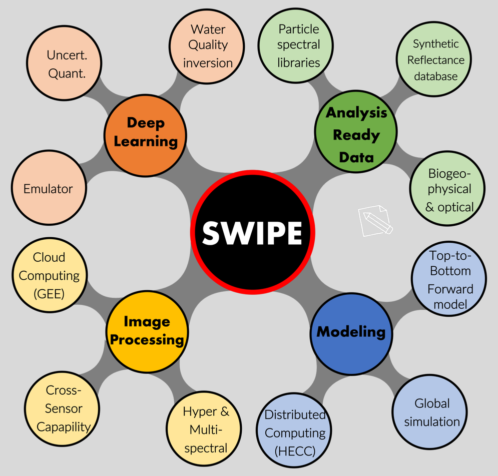

A Computational framework for hyperspectral radiative transfer modeling and deep learning emulation for global water quality applications at scale

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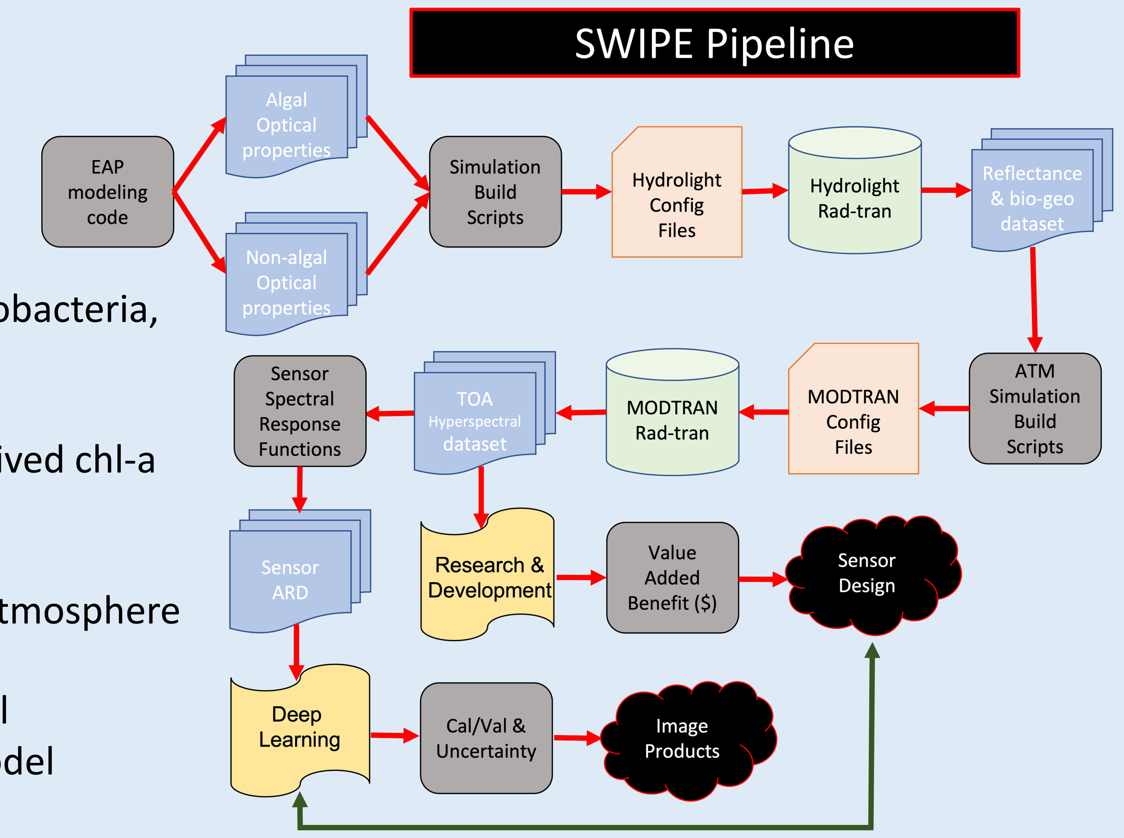
MOTIVATION

Degradation of Earth's inland and coastal water resources due to anthropogenic perturbations and climate anomalies at both local and global scales continues to place human health at substantial risk. There is now a growing necessity to develop pragmatic approaches that allow timely and effective extrapolation of local processes, to spatially resolved global products, and to promote operational and sustainable resource policy management[1]. This presentation will provide updates on NASA's prototype open-source aquatic modeling platform, **Spectral Water Inversion Processor and Emulator (SWIPE)**, which is a comprehensive, multi-faceted modeling platform for **both forward and inverse modeling** of diverse aquatic ecosystems from the **benthos to top-of-atmosphere (TOA).** SWIPE provides a cohesive application which leverages recent advancements in particle modeling, Big Data analytics, and **machine learning** to develop a high-fidelity synthetic training ground for sensitivity studies and algorithm development for multispectral or upcoming hyperspectral missions.

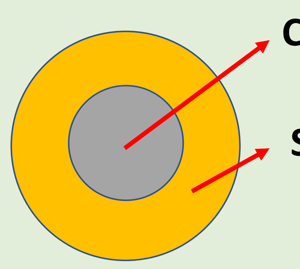
FORWARD MODEL

Processes

- Oligotrophic cases
- Extremely absorbing (CDOM) and extremely scattering cases (Sediment)
- Harmful algal blooms (Cyanobacteria, Marine coastal)
- Optically shallow waters
- Variable functional type derived chl-a fluorescence
- Variable surface sunglint
- NASA AERONET database (atmosphere optical diversity)
- Global benthic mixing model
- Global Adjacency mixing model
- Sensor noise model

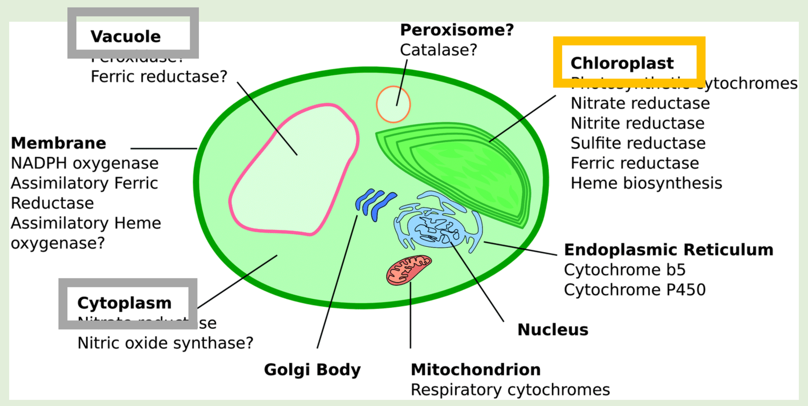


Distributed Equivalent Algal Population (DEAP) 2-Layer Coated Sphere Scattering Model



Core Layer = cytoplasm or vacuole

Shell Layer = Chloroplast (pigments)

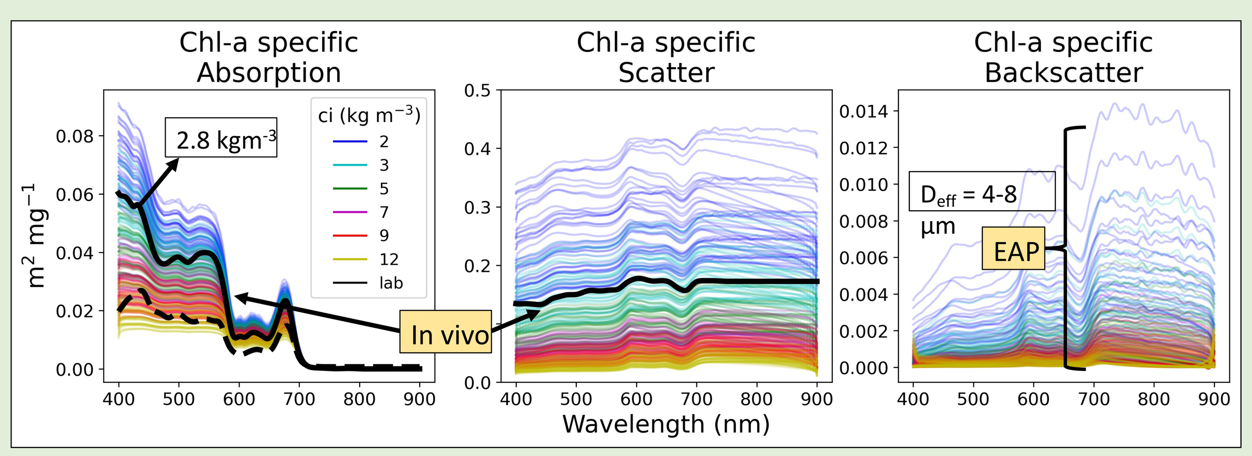


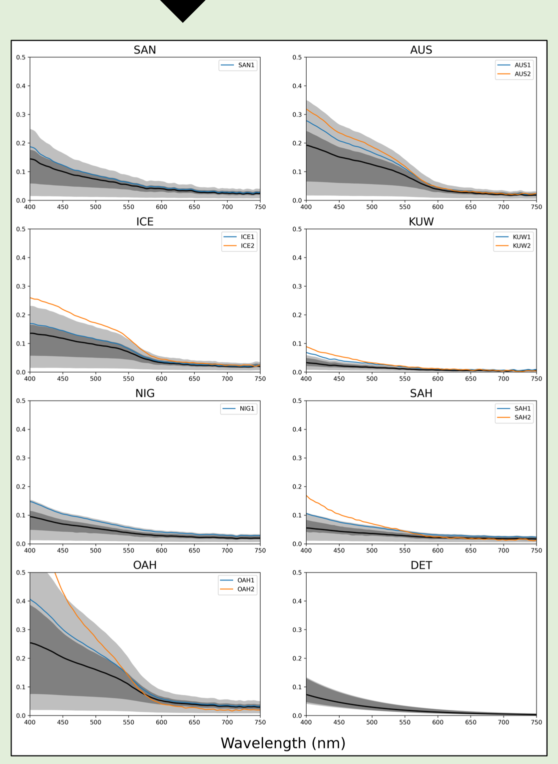
Hyperspectral particle optics for 70+ species of phytoplankton (~16 Classes)
(Example of Rhodophyte *P. Cruentum)*

Seven mineral spectral libraries composed of varying contributions of the major crustal elements:

Al, Fe, Ca, Mg, K, Ti, Ba, Sr, Zn, Mn, Ni, Cr, and V

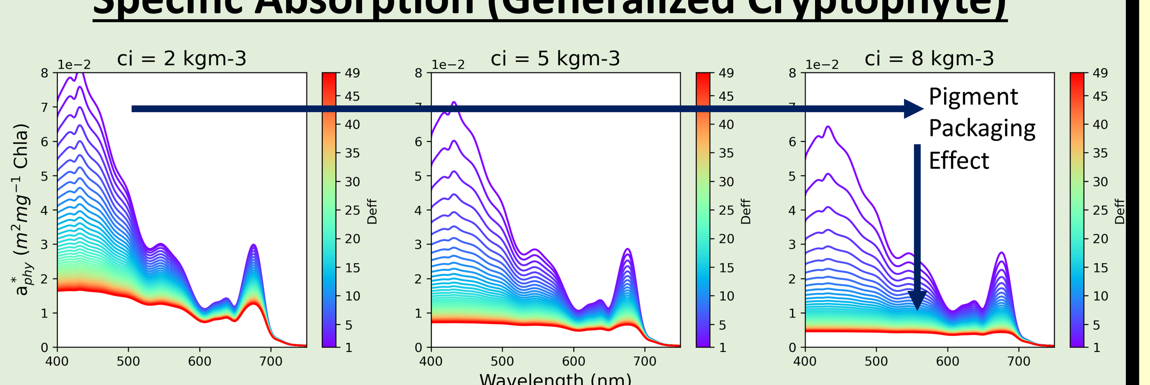
And scaled to different PSDs, particle density, junge distributions





- Population IOPs integrated across entire size distribution – represents combined bulk optical signal for algal assemblage
- incorporates individual biophysical cellular characteristics into assemblage-based optical properties as observable *in situ*
- Facilitates IOP variability as due to environmental forcings[2]

Specific Absorption (Generalized Cryptophyte)

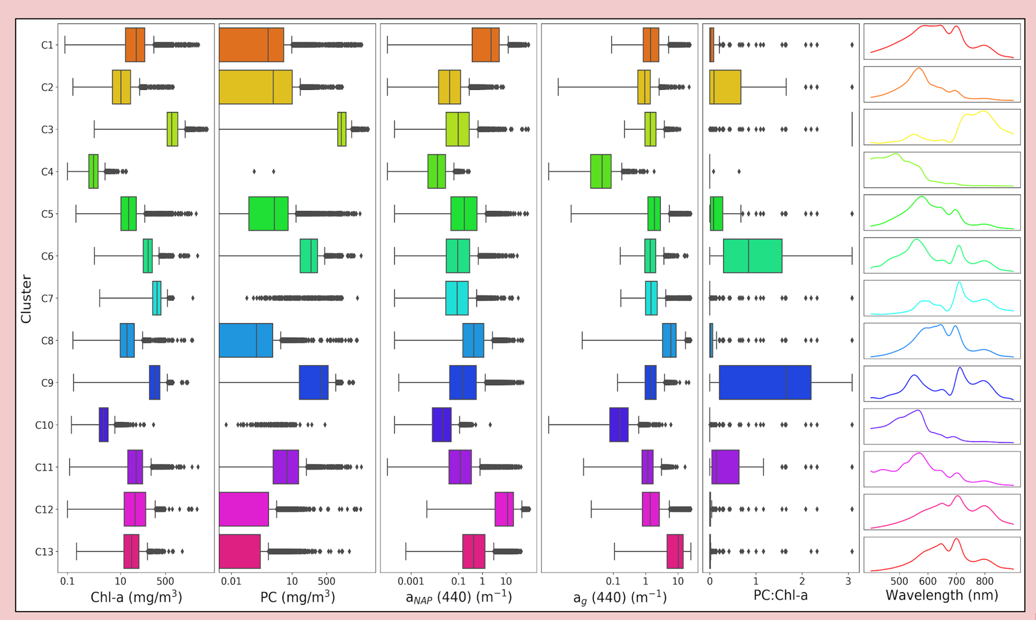


EAP facilitates 4 main drivers of phytoplankton optical variability

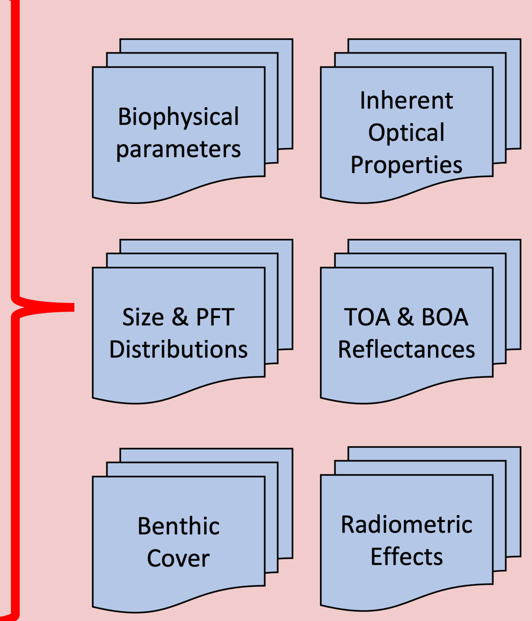
1. Biomass
2. Pigments
3. Cell size
4. Intracellular chl-a (ci)

ANALYSIS READY DATA (ARD)

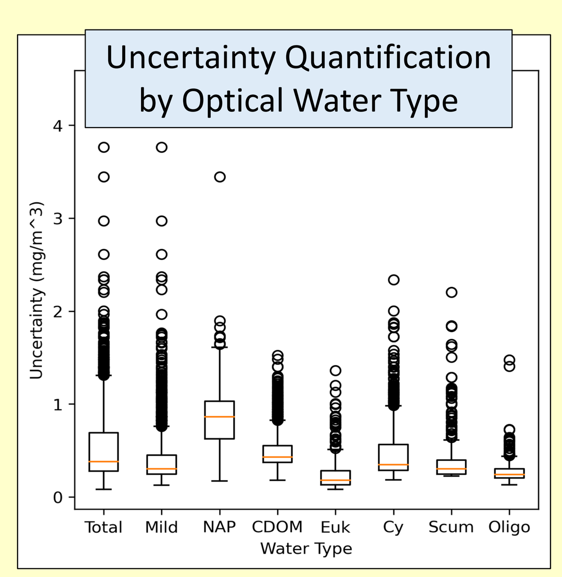
Clustered Hyperspectral (2nm) Reflectance Dataset



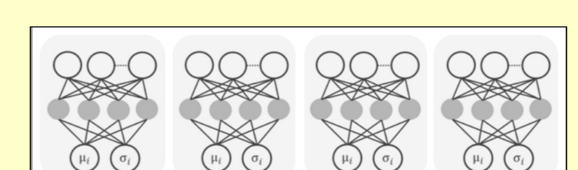
Analysis Ready Data



DEEP LEARNING

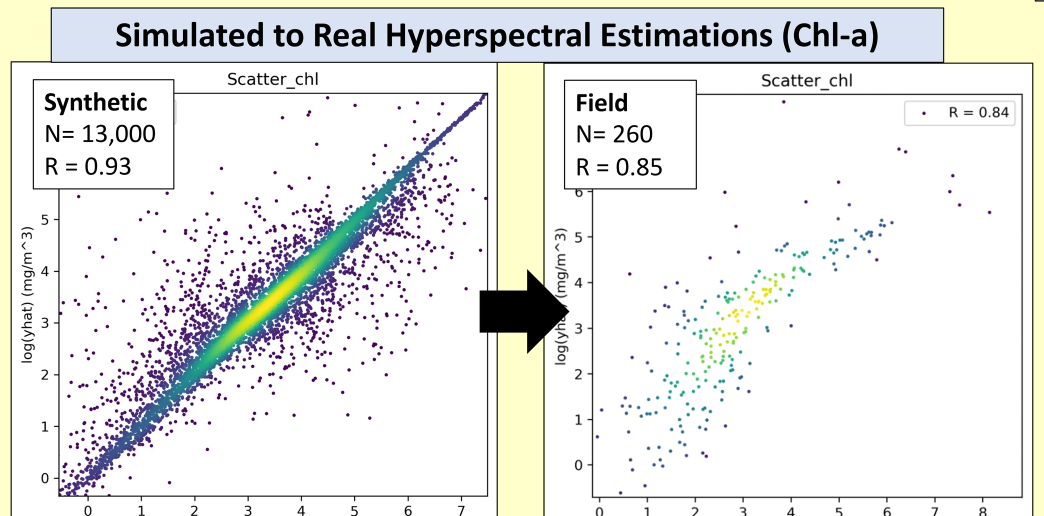


Deep ensemble networks have the potential to provide robust **uncertainty estimates** at a small computational cost. Between leveraging uncertainty quantification and optical water types, we can create more advanced ML models with more **interpretability**

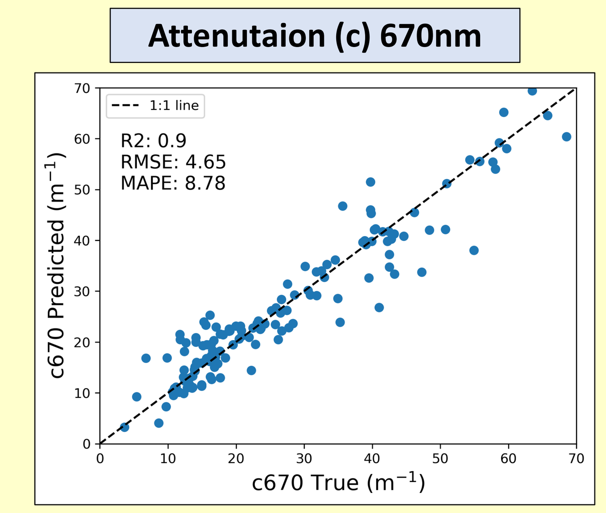


$$p(y|x) = \frac{1}{N}\sum_{i=1}^{N}\phi(y;\mu_i(x),\sigma_i(x))$$

Simulated to Real Hyperspectral Estimations (Chl-a)

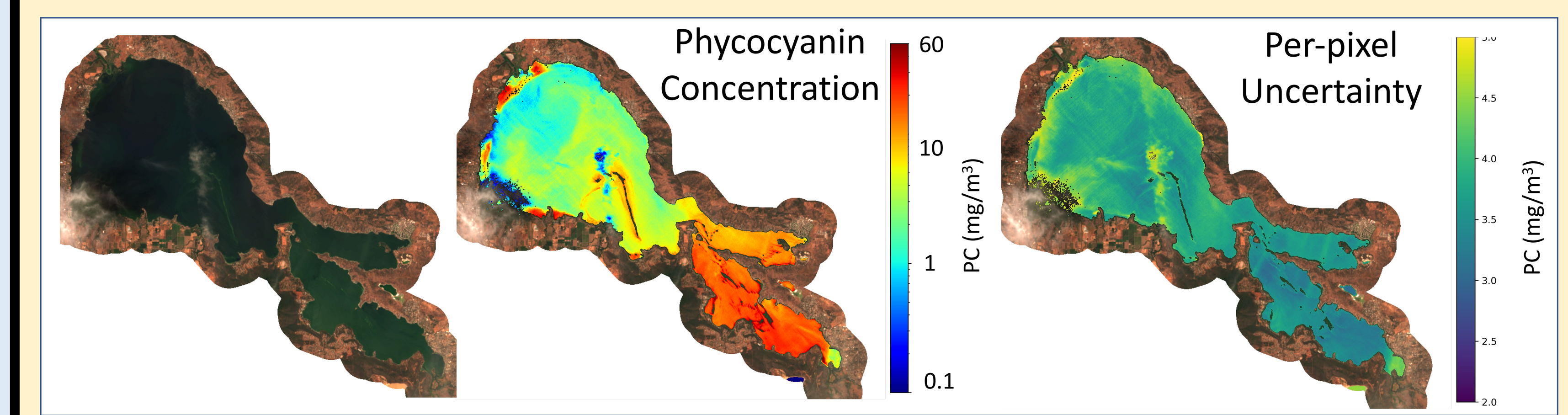


Attenuation (c) 670nm

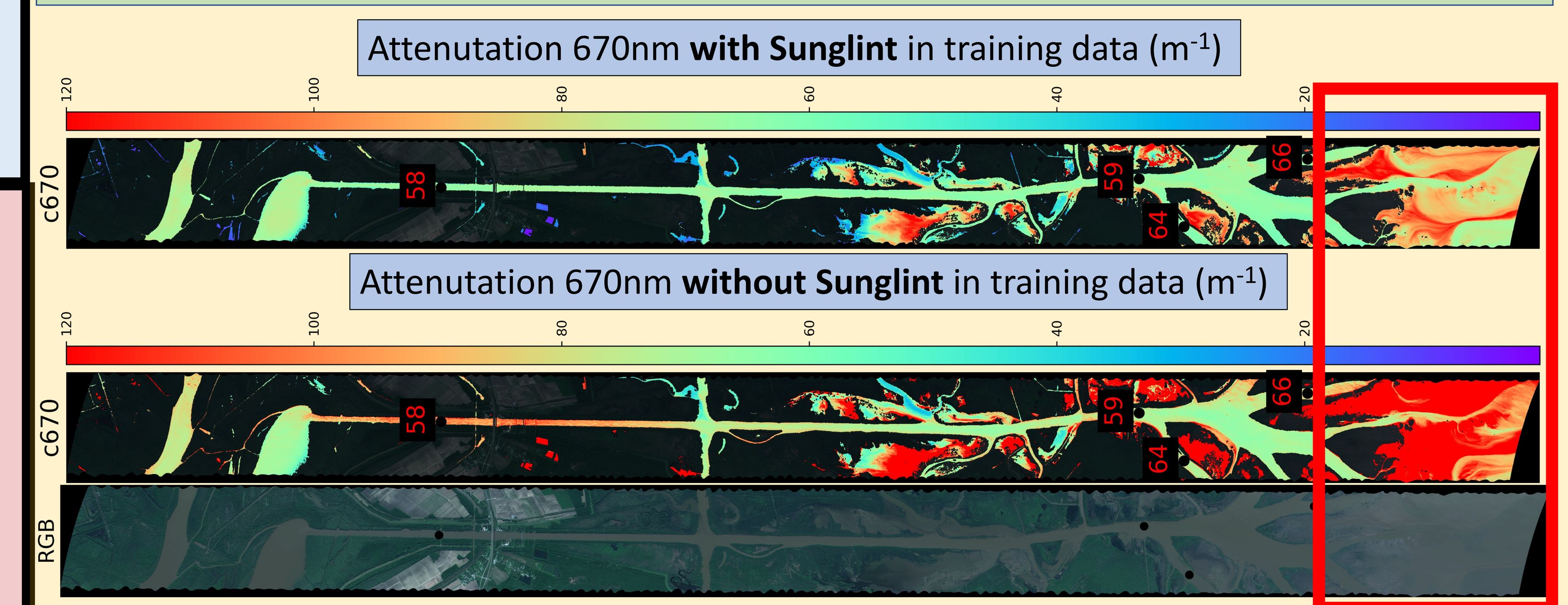


SENSOR AGNOSTIC PROCESSING

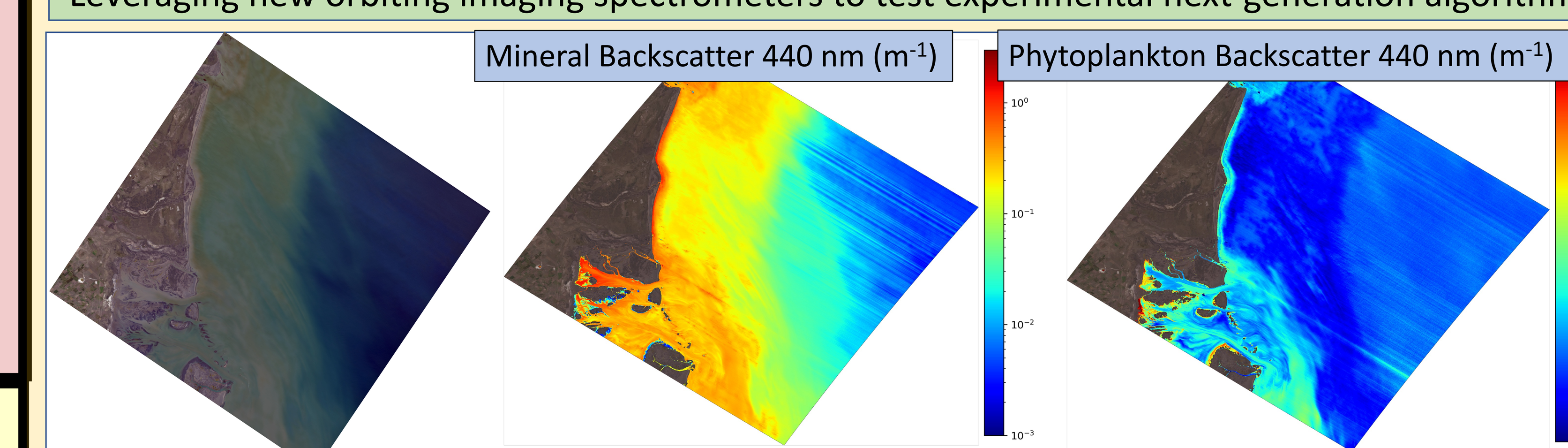
DESIS – Clear Lake, CA USA
Water column constituent estimation with **per-pixel uncertainty**



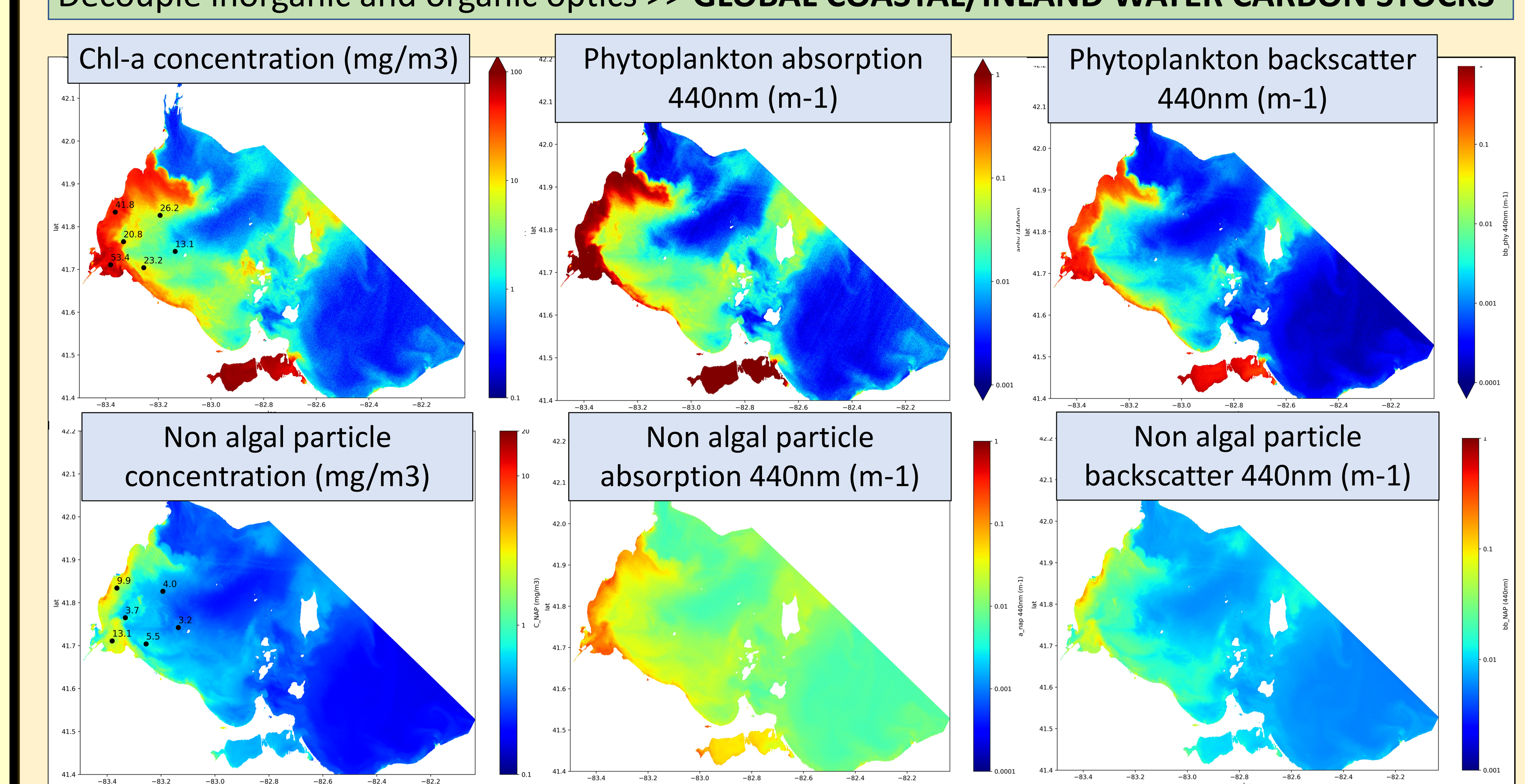
AVIRIS-NG – Mississippi Delta, USA
Beam attenuation 670 nm estimation with **sunglint correction**



EMIT – Bahia Blanca, Argentina
Leveraging new orbiting imaging spectrometers to test experimental next-generation algorithms



HICO – Lake Erie, USA Direct retrieval from top-of-atmosphere
Decouple inorganic and organic optics >> **GLOBAL COASTAL/INLAND WATER CARBON STOCKS**



1. National Academies of Sciences, Engineering, and Medicine. 2018. *Thriving on Our Changing Planet: A Decadal Strategy for Earth Observation from Space*. Washington, DC: The National Academies Press. https://doi.org/10.17226/24938.
2. Lain, L. R., & Bernard, S. (2018). The fundamental contribution of phytoplankton spectral scattering to ocean colour: implications for satellite detection of phytoplankton community structure. *Applied Sciences*, *8*(12), 2681.
3. Kravitz, J., Matthews, M., Lain, L., Fawcett, S., & Bernard, S. (2021). Potential for high fidelity global mapping of common inland water quality products at high spatial and temporal resolutions based on a synthetic data and machine learning approach. *Frontiers in Environmental Science*, *9*, 587660.