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UNCERTAINTY QUANTIFICATION FOR CALIBRATION AND ATMOSPHERE TO ENABLE GLOBAL CROSS-PLATFORM SPECTROSCOPY

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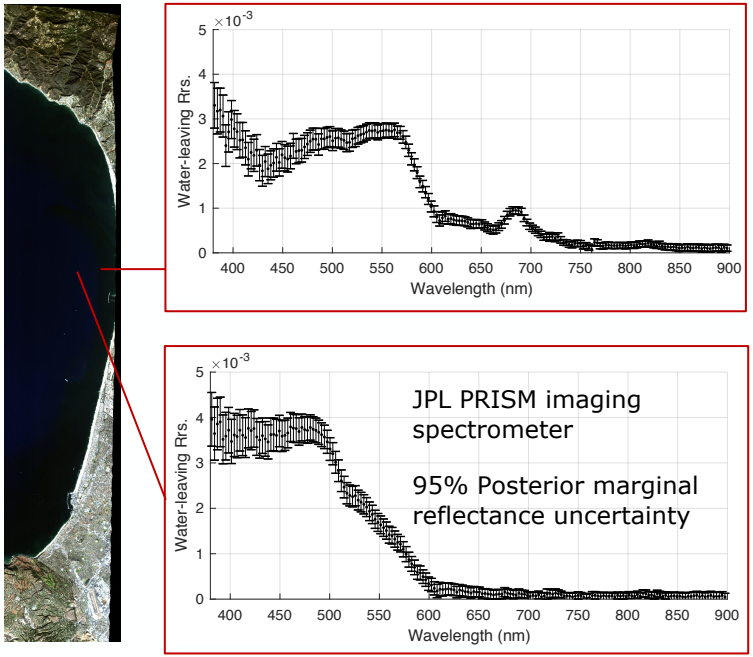
Agenda

1. Motivation and definitions
2. UQ for calibration: challenges, solutions
3. UQ for atmosphere: challenges, solutions
4. Discussion

Uncertainty Quantification (UQ): What?

1. **Define** probability models for instrument and algorithm unknowns
2. **Estimate** and propagate uncertainty across products
3. **Integrate** all available ancillary information using statistical methods
4. **Demonstrate** closure of uncertainty budgets using validation data
5. **Report** uncertainties and covariance for every spectrum (ideally)
6. **Refine** our understanding over time

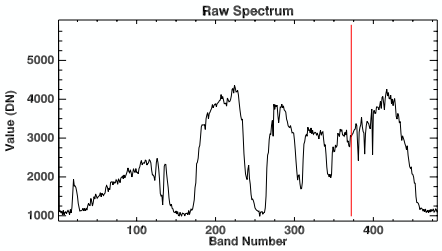


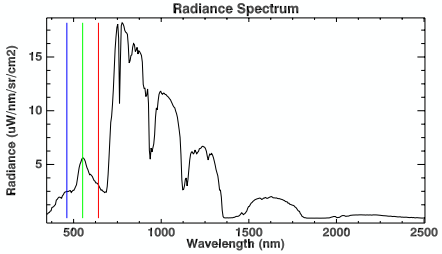
[Frouin et al., Frontiers in Marine Science, in press]

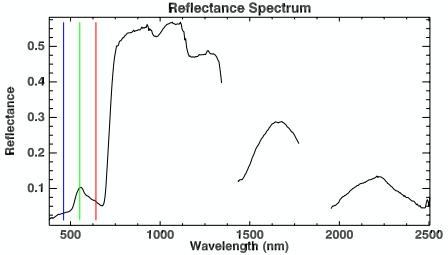
Uncertainty Quantification (UQ): Why?

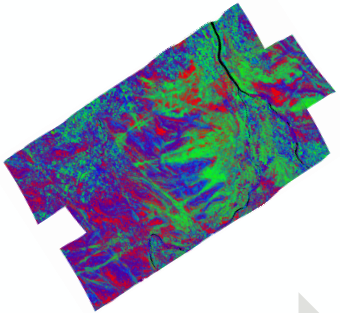
1. **Scientific hypothesis testing**
2. **Formal understanding** of the observation system
3. **Integrating data** from multiple missions
4. **Multi-location and time series data** (acquired under different observation conditions)
5. **Improved retrieval accuracy**
6. **User interpretability** and enhanced decision support

UQ Challenges









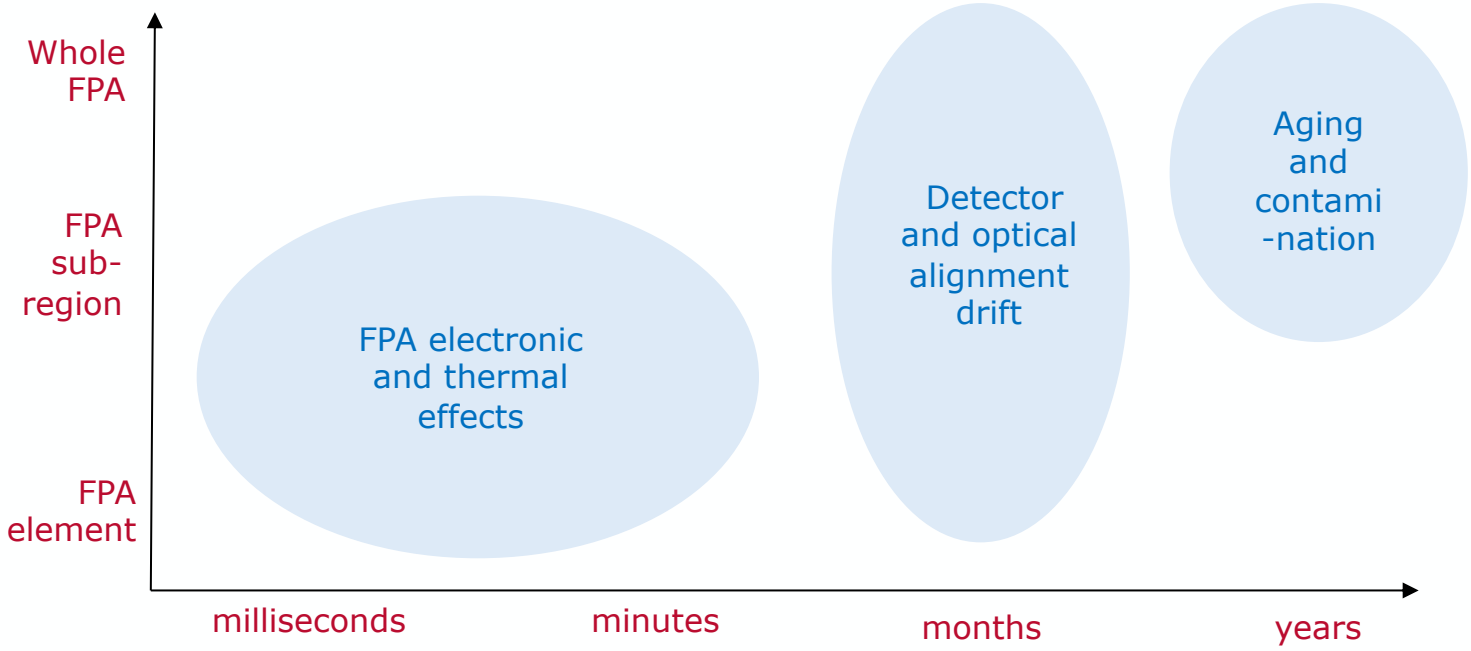
Raw Digital Numbers → **Radiance at sensor** → **Surface Reflectance** → **Geophysical Map**

1. Detector sensitivity drift
2. Transient or systematic electronic effects
3. Long term degradation and contamination
4. Spectral response uncertainty

1. Atmospheric unknowns (aerosol types, gas and particle vertical profiles)
2. Bi-directional reflectance
3. Topographic effects
4. Temporal variability

1. Retrieval models
2. Generalizing local parameterizations
3. Diverse in-situ data sources

UQ for calibration: variability across multiple scales



Calibration uncertainty via physics-based instrument models

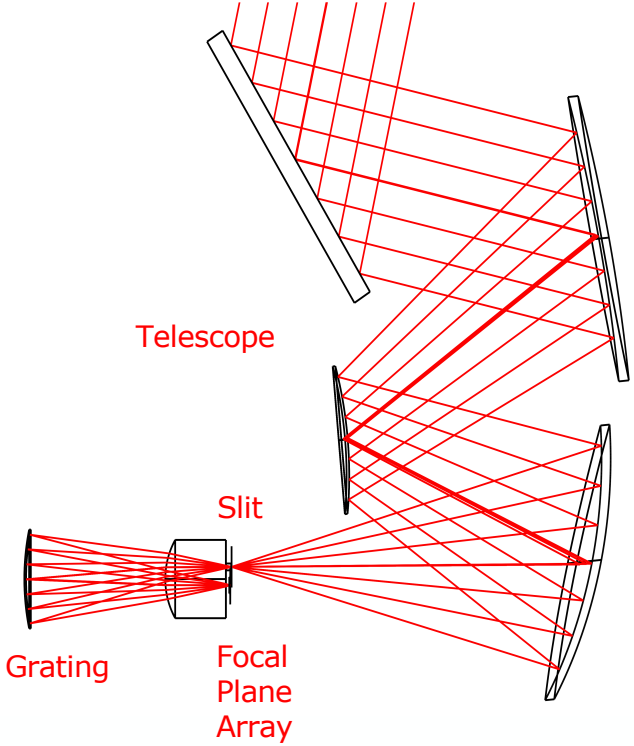
Radiometric uncertainty by forward propagation of photon counting statistics

Fit models by analysis and/or laboratory characterization

SNR is signal-dependent

Pro: SI-traceability; component-wise models; high accuracy

Con: In-flight validation & updates difficult, pathological illumination



Alternative: Empirical noise estimation

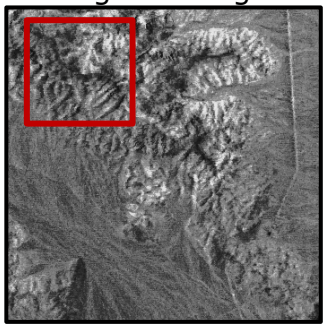
Estimate radiometric uncertainty directly via empirical statistics of flight data

Can exploit scene homogeneity assumptions or reflectance basemaps

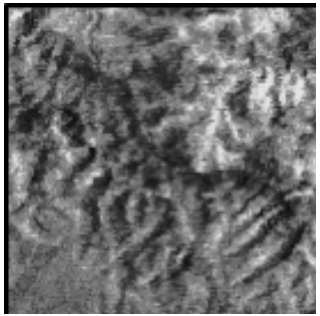
Much easier than vicarious characterization

Not suitable for all scenes

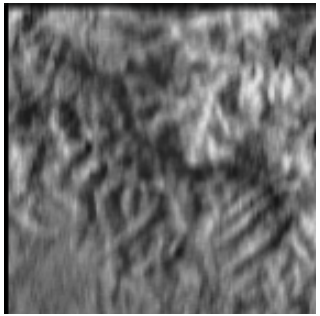
Original Image



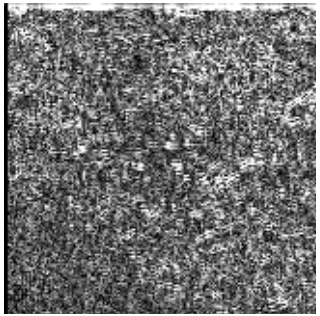
Subset (550 nm)



Smooth scene



Noise contribution

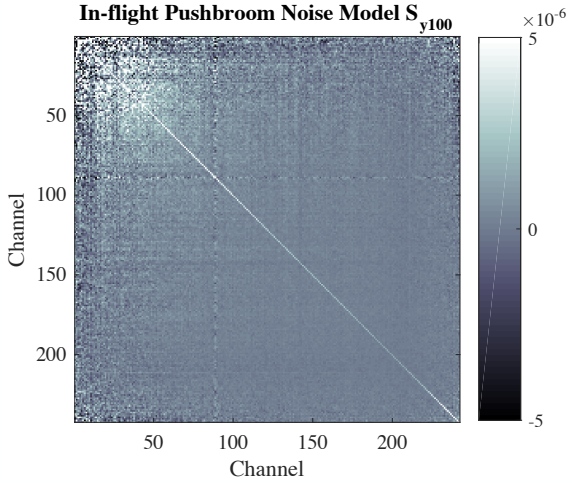


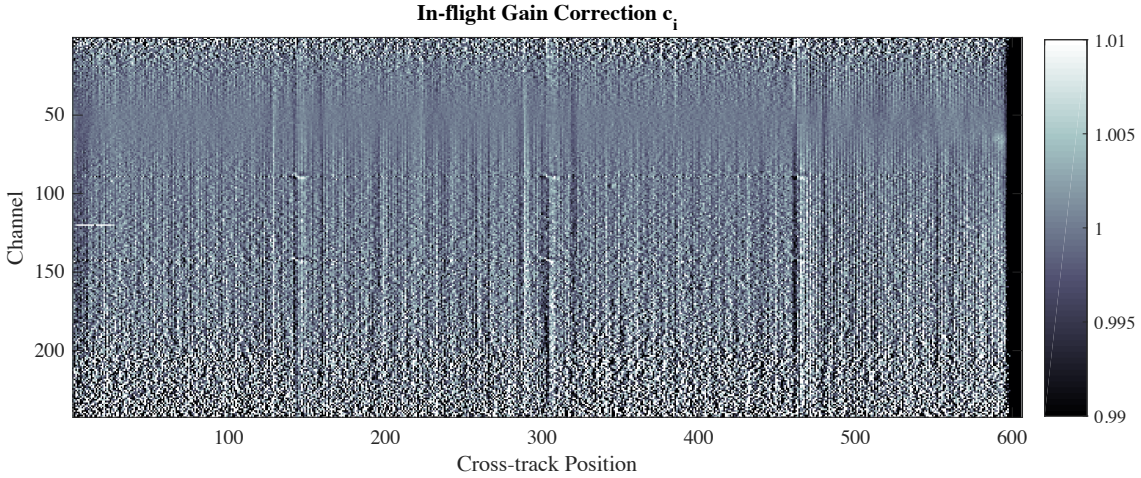
[Thompson et al., *Optics Express* 2017]

Alternative: Empirical noise estimation

Example: in-flight estimates for the PRISM instrument

Permits updated synthetic flat field and per-element instrument noise estimation



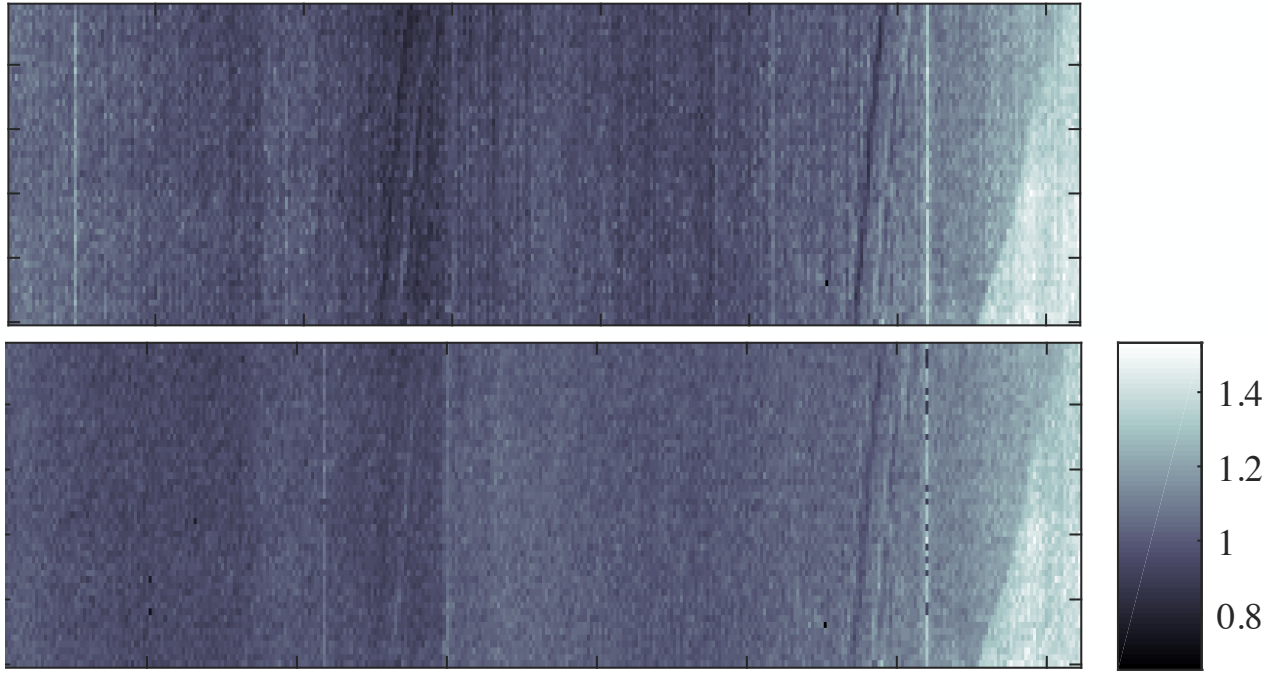


[Thompson et al., *Remote Sensing of Environment* 231, 2019]

Alternative: Empirical noise estimation (contd.)

Original normalized reflectance (510 nm)

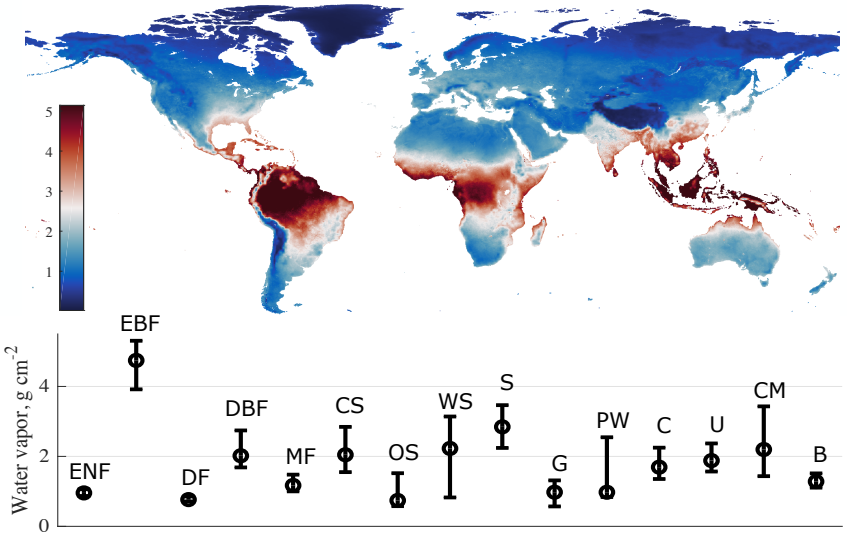
With empirical instrument model



[Thompson et al., *Remote Sensing of Environment* 231, 2019]

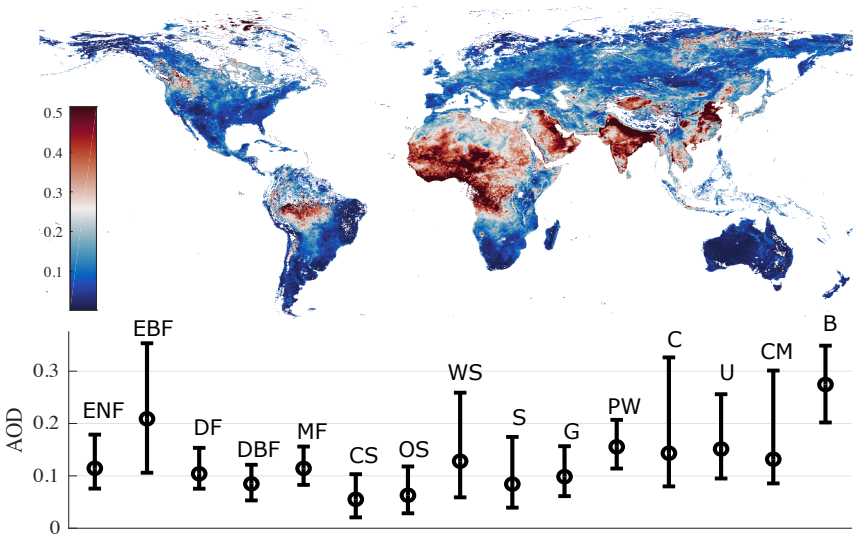
UQ for atmosphere: climatological uncertainties

MODIS average water vapor gm cm^{-2}



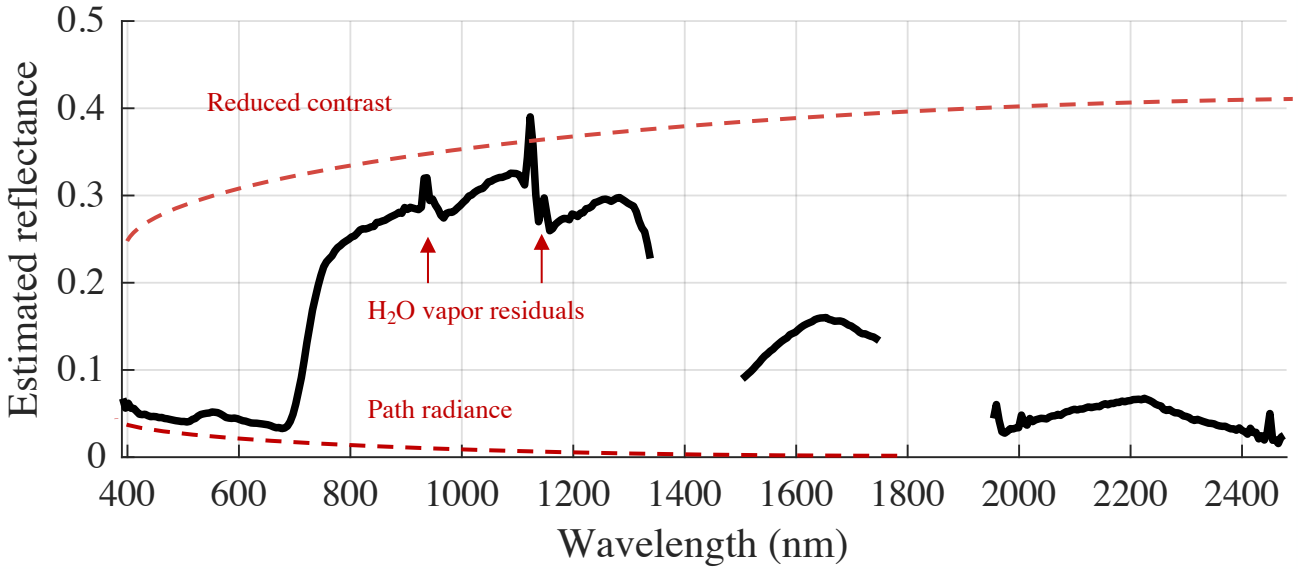
Land cover classification

MODIS average AOD550

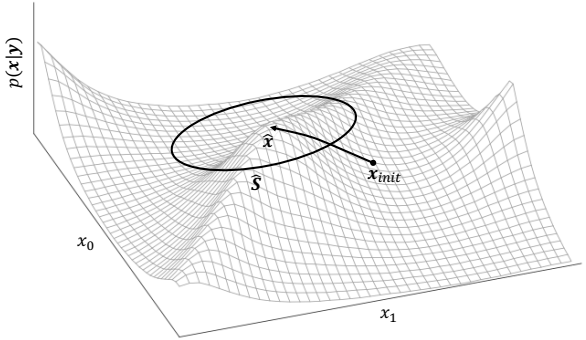


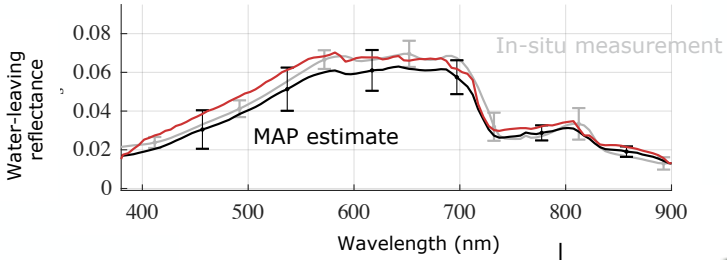
Land cover classification

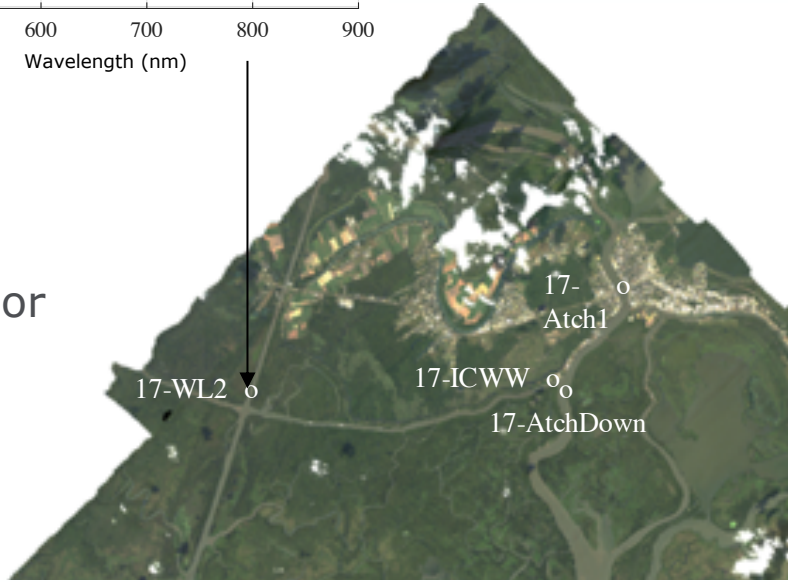
UQ for atmosphere: climatological uncertainties (contd.)



Gaussian posterior distributions







Optimize a state vector **x** defining all surface and atmosphere free parameters

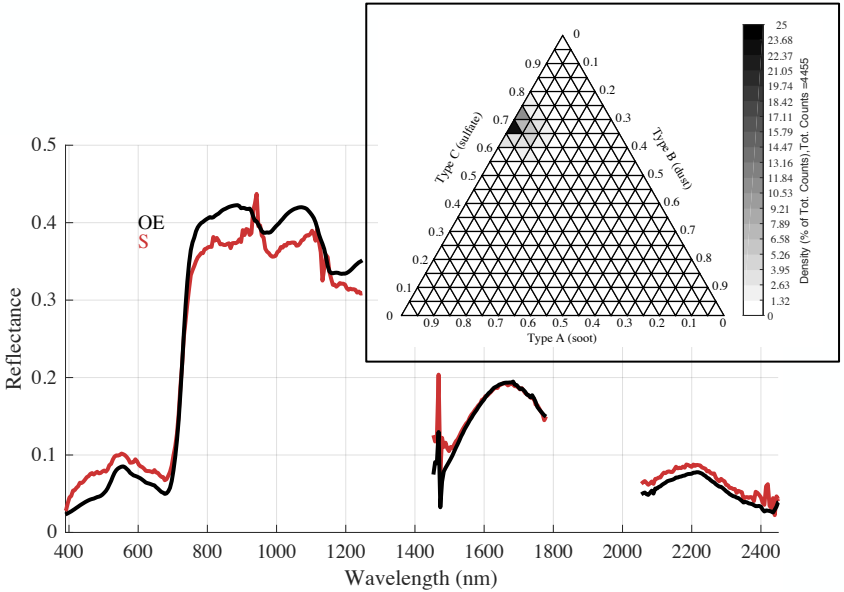
Gradiant-based optimization of cost balancing prior and model match to data

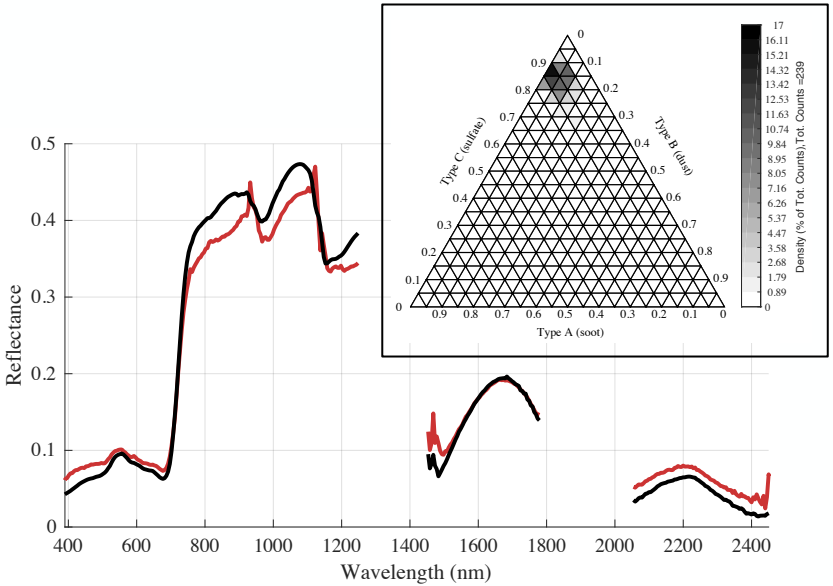
Local linearity of state vector about solution provides uncertainty covariance

[Thompson et al., *Remote Sensing of Environment* 231, 2019]

Gaussian posterior distributions

Simultaneous estimation of surface and atmosphere parameters can account for aerosol distortions

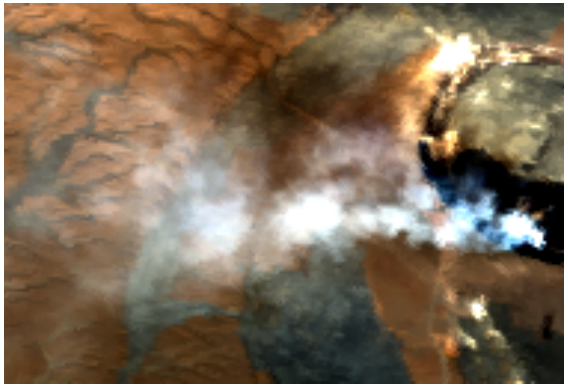




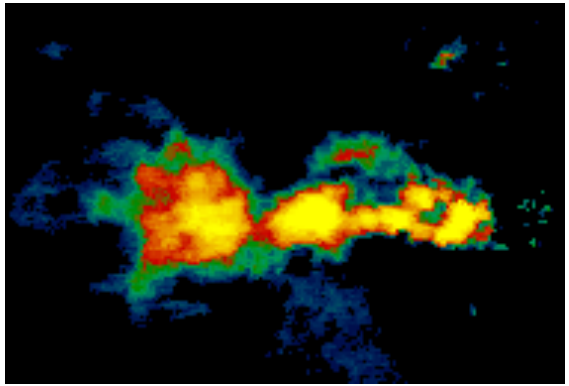
[Thompson et al., *Remote Sensing of Environment, in press*]

Example: AOD Uncertainty

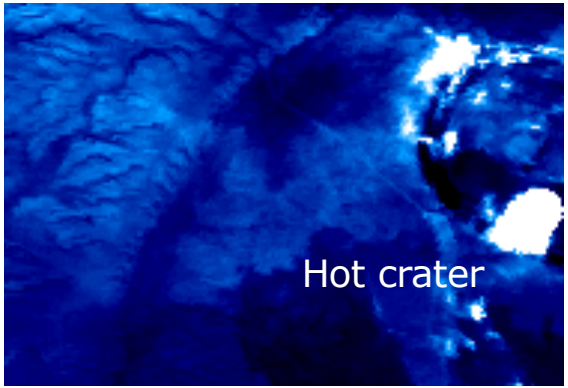
AVIRIS-C
f170127t01p00r16
(visible bands)



Aerosol Optical Depth
at 550 nm



Aerosol Optical Depth
uncertainty

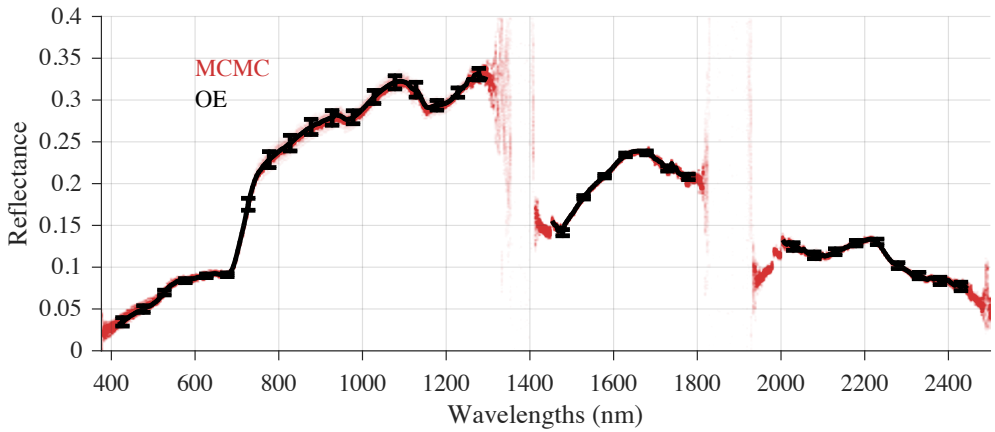


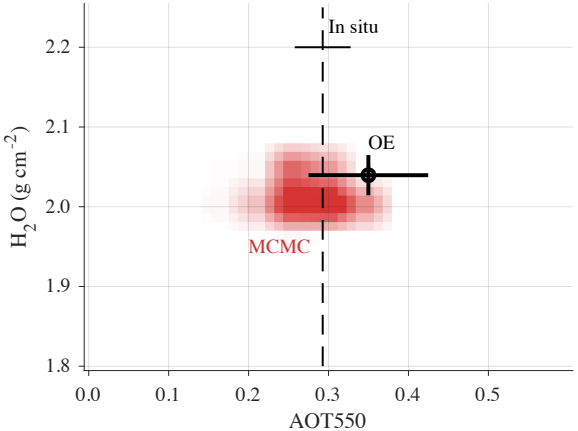
[Realmuto, Thompson et al., *in preparation*]

Sample-based posterior estimation

Monte Carlo estimates are computationally more challenging but capture the full posterior distribution

Linearized estimates work well for reflectance terms



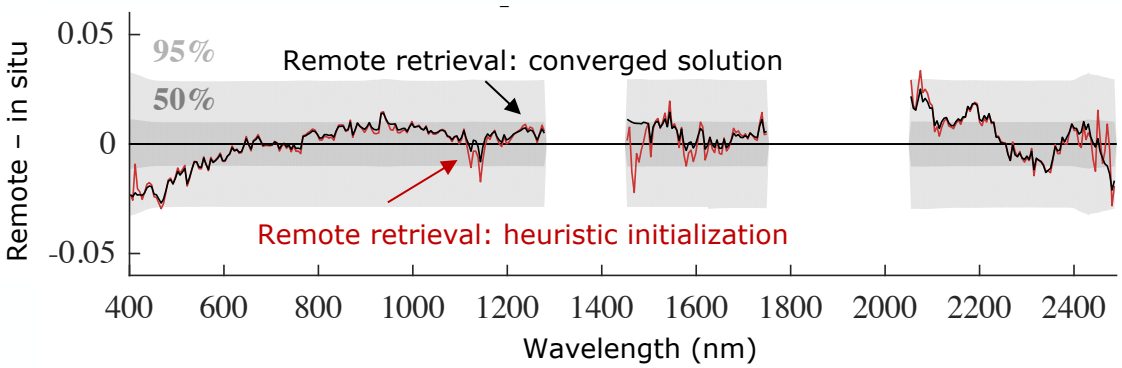


[Thompson et al., *Remote Sensing of Environment* 231, 2019]

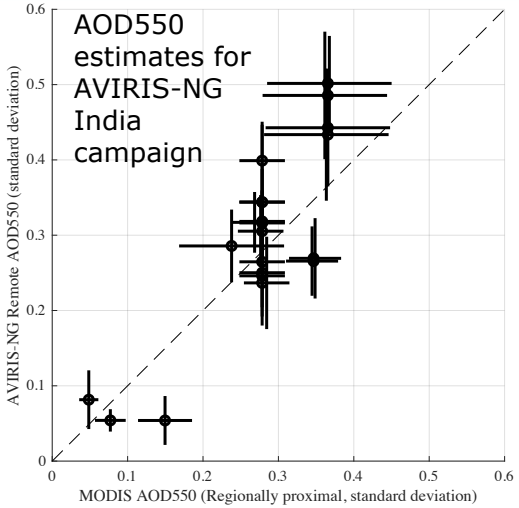
Demonstrating closed uncertainty budgets

Characterize uncertainty via matches to other sensors, vicarious calibration experiments, networks

Requires accounting for uncertainty in two sensors!



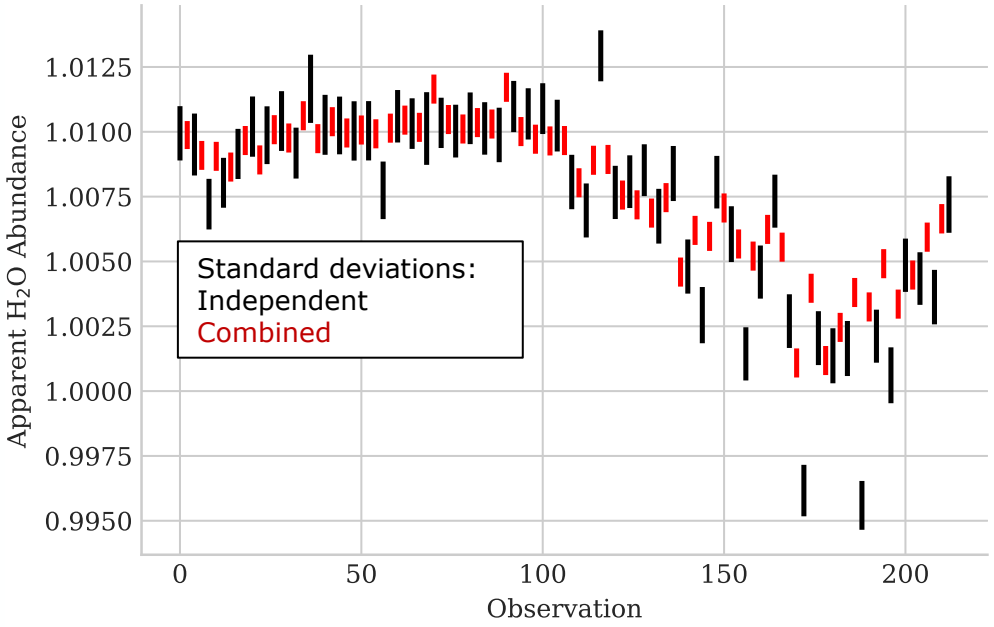
[Thompson et al., *Remote Sensing of Environment* 216, 2018]



[Thompson et al., *Remote Sensing of Environment*, in press]

Combining multiple observations across space and time

- Relate spectra via Markov random fields to capture smooth atmosphere
- For a time series, Kalman smoothing provides a fast optimal dynamic programming solution
- Estimate transition matrices via Expectation Maximization



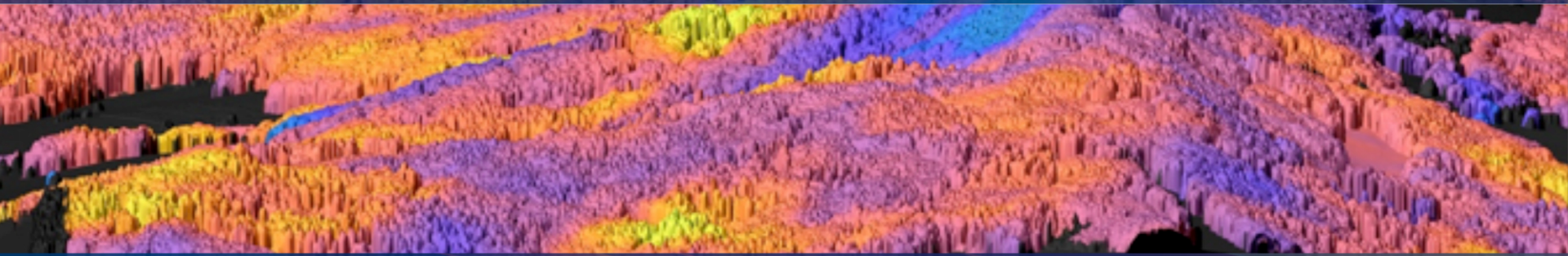
[Swain, Thompson et al., in preparation]

Discussion

How do we report and distribute uncertainties for L1? L2? Beyond?

→ IMAGING SPECTROSCOPY – COOPERATION IN SPACE

From Hyperion & CHRIS via PRISMA & EnMAP to SBG & CHIME



9–11 July 2019 | ESA–ESRIN | Frascati (Rome), Italy