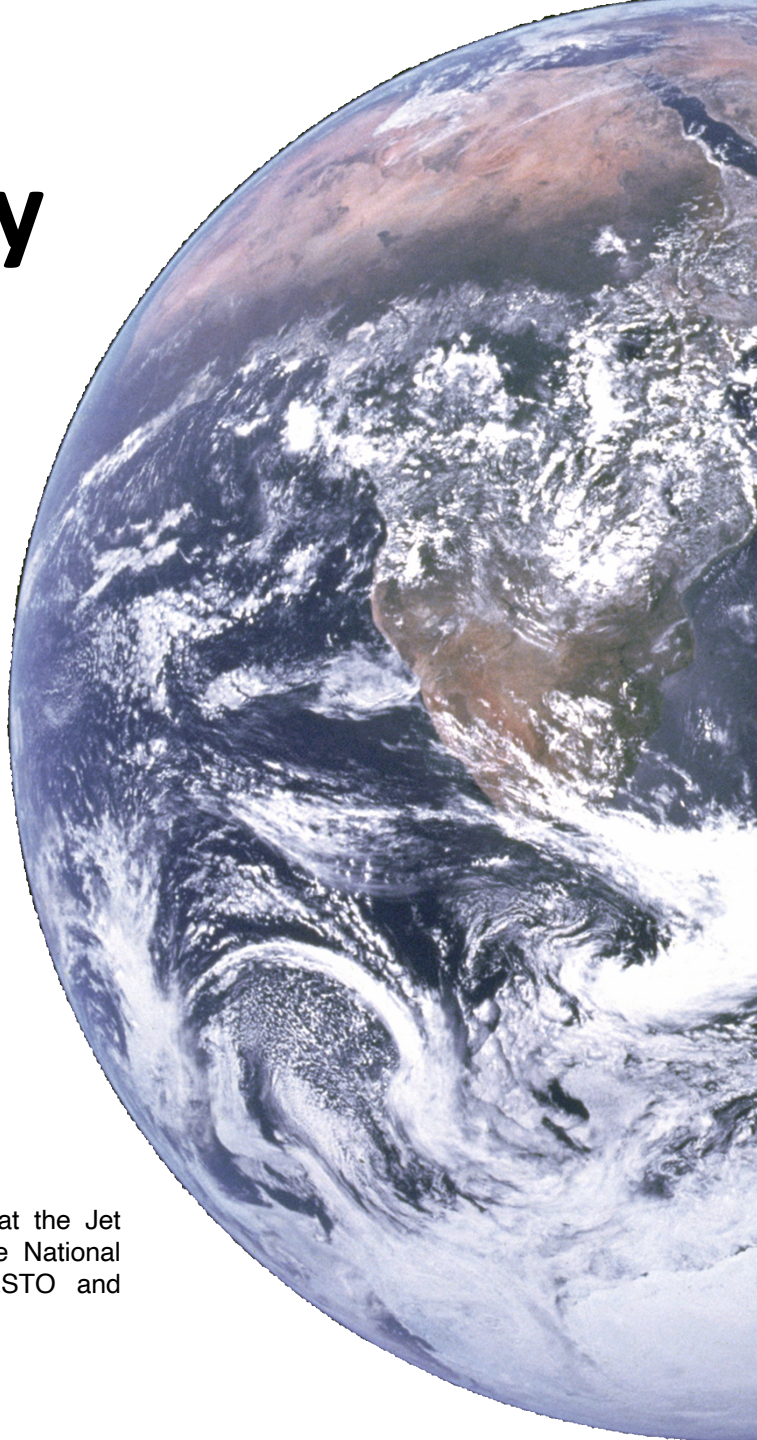
Imaging Spectroscopy for Earth and Planetary Science

David R. Thompson
Jet Propulsion Laboratory, California Institute of Technology



Jet Propulsion Laboratory
California Institute of Technology

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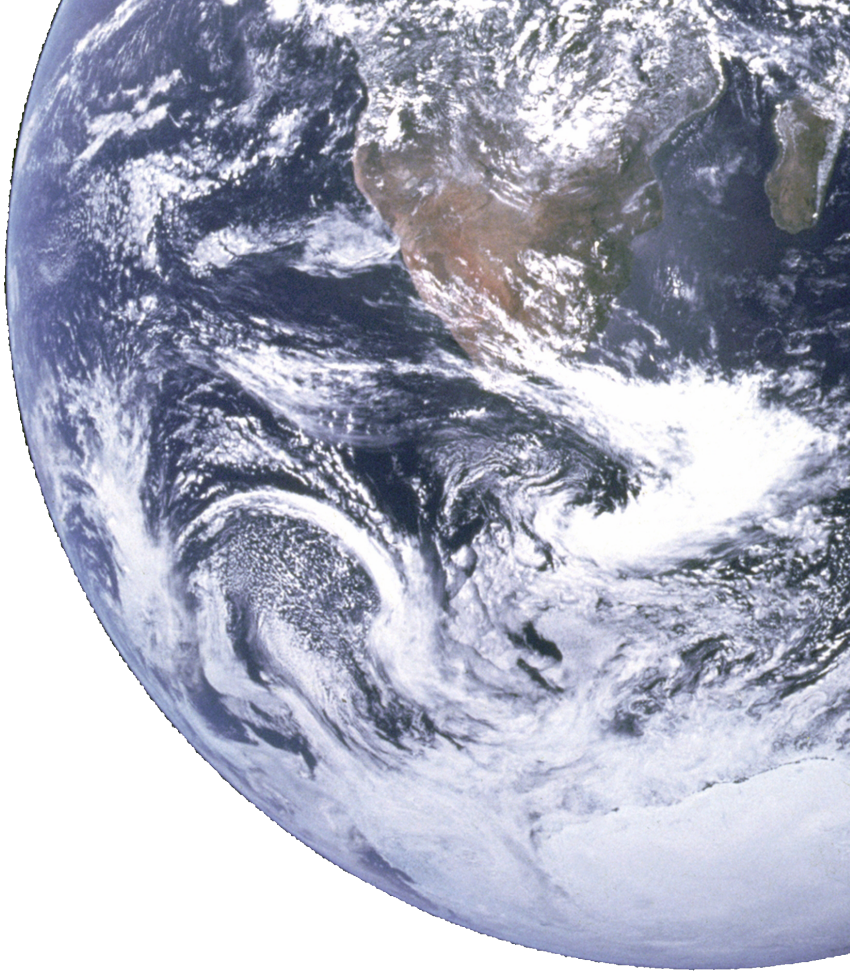
Agenda

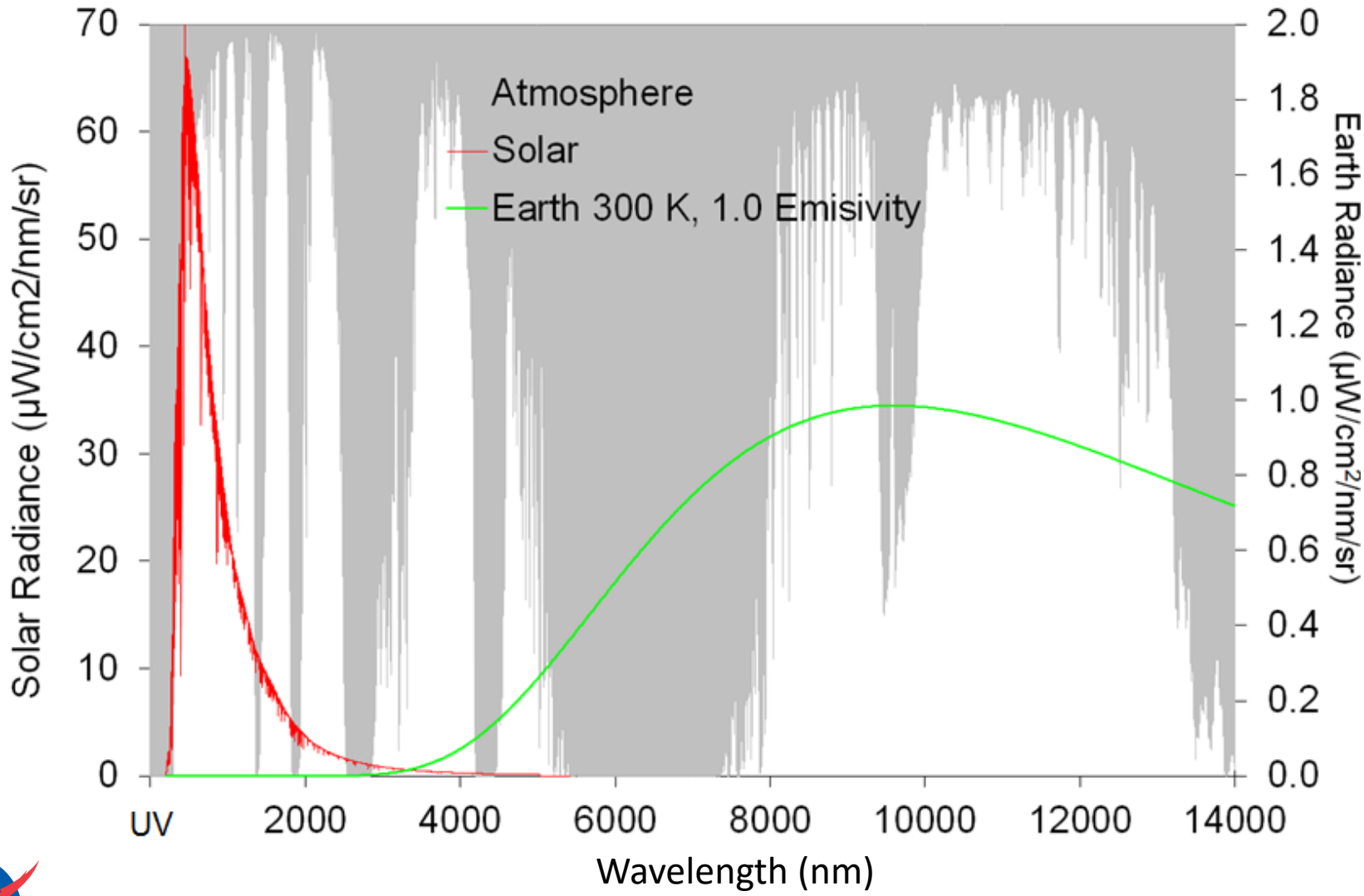
Measurement Method

Science Themes

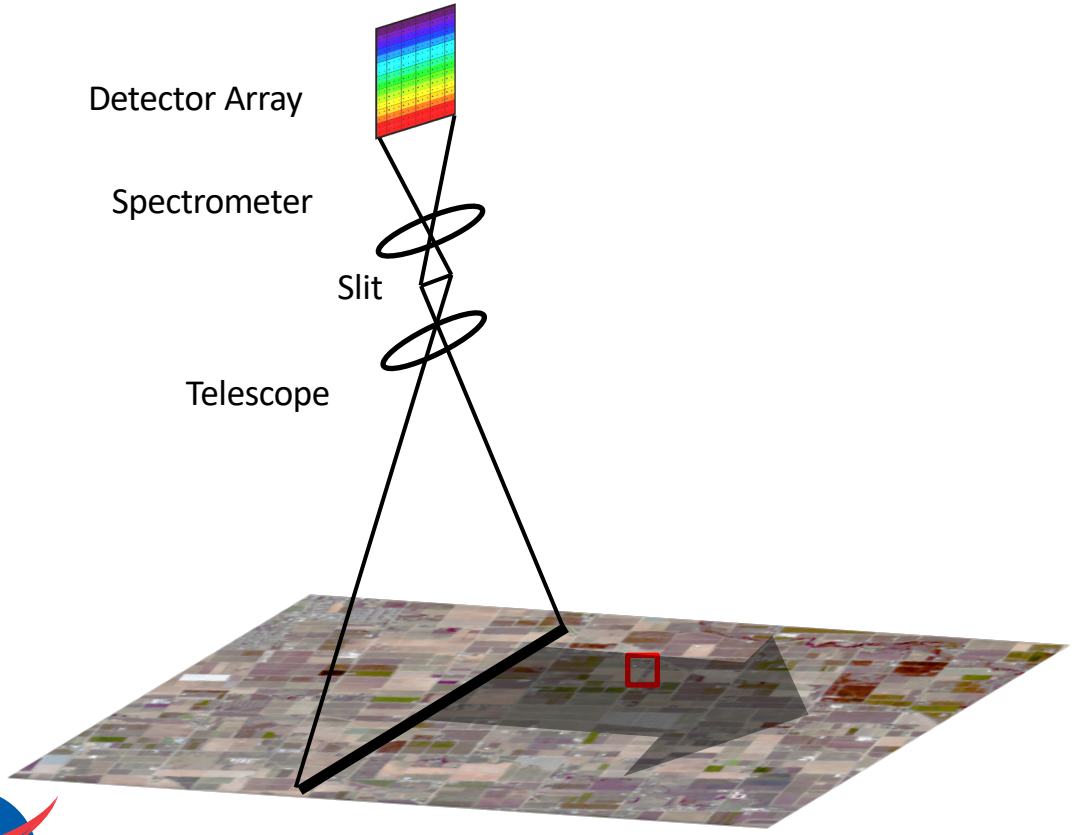
Deep dive: Bayesian Atmospheric Correction



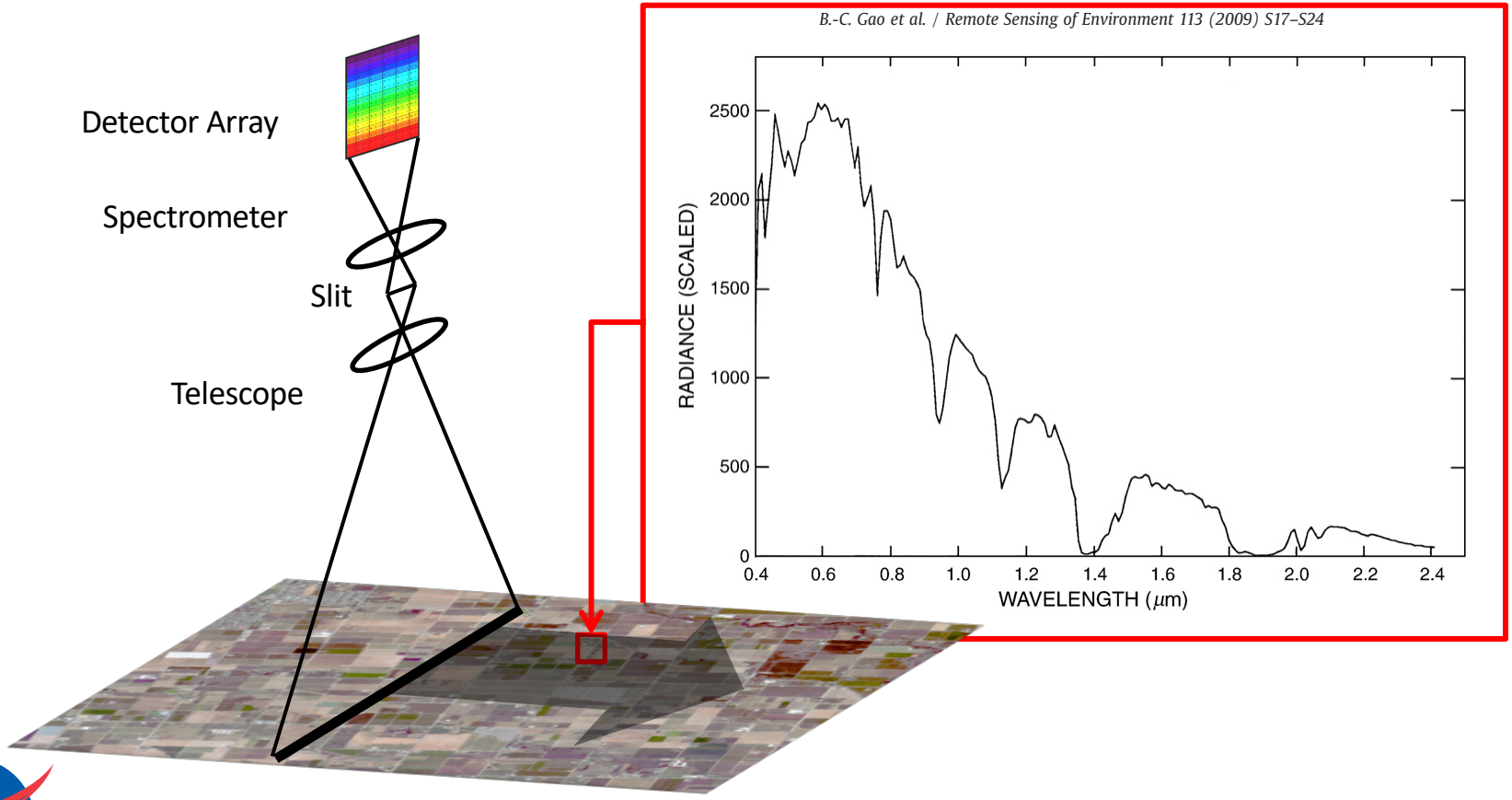
Dramatis Personae



Imaging spectroscopy – 100s of parallel spectrometers



Imaging spectroscopy – 100s of parallel spectrometers



Imaging spectroscopy at JPL

1982

1986

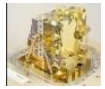
1989

1997

2000

1998

2005


2009

2008

24 Months

- First Imaging Spectrometer AIS flights in 1982
- AVIRIS imaging spectrometer > 1000 refereed journal articles
- NIMS imaging spectrometer to Jupiter
- VIMS imaging spectrometer to Saturn
- MICAS Miniature Integrated Camera and Imaging Spectrometer to Comet
- Hyperion-Earth, CRISM-Mars and ARTEMIS-Earth imaging spectrometers (gratings, designs, calibration, science)
- NASA Moon Mineralogy Mapper (M3)
- > 7 Airborne/Rover-type Imaging Spectrometer operating at cryogenic temperature and in a vacuum (2005-2015)

MaRS 2005

24 Months

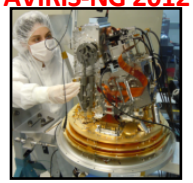
24 Months

CAO 2010

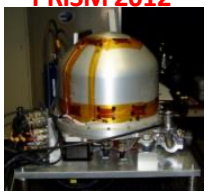
< 18 Months

MSS 2011

AVIRIS-NG 2012

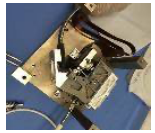


PRISM 2012

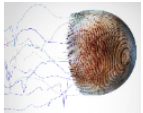


UCIS 2013

ESWIRS 2014

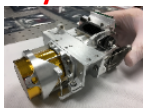


MISE 2015



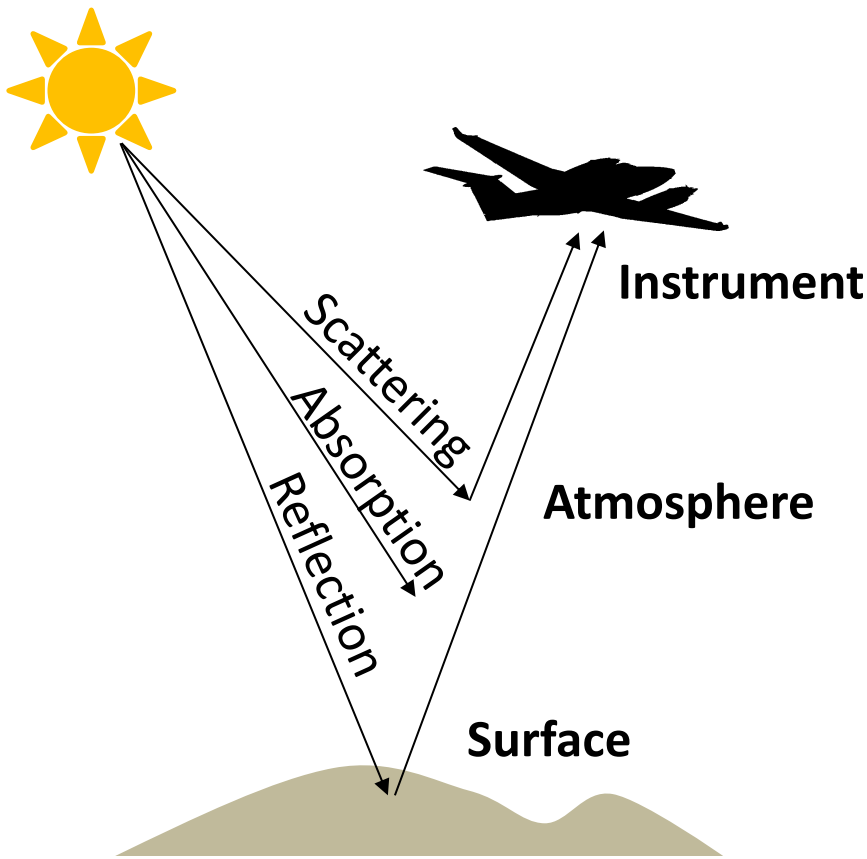
CWIS 2016

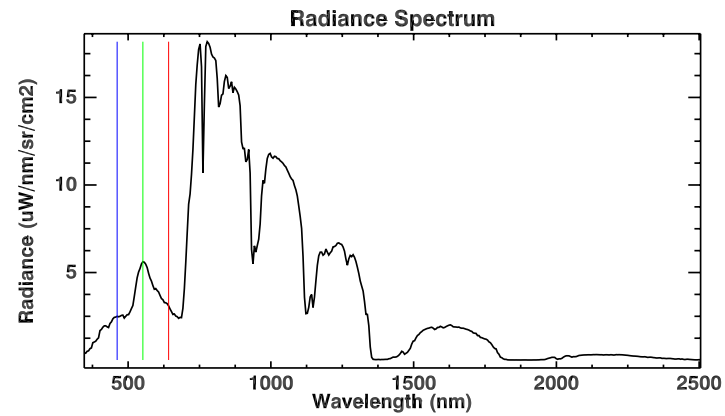
VS-Dyson 2017

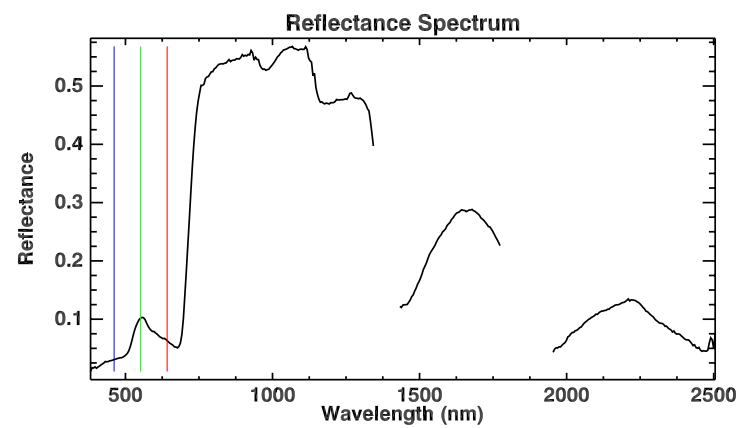


From radiance to reflectance

[Thompson et al., RSE 2015; Thompson et al., RSE 2018]







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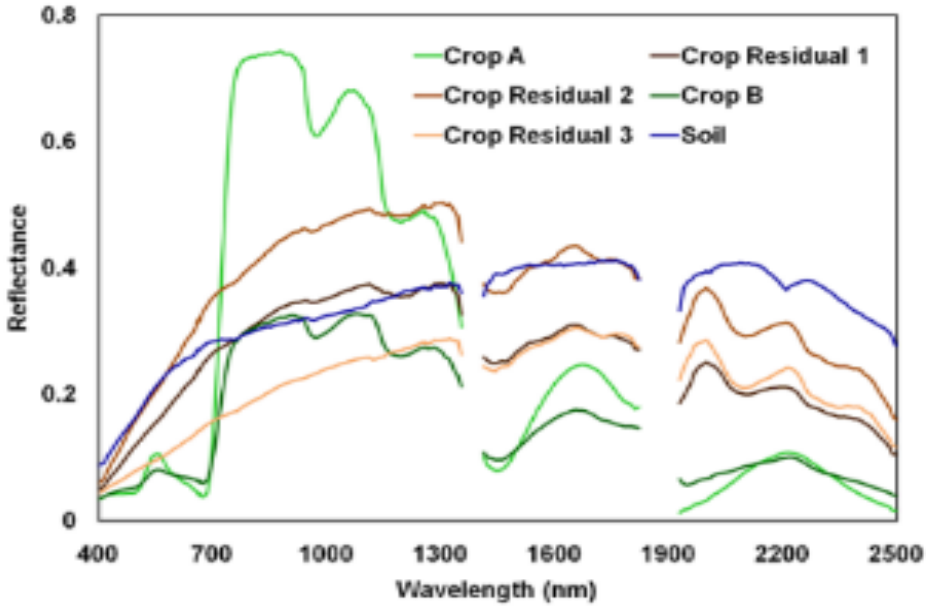
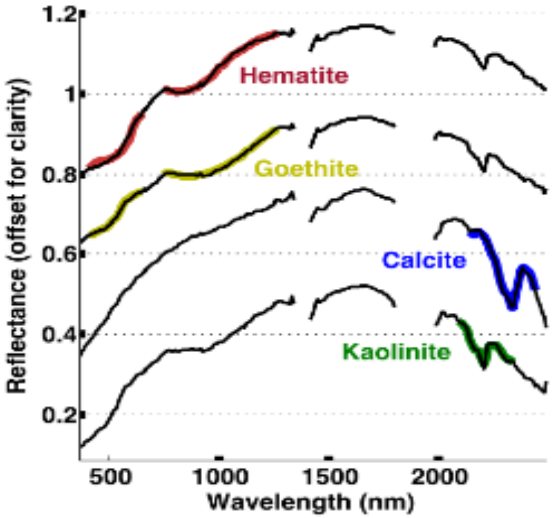
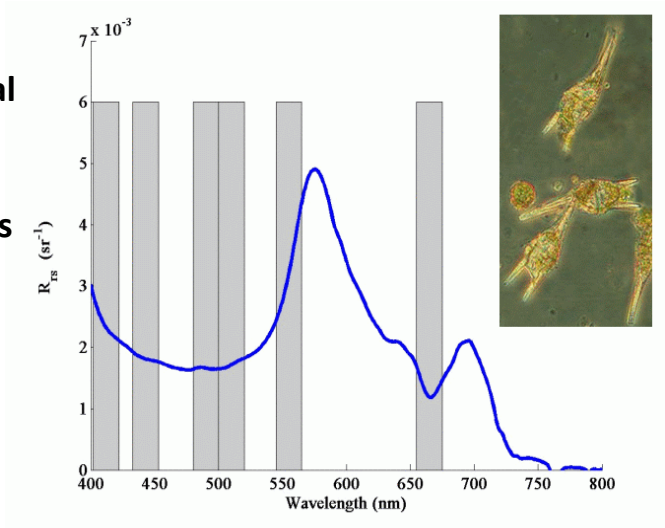
Agriculture and Terrestrial Ecosystems



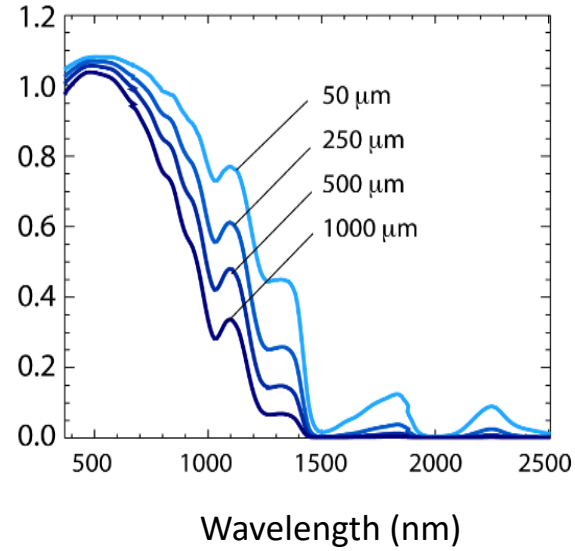
Geology, Soils, Surface Composition



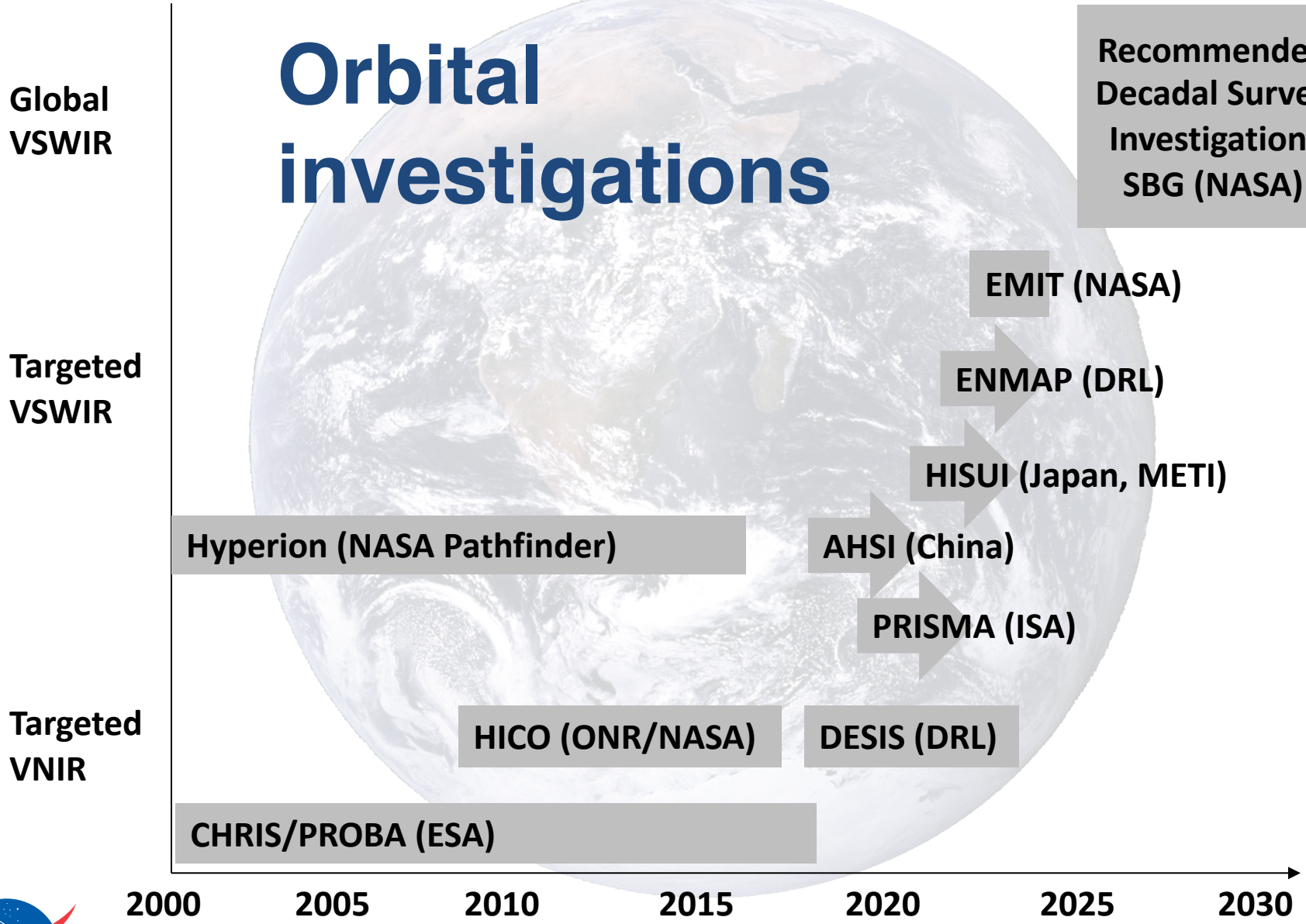
Coastal and Inland Waters

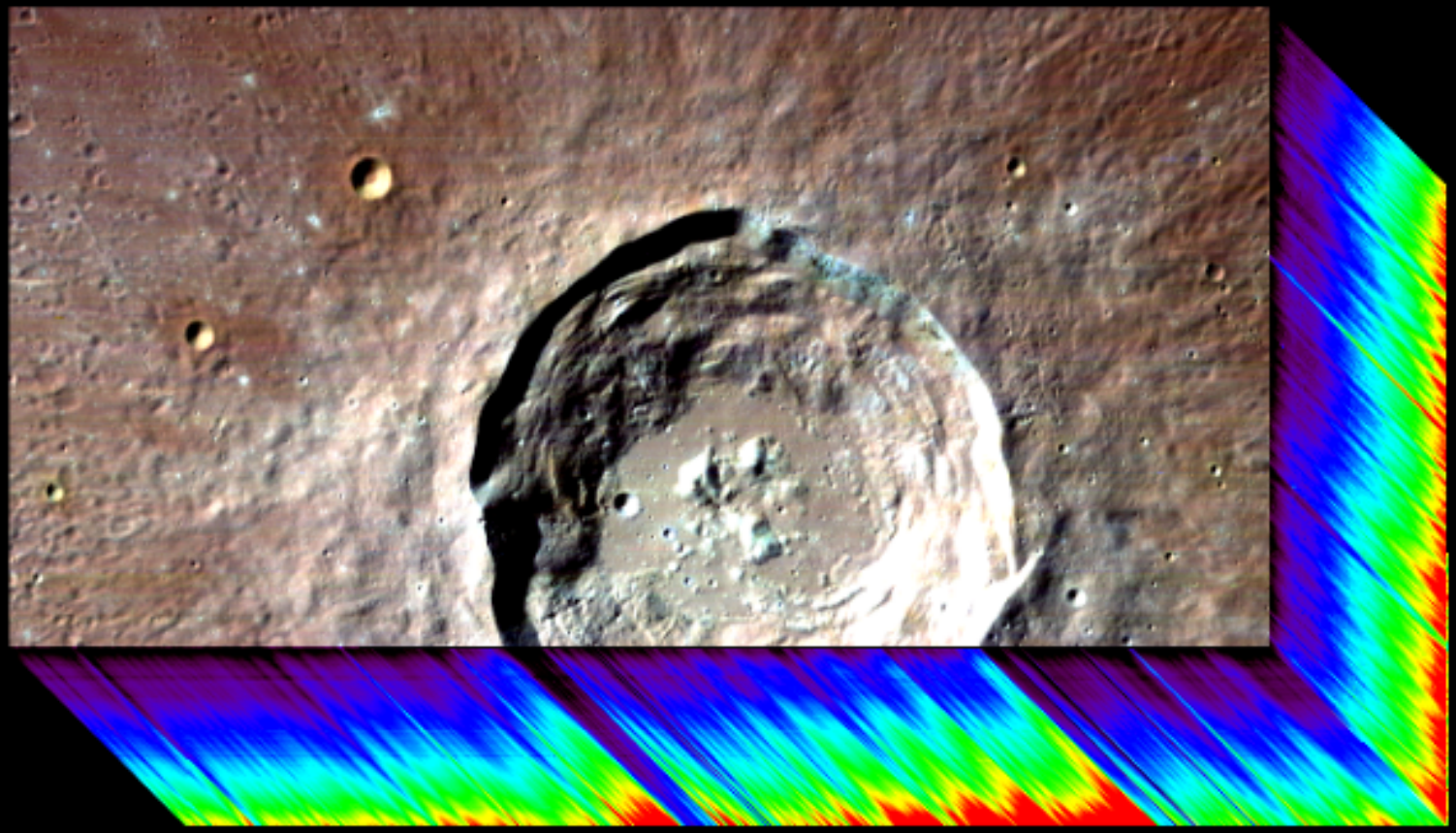


Snow and Ice



Orbital investigations





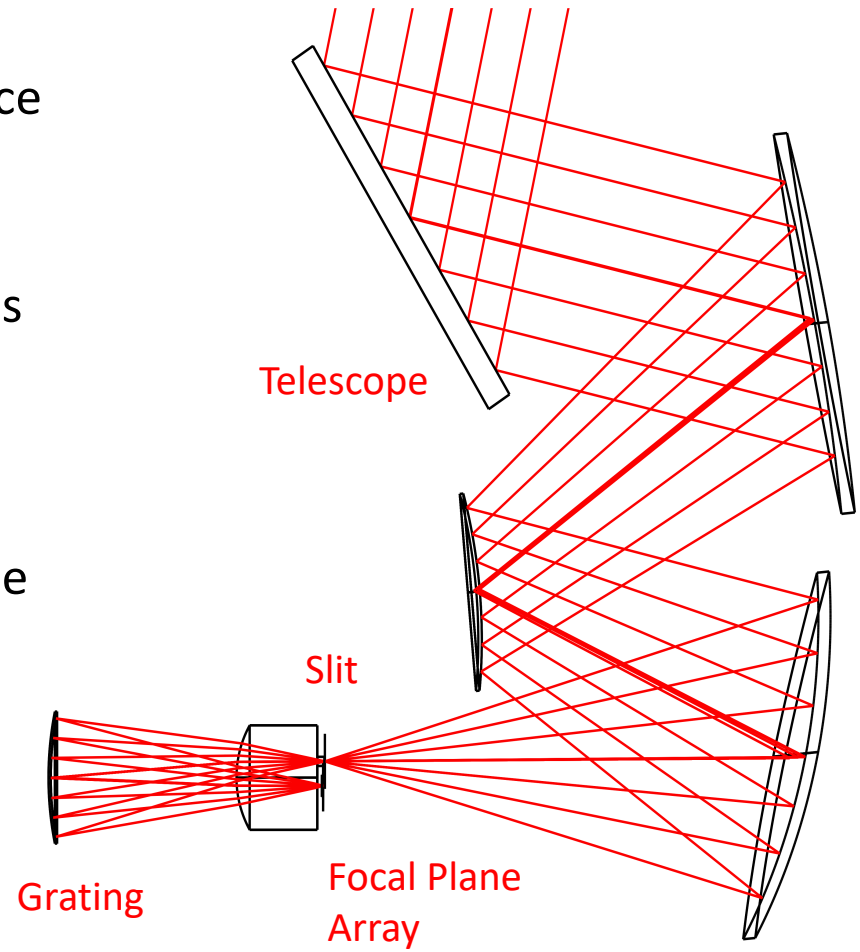
Special needs of remote Earth science

High accuracy: e.g. sub-percent surface reflectance

Physical interpretability: Output reported in physical units of quantities measurable *in situ*, and traceable to rigorous physical models

Rigorous uncertainty propagation: Respect input noise, report confidence intervals

Generalizability: should apply across different new locales, new spatiotemporal sampling



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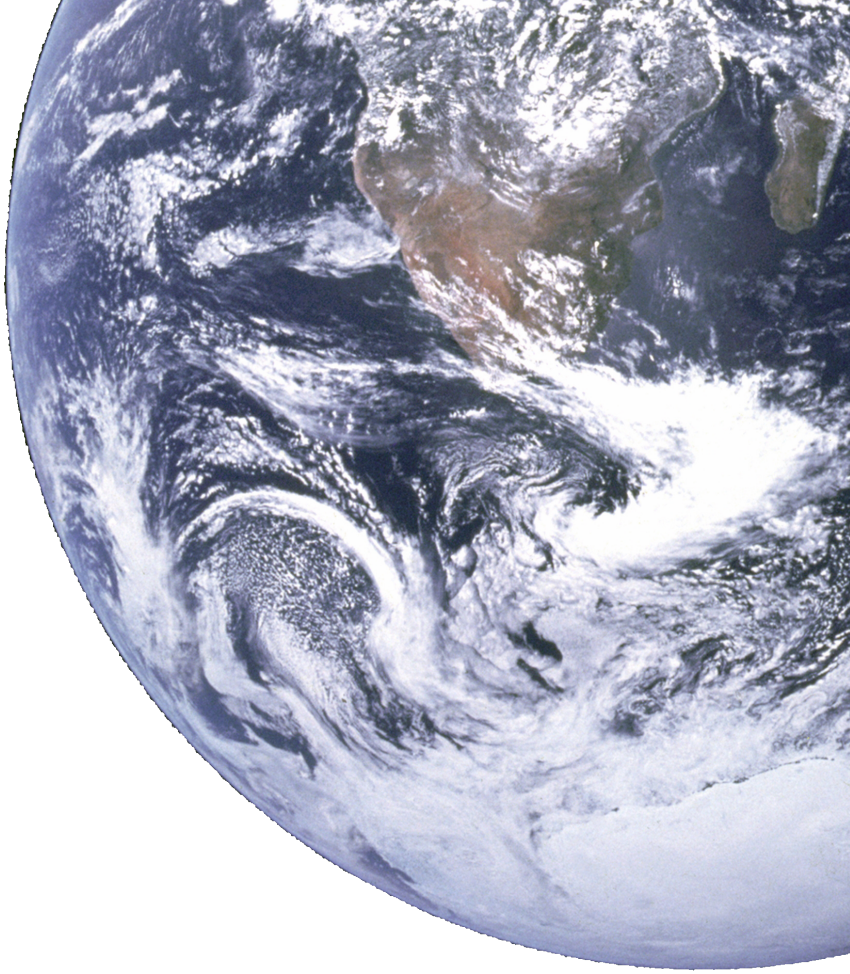
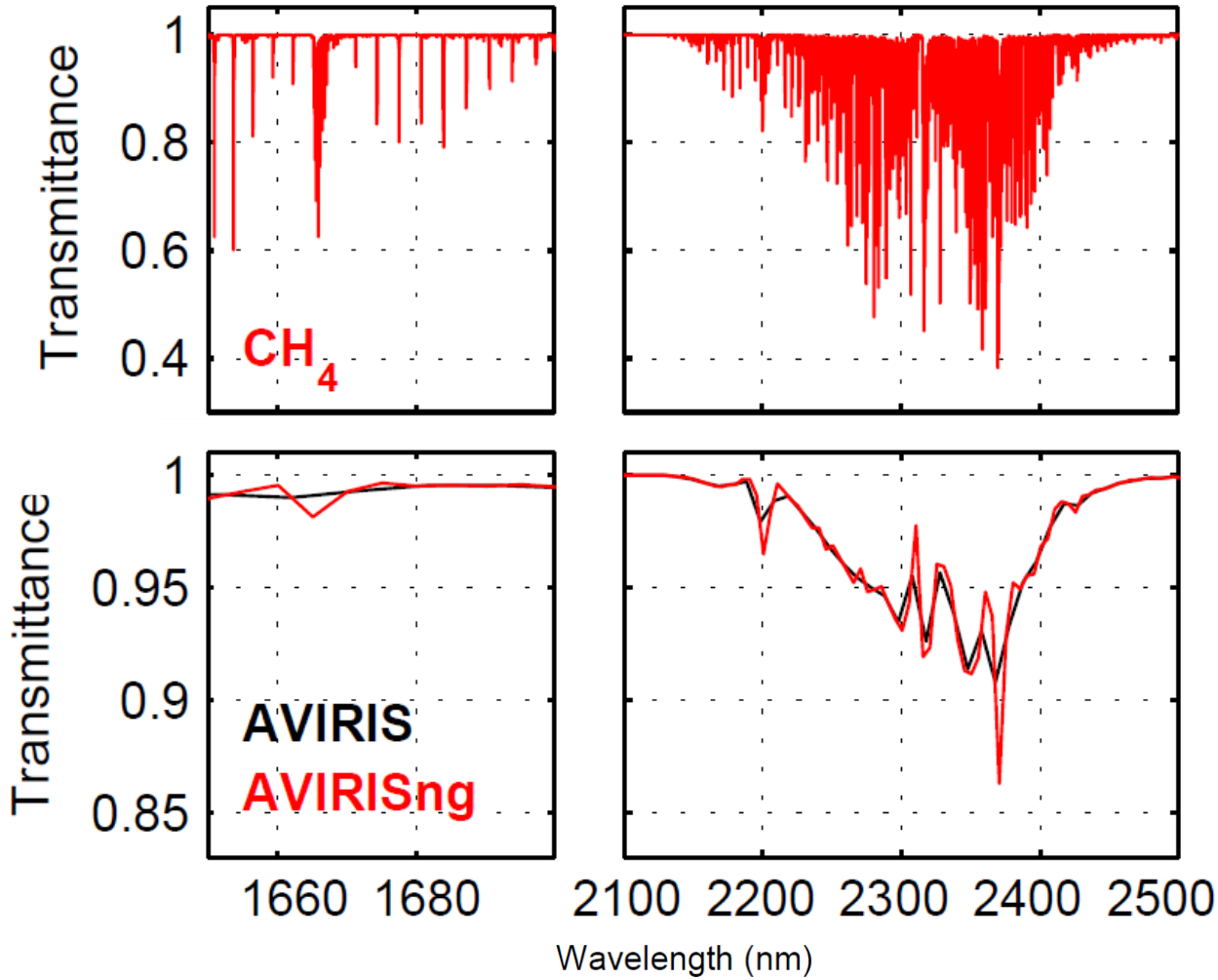


Localized greenhouse sources



Localized greenhouse sources

Matched filter applied independently in each column

$$\hat{\alpha}(\mathbf{x}) = (\mathbf{x} - \mu)^T \Sigma^{-1} \mathbf{t} / (\mathbf{t}^T \Sigma^{-1} \mathbf{t})$$

Mixing ratio length

Tested spectrum

Background mean

Background covariance

target

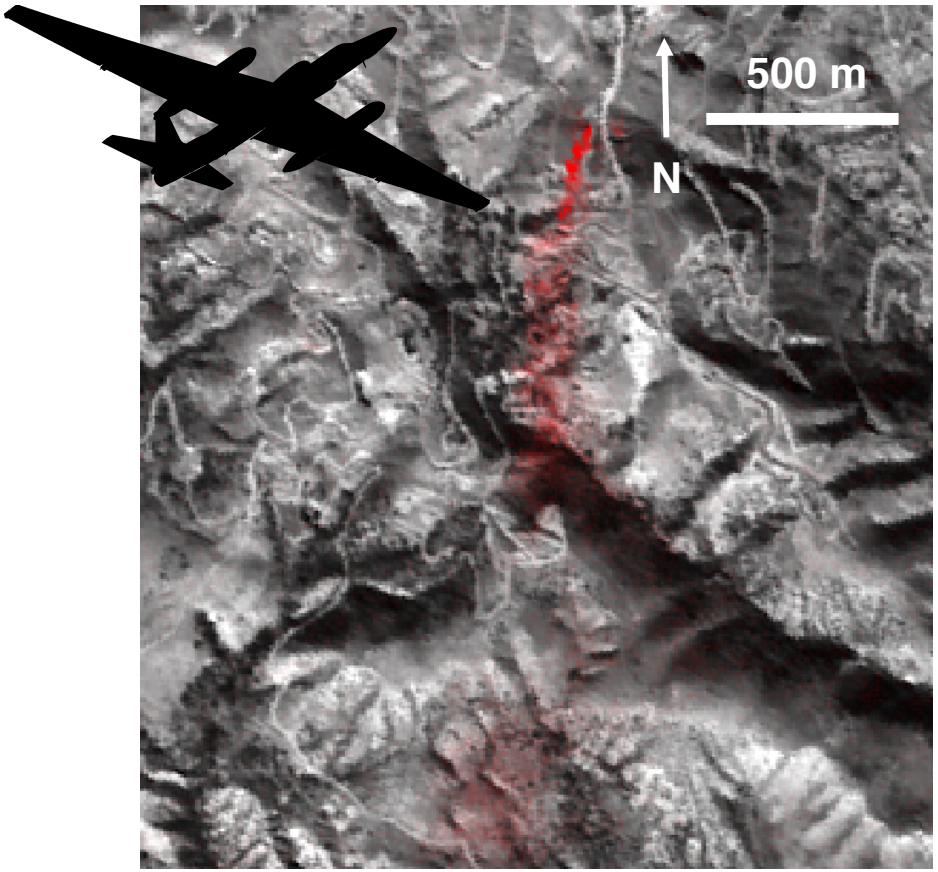
Using the target signature

$$\mathbf{t} = \partial \mathbf{x} / \partial \ell = -\mu e^{-\kappa \ell} \kappa = -\mu \kappa$$

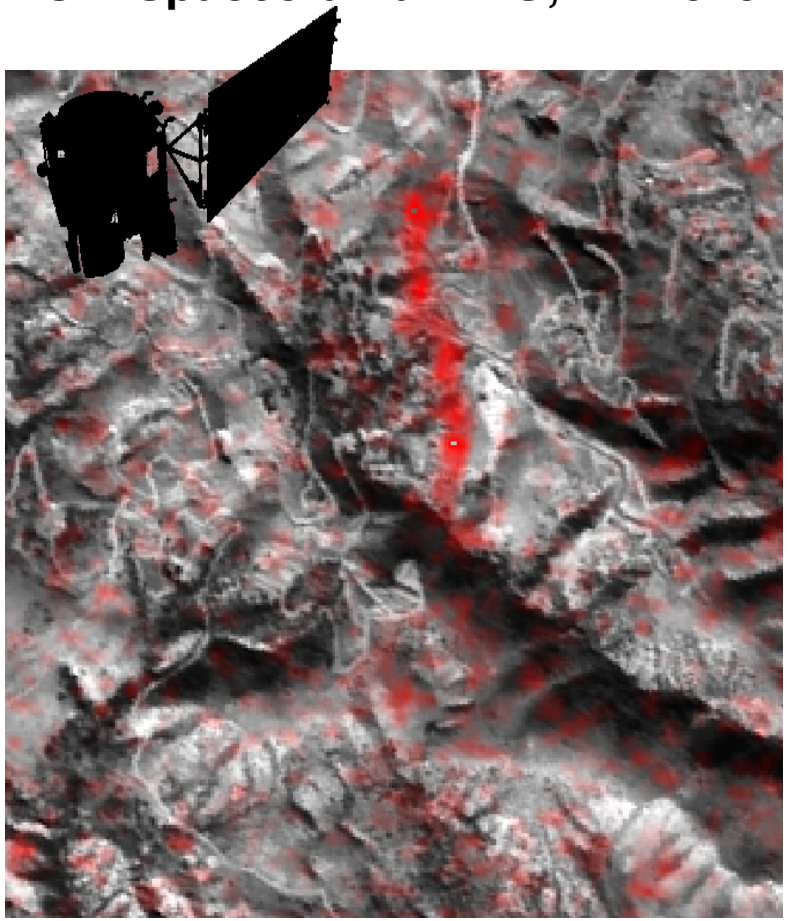
Unit absorption coefficient

Aliso canyon gas storage leak

ER-2 at 6.6 km altitude, 1/12/2016



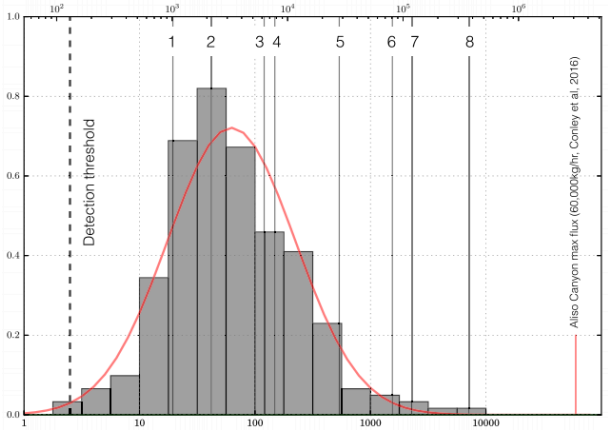
EO-1 Spacecraft at LEO, 1/1/2016

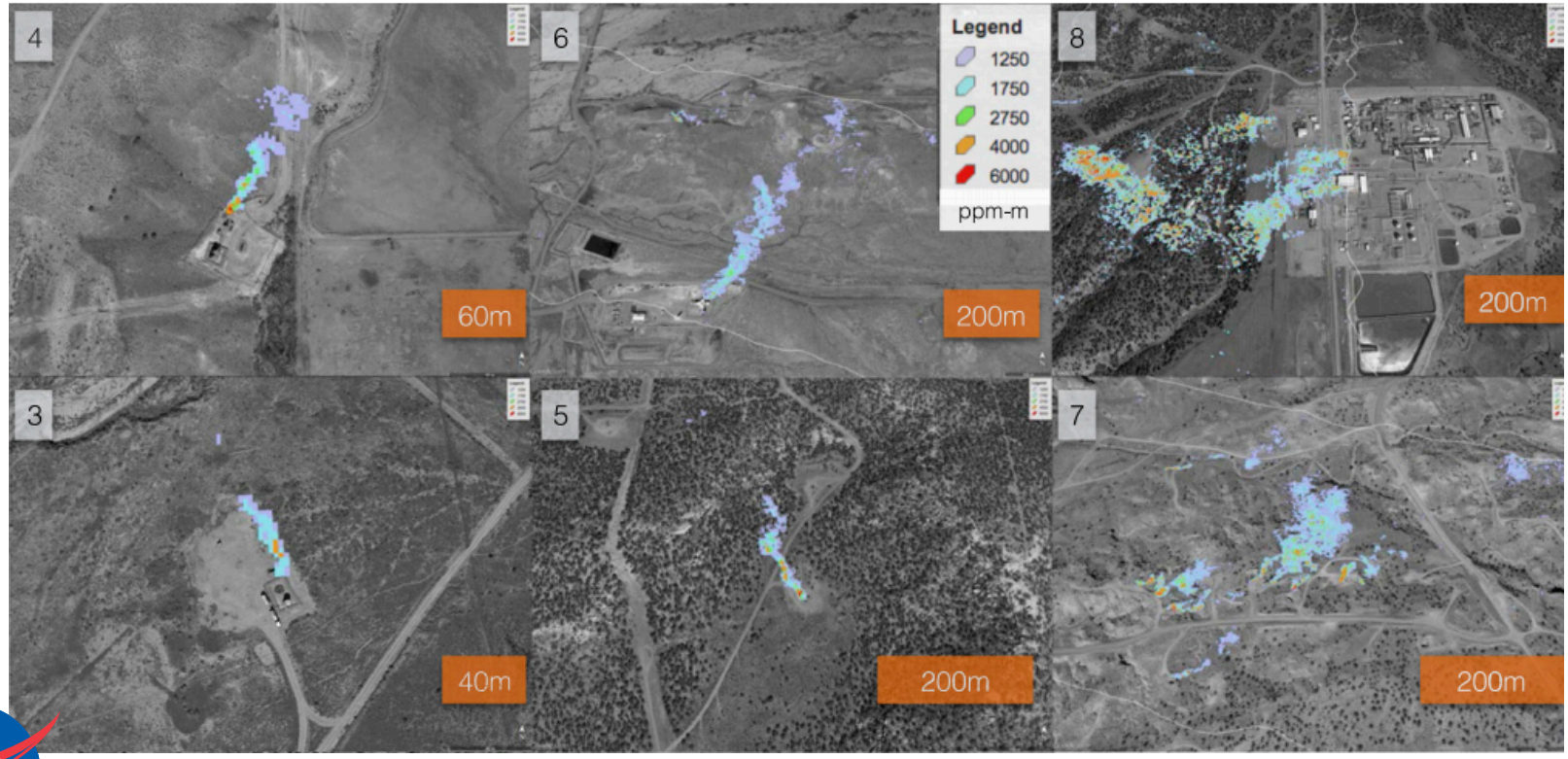


Thompson et al., *Geophys. Res. Lett.* (2016)

Fugitive CH_4 emissions at Four Corners, NM

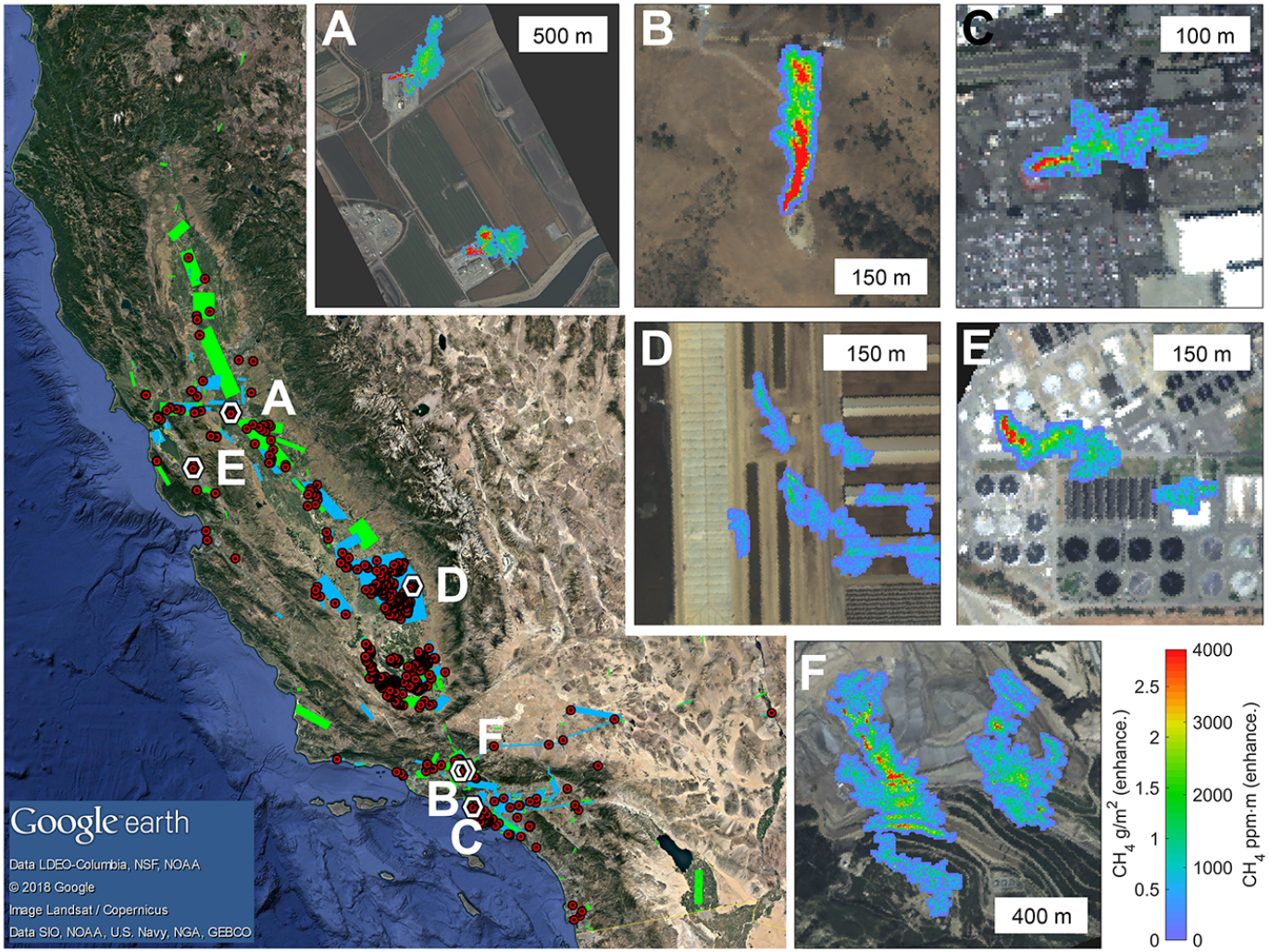
Frankenberg, Thorpe, Thompson et al., PNAS 2016

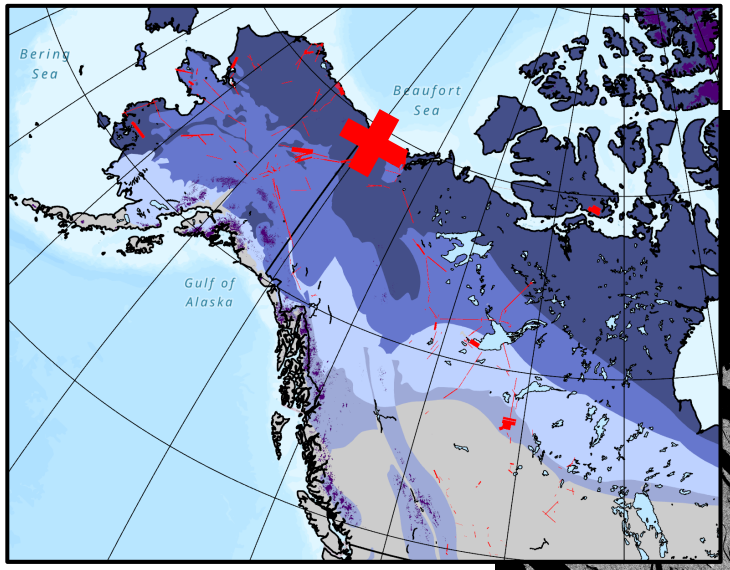


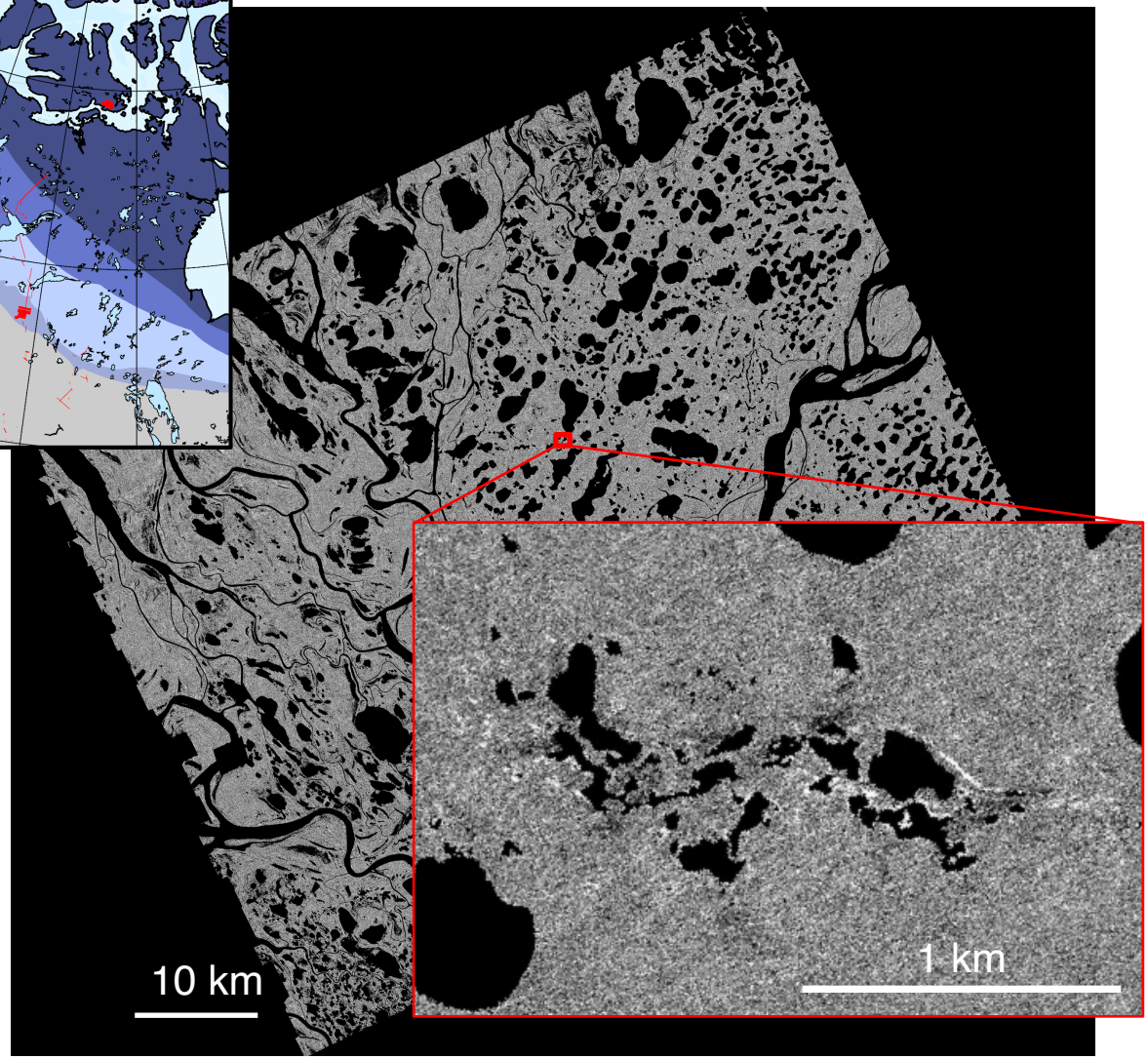


CH_4 in California

Duren et al. (in review), Thorpe et al. (2016), Thompson et al. (2015)





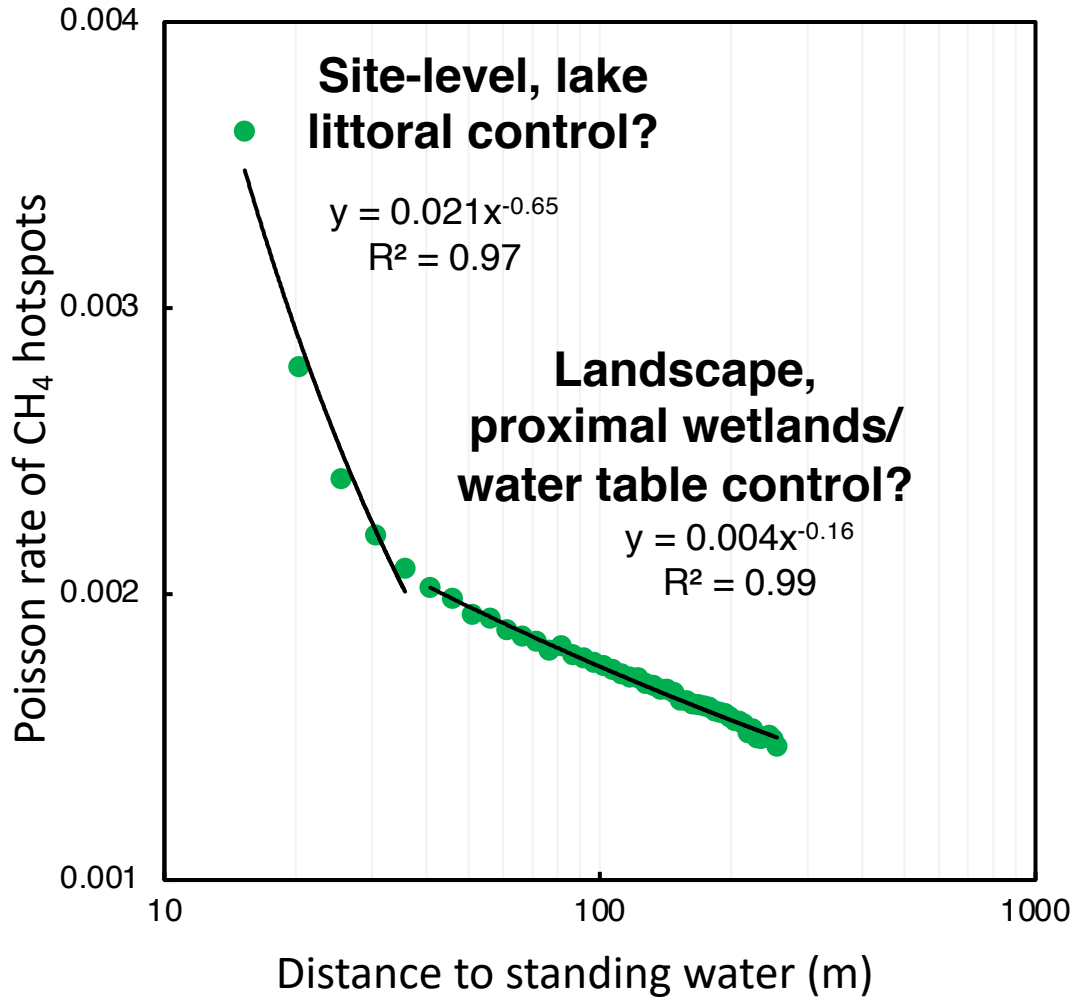


Arctic CH_4 Emissions

Elder, Thompson, et al. (in preparation)
Analysis of AVIRIS-NG data from the ABoVE campaign, PI: Chip Miller

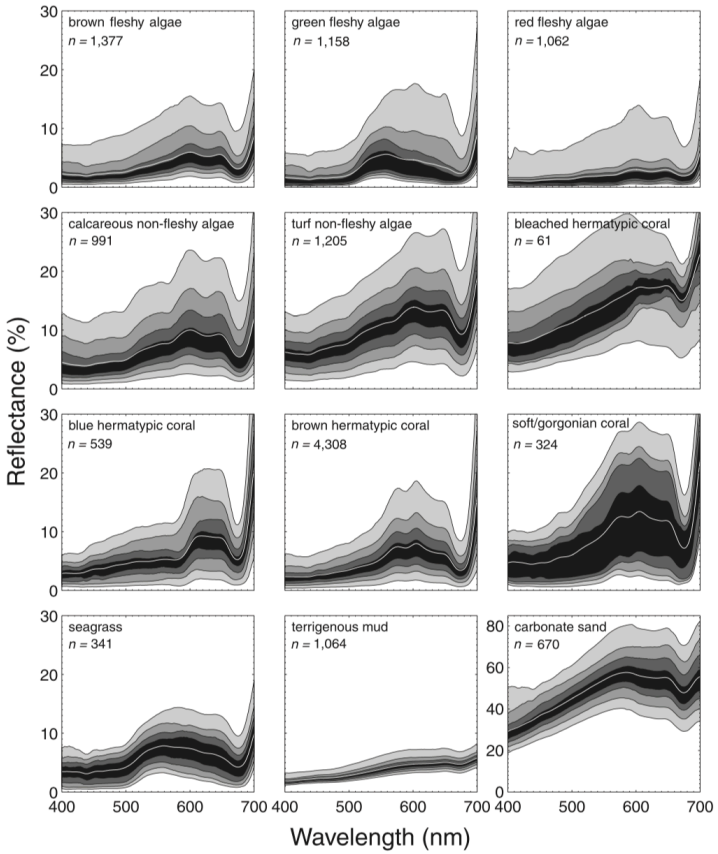
Arctic-wide statistics reveal a two component power law

Elder, Thompson, et al. (in preparation) Analysis of AVIRIS-NG data from the ABoVE campaign
PI: Chip Miller

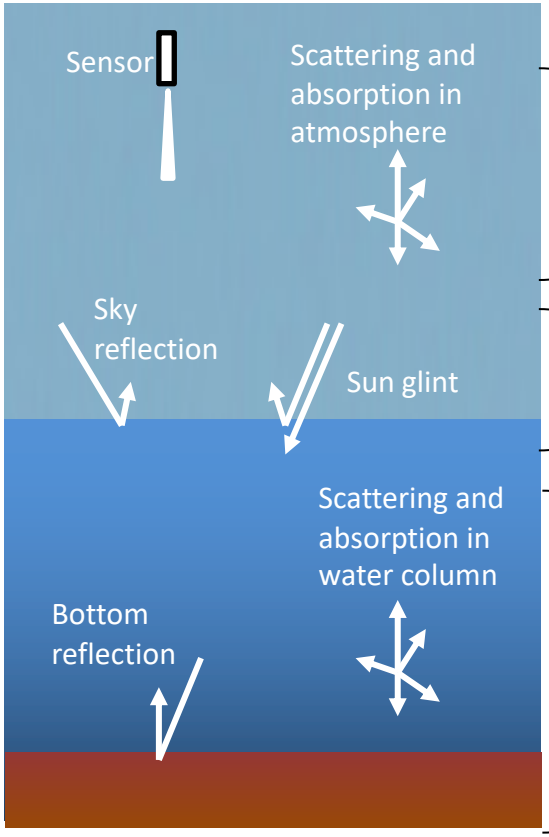


The CORAL EV-S mission

PI: Eric Hochberg (BIOS) Deputy PI: Michelle Gierach (JPL)



Hochberg et al., *Remote Sensing of Environment* 2003



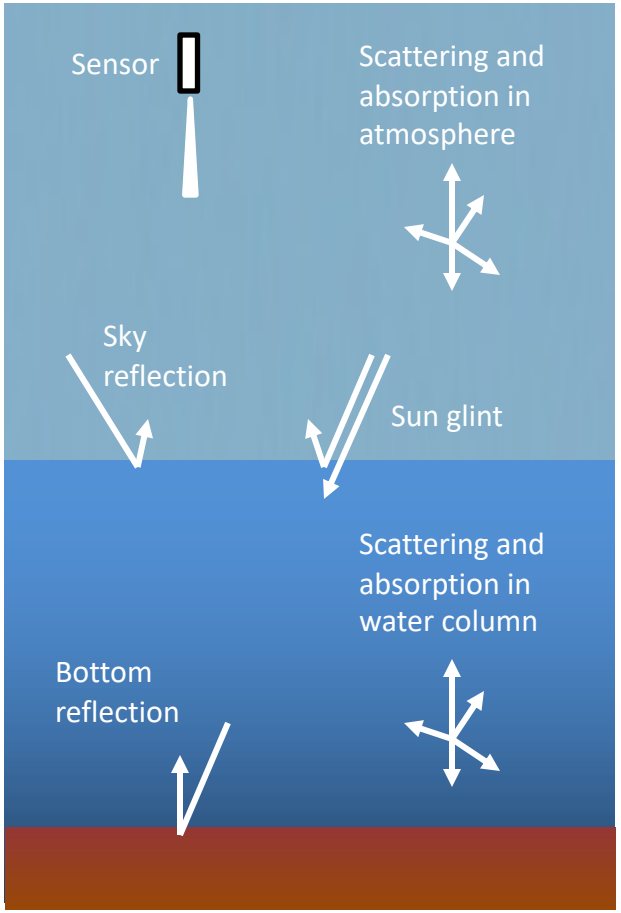
Step 1
Aerosol optical depth τ
Aerosol type ζ
Water leaving reflectance R_{rs}

Step 2
Glint-corrected Rrs_0

Step 3
Backscatter b_b
Attenuation K_d
Depth H
Benthic reflectance R_b

Thompson et al., *Remote Sensing of Environment* 2017

Estimating Benthic Reflectance



Retrieved quantities

Step 1
Aerosol optical depth τ
Aerosol type ζ
Water leaving reflectance R_{rs}

Step 2
Glint-corrected Rrs_0

Step 3
Backscatter b_b
Attenuation K_d
Depth H
Benthic reflectance R_b

Graphic inspired by [Kirk, 2011].

Procedure

Posit the relation [Maritorena et al., 1994]:

$$Rrs_0 = R_{inf} + (R_b - R_{inf})\, e^{-2K_d H}$$

bb / ($2K_d$)

Benthic reflectance

Attenuation

Depth

Procedure

Posit the relation [Maritorena et al., 1994]:

$$Rrs_0 = R_{inf} + (R_b - R_{inf})\, e^{-2K_d H}$$

bb / ($2K_d$)

Benthic reflectance

Attenuation

Depth

Problem: underdetermined

K_d, bb, and R_b yield (3N + 1) parameters for just N measurements

Procedure

Posit the relation [Maritorena et al., 1994]:

$$Rrs_0 = R_{inf} + (R_b - R_{inf})\, e^{-2K_d H}$$

bb / ($2K_d$) — Benthic reflectance — Attenuation — Depth

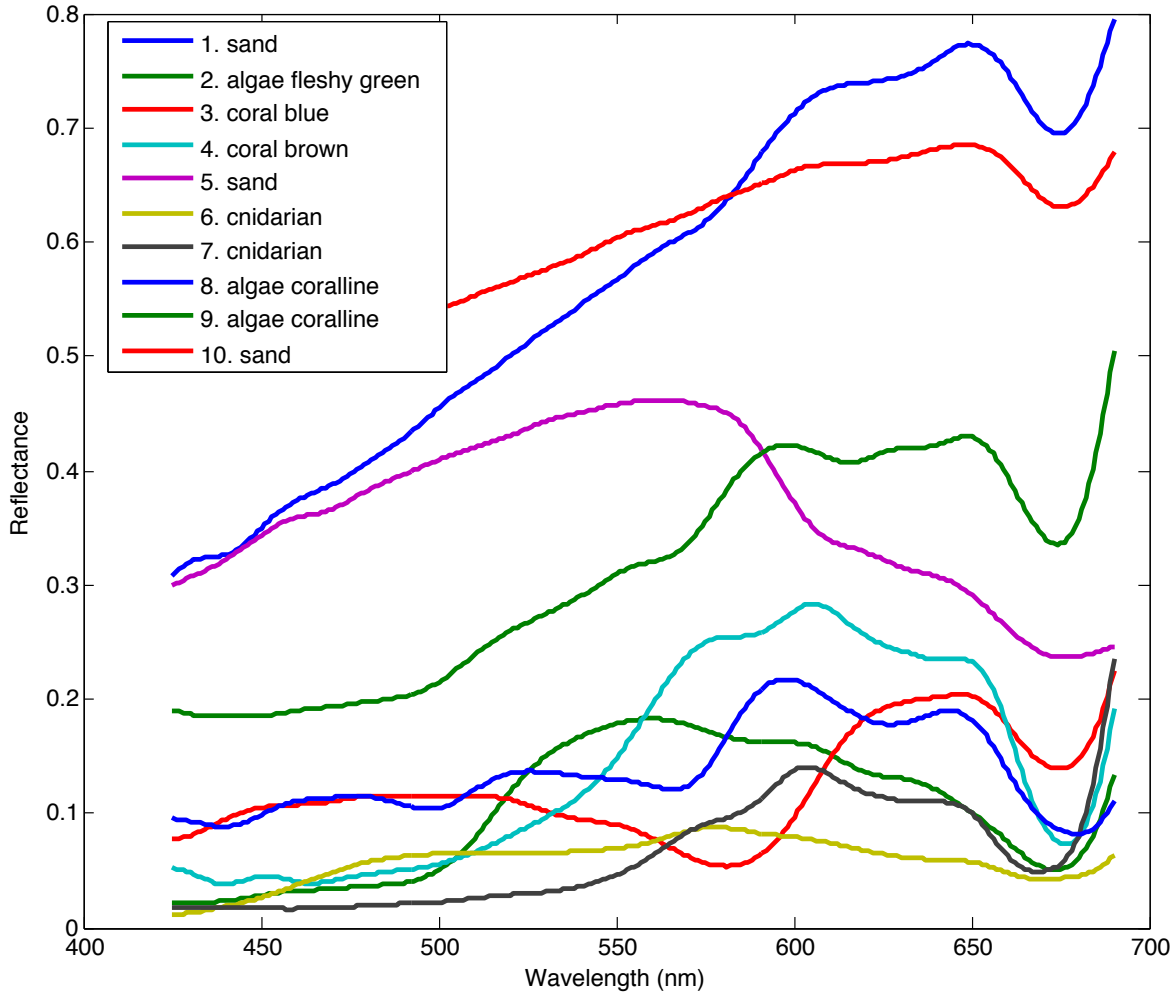
Problem: underdetermined

K_d, bb, and R_b yield (3N + 1) parameters for just N measurements

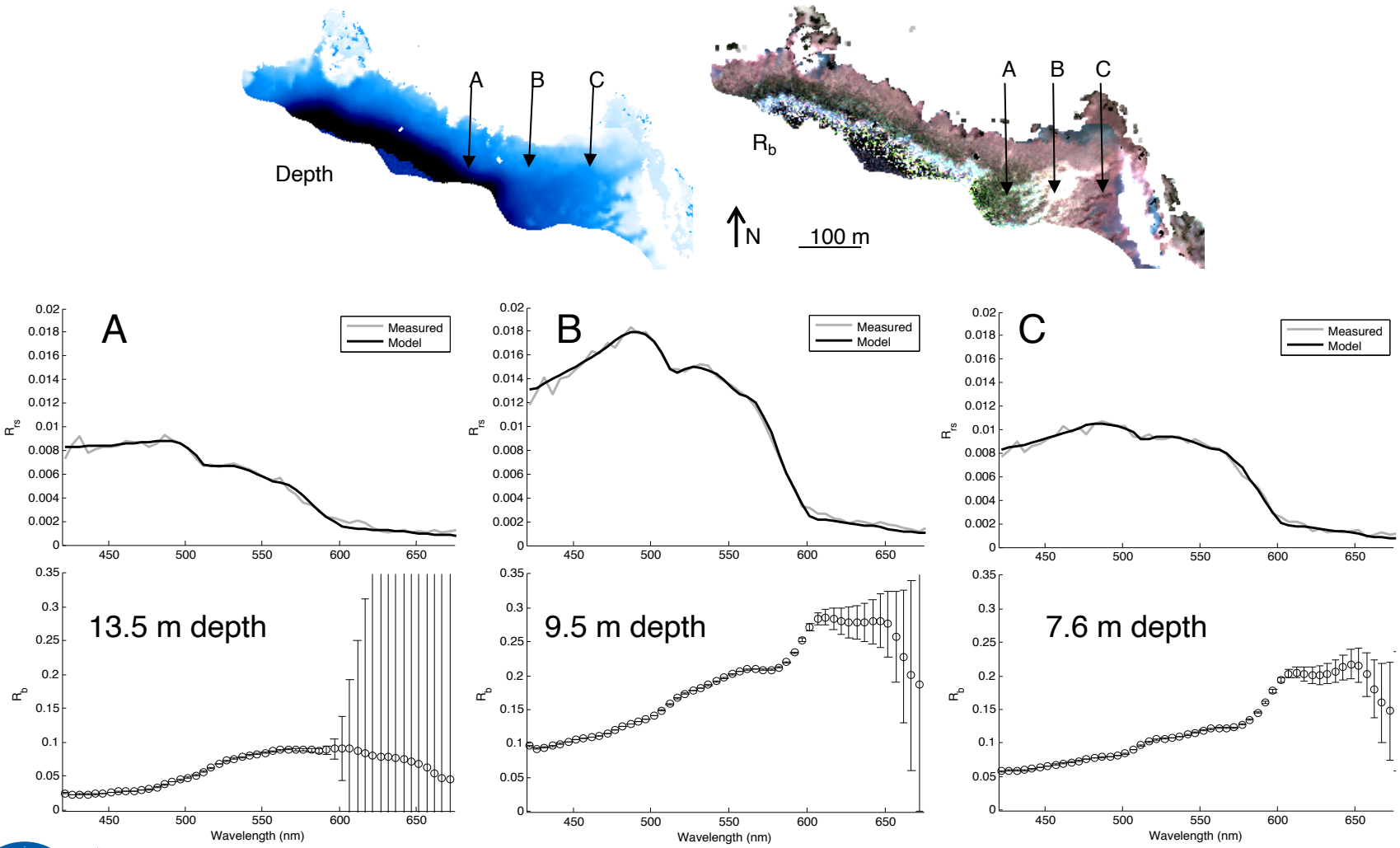
Solution: represent as linear mixtures

Parameterize K_d, bb, and R_b as nonnegative linear combinations of endmember spectra, and retrieve mixing coefficients (~20 DOF)

Example of R_b endmember library

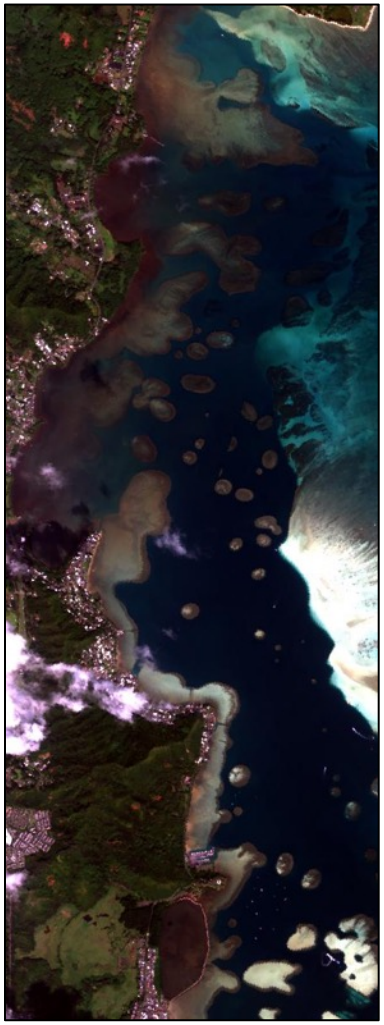


R_{rs} vs. bottom reflectance result

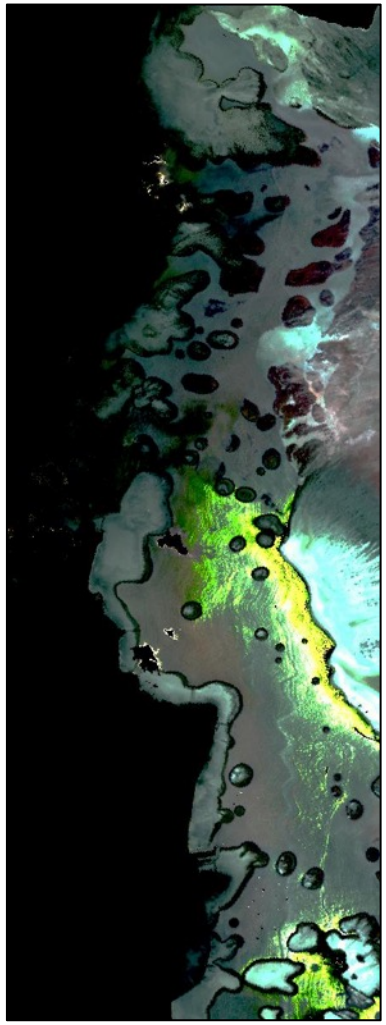


Airborne VSWIR data collected by the Carnegie Airborne Observatory

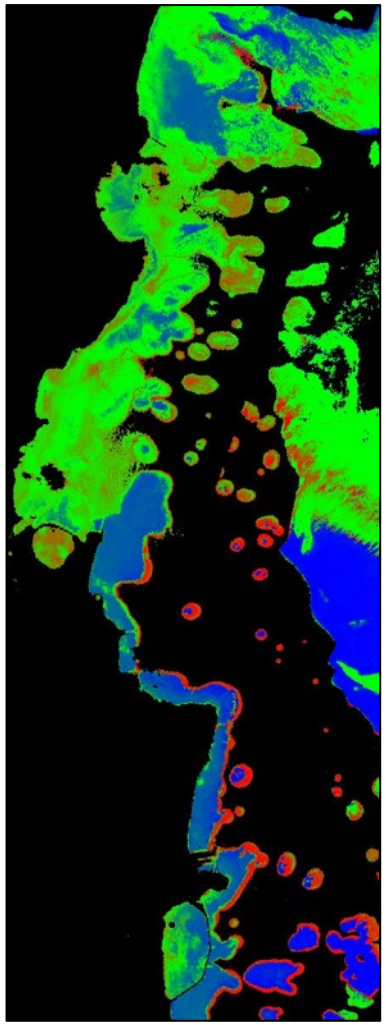
Water-leaving Reflectance



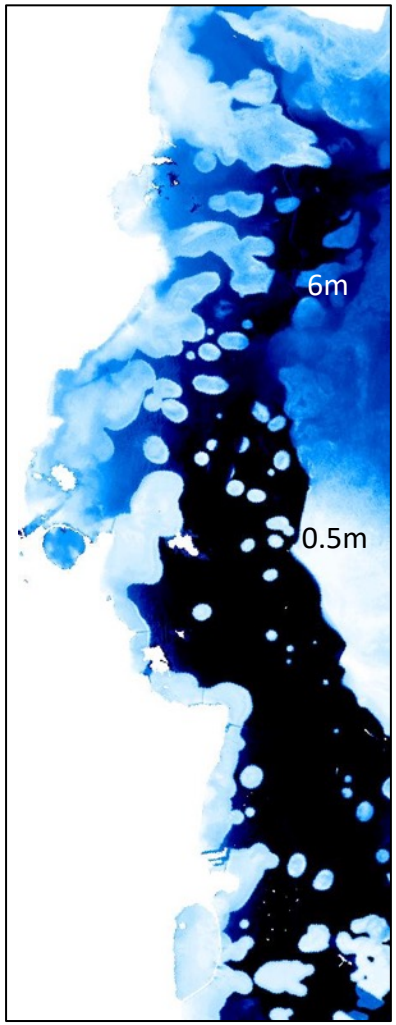
Rb



Benthic Cover



Depth



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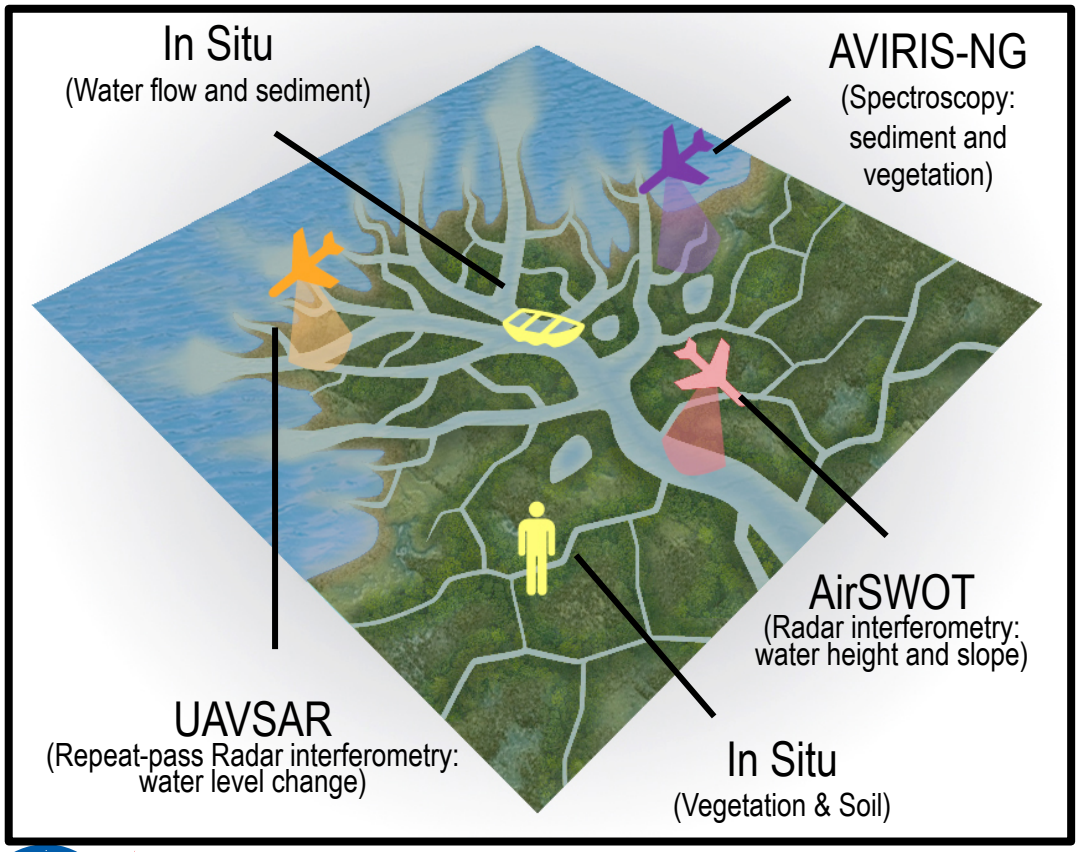
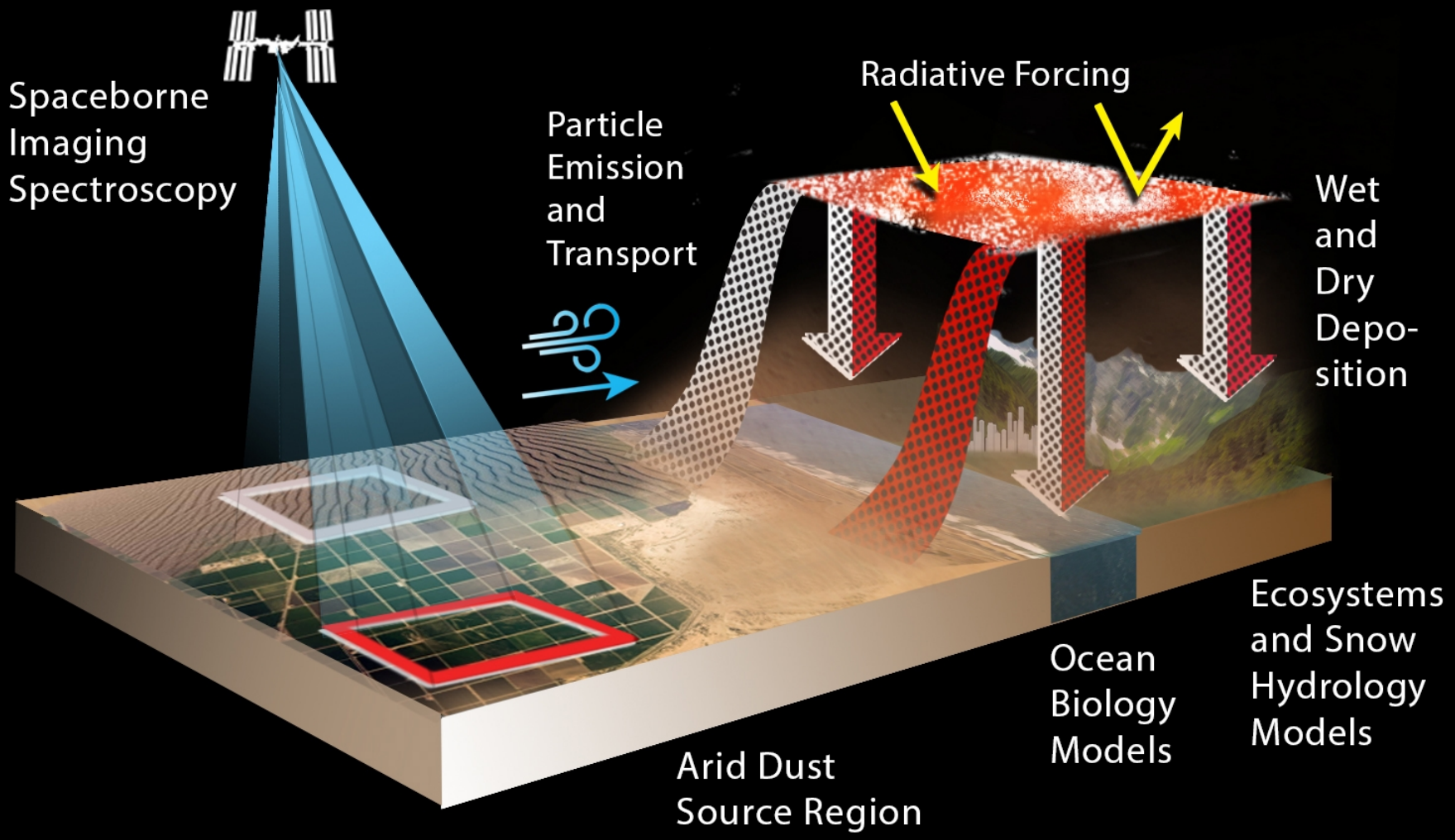
Delta-X EV-S mission PI: Marc Simard

Urgency: If ignored, Relative Sea Level Rise (RSLR) will very soon have devastating consequences on the livelihood of the half billion people that live in these low-lying coastal regions. Nearly all the world's major river deltas are threatened along with the services they provide: flood protection, carbon sequestration, biodiversity and food supply.

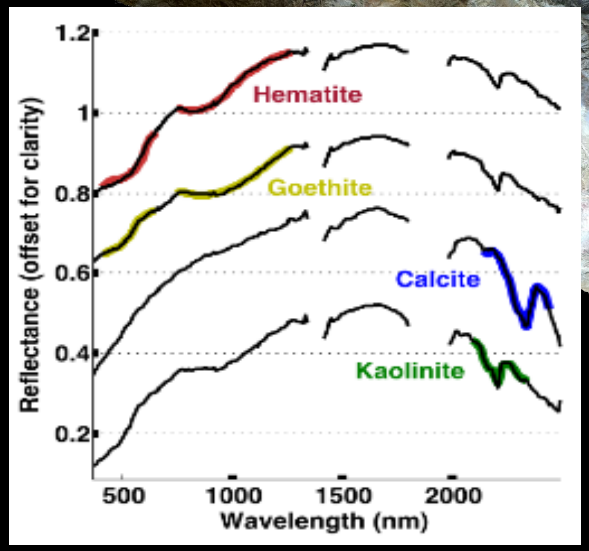


Delta-X Science Question: Will river deltas completely drown, or some parts of these deltas accumulate sufficient sediments and produce enough plants to keep pace with RSLR ?

Launching 2021: EMIT

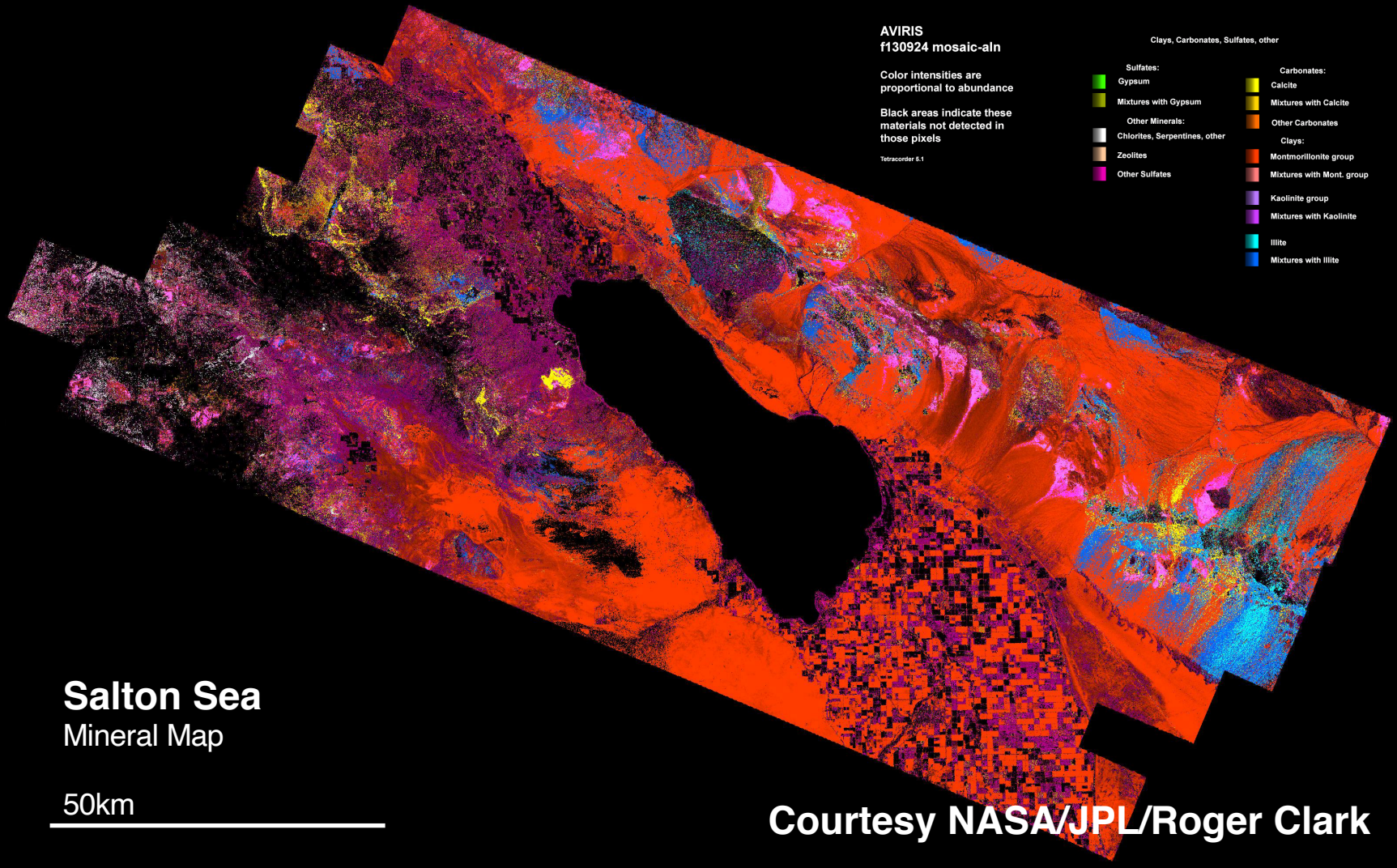


Salton Sea, CA (AVIRIS instrument)



Courtesy NASA/JPL/Roger Clark

Salton Sea, CA (AVIRIS instrument)



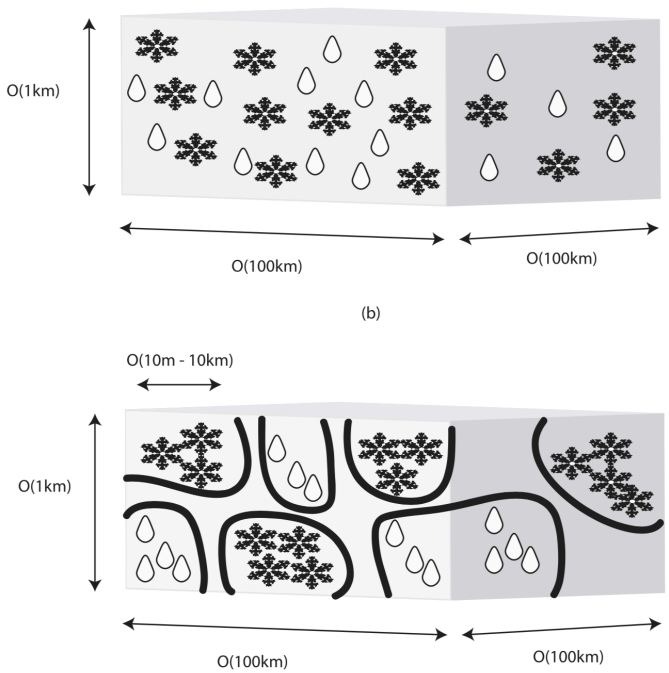
Salton Sea
Mineral Map

50km

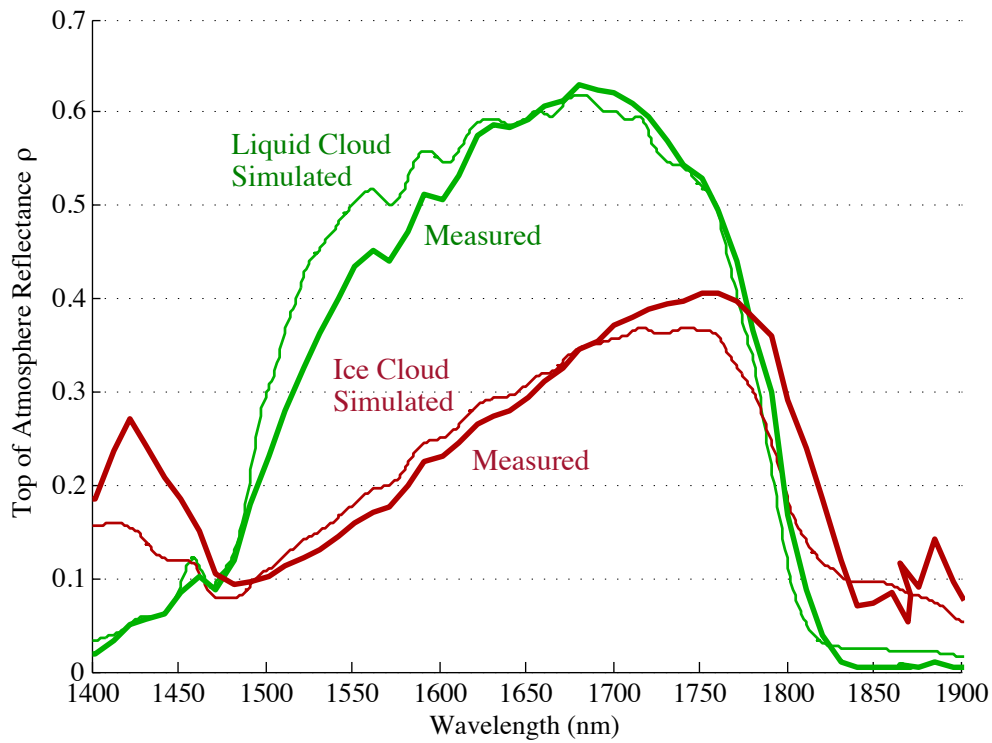
Courtesy NASA/JPL/Roger Clark

Cloud optical properties at high spatial resolution

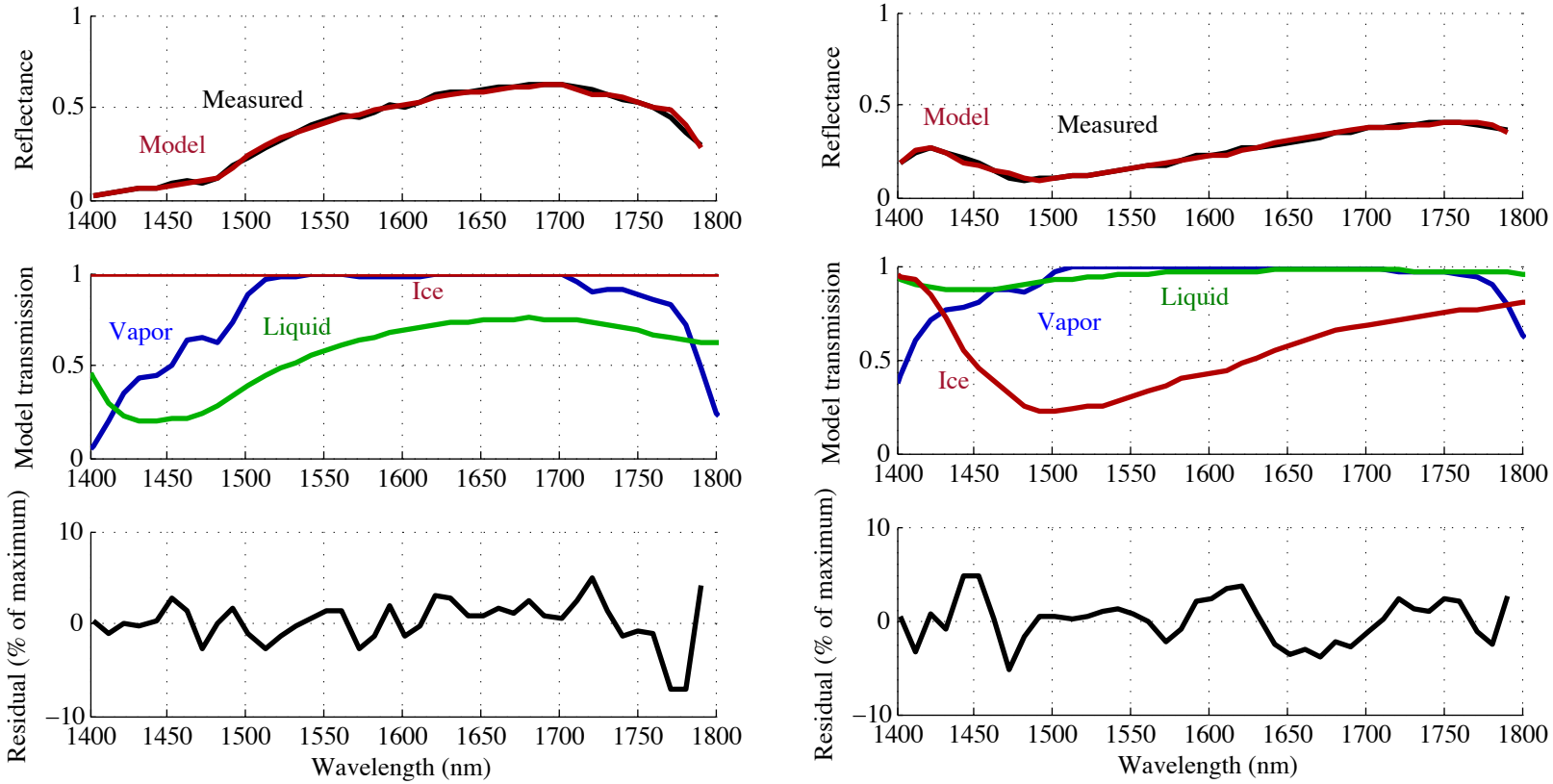
[Thompson et al., JGR 2016; Thompson et al., AMT 2018]



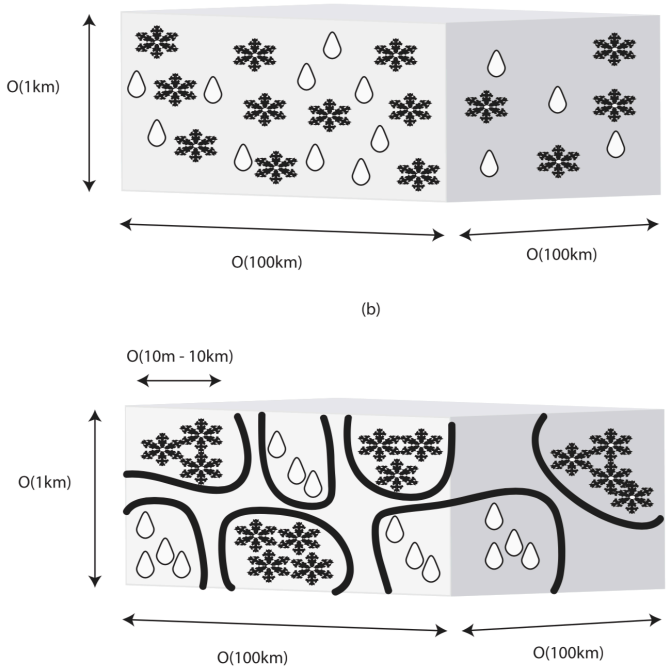
Tan and Storelvmo, Journal of the Atmospheric Sciences, 2016



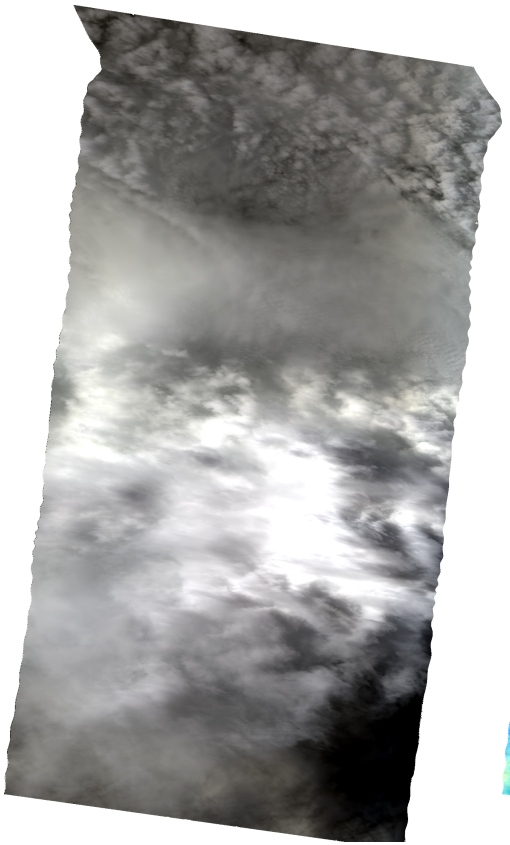
Fits of liquid and ice cloud spectra



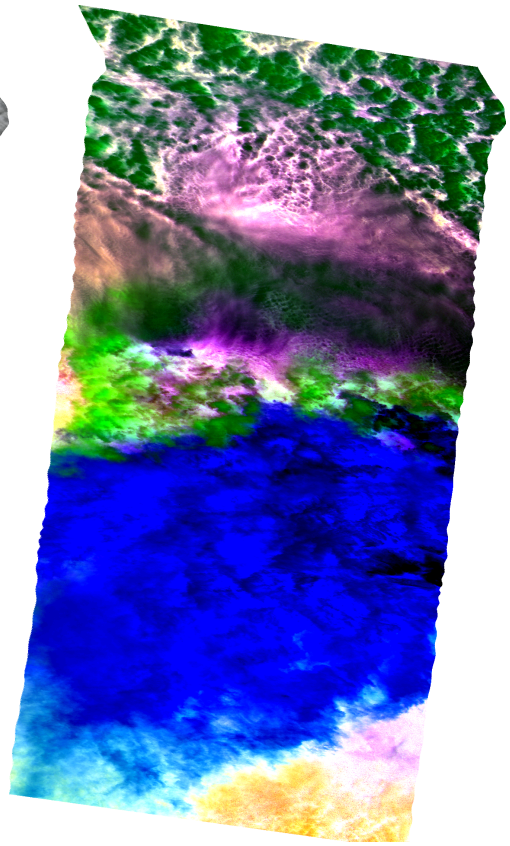
Cloud optical properties at high spatial resolution



Tan and Storelvmo, Journal of the Atmospheric Sciences, 2016

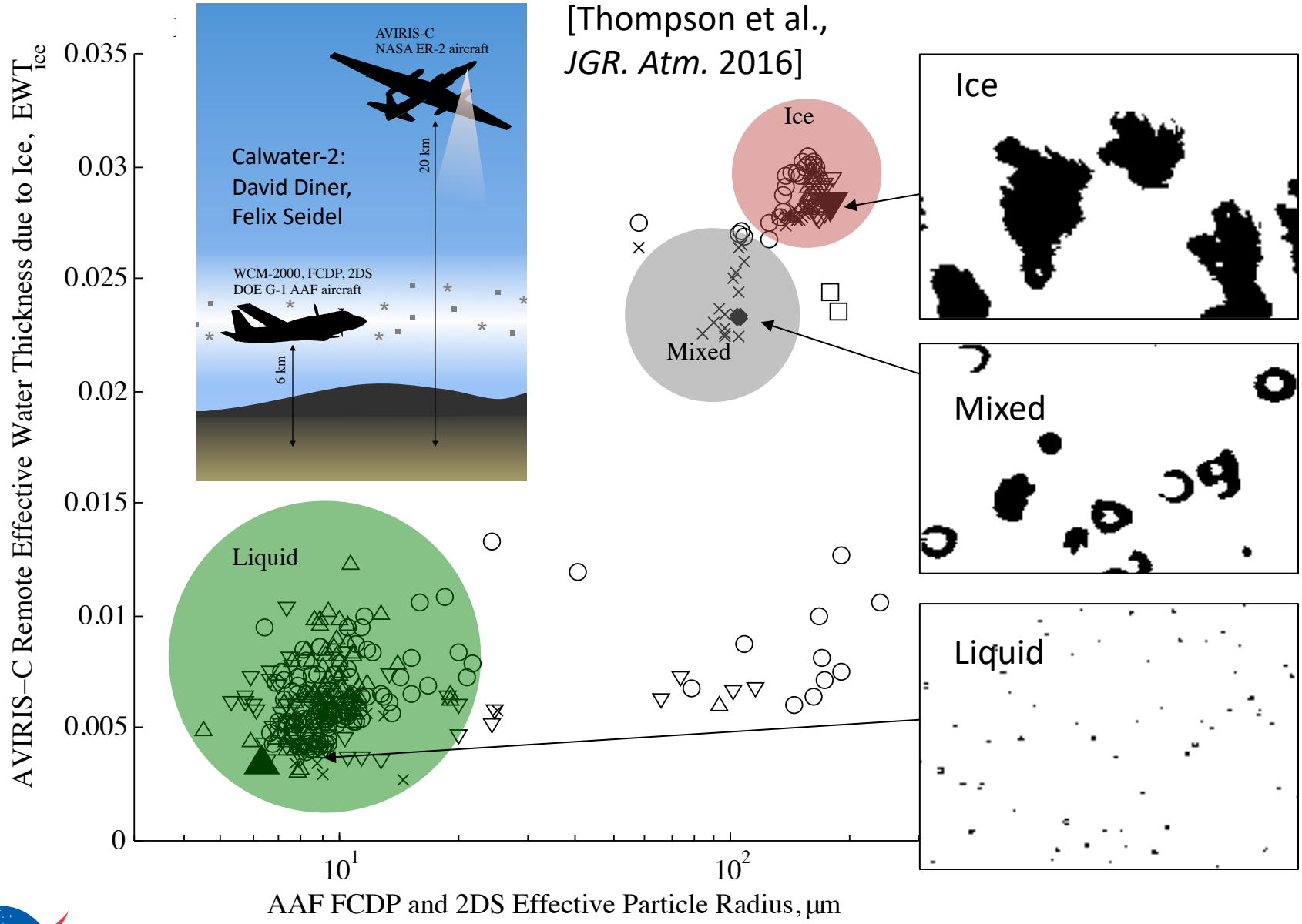


RGB Image



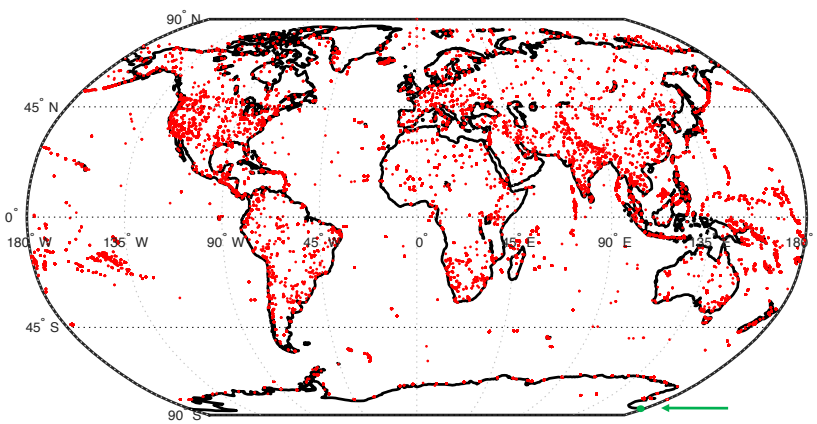
Ice Liquid Vapor

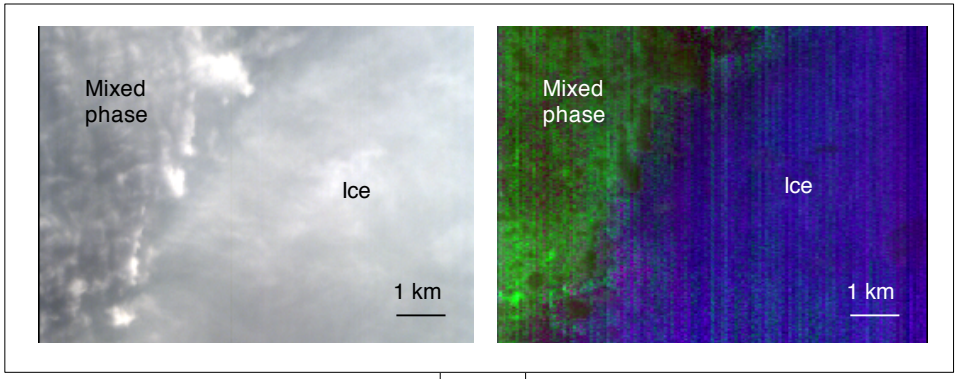
[Thompson et al., *JGR. Atm.* 2016]

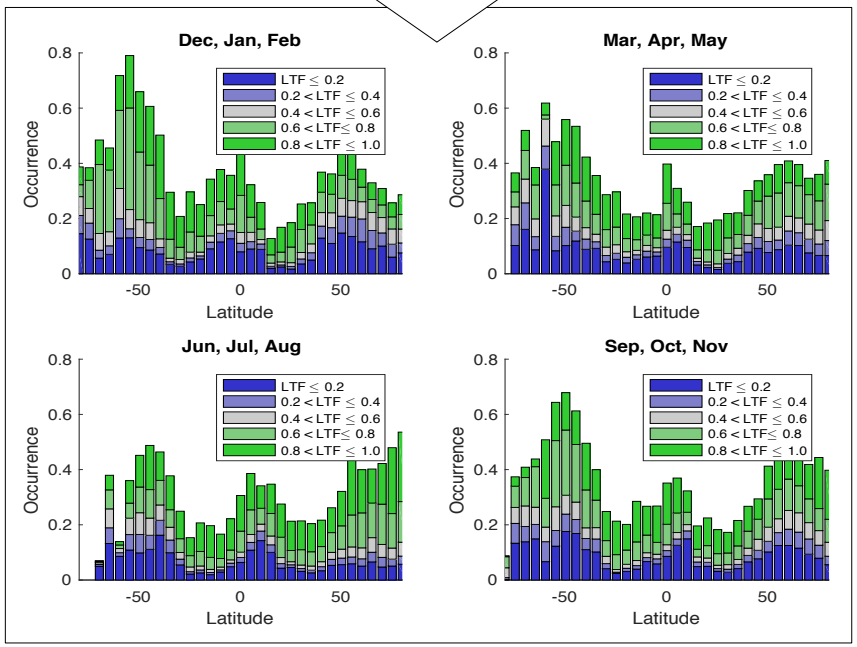


Global cloud survey by Hyperion on EO-1

[Thompson et al., AMT 2016]







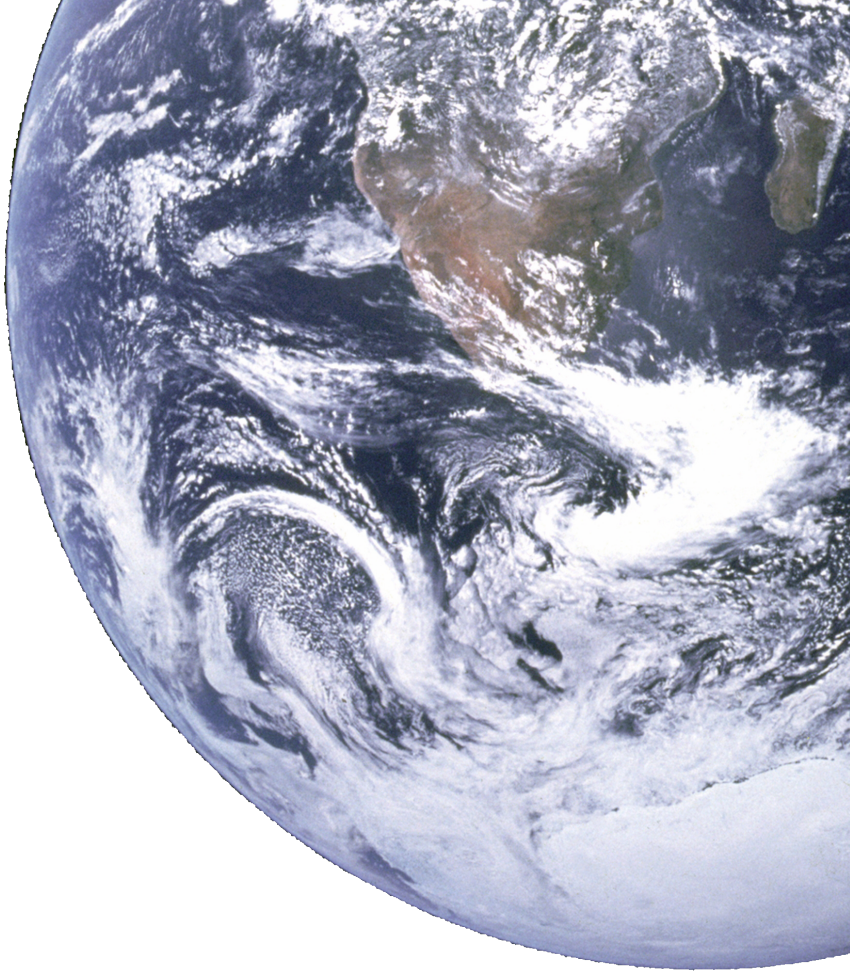
Top: Example Hyperion data showing visible RGB channels (left) and associated thermodynamic phase map. **Bottom:** Zonal variability of liquid phase (dark green), ice phase (dark blue), and intermediate phases.

Agenda

Measurement Method

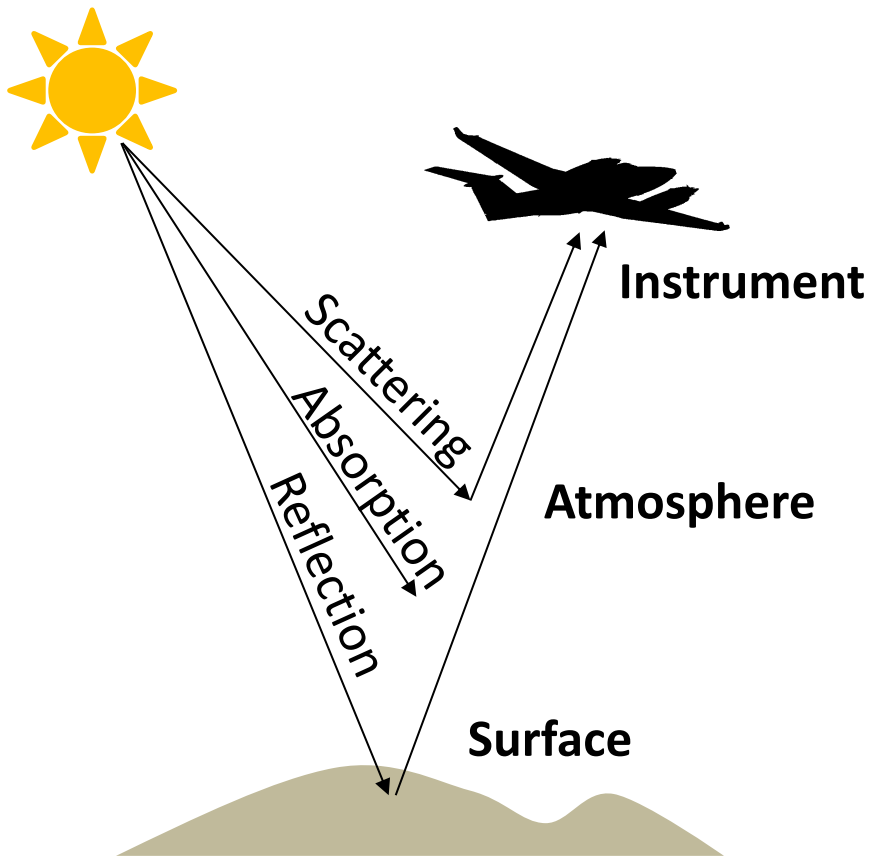
Science Themes

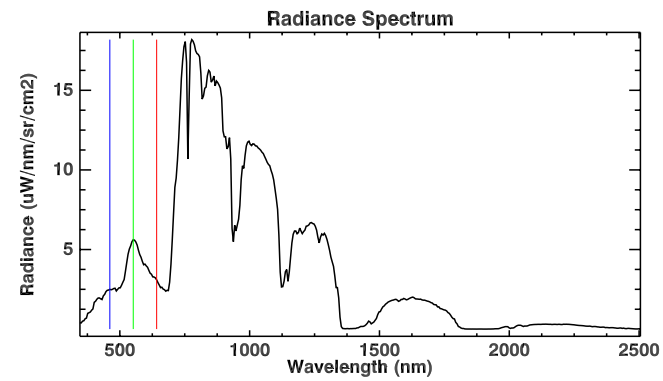
Deep dive: Bayesian Atmospheric Correction

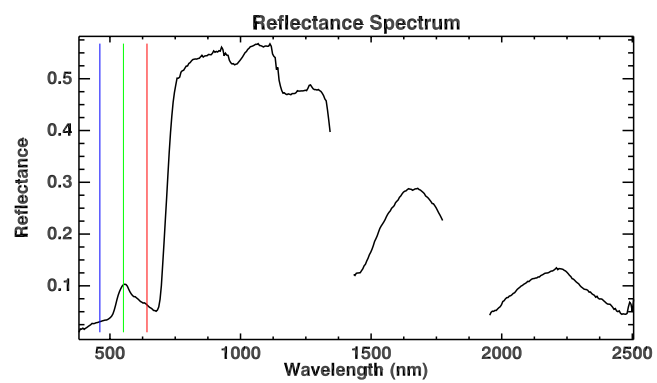


Atmospheric correction

[Thompson et al., RSE 2015; Thompson et al., RSE 2018, Thompson et al., RSE 2019a, Thompson et al., RSE 2019b]





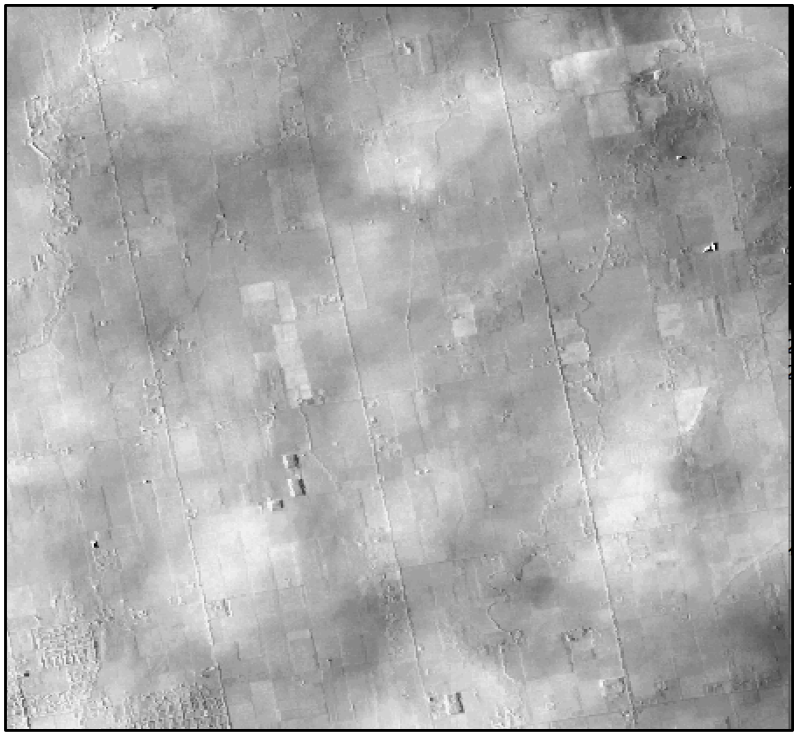


david.r.thompson@jpl.nasa.gov

Atmosphere varies over short spatiotemporal scales

"AVIRIS Classic" imaging spectrometer, visible wavelengths

Retrieved Water vapor
[Thompson et al., *Surv. Geohysics,* 2018]

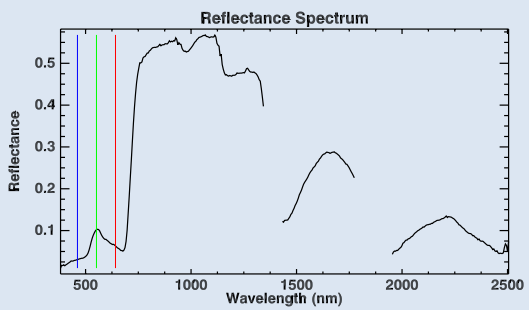


The “forward problem”

State vector

$$\mathbf{x} \in \mathbb{R}^N$$

$$\mathbf{x} = \begin{bmatrix} \text{Surface parameters} \\ \cdots \\ \text{Atmosphere parameters} \\ \cdots \\ \text{Instrument parameters} \\ \cdots \end{bmatrix}$$



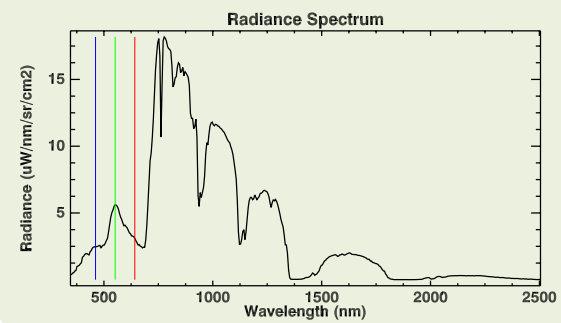
Forward model

$$F(\mathbf{x}) : \mathbb{R}^N \mapsto \mathbb{R}^M$$

Measurement

$$\mathbf{y} \in \mathbb{R}^M$$

$$\mathbf{y} = \begin{bmatrix} \text{Calibrated at-aperture} \\ \text{radiance measurements} \end{bmatrix}$$

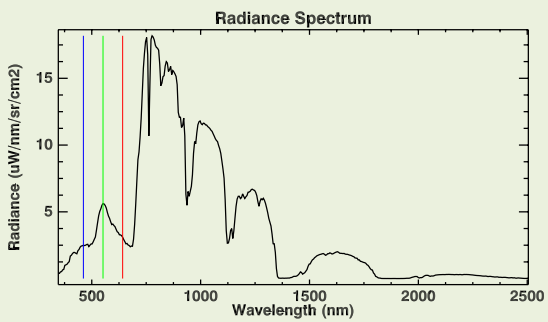


The “inverse problem”

Measurement

$$\mathbf{y} \in \mathbb{R}^M$$

$$\mathbf{y} = \begin{bmatrix} \text{Calibrated at-aperture} \\ \text{radiance measurements} \end{bmatrix}$$



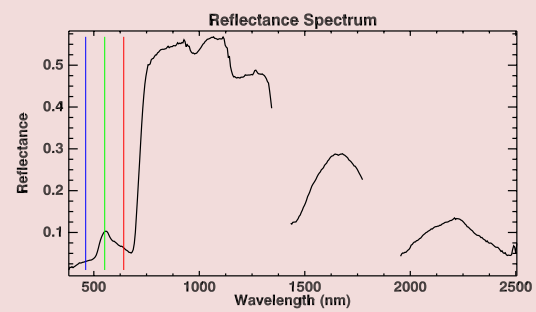
Inversion algorithm

$$R(\mathbf{y}) : \mathbb{R}^M \mapsto \mathbb{R}^N$$

Estimated state vector

$$\hat{\mathbf{x}} \in \mathbb{R}^N$$

$$\hat{\mathbf{x}} = \begin{bmatrix} \text{Estimated} \\ \text{surface parameters} \\ \cdots \\ \text{Estimated} \\ \text{atmosphere parameters} \\ \cdots \\ \text{Estimated} \\ \text{instrument parameters} \\ \cdots \end{bmatrix}$$



Maximum *A Posteriori* solution

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$

Maximum *A Posteriori* solution

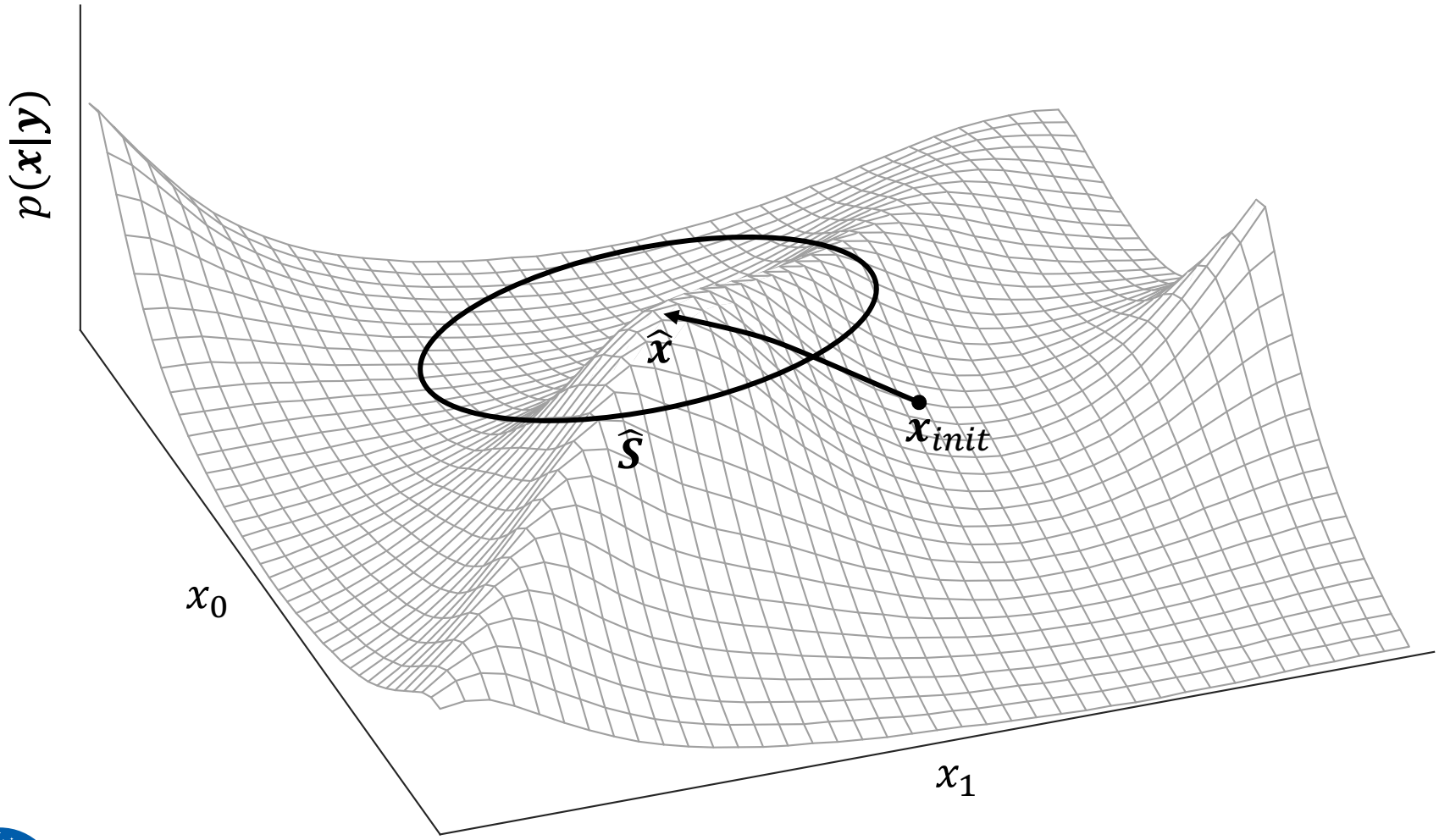
$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$

The *Maximum A Posteriori* estimation is equivalent to the optimization:

$$\underbrace{\chi^2(\mathbf{x})}_{\text{Cost}} = \underbrace{(\mathbf{F}(\mathbf{x}) - \mathbf{y})^{\mathbf{T}}\, \mathbf{S}_{\boldsymbol{\epsilon}}^{-1}\, (\mathbf{F}(\mathbf{x}) - \mathbf{y})}_{\text{Model match to measurement}} + \underbrace{(\mathbf{x} - \mathbf{x}_{\mathbf{a}})^{\mathbf{T}}\, \mathbf{S}_{\mathbf{a}}^{-1}\, (\mathbf{x} - \mathbf{x}_{\mathbf{a}})}_{\text{Bayesian prior}}$$

… we can solve it by conjugate gradient descent.

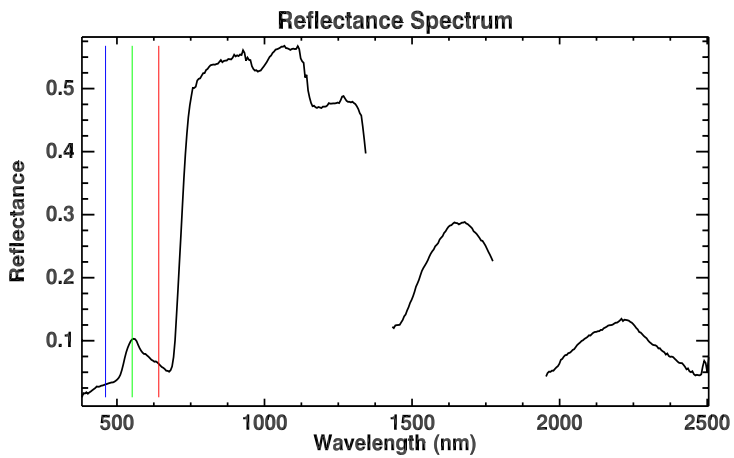
Maximum A Posteriori estimation

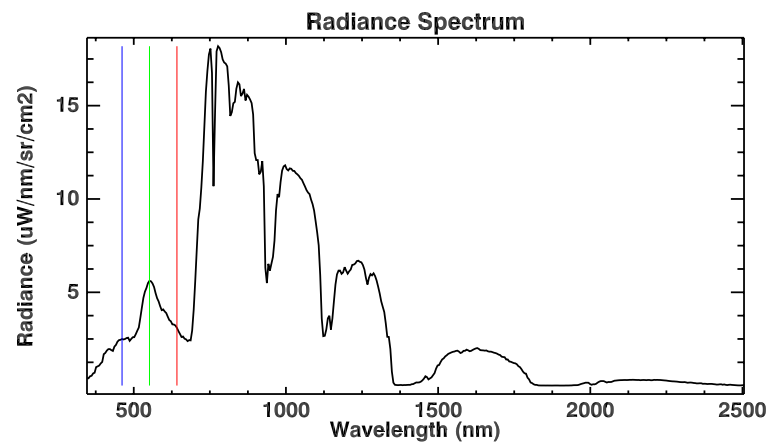


Iterative simultaneous estimation of atmosphere and surface

1. Predict radiance

$$\mathbf{y} = \mathbf{F}(\mathbf{x}) + \epsilon$$





2. Optimize state vector

$$\underbrace{\chi^2(\mathbf{x})}_{\text{Cost}} = \underbrace{(\mathbf{F}(\mathbf{x}) - \mathbf{y})^{\mathbf{T}}\, \mathbf{S}_{\epsilon}^{-1}\, (\mathbf{F}(\mathbf{x}) - \mathbf{y})}_{\text{Model match to measurement}} + \underbrace{(\mathbf{x} - \mathbf{x}_{\mathbf{a}})^{\mathbf{T}}\, \mathbf{S}_{\mathbf{a}}^{-1}\, (\mathbf{x} - \mathbf{x}_{\mathbf{a}})}_{\text{Bayesian prior}}$$

Case study

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

- In-situ AOD via Reagan sunphotometers
- In-situ surface reflectance via ASD Fieldspec

Jet Propulsion Laboratory

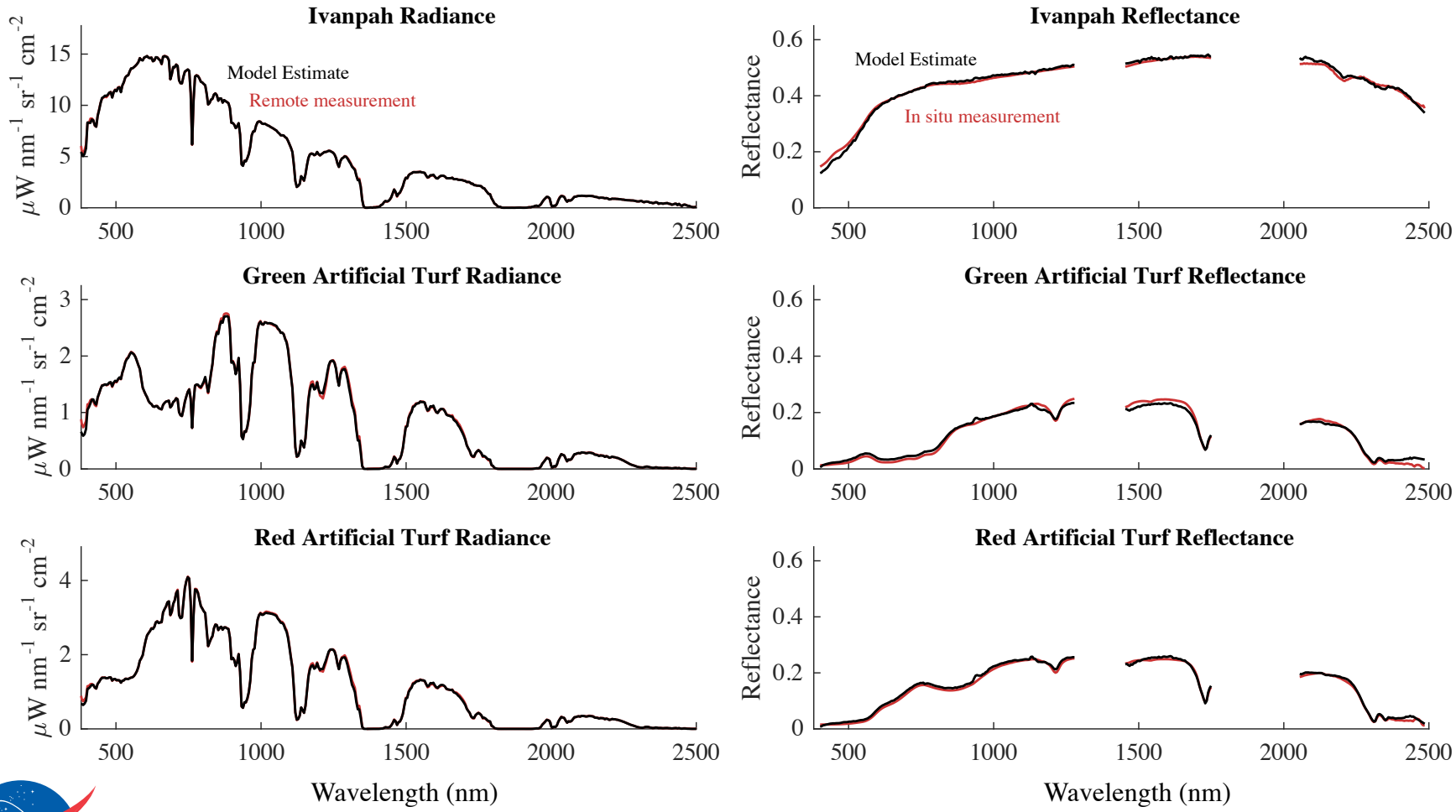
Ivanpah Playa

California Institute of Technology

From Thompson et al., RSE 2018.

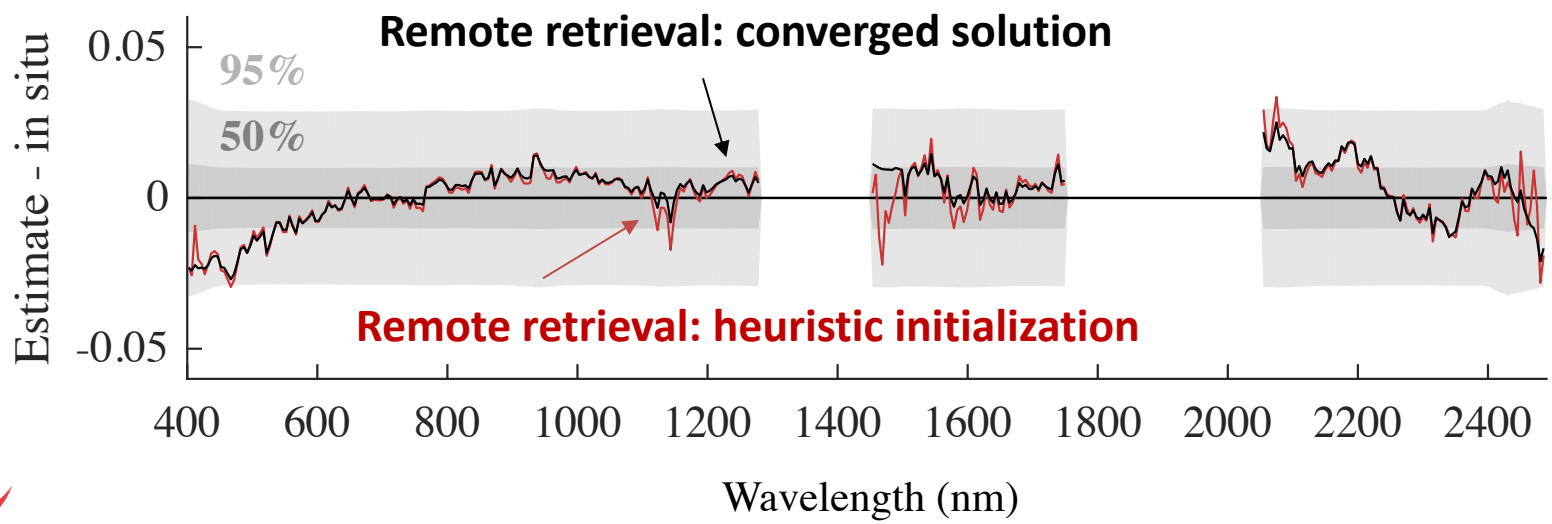
Reflectance estimate vs. in situ

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



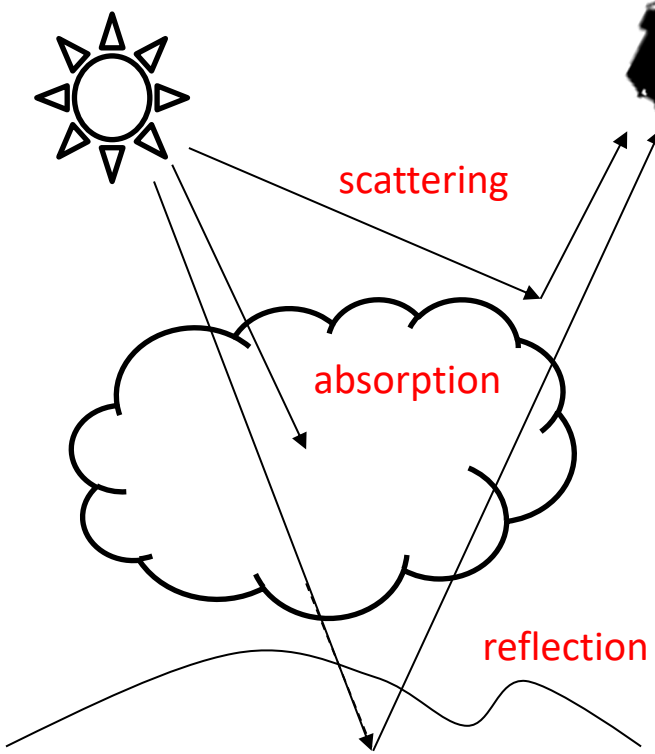
Posterior uncertainty compared to actual discrepancies

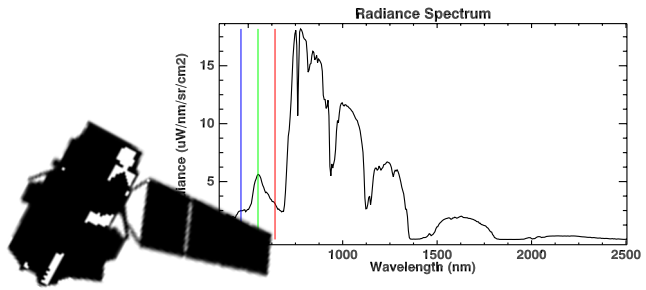
[Thompson et al., *Remote Sensing of Environment* 2018]

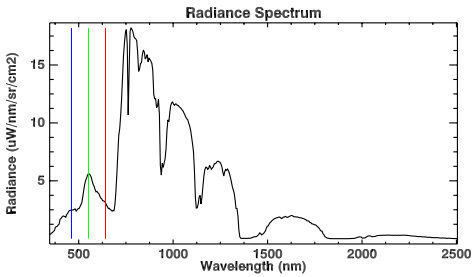


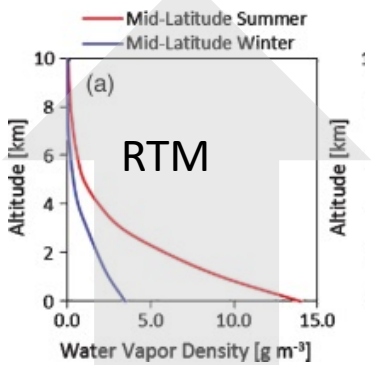
Speeding up the forward model

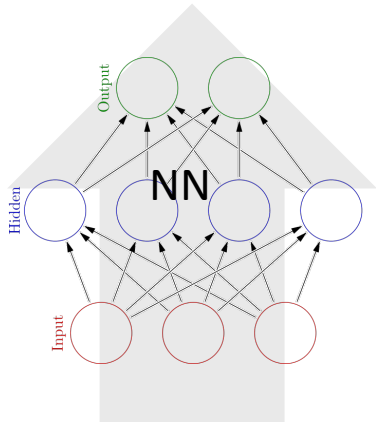
images: Mishra et al., Heliyon 2015, wikimedia

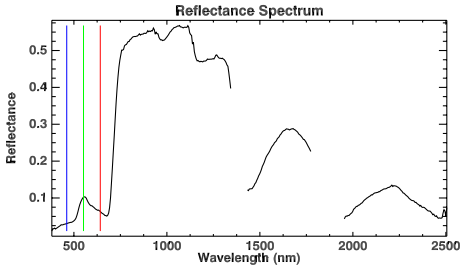


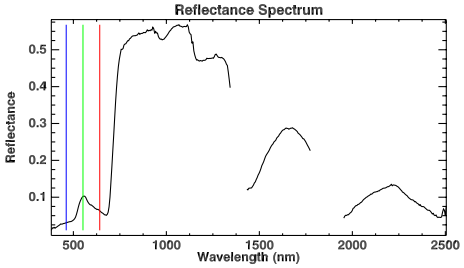




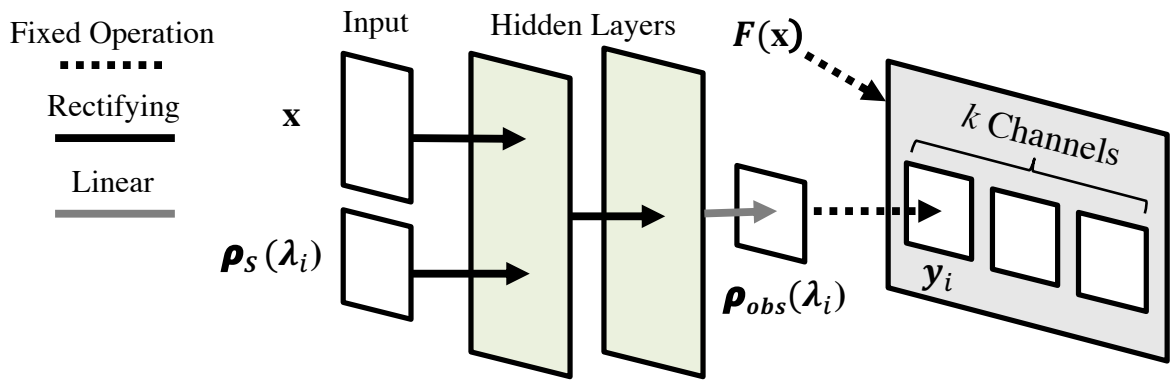






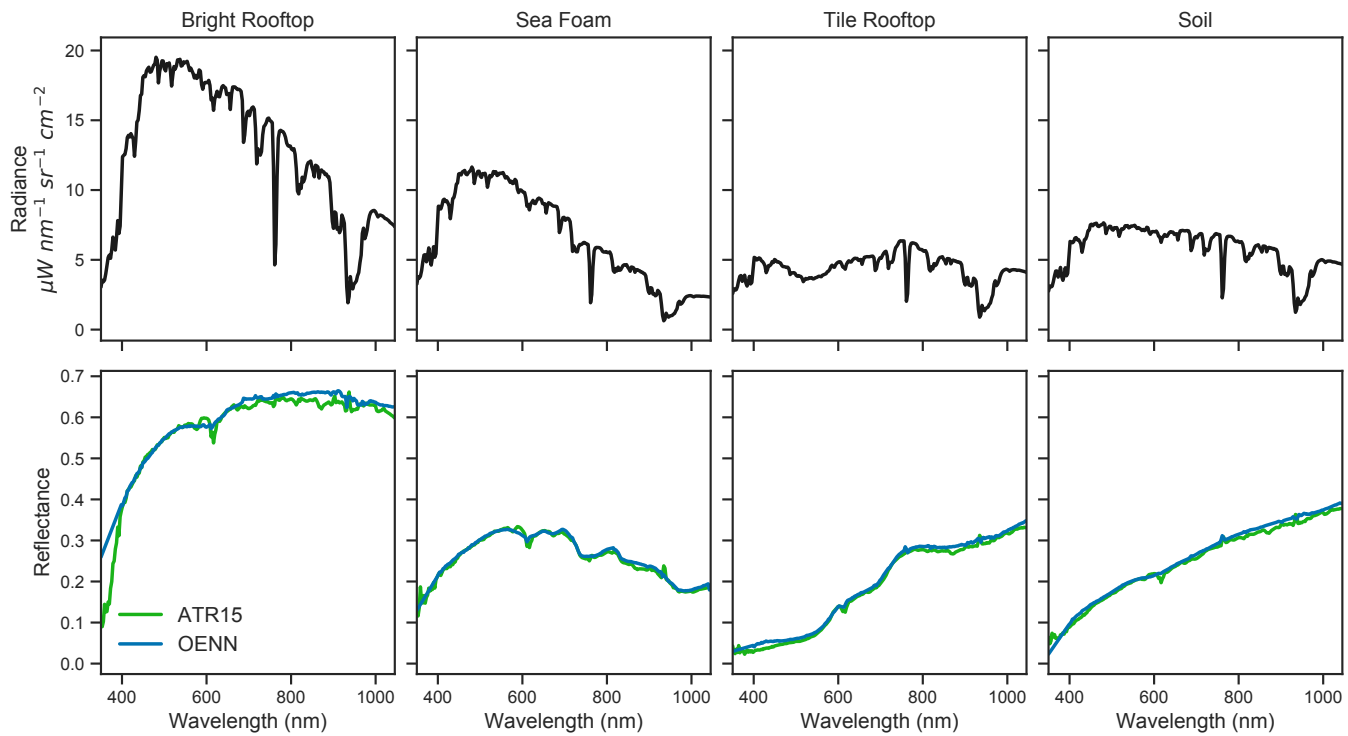


Radiative transfer emulation

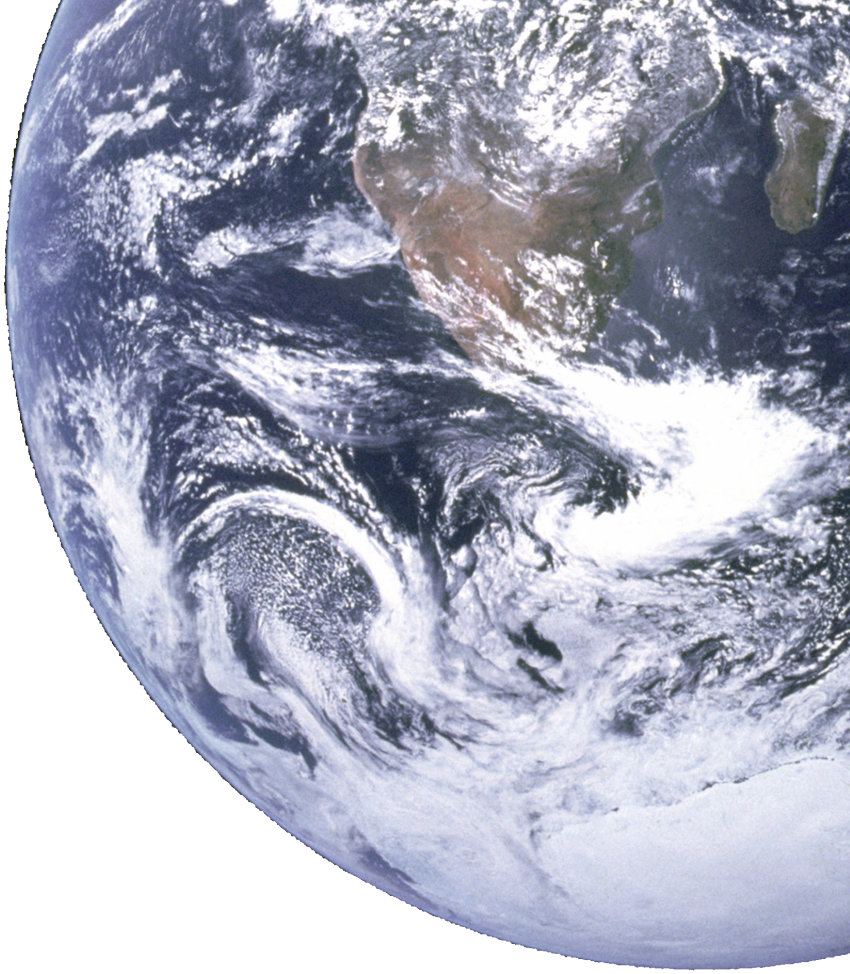


Four orders of magnitude speed improvement at negligible accuracy penalty!

[Bue et al., *Atmos. Meas. Tech.* 2019]



Summary



Imaging spectroscopy:

- **Is statistically rigorous and quantitative**
- **Reveals physical and chemical processes in the environment**
- **Has unique accuracy and generalizability needs**

Get ready for global-scale spectroscopy datasets

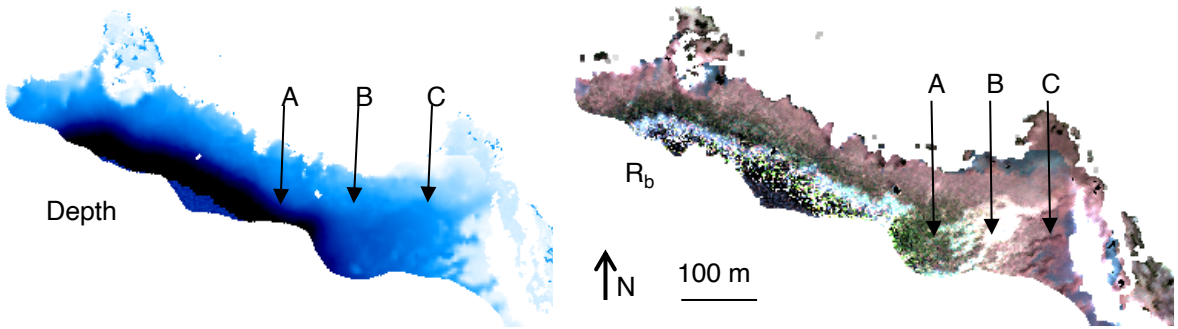
Your help will be critical

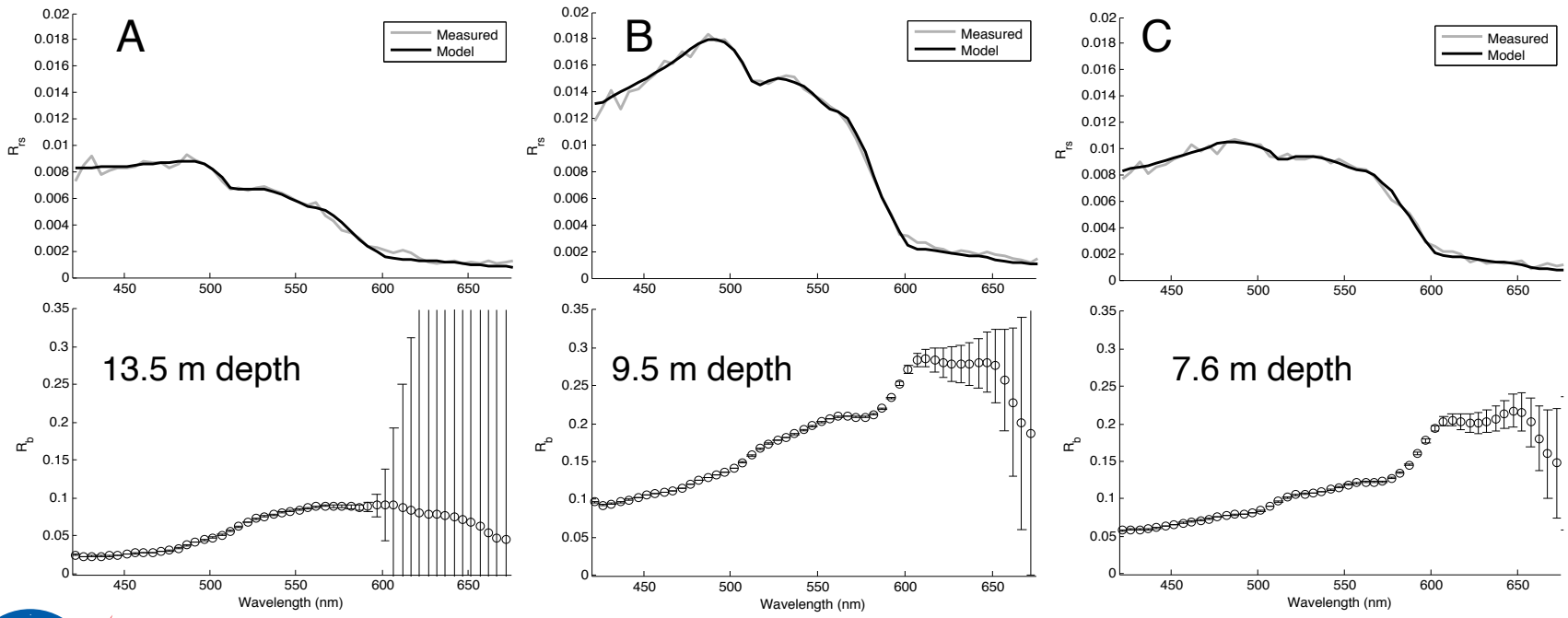
With due thanks to:

- **Kevin Bowman** (JPL), for much of the source material in these slides
- **Clive D. Rogers,** for theoretical foundations, approach and notation (e.g. *Inverse Methods for Atmospheric Sounding, Theory and Practice*, 2000).
- **NASA Earth Science** for sponsorship of AVIRIS-NG and the AVIRIS-NG India investigation and analysis.
- **The JPL Research and Technology Development and NASA Center Innovation Fund Programs**
- **The JPL Office of Chief Scientist and Technologist**
- **Other coinvestigators, coauthors and colleagues** including Amy Braverman, Jonathan Hobbs, Robert Spurr, Steven Massie, Bruce Kindel, Manoj Mishra, et cetera.
- **The NSF National Robotics Initiative**

Backup

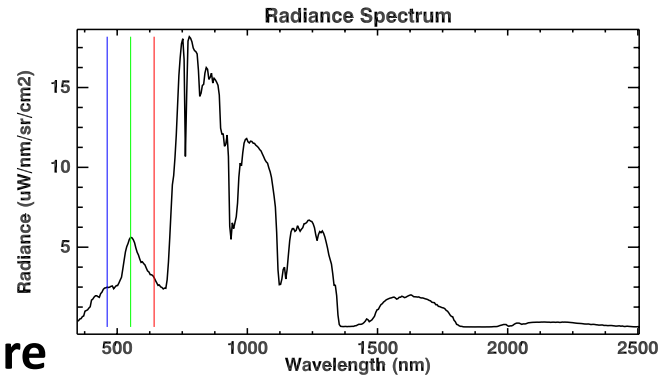
Sensitivity and depth



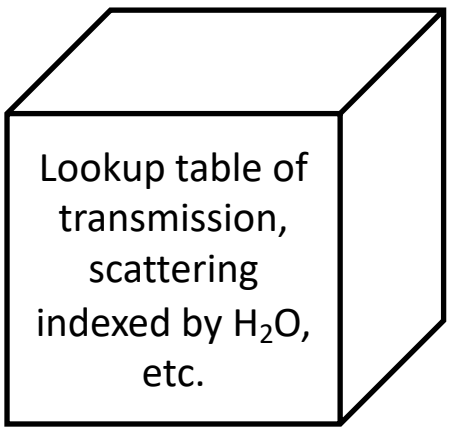


Airborne VSWIR data collected by the Carnegie Airborne Observatory

Conventional atmospheric correction: A sequential process



2. Estimate atmosphere (typically by band ratios)



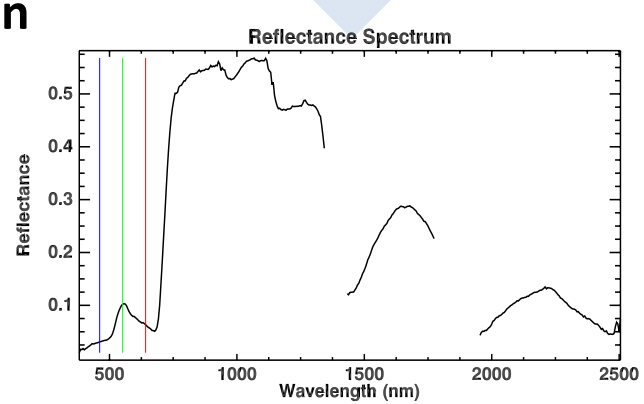
1. In advance, do RTM calculations

measurement

reflectance

$$\rho^*_{obs} = \rho_a + \frac{T\rho_s}{1 - S\rho_s}$$

3. Algebraic Inversion



Ongoing: *Optimal Estimation* for iterative fits of surface and atmosphere

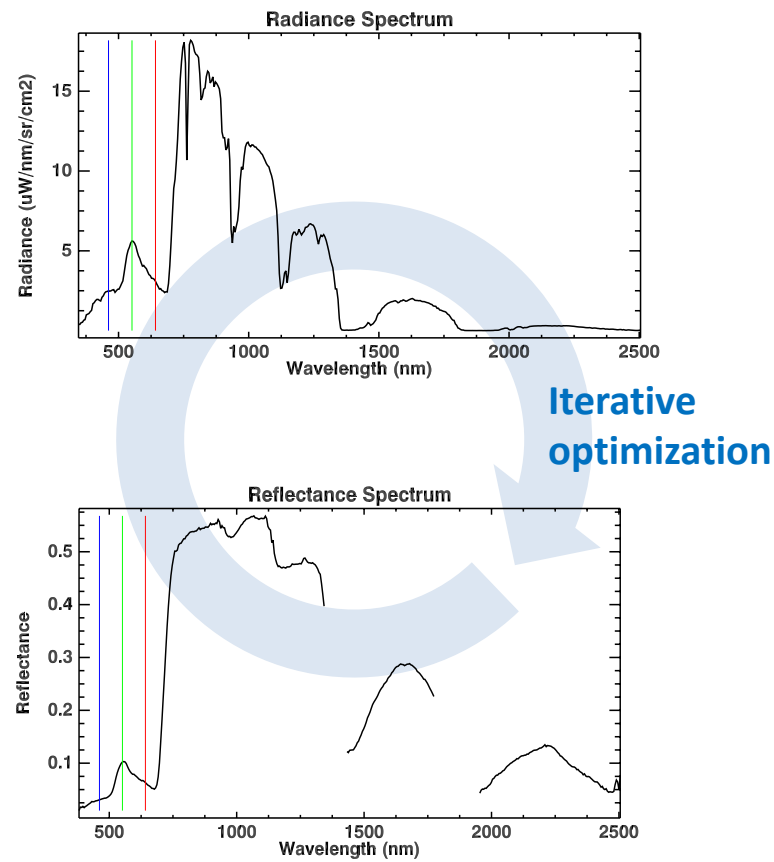
[Thompson et al., *Remote Sensing of Environment* 2018]

Bayesian *Maximum a Posteriori* estimate using a combined model of surface, atmosphere, instrument

Improves atmospheric correction accuracy

Rigorous uncertainty accounting

Optimal weighting of information from instrument vs. domain knowledge



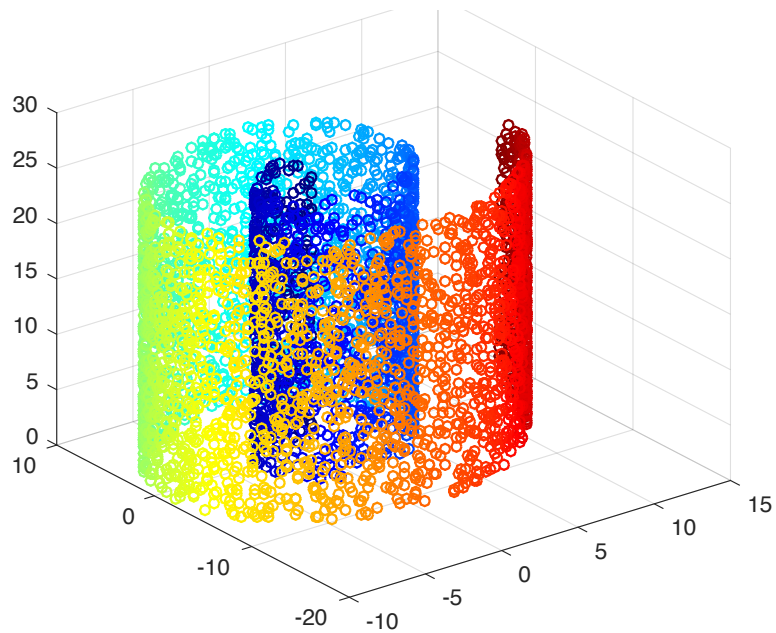
https://github.com/isofit/isofit

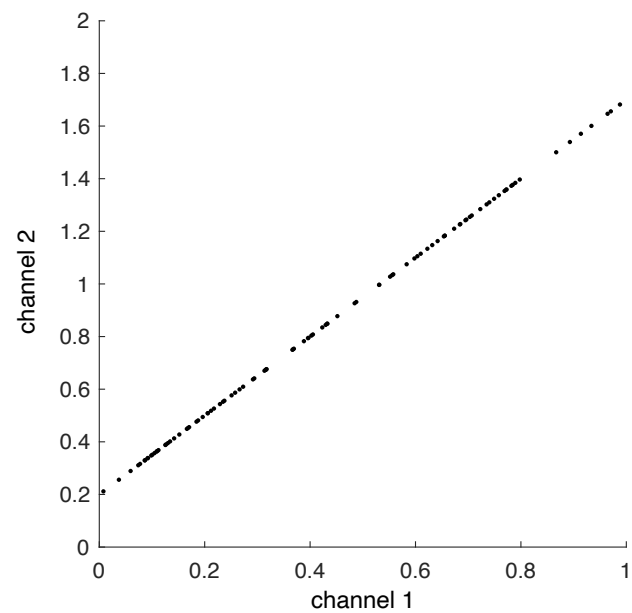
Limitations of conventional methods

1. Limited size of state vector that can be represented in the lookup table
2. Algebraic approximate solutions are less accurate for extreme geometries
3. Do not couple surface and atmosphere
4. Estimate atmosphere and surface sequentially, making it difficult to disambiguate atmospheric effects from surface effects
5. **Disregard uncertainties**

Intrinsic dimensionality

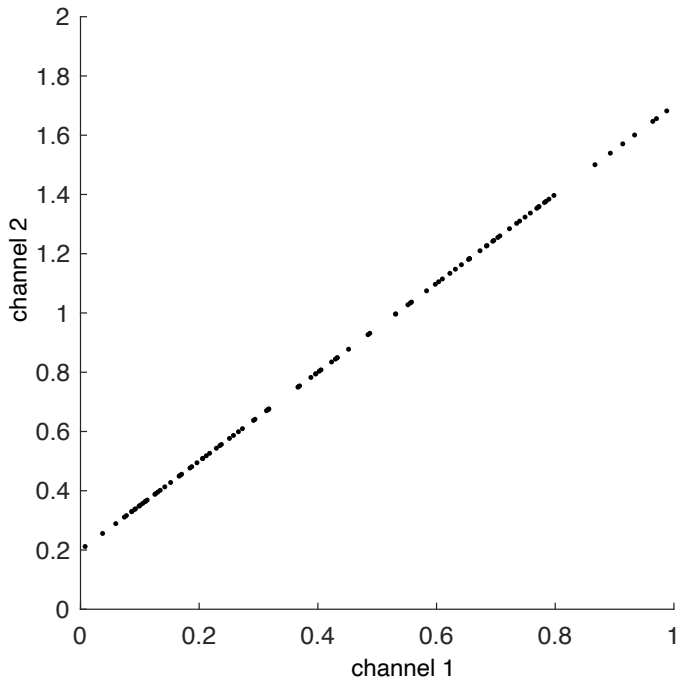
- The degrees of freedom in a process under study
- Quantifies the measurable diversity in a dataset

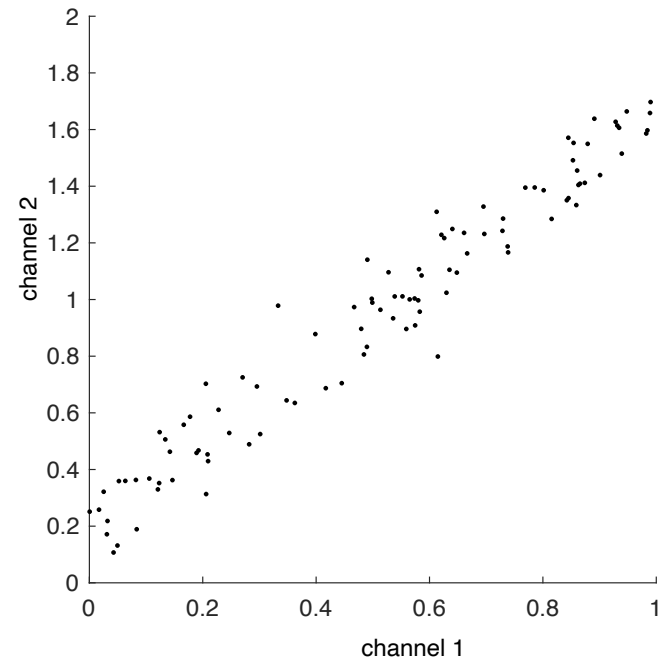




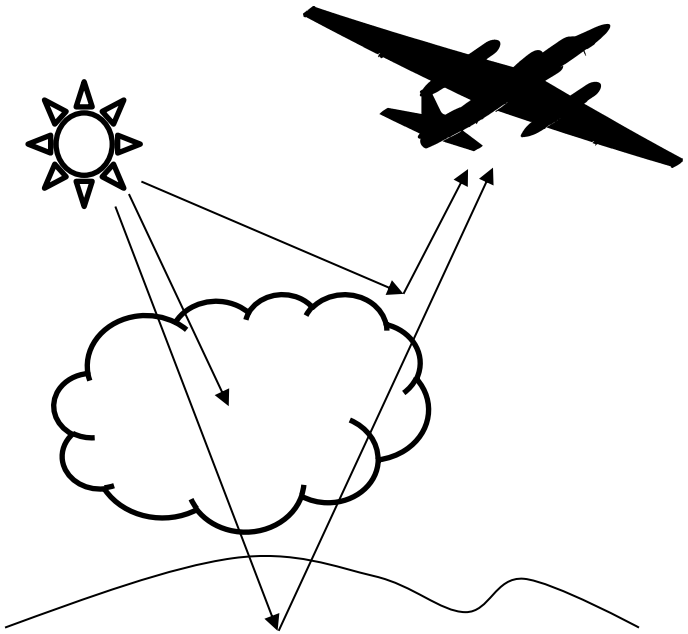
Laplacian Eigenmap code via Kye Taylor, Mathworks file exchange

Dimensionality estimates must account for measurement noise





Laplacian Eigenmap code via Kye Taylor, Mathworks file exchange



Model components

Pre-defined

Statistical, fit to data

Retrieved in the inversion

Instrument: AVIRIS-NG

- Instrument model with Wavelength- and signal-dependent SNR
- Photon shot & read noise
- Uncorrelated calibration uncertainty
- Systematic calibration / RT uncertainty

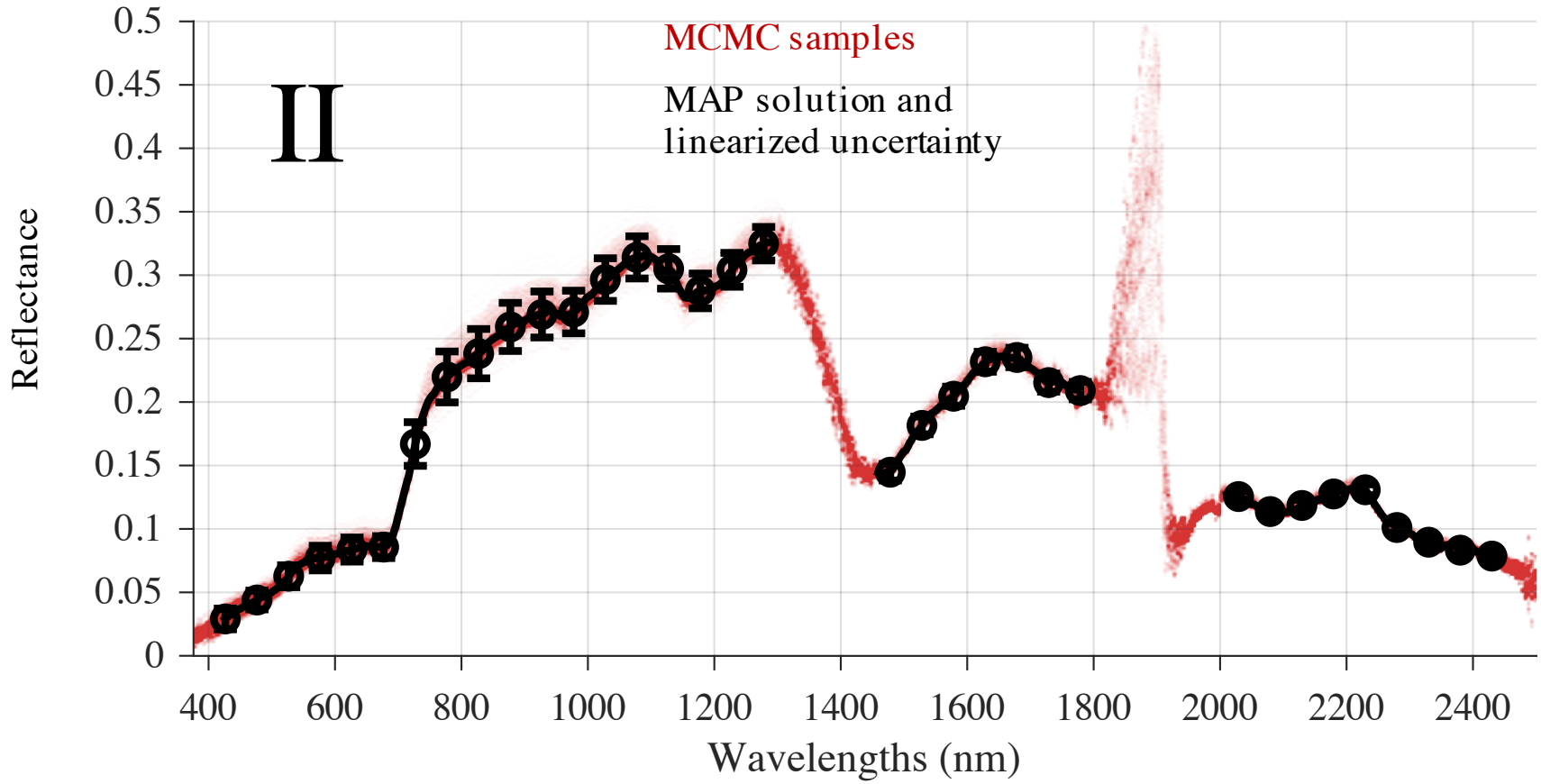
Atmosphere: MODTRAN 6.0 RTM

- DISORT MS, Correlated-k
- Rural aerosol model
- broad prior uncertainties
- Unmodeled unknowns, including H_2O absorption coefficients
- H_2O, AOD retrieved

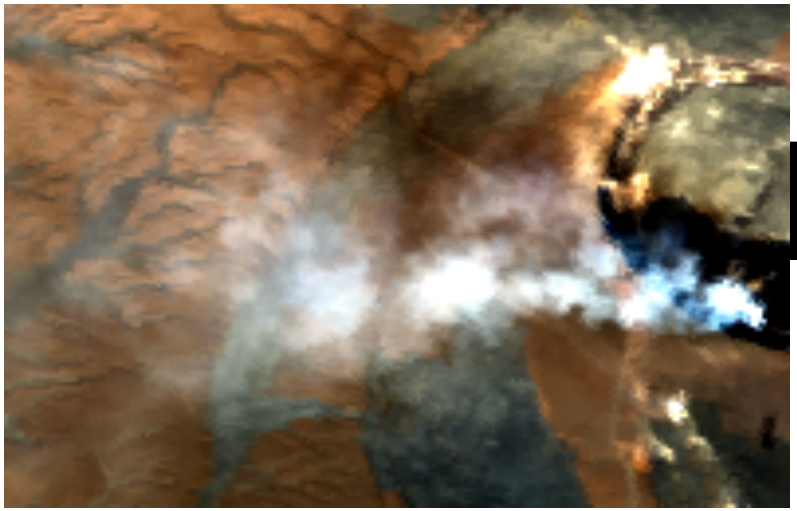
Surface: Multi-component Multivariate Gaussians

- Prior based on universal library, highly regularized to permit accurate retrieval of arbitrary shapes
- Reflectance estimated independently in every channel

Maximum A Posteriori vs. MCMC

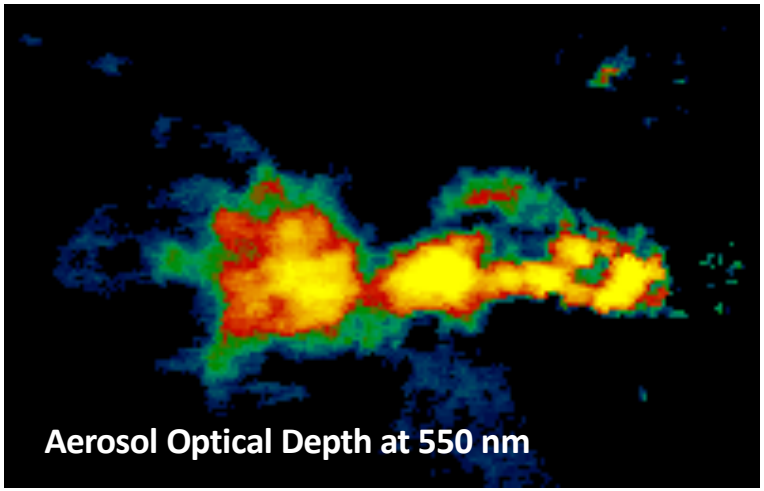


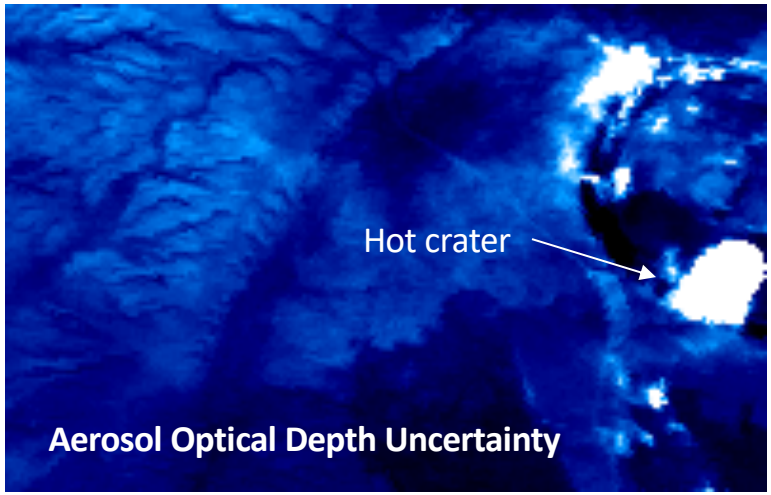
Aerosol mapping examples (Hawaii campaign)



AVIRIS-C f170127t01p00r16
(subset, visible bands)

Combined estimate of H_2O vapor, AOT, surface reflectance and temperature





Variability due to measurement noise vs. unknown state parameters

Total observation noise

Jacobian WRT unknowns

$$\mathbf{S}_\epsilon = \mathbf{S}_y + \mathbf{K}_b \mathbf{S}_b \mathbf{K}_b^T$$

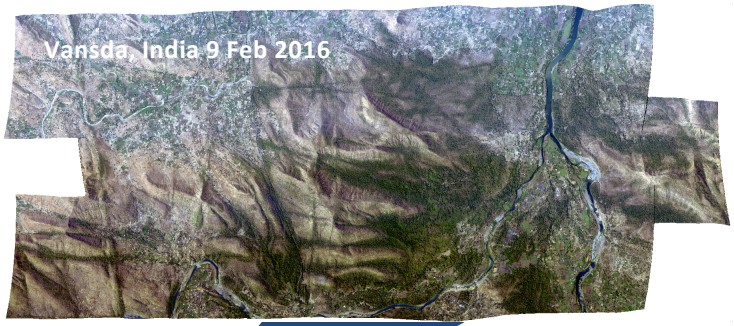
Measurement noise (instrument effects)

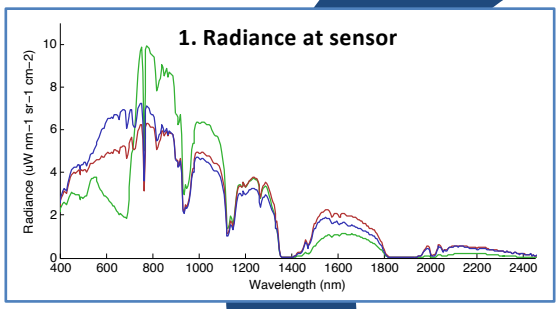
- Photon noise
- Read noise
- Dark current noise

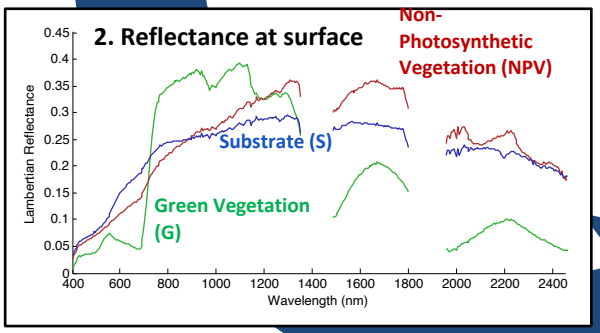
Unknown parameters in the observation system

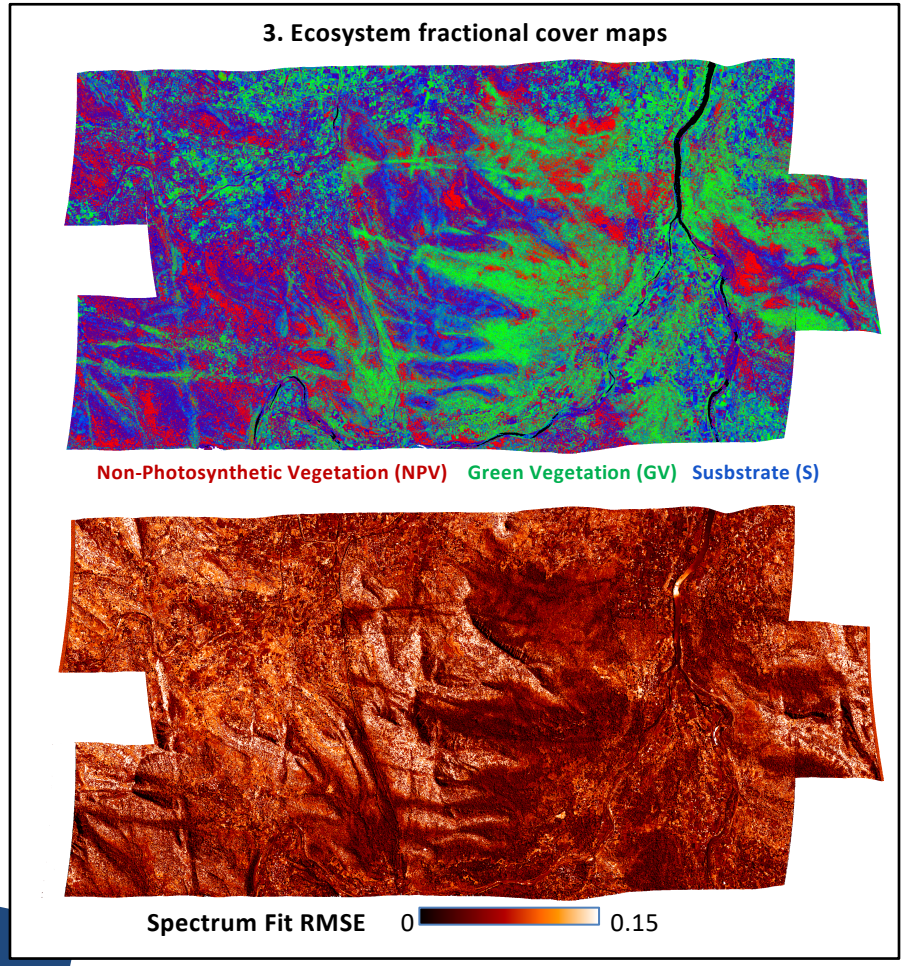
- Sky view factor
- H_2O absorption coefficient intensity
- Systematic radiative transfer error
- Uncorrelated radiative transfer error

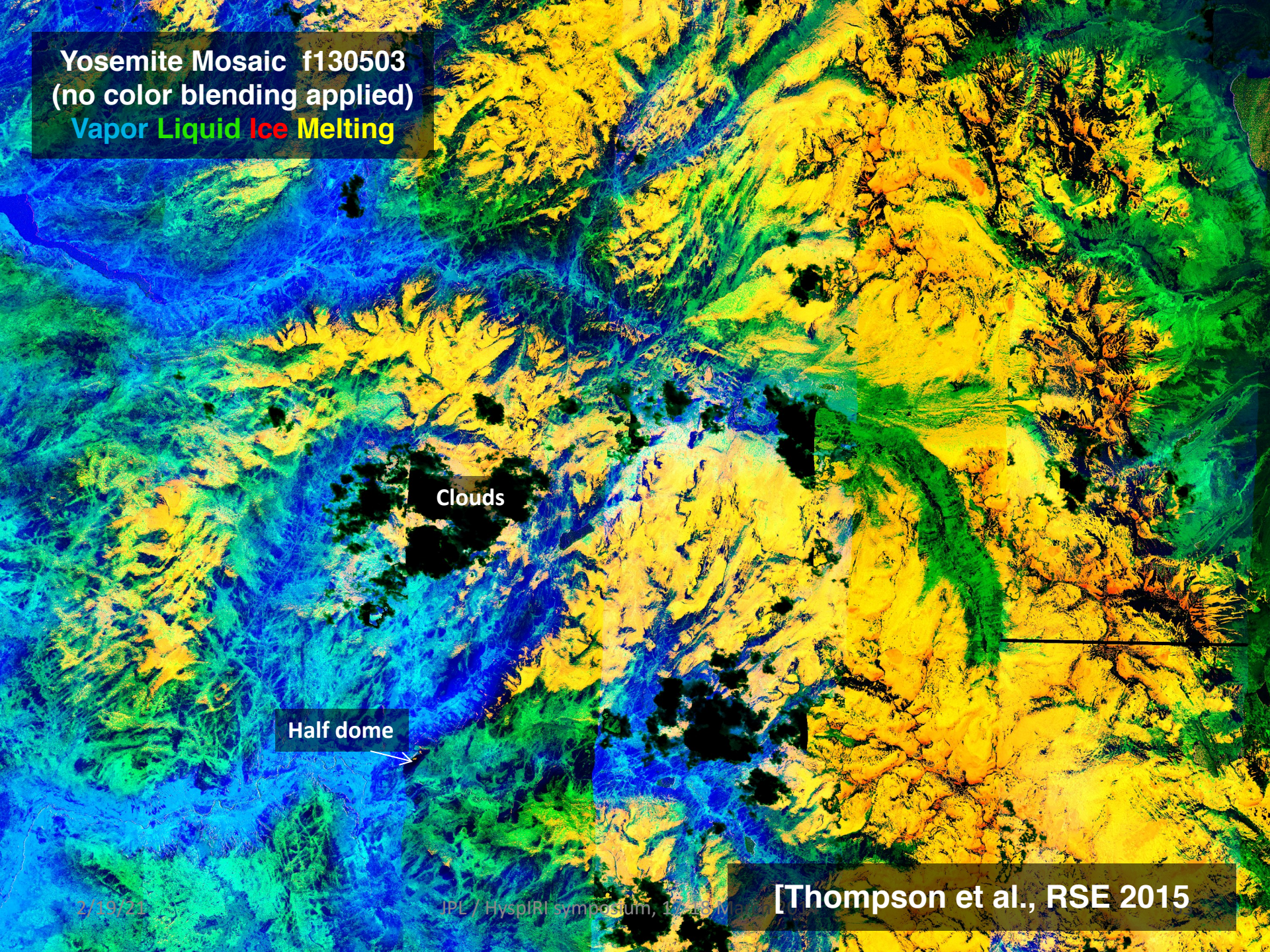
Measuring subpixel coverage





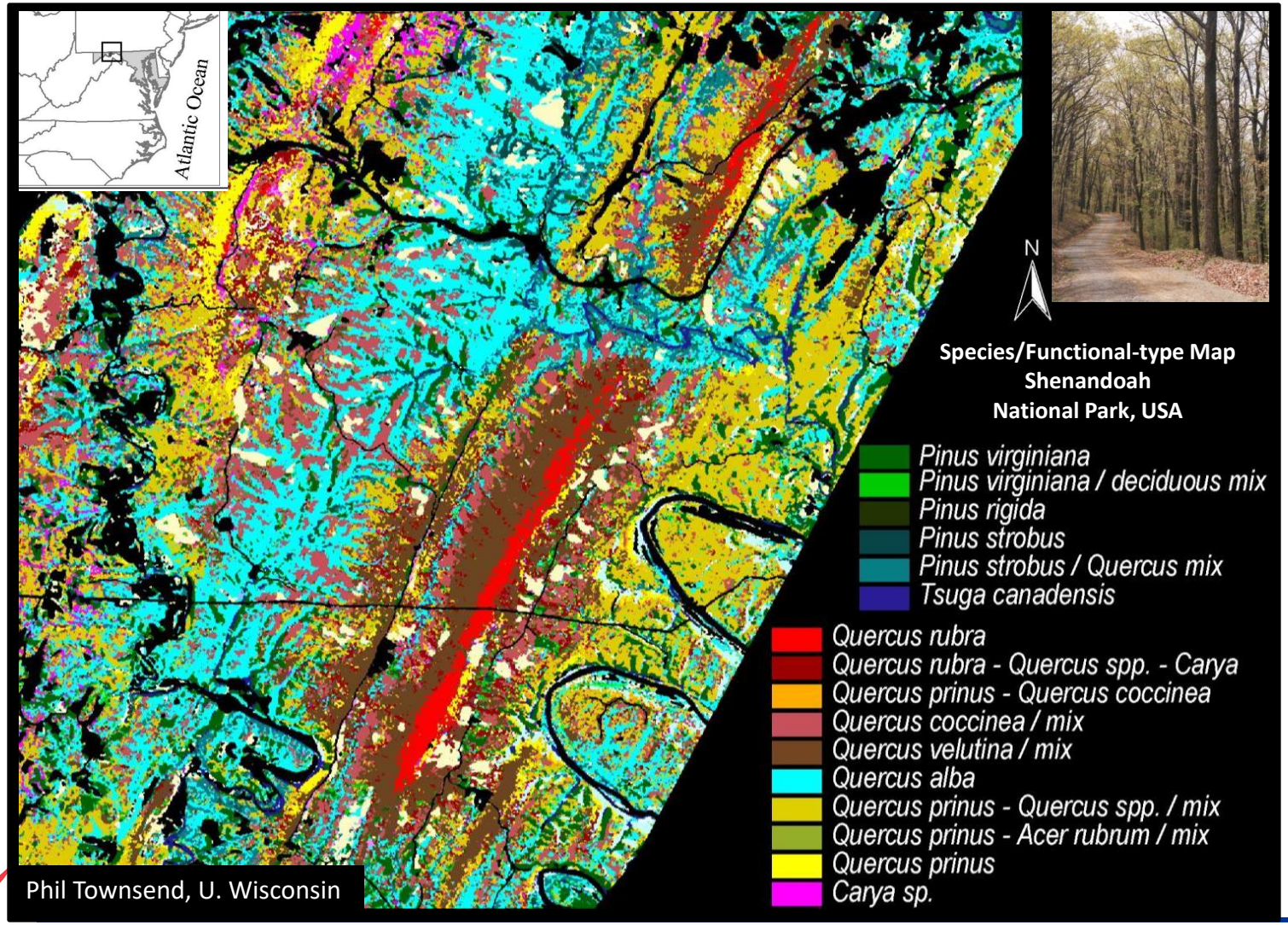






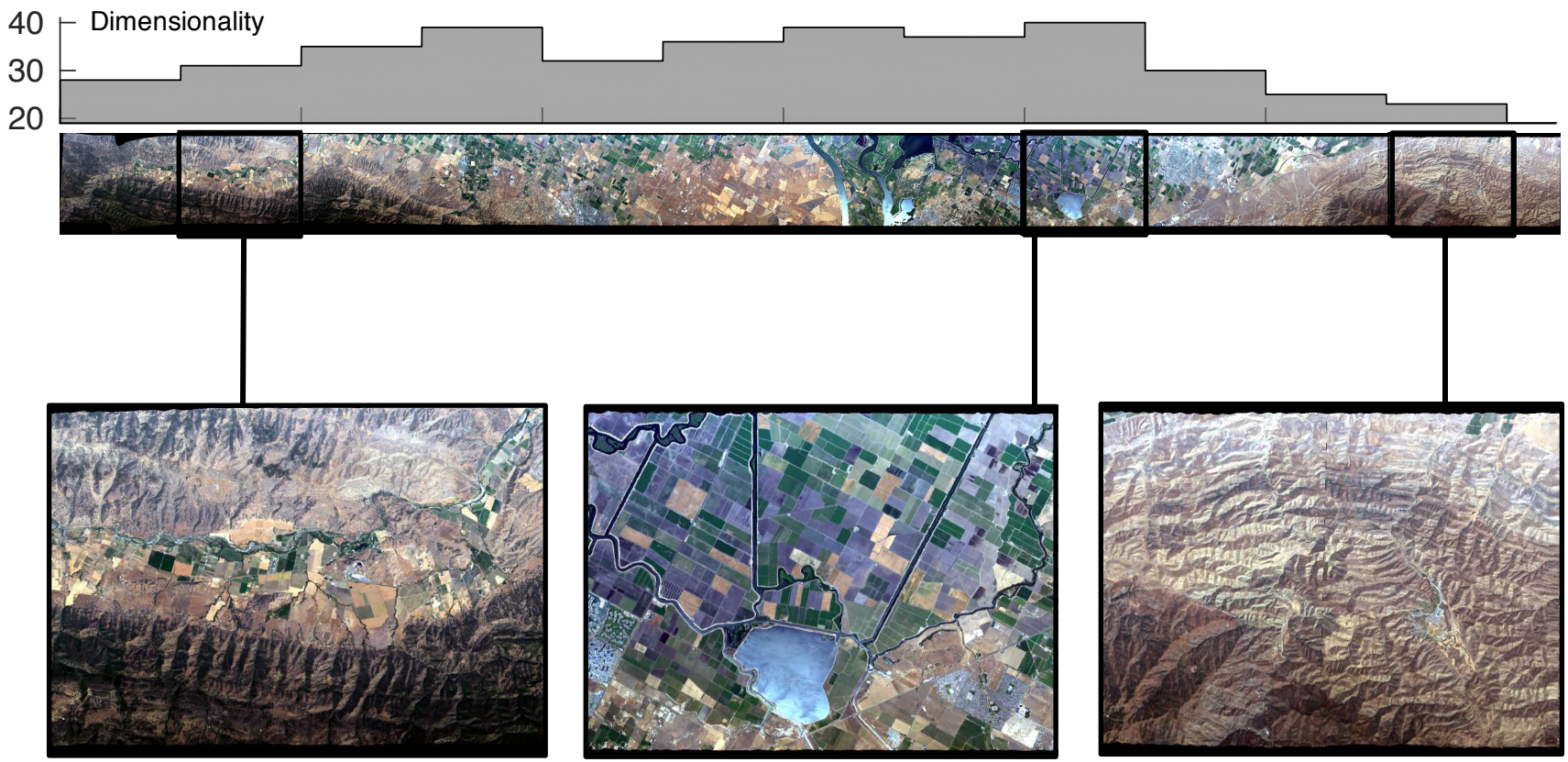
[Thompson et al., RSE 2015

Shenandoa species maps



Phil Townsend, U. Wisconsin

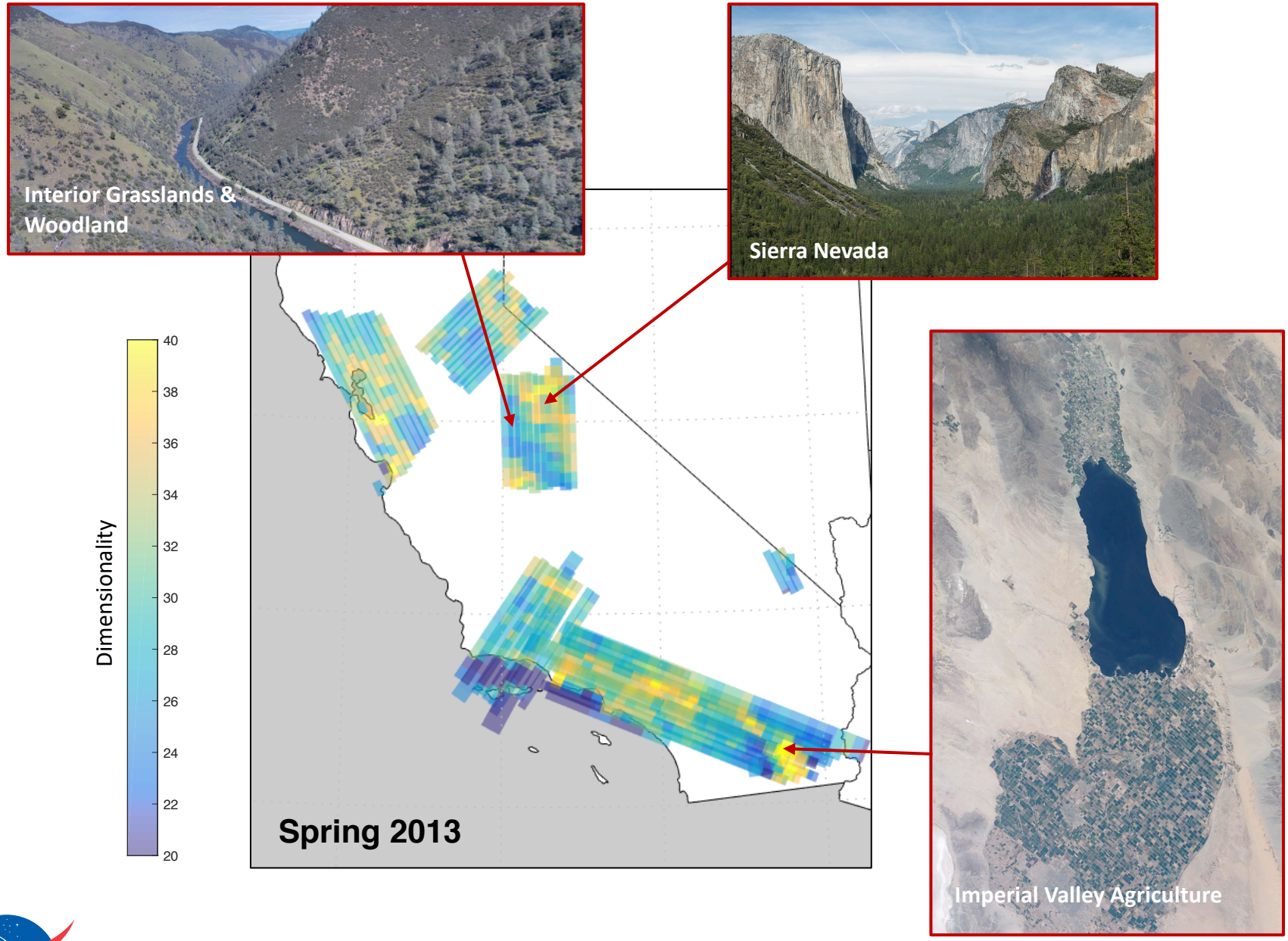
High Intrinsic Dimensionality



River Valley, Dimensionality 31

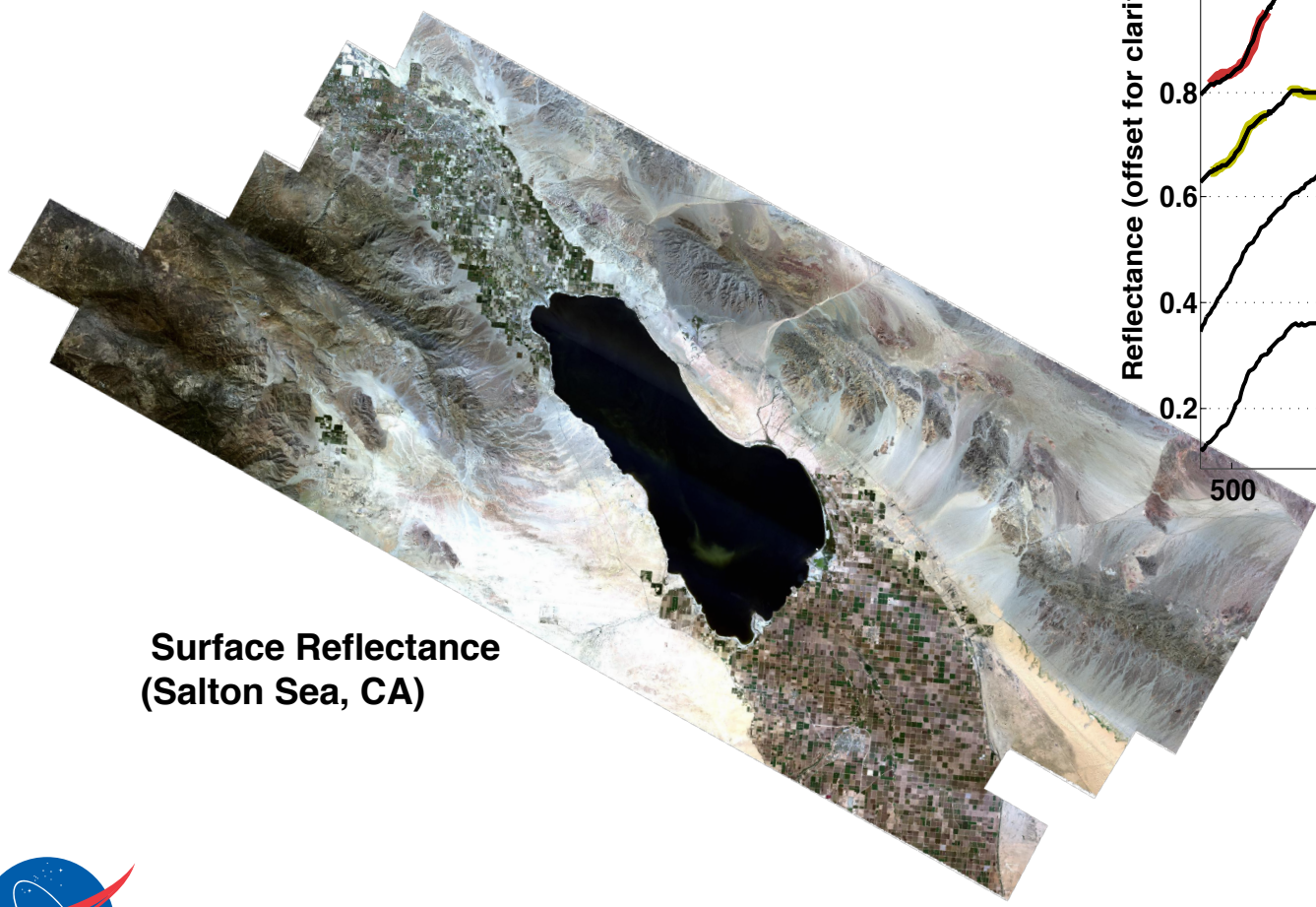
Cropland/Urban, Dimensionality 40

Barren, Dimensionality 23

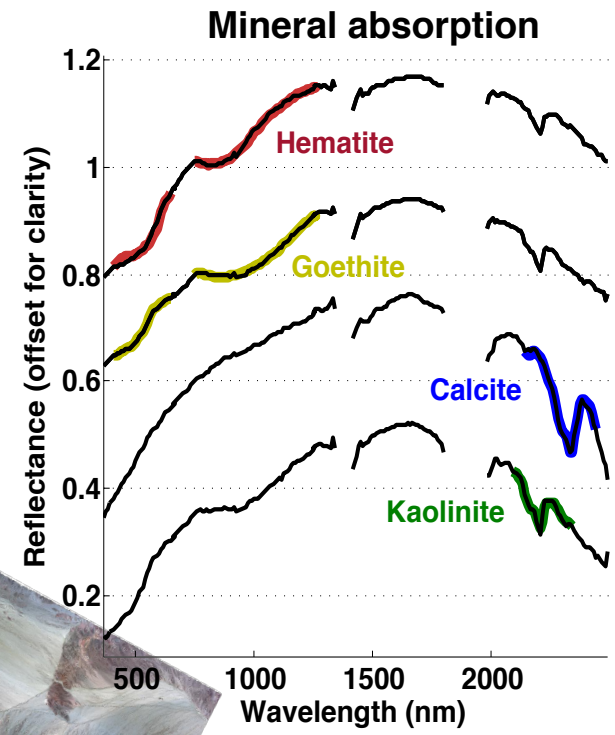


Images: Google / NASA / Sierra Nevada Photo by DAVID ILIFF. License: CC-BY-SA 3.0

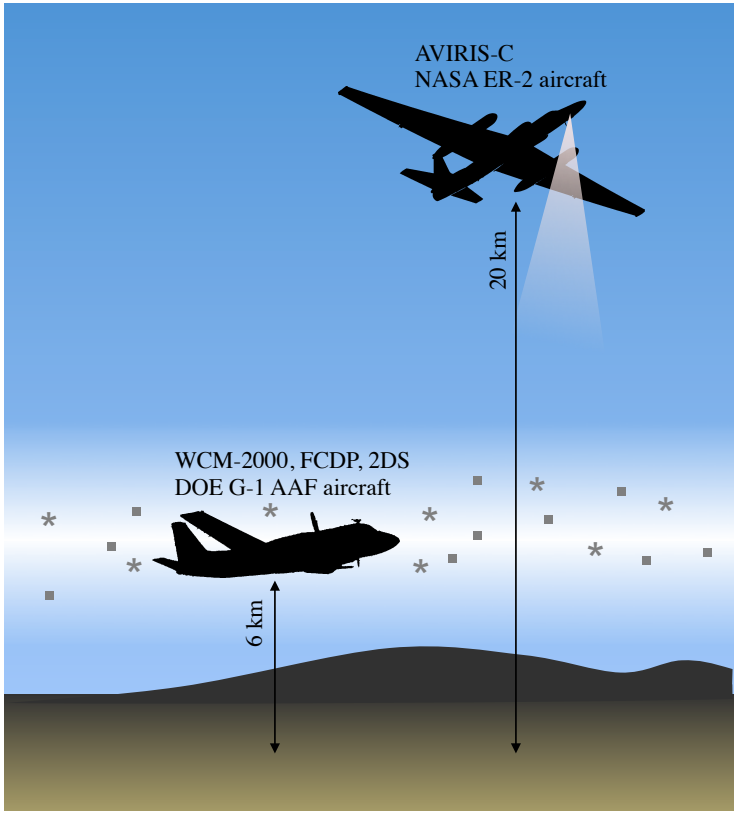
Geologic maps for the EMIT mission

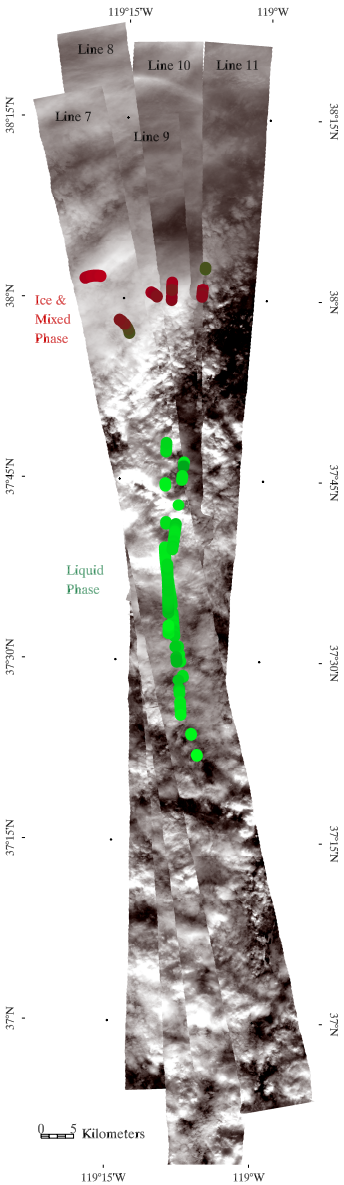


Surface Reflectance
(Salton Sea, CA)

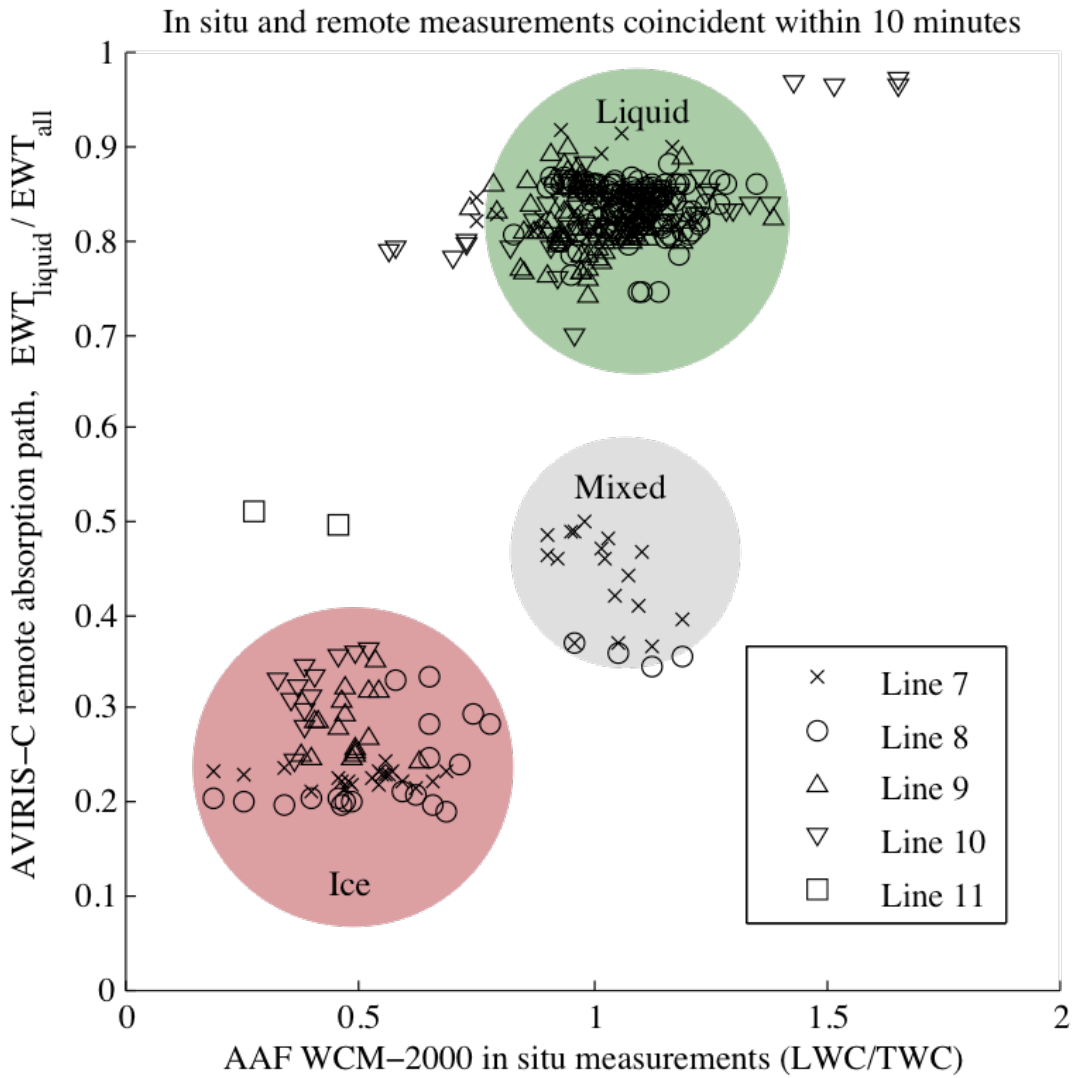


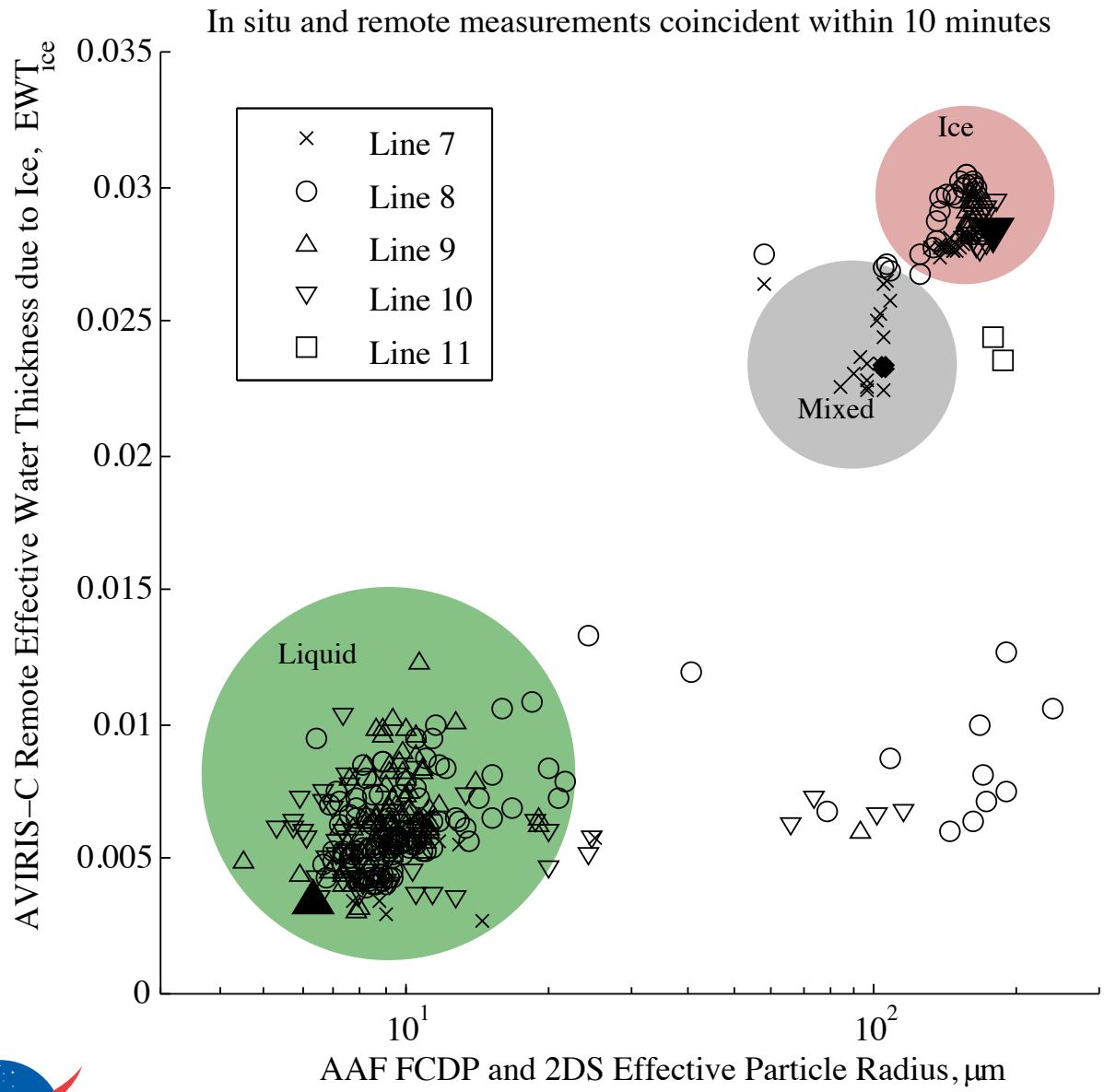
Coincident multi-aircraft measurement

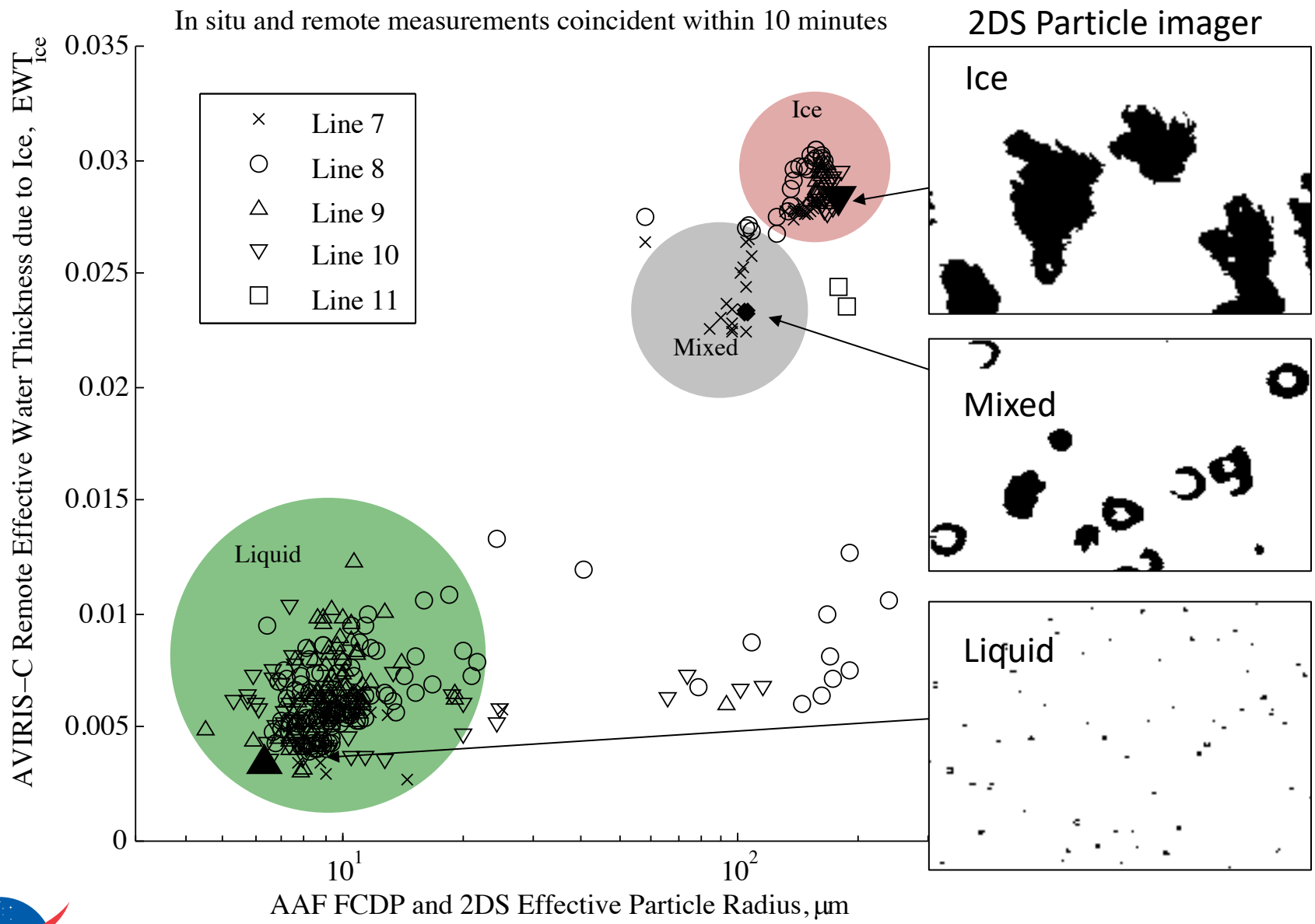




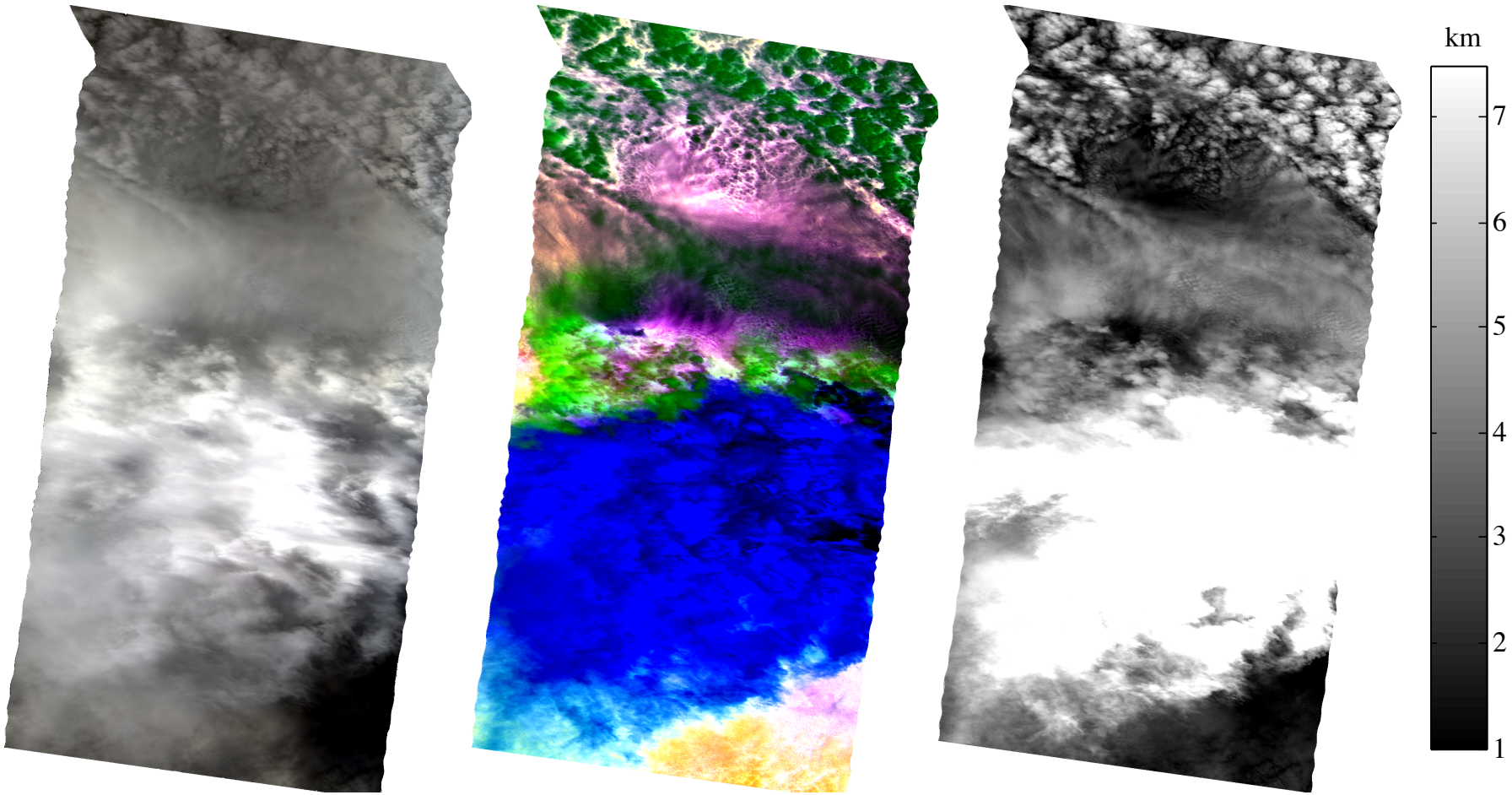
In situ corroborates remote data




In situ and remote measurements coincident within 10 minutes
AVIRIS–C Remote Effective Water Thickness due to Ice, EWT_{ice}
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
Line 7
Line 8
Line 9
Line 10
Line 11
Ice
Mixed
Liquid
10^1
10^2
AAF FCDP and 2DS Effective Particle Radius, μm


In situ and remote measurements coincident within 10 minutes
2DS Particle imager
AVIRIS–C Remote Effective Water Thickness due to Ice, EWT_{ice}
AAF FCDP and 2DS Effective Particle Radius, µm
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
10^1
10^2
Line 7
Line 8
Line 9
Line 10
Line 11
Ice
Mixed
Liquid
Ice
Mixed
Liquid

Remote sensing of cloud phase

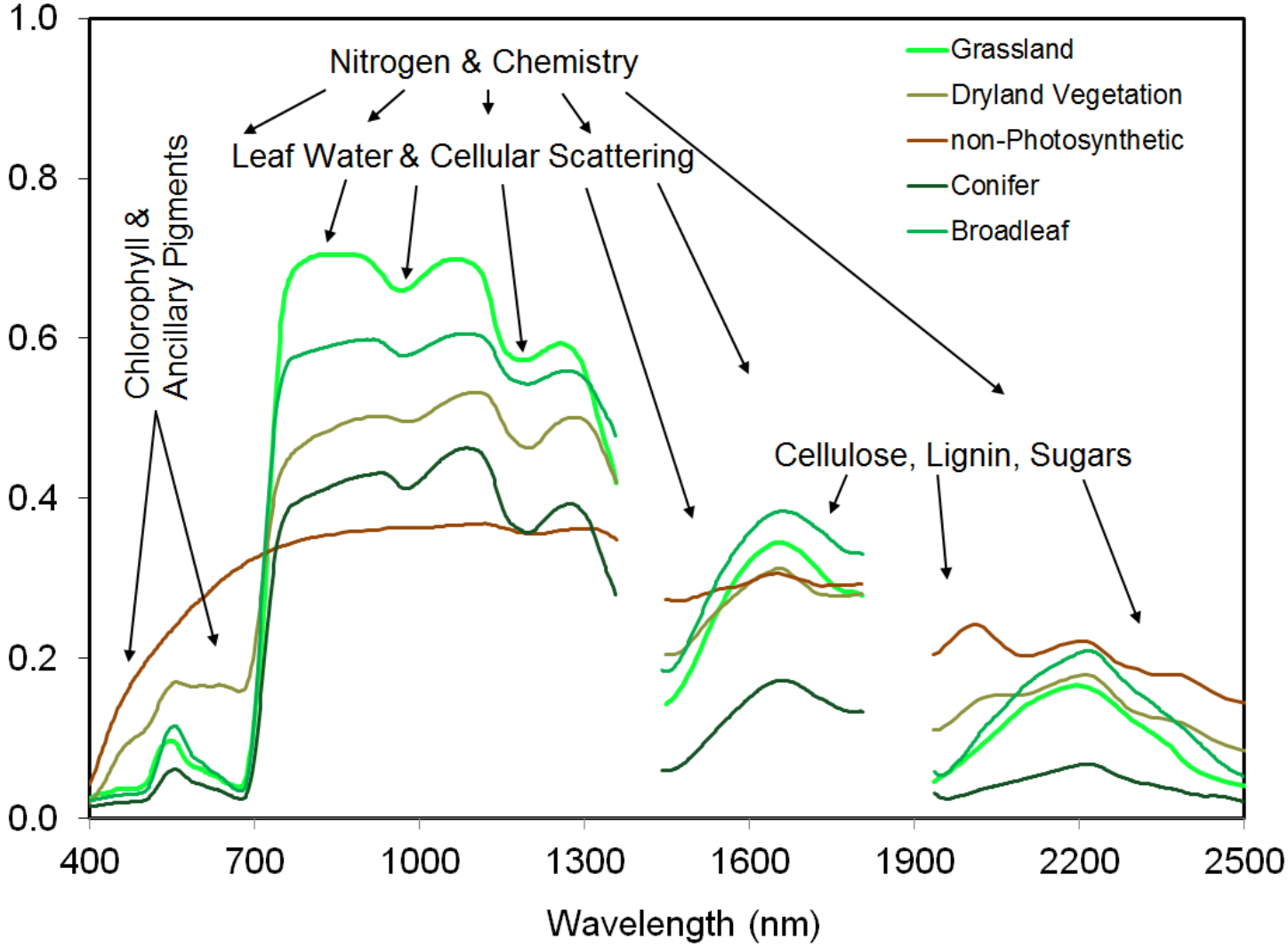


RGB Image

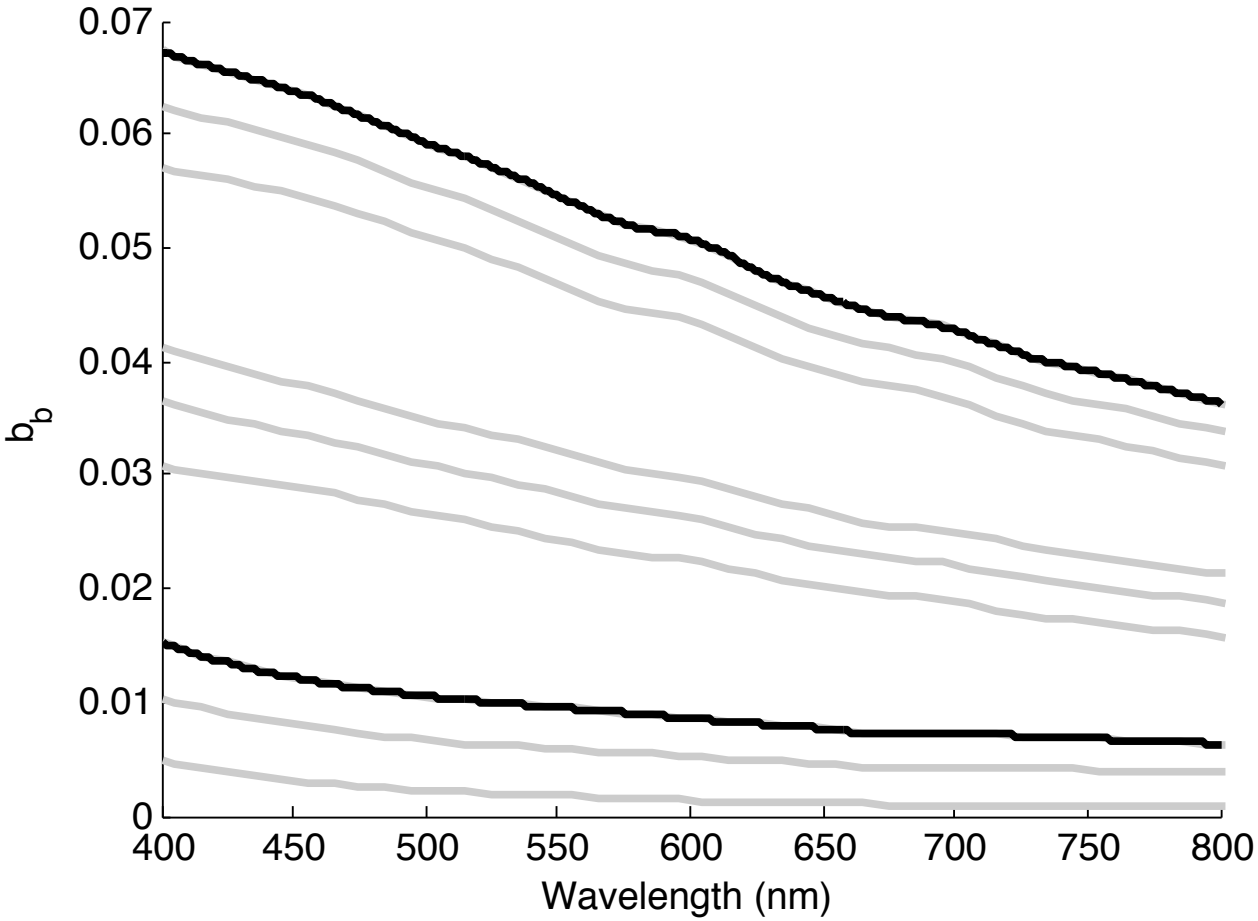
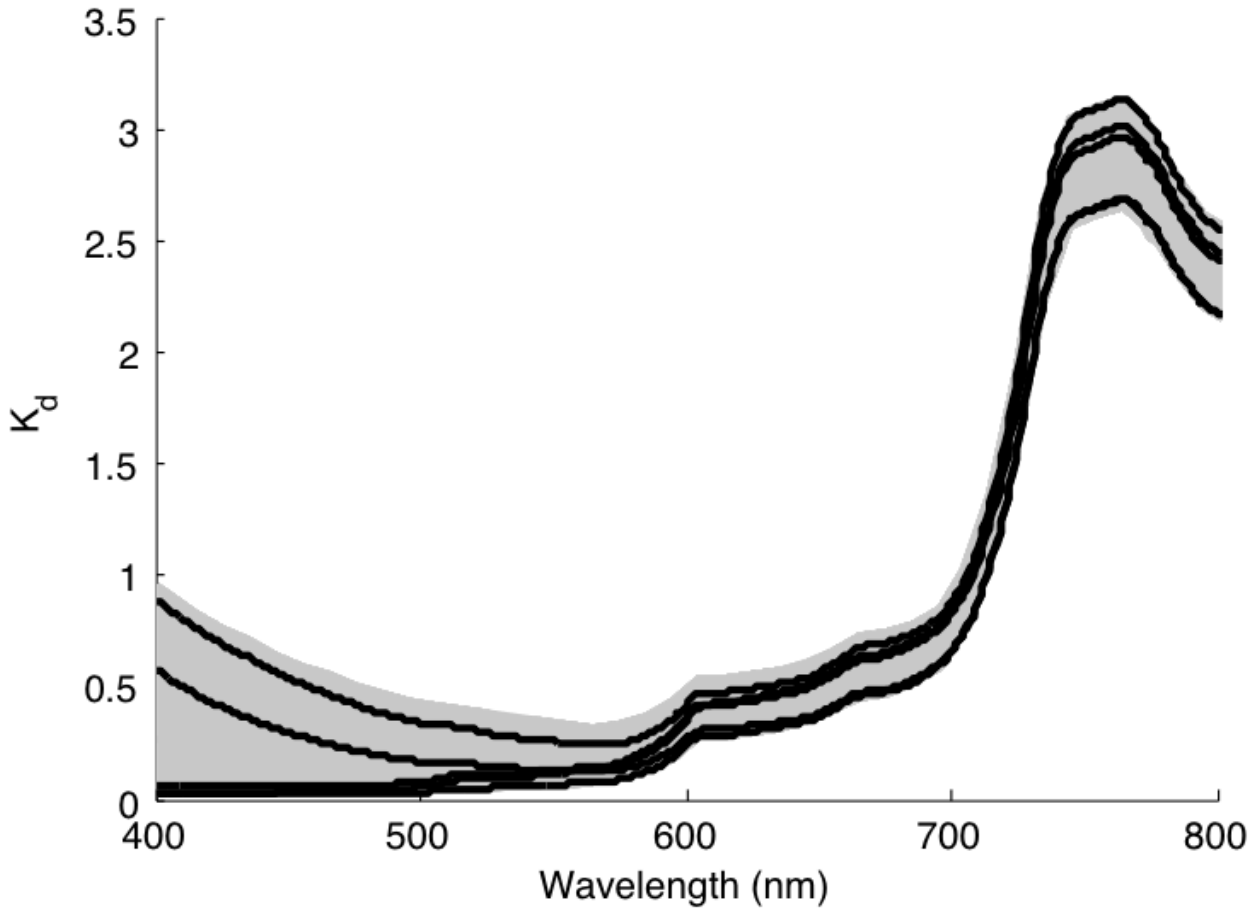
Ice Liquid Vapor

Pressure Altitude

Vegetation signatures



Example of b_b endmember library



Example of K_d endmember library