Development of Robust Spectral Derivative Algorithms for Phytoplankton Pigment Concentrations on Local to Global Scales

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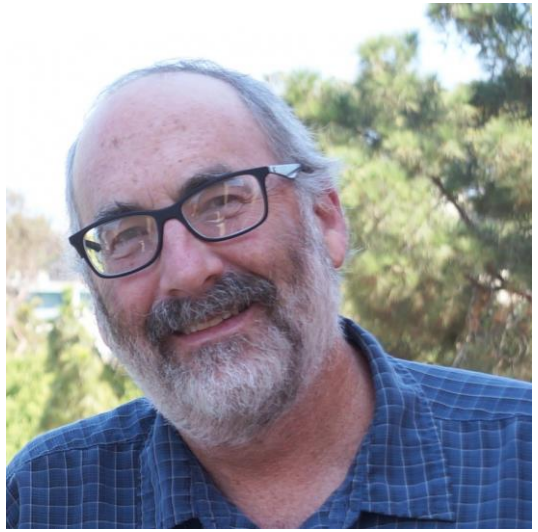
Team:



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PI – Project Lead
Modeling

Stéphane Maritorena
Co-PI – Inverse modeling
of hyperspectral $R_{rs}(\lambda)$

Dr. Dylan Catlett
Coastal PFTs
& genomics

Sasha Kramer
Global PFTs

Goal:

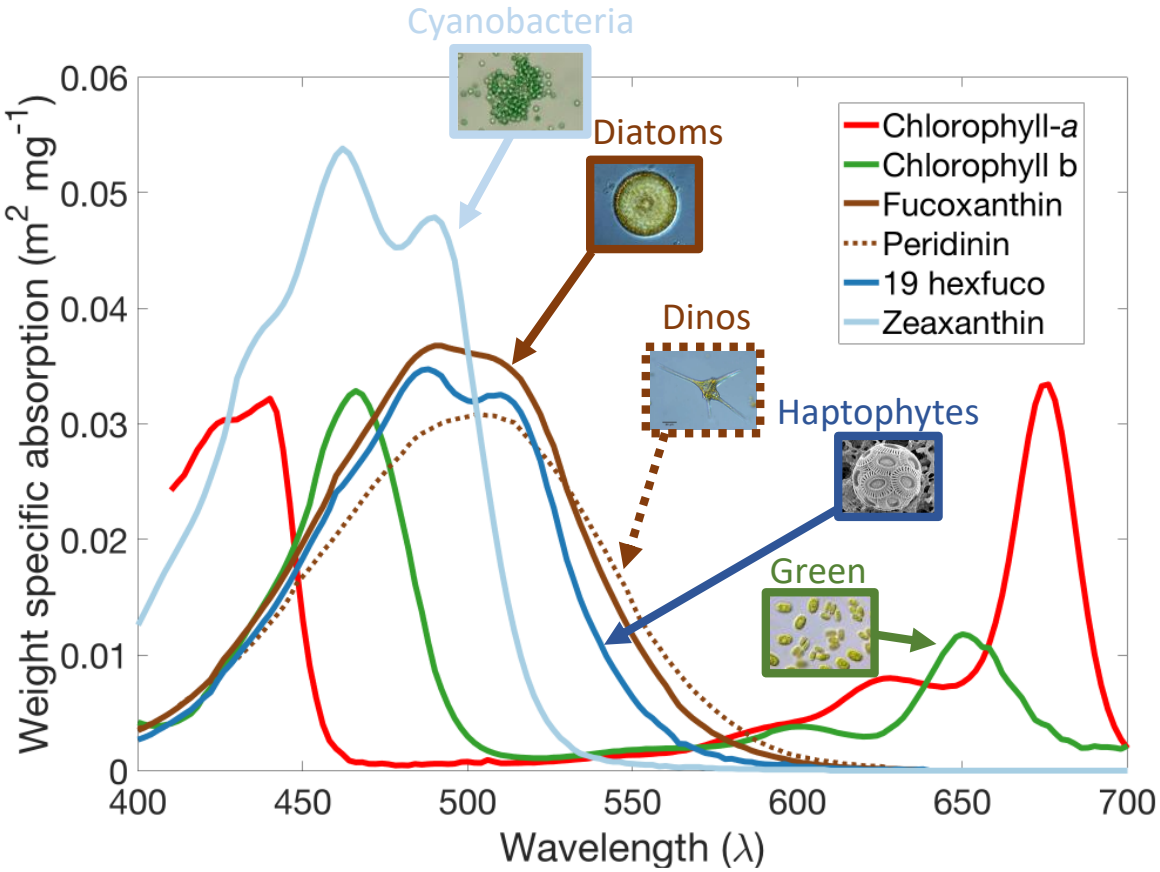
- Develop robust spectral methods for quantifying chemo-taxonomic marker phytoplankton pigments for PACE

Approach:

- Take advantage of the “spectral gap” between phytoplankton IOPs (≤ 100 nm) & the other IOPs (>> 100nm)
- Apply statistical methods that account for covariability among pigments and their spectral signatures
- Focus on retrieving chemotaxonomic marker pigments on both local (Santa Barbara Channel, CA) and global scales
- Assess the degree to which pigment biomarkers represent phytoplankton community structure by comparing pigment & genomic meta-barcoding assessments

The “Spectral Gap” Hypothesis

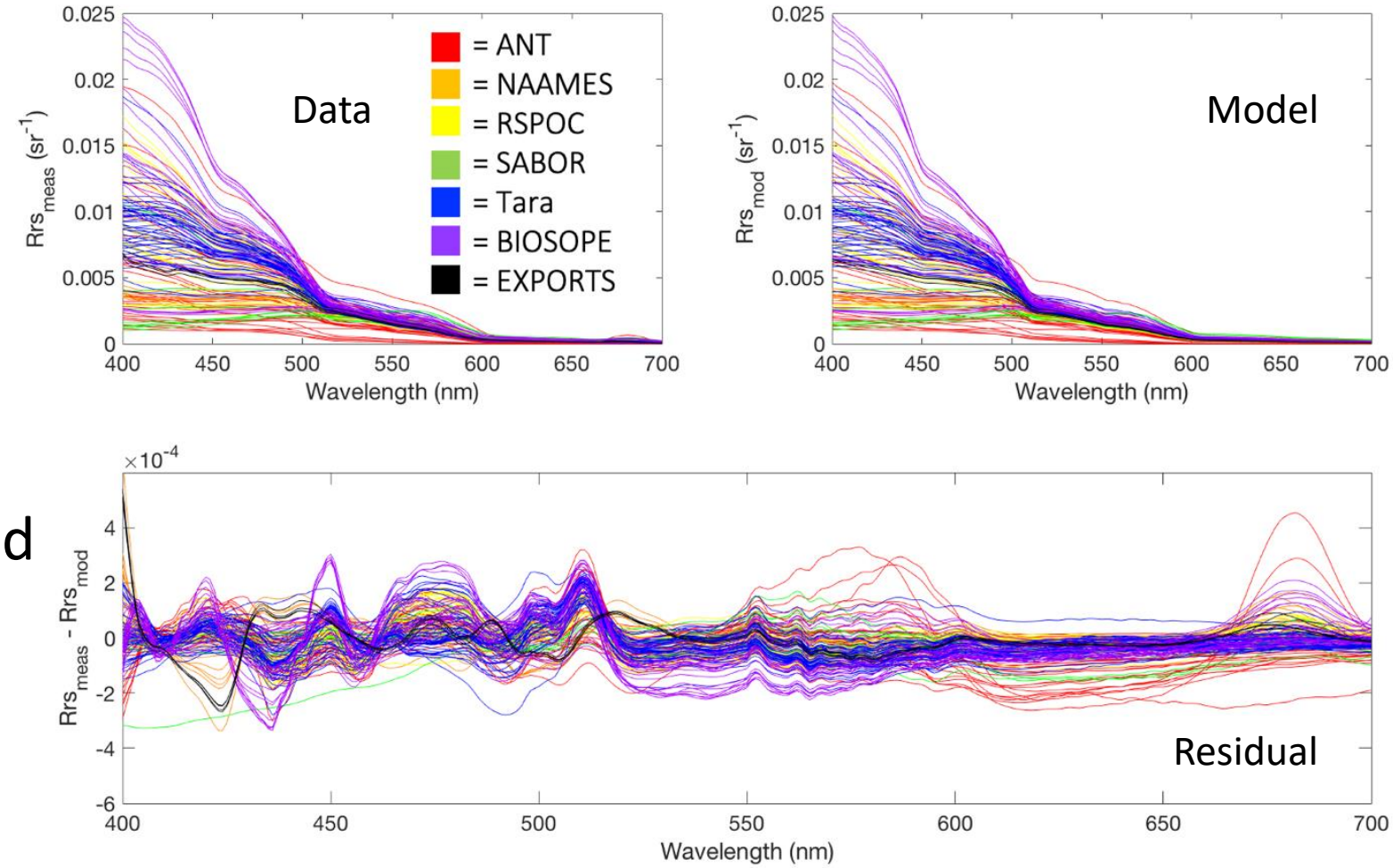
- Phytoplankton $a_{ph}(\lambda)$ spectra vary on scales ≤ 100 nm
- CDOM, $a_{det}(\lambda)$ & $b_{bp}(\lambda)$ vary on much longer spectral scales
- Water IOPs are known



- Suggests that phytoplankton signatures can be assessed by focusing on spectral scales less than 100 nm -> spectral derivative methods

Modeling Global Pigments Using Rrs(λ) Residuals

- Use IOP inversion model to model hyperspectral Rrs(λ) estimates from Rrs(λ) obs
- Calculate residual Rrs(λ) spectra from the obs-model difference
- First order effects of the dominant IOPs will be removed
- Rrs(λ) residual spectra should provide information about phytoplankton community composition



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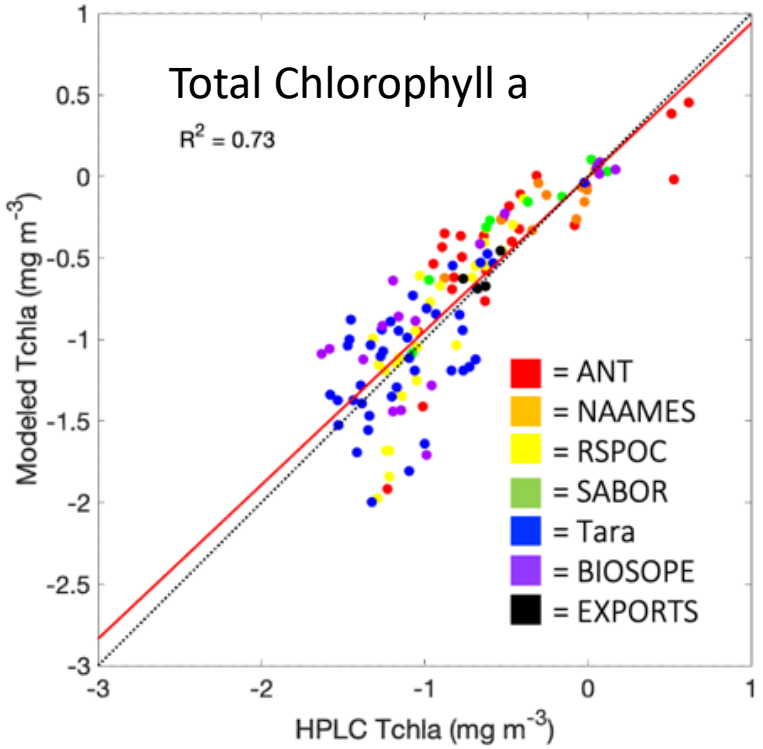
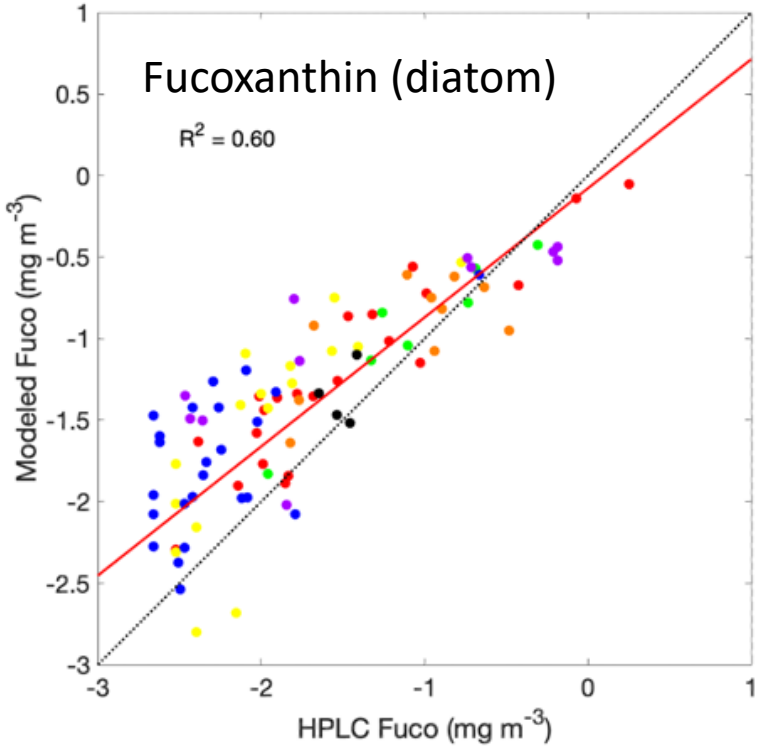
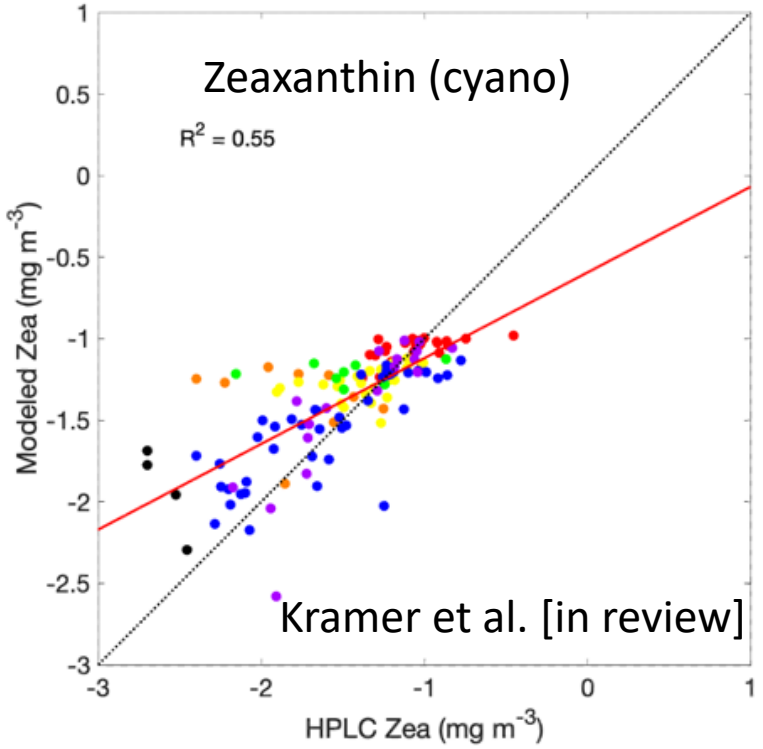
Modeling Global Pigments Using Rrs(λ) Residuals

- Model pigment concentrations using Rrs(λ) residuals & its 2nd derivative
- Principle component regression is used to reduce influences of collinearity
- Results show promise – emphasize need for more high quality data (N = 145)!!!
- Illustrates importance of the entire solar spectrum (not just where pigments are…)

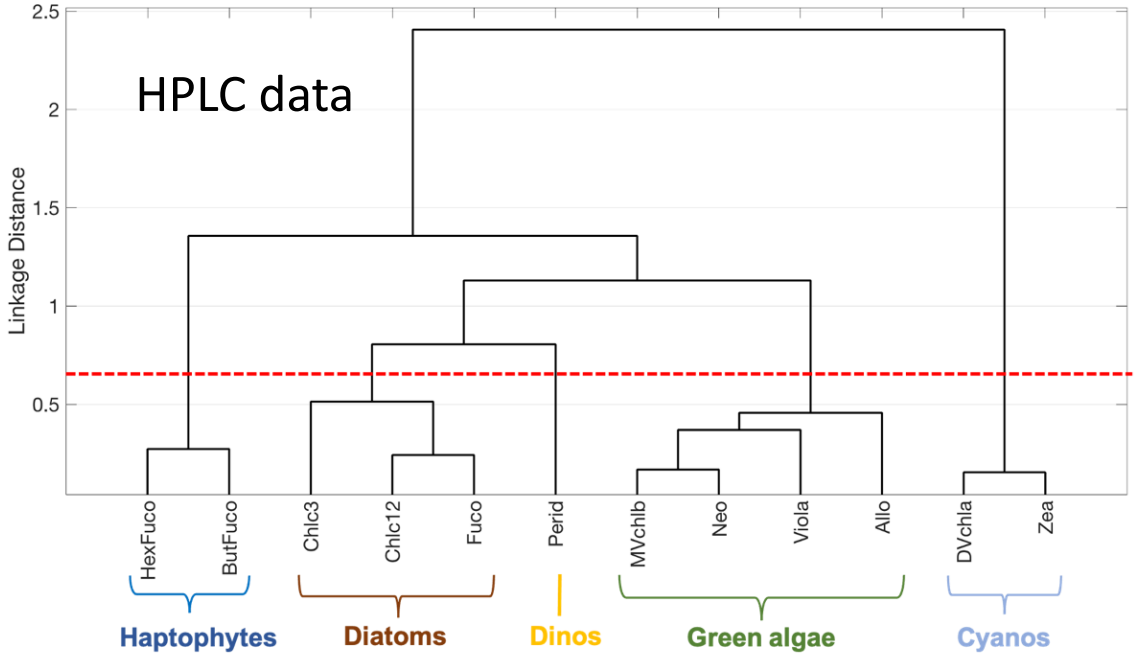


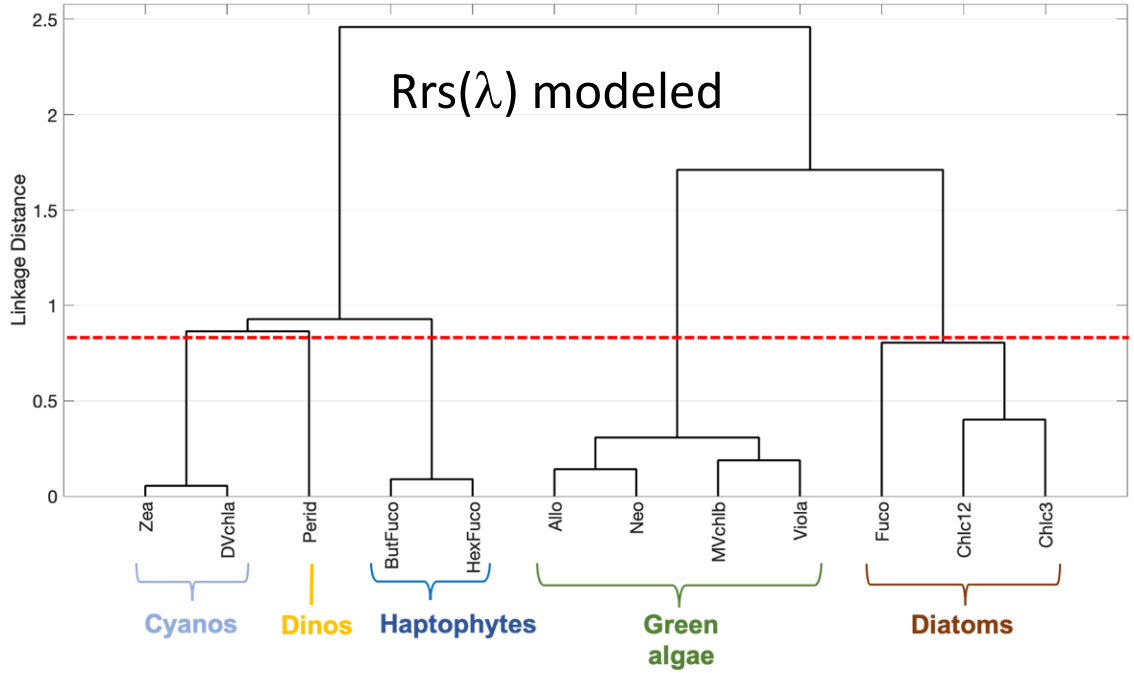




Modeling Global Pigments Using Rrs(λ) Residuals

Hierarchal clustering of TotChla-normalized phytoplankton pigment concentrations





- Rrs(λ) modeling recovered the observed covariability among pigments
- Again demonstrates that there are a limited number of phytoplankton groups that can be retrieved from optical data

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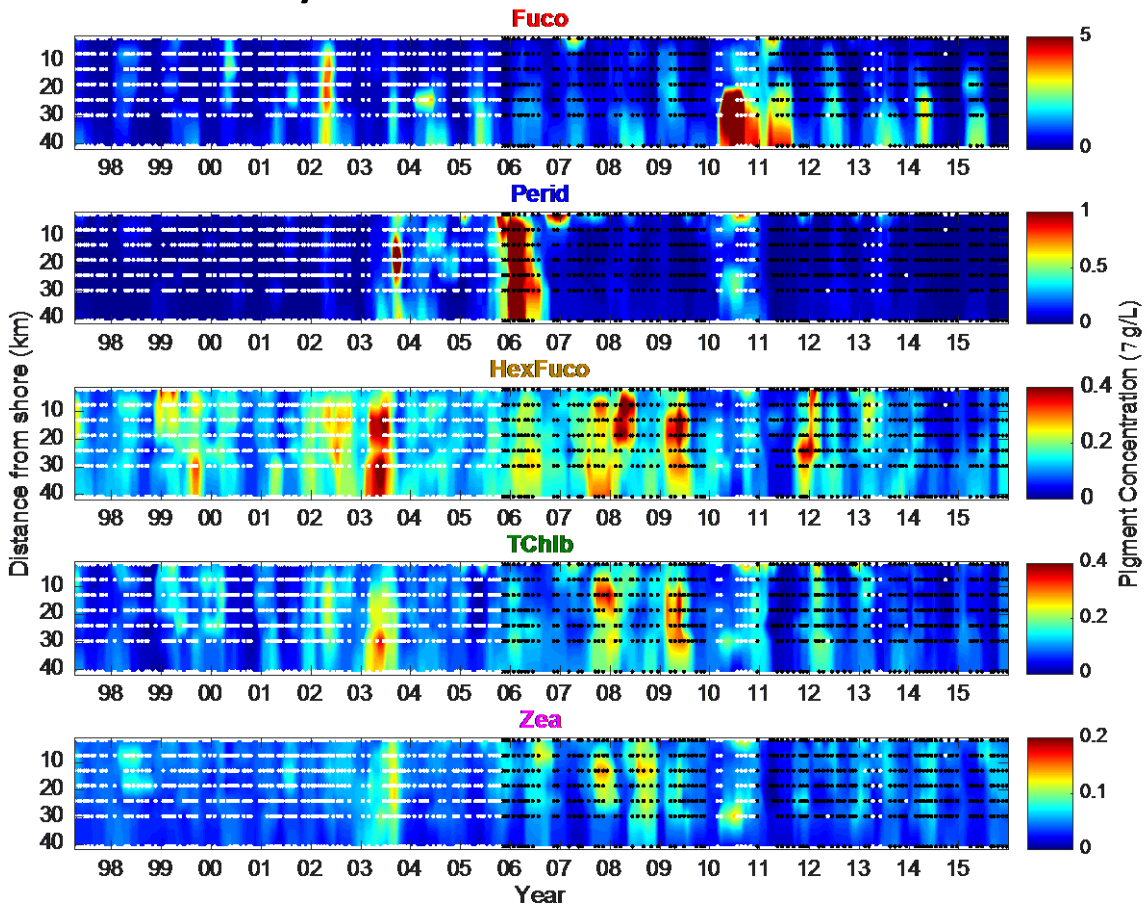
Local Data – Plumes and Blooms (PnB) Time Series

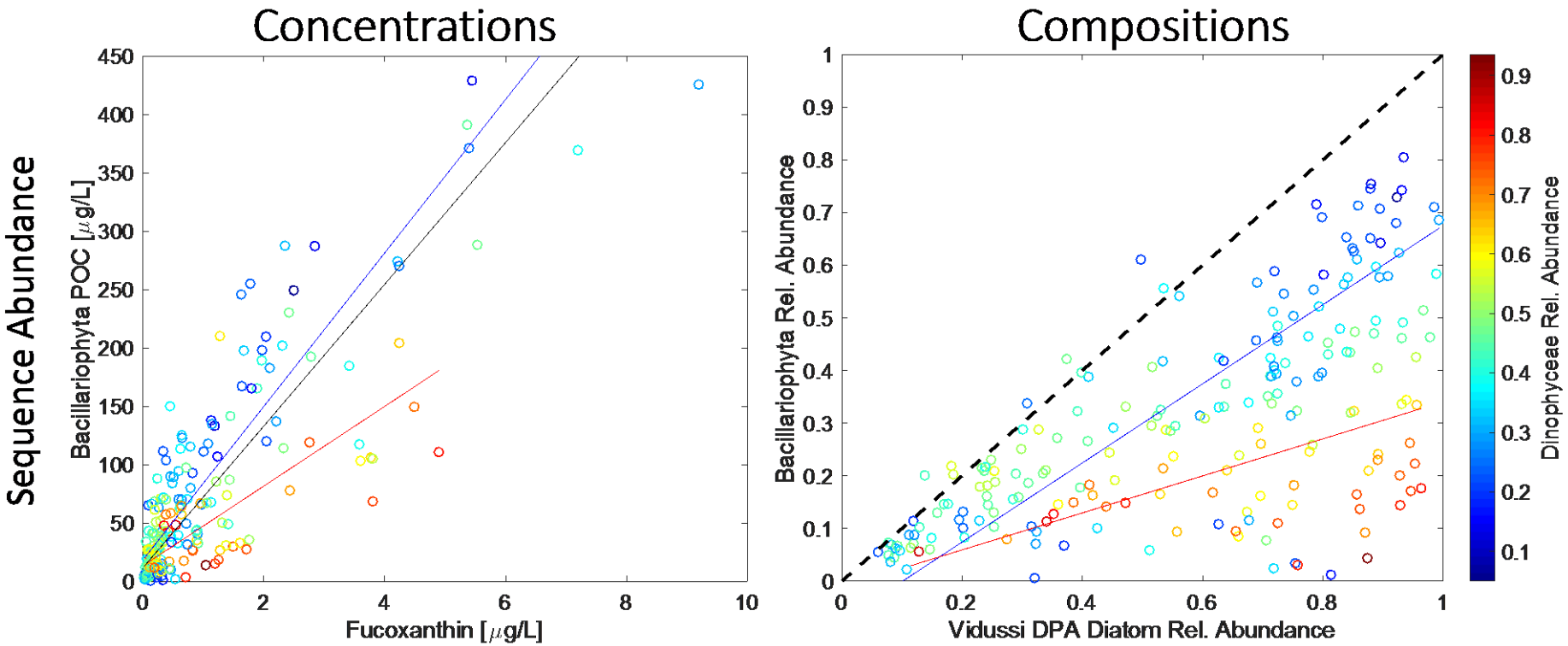
- Santa Barbara Channel, California (in collaboration with NOAA CINMS)
- 7 stations - ~10 one-day cruises per year – 20+ year time series
- Reconstructed marker pigments from $a_{ph}(\lambda)$ spectra
- Extended PFT info over the entire PnB time series
- Enabled assessment of the climate-oceanographic controls on phytoplankton group dynamics on seasonal to decadal time scales
- Trying to restart hyperspectral $Rrs(\lambda)$ observations



Catlett et al. *Progress in Oceanography* [2021]

What do pigments tell us about phytoplankton groups?

- Nearly 4 years of paired pigment – 18S amplicon sequence obs from PnB (N=215)
- Correspondence between “diatom” group assessments is good when dinoflagellate contributions are small (see colors)
- Illustrates that pigment biomarkers are imperfect tools for assessing phyto groups



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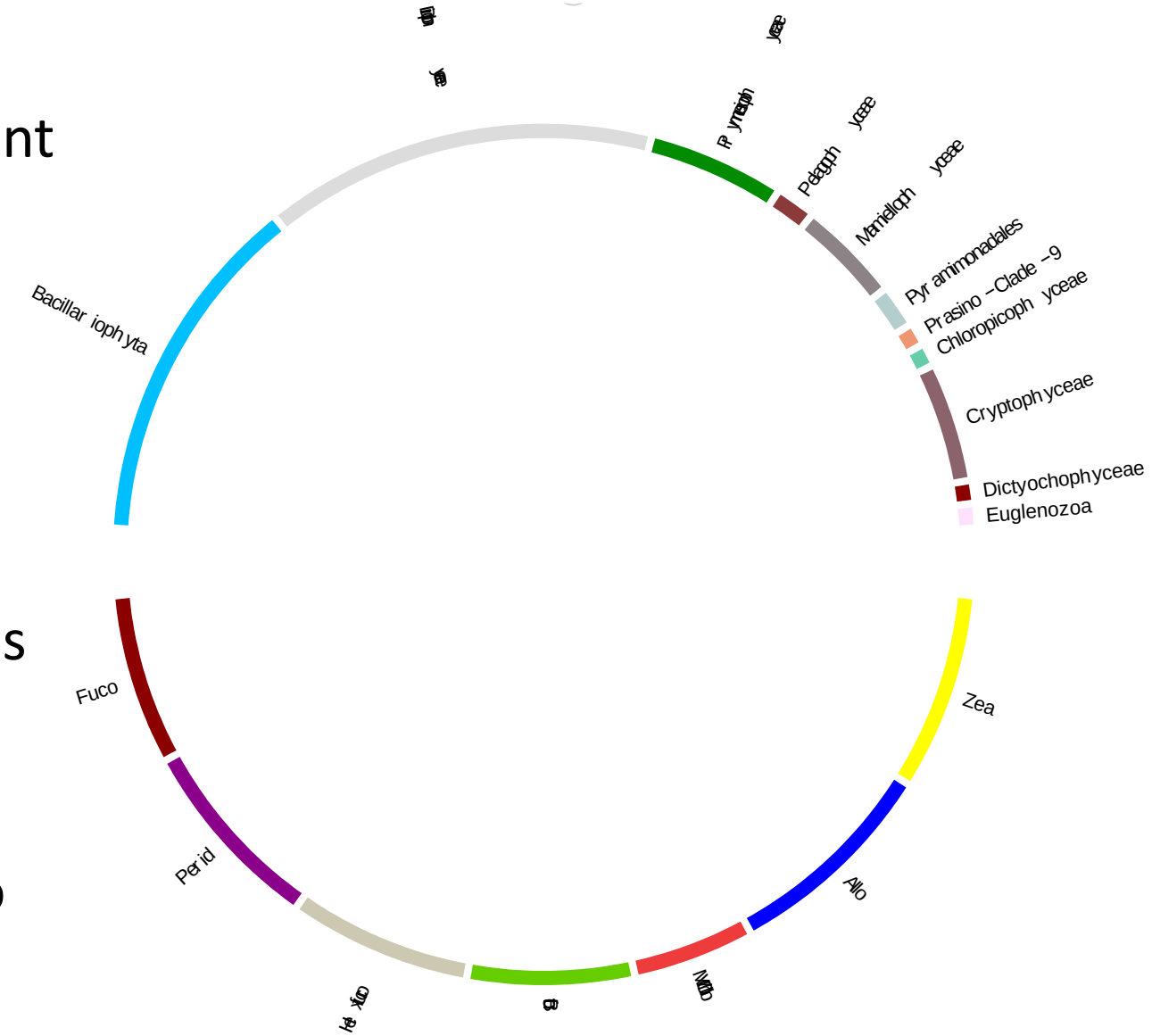
What do pigments tell us about phytoplankton groups?

- Positive associations between seven biomarker pigment (lower) & dominant phytoplankton amplicon sequence (upper) abundances
- Illustrates that pigments provide “mixed” information about phytoplankton community structure
- Changes in pigment to amplicon ratios are also found demonstrating the influences of photoacclimation
- Now, we (Sasha) are extending this to global scales



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Next Steps…

- Complete global analyses comparing pigment & amplicon sequence assessments of phytoplankton composition
- Include new hyperspectral RRs(λ) observations in our global analysis as they become available & make these data available
- Restart PnB's hyperspectral RRs(λ) sampling (love to borrow / rent a HyperTSRB…)
- Suggest the RRs(λ) residual spectra as a data product for PACE – could be useful for assessing community shifts…
- ??