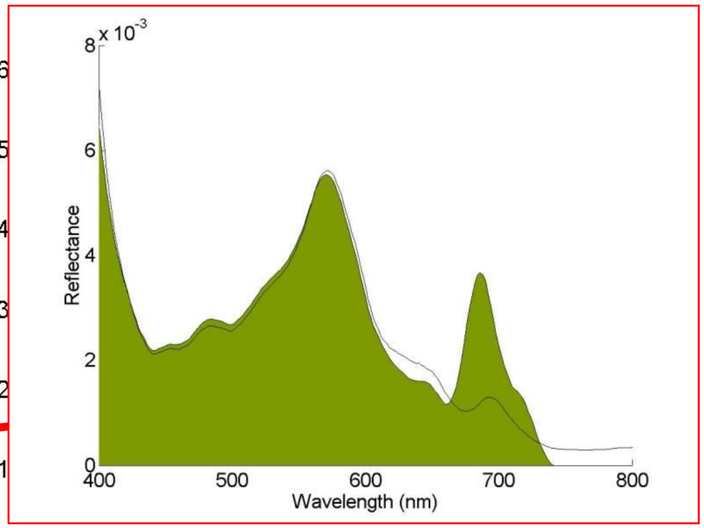
“Pre-bloom” condition

Examples from South African Time Series



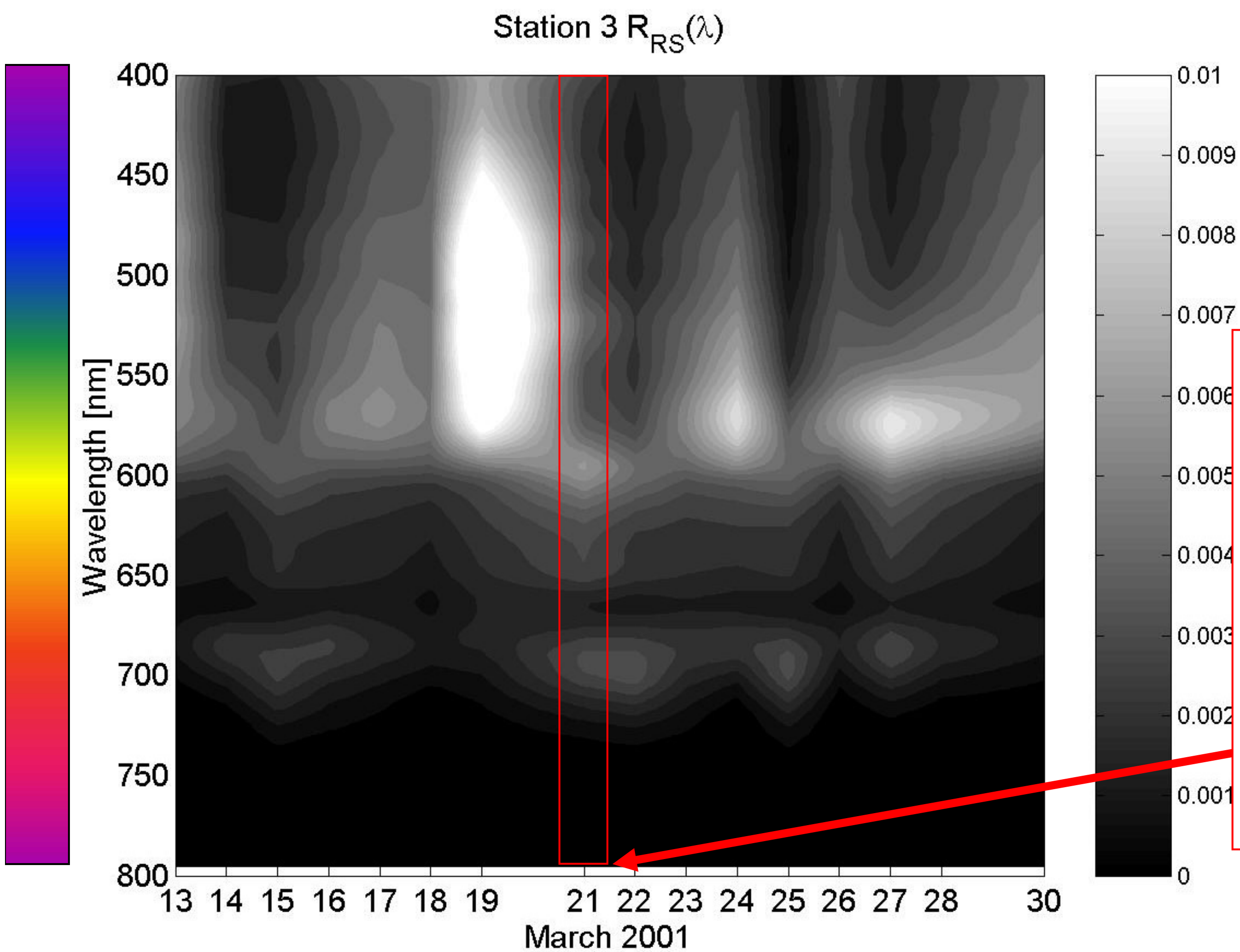
Measured

Modeled (line)

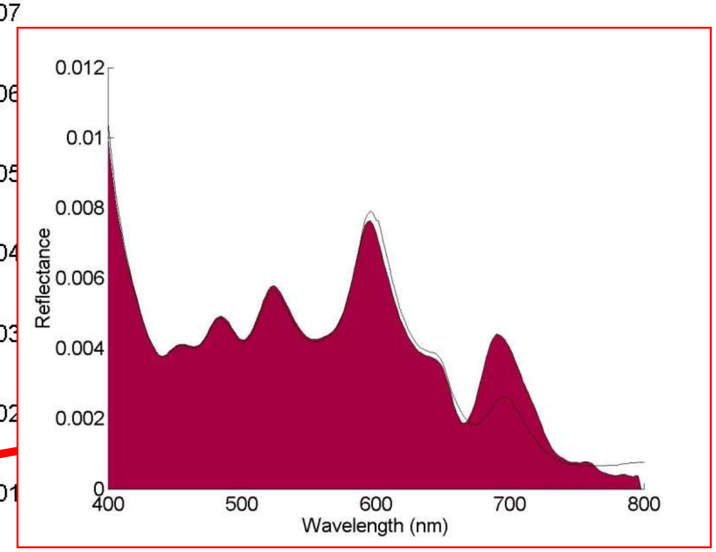


Diatom bloom

Examples from South African Time Series



Measured
Modeled (line)

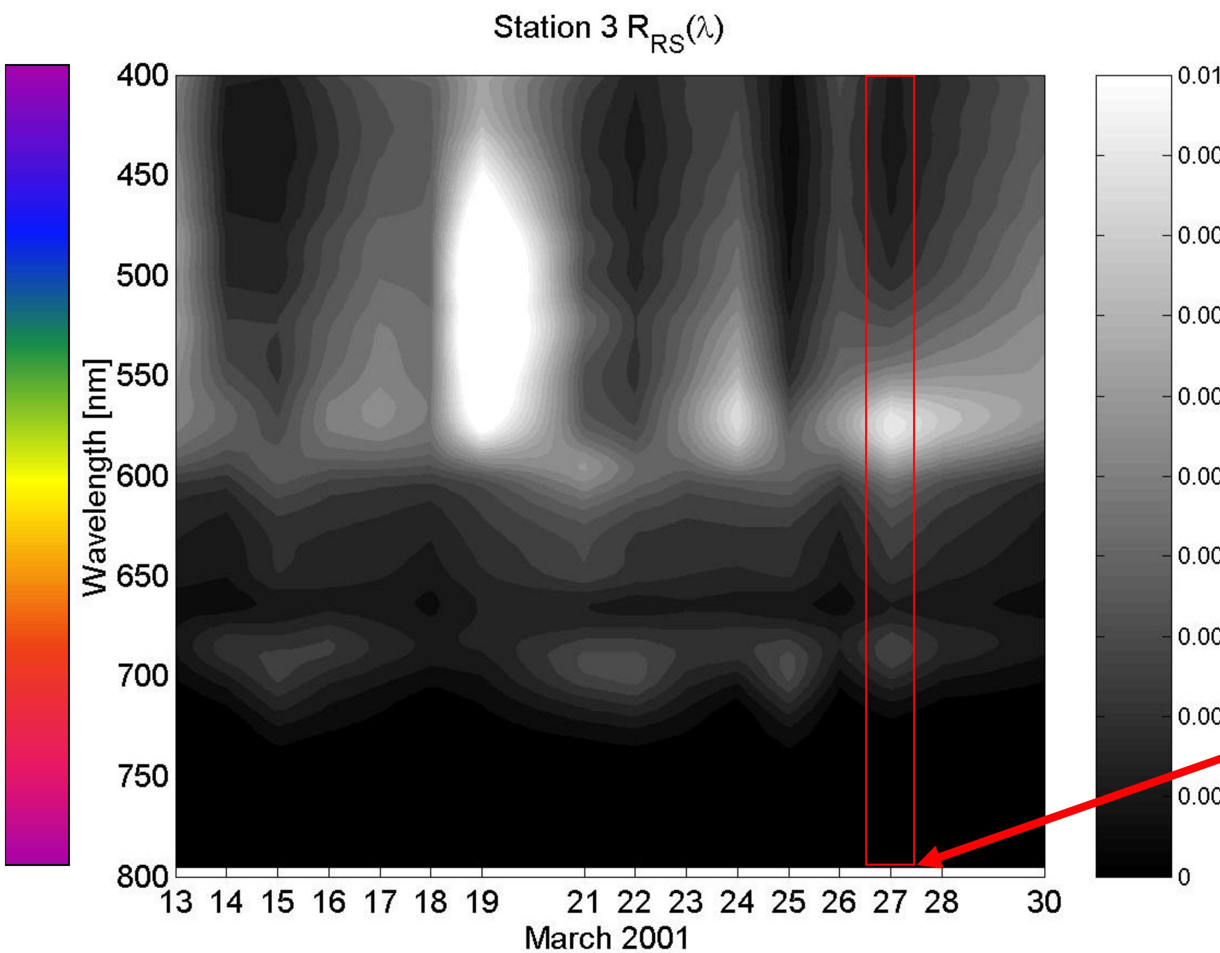


Mesodinium bloom

Examples from South African Time Series

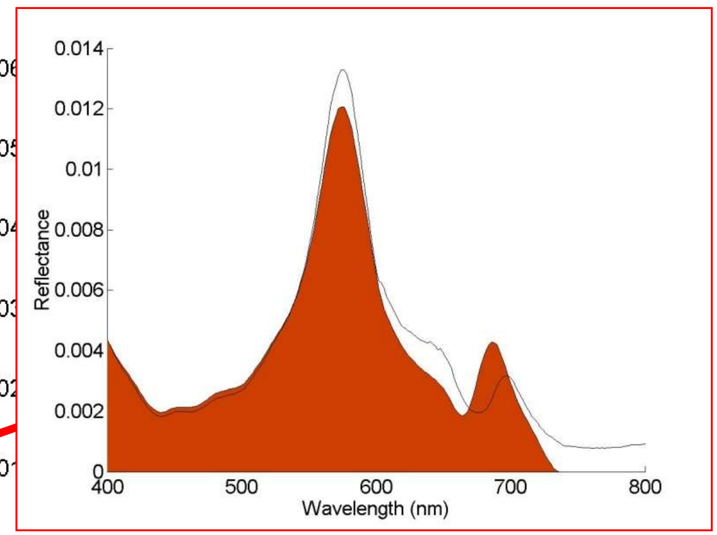
the differences in ocean color are due to differences in pigmentation,

so we can retrieve species information



Measured

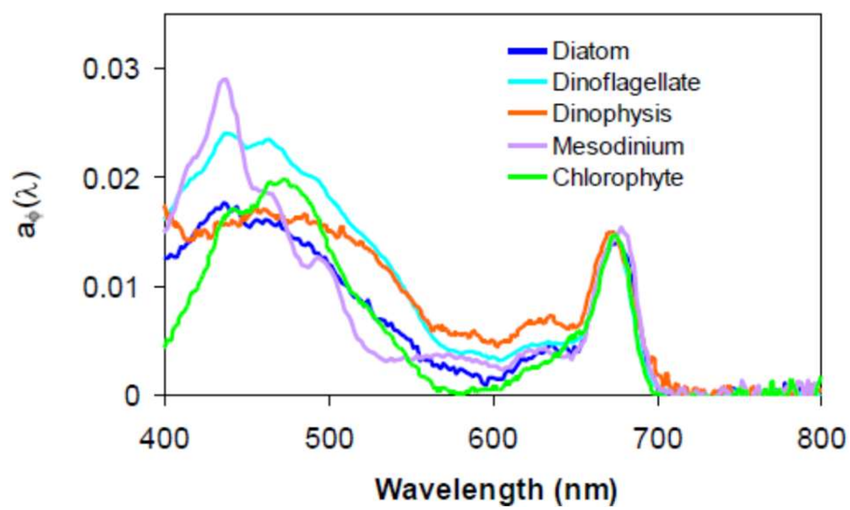
Modeled (line)

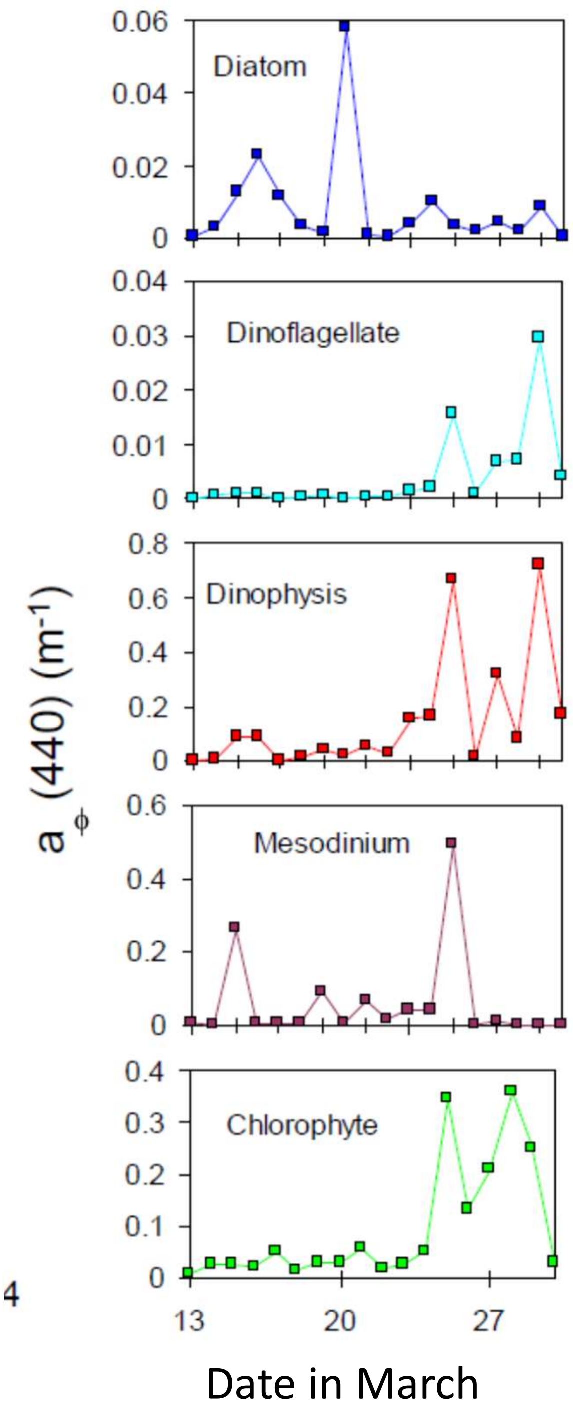


Dinophysis bloom

Inversion Modeling for Phytoplankton Functional Types: South African Red Tide (Roesler et al 2004)

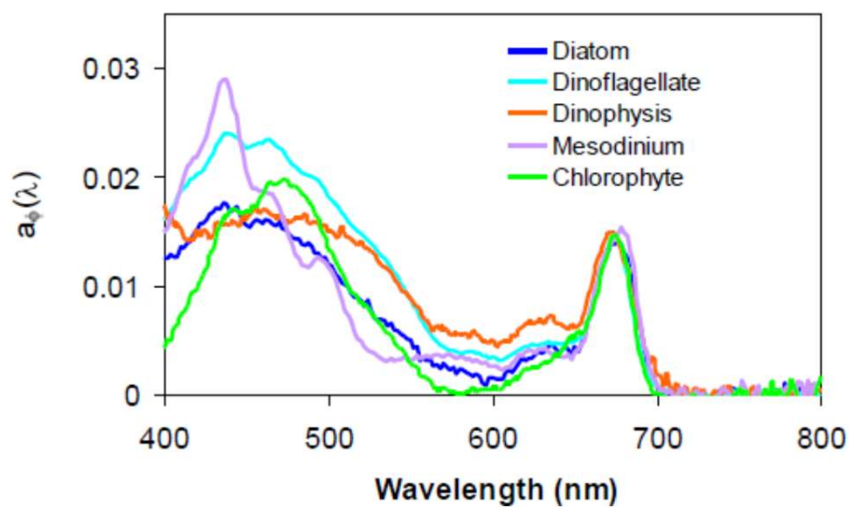
- Validation
  - Daily microscopic cell counts (Grant Pitcher)
  - Converted cell counts to absorption coefficients for each species using mean cell size and intracellular pigment concentrations (Bricaud and Morel approach), measured a_{ph}

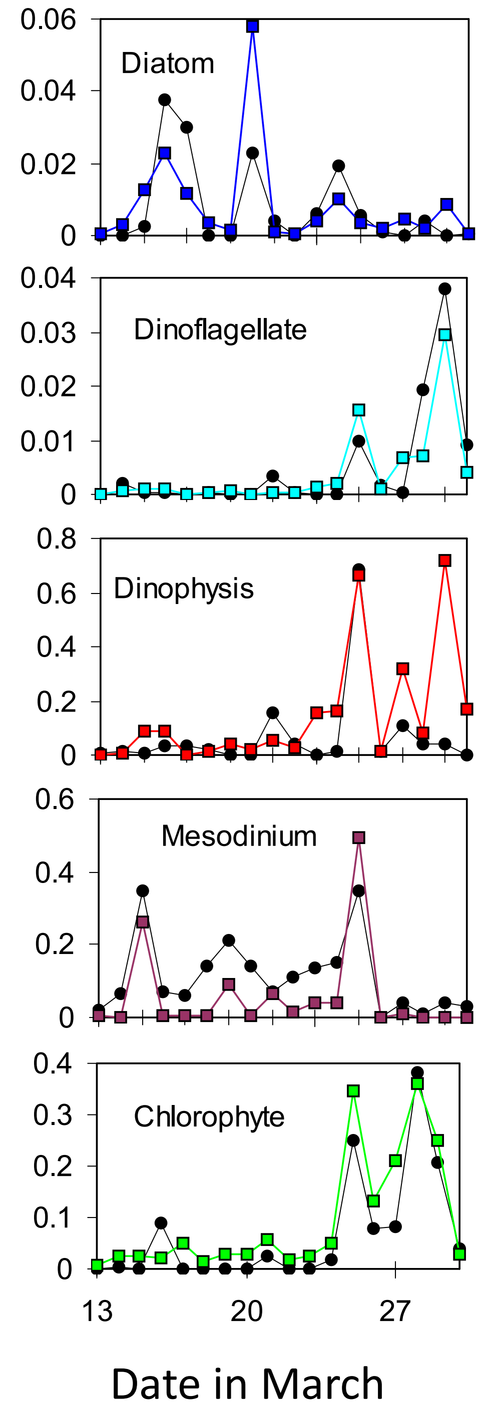




Inversion Modeling for Phytoplankton Functional Types: South African Red Tide (Roesler et al 2004)

- 5-phytoplankton eigenvectors, PFTs
- estimate time series of PFT contributions (black symbols) by inversion
- compare with time series of microscopic estimates (colored symbols)
- model resolved accurate proportions of each species/group even over large range of PFTs





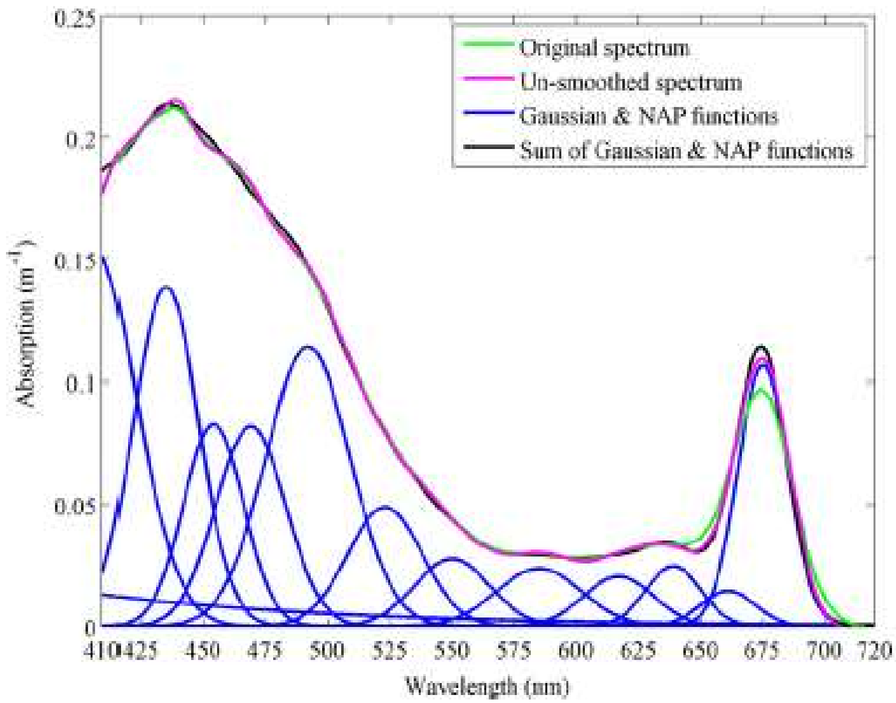
Example 2: Hyperspectral Inversion to pigments

- is an overconstrained problem (many more measured wavelengths than unknown eigenvalues)
- allows resolution of spectral gradients in $R(\lambda)$, hence spectral gradients in $a(\lambda)$
- This spectral resolution is what makes this approach sensitive to variations in pigment-based phytoplankton taxonomy
- By using pigment-based taxonomic eigenvectors, PFTs can be estimated
- But the PFT absorption spectra must be distinct and sufficiently large to impact the R spectrum

Hyperspectral Inversion of PFTs
Chase et al. 2013 and 2017

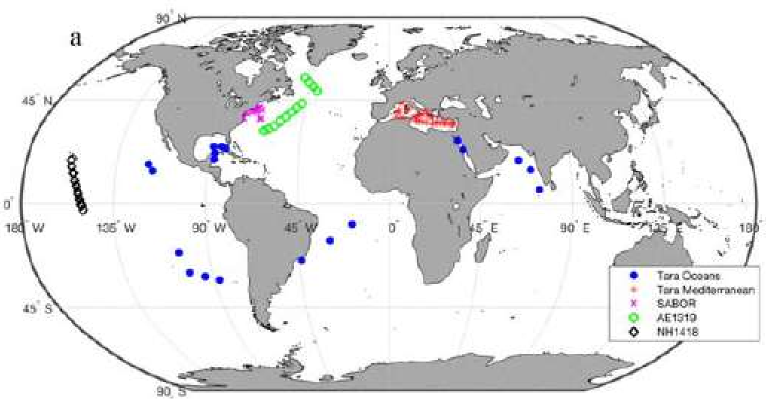
- Decompose particulate absorption into contributions by
  - Each pigment modeled analytically by one or more Gaussian curves
  - NAP exponential

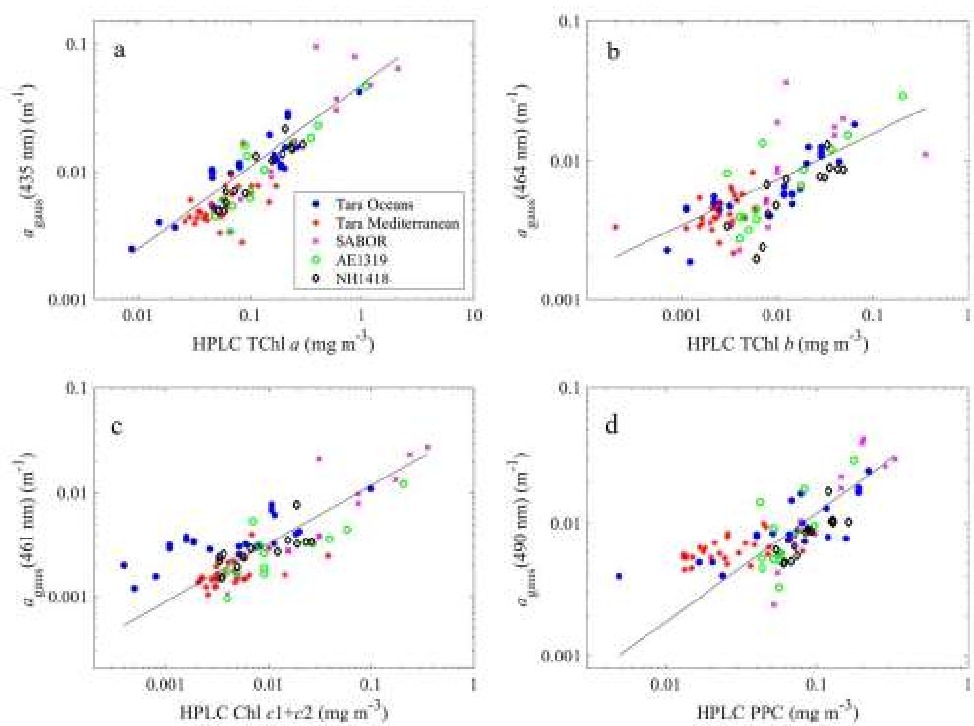
A. Chase et al. / Methods in Oceanography 7 (2013) 110–124



Hyperspectral Inversion of PFTs
Chase et al. 2013 and 2017

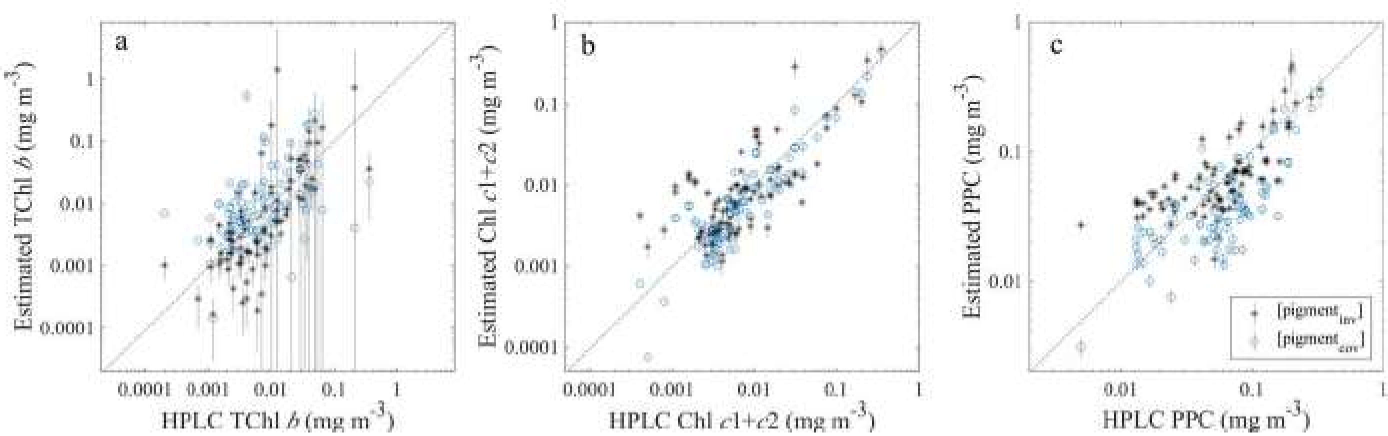
- Use Gaussians as basis vectors for the inversion
  - How well does the inversion estimate of the absorption Gaussian relate to associated HPLC pigment?
  - 8 Gaussians used
  - 4 showed significance





Hyperspectral Inversion of PFTs Chase et al. 2013 and 2017

- Use Gaussians as basis vectors for the inversion
  - Is the inversion result more robust than simply using covariability between Tchla and other pigments?
  - Similar errors → but one is empirical (chl cov) one allows for independence (chl-indep pigments)



Questions?

- Why is the water red during a red water HAB event?
- Now we will reformulate the reflectance equation to exploit the b_b eigenvector to obtain information on $c(\lambda)$, $b_b(\lambda)$, b_b/b

Example 3: Reformulate the reflectance equation to retrieve more information

- Magnitude and slope of beam c
- Backscattering spectrum
- Backscattering ratio

GEOPHYSICAL RESEARCH LETTERS, VOL. 30, NO. 9, 1468, doi:10.1029/2002GL016185, 2003

Spectral beam attenuation coefficient retrieved from ocean color inversion

Collin S. Roesler
Bigelow Laboratory for Ocean Sciences, West Boothbay Harbor, Maine, USA

Emmanuel Boss
School of Marine Sciences, University of Maine, Orono, Maine, USA

Roesler and Boss 2003 GRL:

Semianalytic inversion to retrieve beam attenuation

$$R(\lambda) = \frac{f}{Q} \frac{b_{bw} + b_{bp}}{a_w + a_{phyt} + a_{CDOM} + a_{nap} + b_{bw} + b_{bp}}$$

let $b_{bp} = \tilde{b}_{bp}\, b_p$

where $\tilde{b}_{bp}$ is the particle backscattering ratio

so $b_{bp}(\lambda) = \tilde{b}_{bp}\, b_p(\lambda)$

therefore $b_{bp}(\lambda) = \tilde{b}_{bp} \left(c_p(\lambda) - a_p(\lambda) \right)$

What do we know about the particle backscattering ratio?

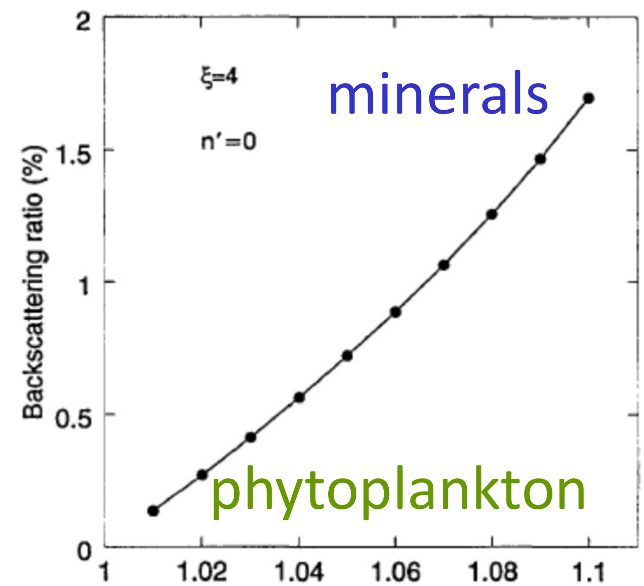
Effect of the particle-size distribution on the backscattering ratio in seawater

7070 APPLIED OPTICS / Vol. 33, No. 30 / 20 October 1994

Osvaldo Ulloa, Shubha Sathyendranath, and Trevor Platt

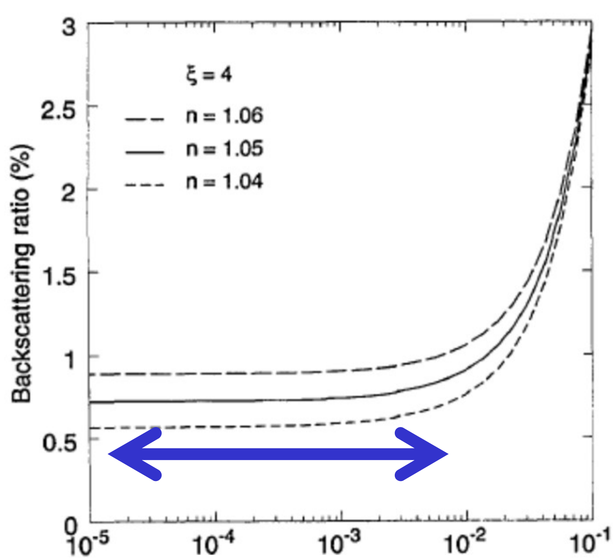
Varies with real
Index of refraction

$\tilde{b}_{b_p}$



n index of refraction

$\tilde{b}_{b_p}$



n’ imaginary index of refraction (absorption)

Independent of imaginary
Index of refraction
→ independent of absorption
so not strongly spectral

$$b_{bp}(\lambda) = \tilde{b}_{bp}\left(c_p(\lambda) - a_p(\lambda)\right)$$

we know $a_p(\lambda) = a_{phyt}(\lambda) + a_{nap}(\lambda)$

and $c_p(\lambda)$ is a smoothly varying function

$$c_p(\lambda) = c_p(\lambda_{ref})\left(\frac{\lambda}{\lambda_{ref}}\right)^{\gamma}$$

so

$$b_{bp}(\lambda) = \tilde{b}_{bp}\left(c_p(\lambda_{ref})\left(\frac{\lambda}{\lambda_{ref}}\right)^{\gamma} - a_{phyt}(\lambda) - a_{nap}(\lambda)\right)$$

Regression Model

$$R(\lambda) = \frac{f}{Q}\frac{b_b}{a + b_b}$$

Where

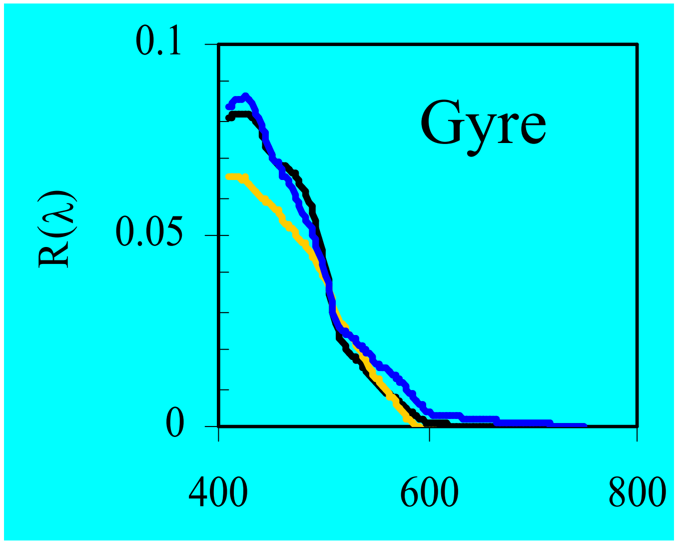
$$\frac{f}{Q} = A_{\frac{f}{Q}}$$

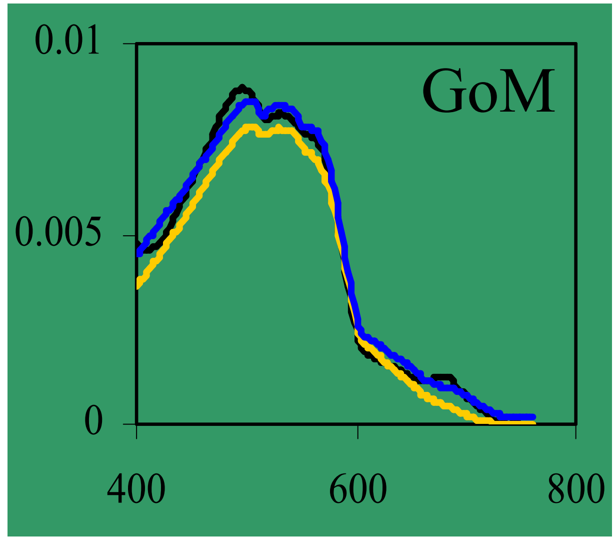
$$b_b(\lambda) = b_{bw}(\lambda) + A\tilde{b}_{bp}\left(Ac_p(\lambda_{ref})\left(\frac{\lambda}{\lambda_{ref}}\right)^{A\gamma} - A_{phyt}\hat{a}_{phyt}(\lambda) - A_{nap}\hat{a}_{nap}(\lambda)\right)$$

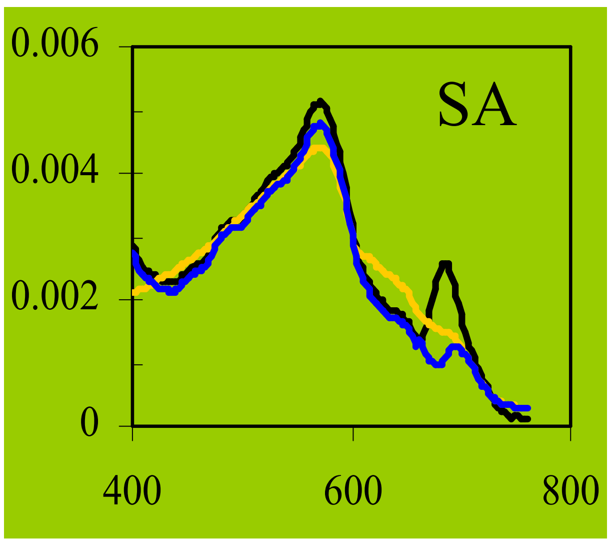
$$a(\lambda) = a_w(\lambda) + A_{phyt}\hat{a}_{phyt}(\lambda) + A_{nap}\hat{a}_{nap}(\lambda) + A_{CDOM}\hat{a}_{CDOM}(\lambda)$$

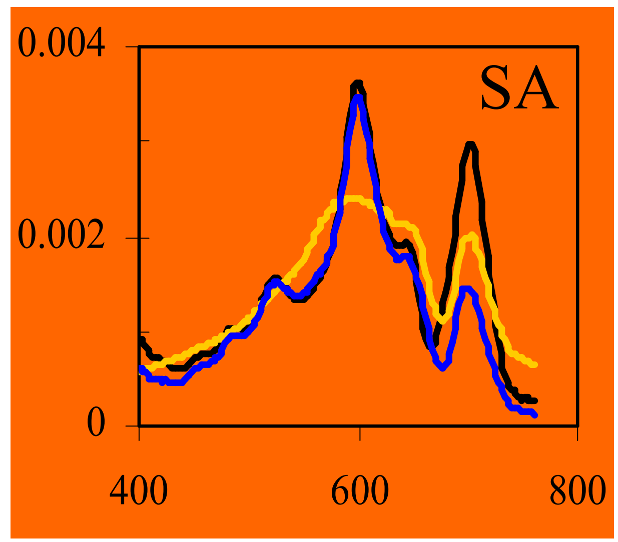
7 unknowns, 3 absorption eigenvectors

Results: Model fit to reflectance





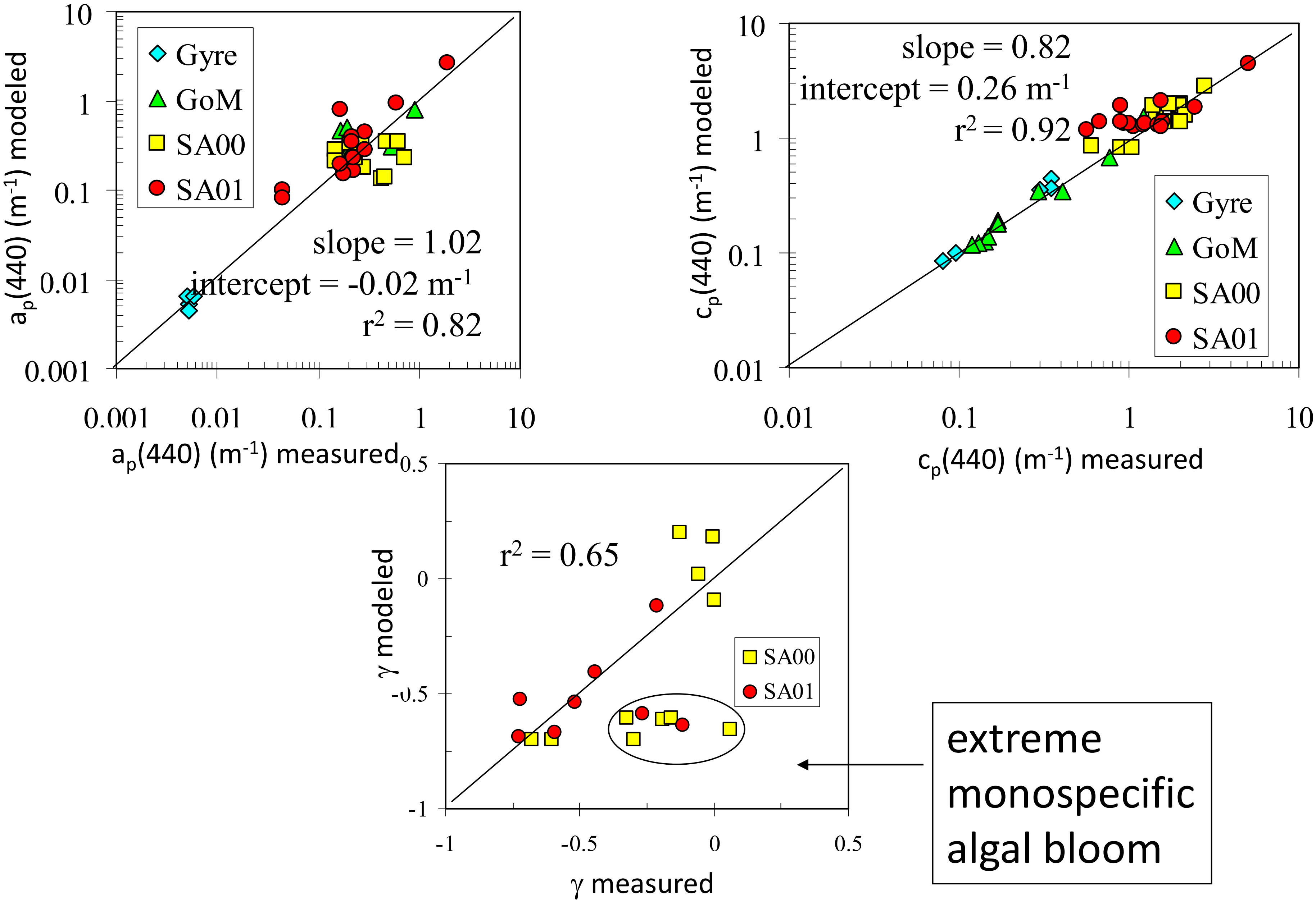




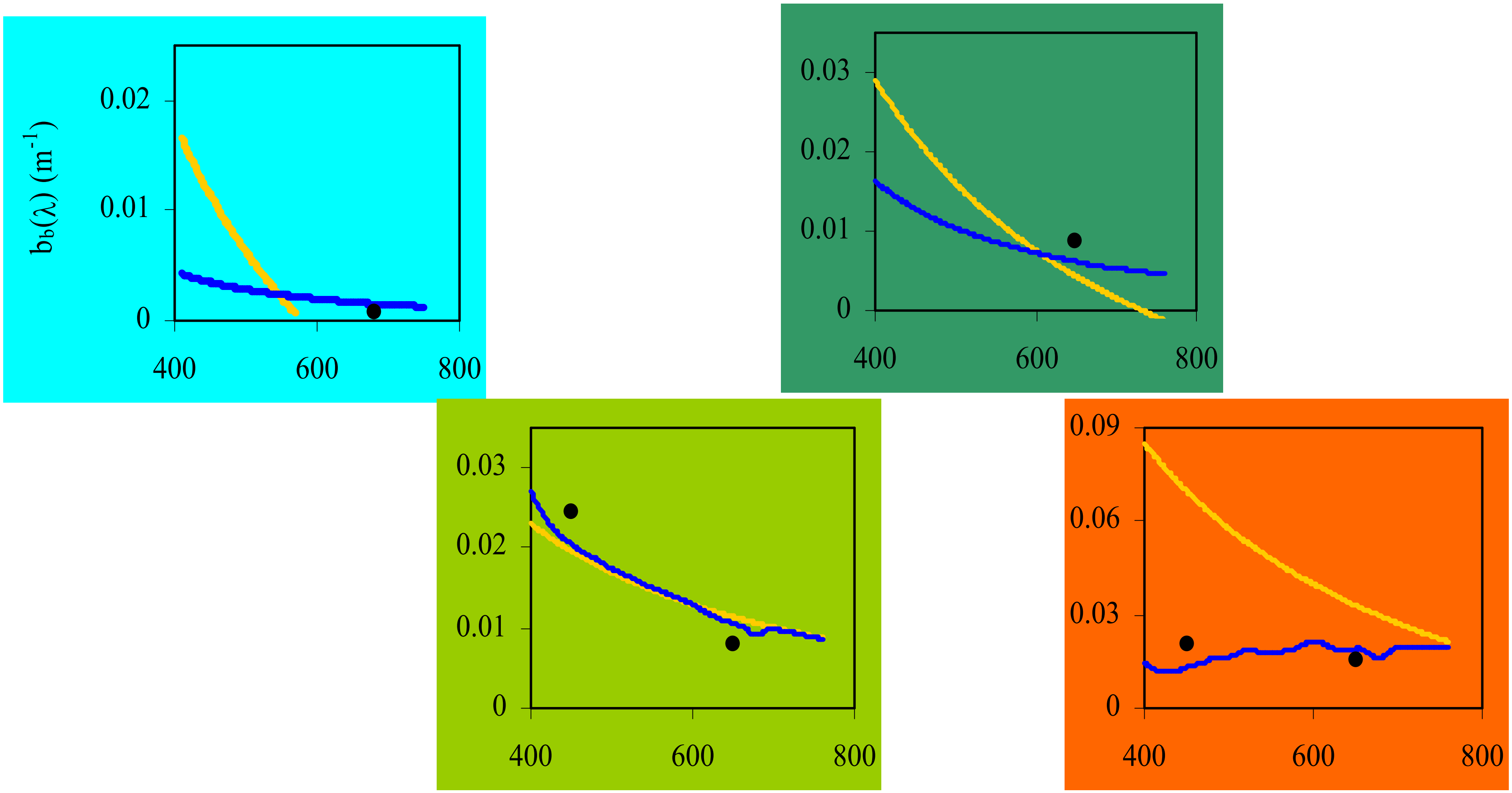
Standard Model Fit

Better fit with c-model

Results: **Validate** with measured IOPs



Results: **Validate** with measured IOPs



c-model realistic spectrum, spectral features under high absorption conditions as predicted by Mie theory.

So spectral backscattering and beam c **seem to be** retrievable from R

- More sensitive to starting values (use OC chl to estimate order of magnitude)
- Better to assume smooth power function for c than b_b
- Separates CDOM from NAP due to differential impact on backscattering
- Useful for carbon models (DOC vs POC)

Questions?

- Which quantity would you most want to retrieve from space: c, $c(\lambda)$, $b_b(\lambda)$, b_b/b?
- Now I will show an example of Linear Matrix Inversion (approach of Hoge and Lyon 1996) which allows for uncertainty estimates in the retrievals

Example 4: Linear matrix inversion

- This is linear??

$$R(\lambda) = \frac{f}{Q} \frac{b_{bw} + b_{bp}}{a_w + a_{phyt} + a_{CDOM} + a_{nap} + b_{bw} + b_{bp}}$$

$$a_w + a_{phyt} + a_{CDOM} + a_{nap} + b_{bw} + b_{bp} = \frac{f}{QR(\lambda)}(b_{bw} + b_{bp})$$

$$a_{phyt} + a_{CDOM} + a_{nap} + \left(1 - \frac{f}{QR(\lambda)}\right)b_{bp} = \frac{f\, b_{bw}}{QR(\lambda)} - (a_w + b_{bw})$$

$$A_{phyt} a_{phyt} + A_{CDOM} a_{CDOM} + A_{nap} a_{nap} + A_{bbp} b_{bp} = \left(\frac{f}{QR(\lambda)} - 1\right) b_{bw} - a_w$$

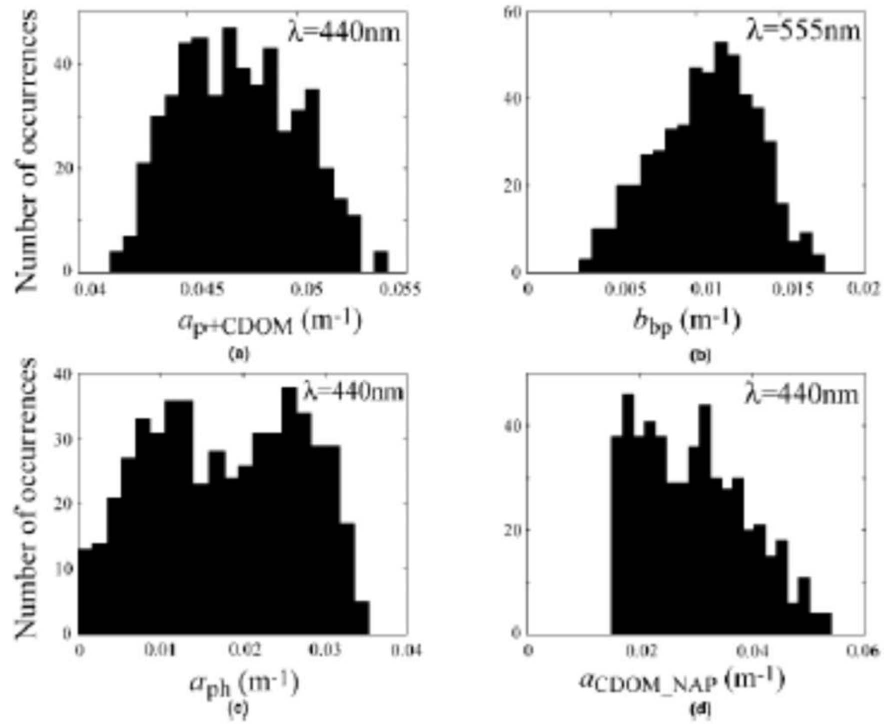
(unknowns) (knowns)

Because it is linear

- Regression yields exact solution
- Fast (good for image processing)
- Allows for computation of uncertainties in retrieved IOPs (when system is overconstrained)
- based upon our uncertainties in
  - Measured Rrs
  - Spectral shapes of basis vectors

Linear Matrix Inversion

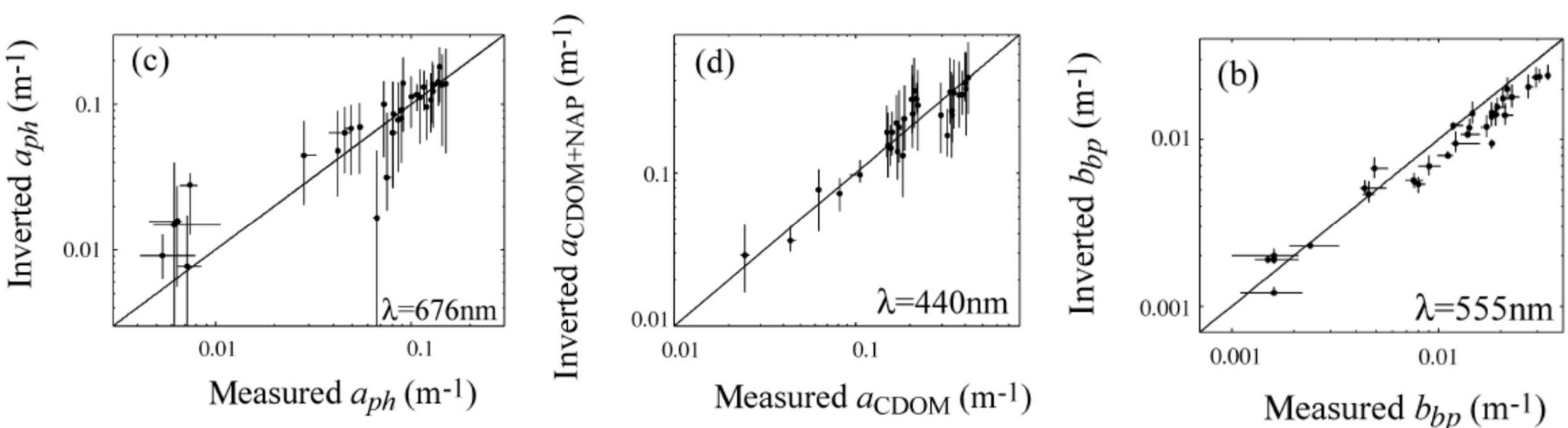
- For each eigenvector (component IOPs), define **range** in spectral shapes
- For each measured R(λ)
  - Perform LMI for every possible combination of eigenvectors (think nested loops in code)
  - Allow statistics to determine most likely estimate and uncertainties (note ranges are small!)

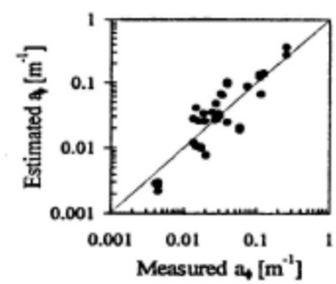


Wang, Boss, Roesler 2005

Determining uncertainties
Linear Matrix Inversion

- Each R spectrum inverted hundreds (thousands) of times
- Average estimate of each eigenvalue comes with uncertainties (errorbars)
- Non-linear inversion yields single eigenvalue for each R





Wang et al 2005

Questions?

- Why do we care about uncertainties in our retrieved eigenvalues?