Uncertainty Quantification Activities of Geophysical Retrievals within the PACE Mission

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Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) Mission

- Primary instrument is the Ocean Color Instrument (OCI) hyperspectral scanning radiometer
- 2 Contributed multi-angle polarimeters: HARP-2, SPEXone

https://pace.gsfc.nasa.gov/

Required OCI Science (ocean) Products

Data Product	Baseline Uncertainty $\Delta\rho_w$
Water-leaving reflectances centered on (±2.5 nm) 350, 360, and 385 nm (15 nm bandwidth)	0.0057 or 20%
Water-leaving reflectances centered on (±2.5 nm) 412, 425, 443, 460, 475, 490, 510, 532, 555, and 583 (15 nm bandwidth)	0.0020 or 5%
Water-leaving reflectances centered on (±2.5 nm) 617, 640, 655, 665 678, and 710 (15 nm bandwidth, except for 10 nm bandwidth for 665 and 678 nm)	0.0007 or 10%

these are required for science goal success & drive OCI design

Additional required products to be generated
Chlorophyll concentration
Spectral diffuse attenuation coefficients
Spectral absorption coefficients (phytoplankton, CDOM+NAP)
Spectral backscattering coefficients
Fluorescence line height

Atmospheric Correction using OCI alone

*Better characterization of aerosols using MAP

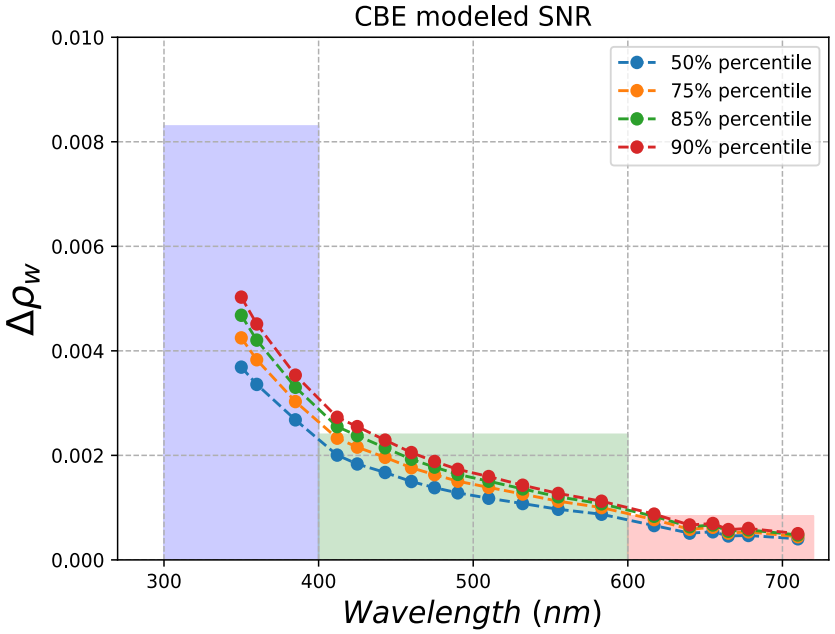
Each uncertainty requirement is defined as the maximum of the absolute and relative values for Level-2 satellite data processing (geophysical values in the original satellite coordination system). These requirements are defined for **≥ 50% of the observable deep ocean** (≥ 1000 m).

*L1 requirements also exist for atmospheric products

Data product uncertainties

$$\rho_w = \pi \, Rrs$$

- Comments on how to proceed with uncertainty metrics
  - Possibilities for generating them
  - Limitations in generating them
  - What spectral ranges (when appropriate)?
  - How to maximize information & minimize file sizes / computational burdens?



Uncertainty in ocean reflectance after the Atmospheric Correction

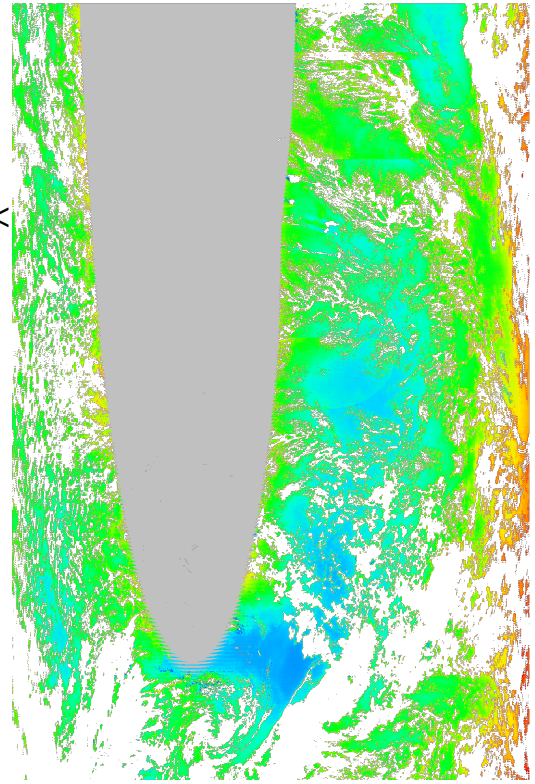
Surface glint

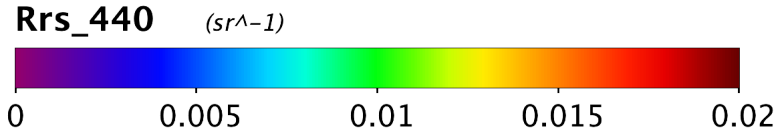
Rrs(440)

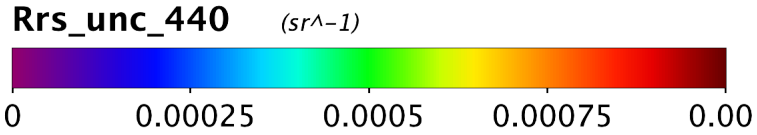
Cloud covered pixels

One goal is to retrieve Rrs_unc_440 < 0.000636 sr-1

Rrs(440) uncertainty







A main goal for PACE is to provide pixel-level uncertainty

PACE science and applications team Working group goals

- To **assess** various sources of uncertainty relevant to the PACE mission
- To **document** what is currently known and is unknown
- To **identify** what poorly-known aspects we can make progress on before/during PACE's lifetime
- To **suggest** appropriate methods for uncertainty propagation and metrics for validation, together with their limitations
- To **encourage** and **guide** the community on formulating the above
- To **report** back to the broader team and the community via Tech Memo/paper(s)

Working group discussions and report outline

1. Definitions and terminology

Uncertainty terminology:

- Generally following ISO Guide to Uncertainty in Measurement (GUM): https://www.iso.org/sites/JCGM/GUM-introduction.htm
- Distinction between uncertainty and error, accuracy and precision

2. Instrument-related uncertainties

- Radiometric
- Non-radiometric

3. Uncertainties in the L2 retrieval process

- Forward model uncertainties
- Inversion-related uncertainties
- Categorical or non-Gaussian errors (e.g. land/ocean or cloud mask misidentification)

4. Propagating uncertainties from L1 to L2

- Discuss various techniques (OE, MCMC, AI/ML, empirical)
- Highlight strengths and limitations
- Assumptions, practicality
- Possibly provide an example with flow chart/pseudocode
- Options if you can't/won't do forward propagation

5. Validating retrievals and uncertainty estimates

- Validating retrievals
- Validating L2 uncertainty estimates
- Understanding and communicating the results
- Assessing retrievals/uncertainties if we don't have a comparison data source

6. Towards level 3 uncertainties and beyond