ReFRACtor

Reusable FRamework for Atmospheric Composition

ROSES 16-AIST-0019

Jet Propulsion Laboratory
California Institute of Technology

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1. Jet Propulsion Laboratory, California Institute of Technology.

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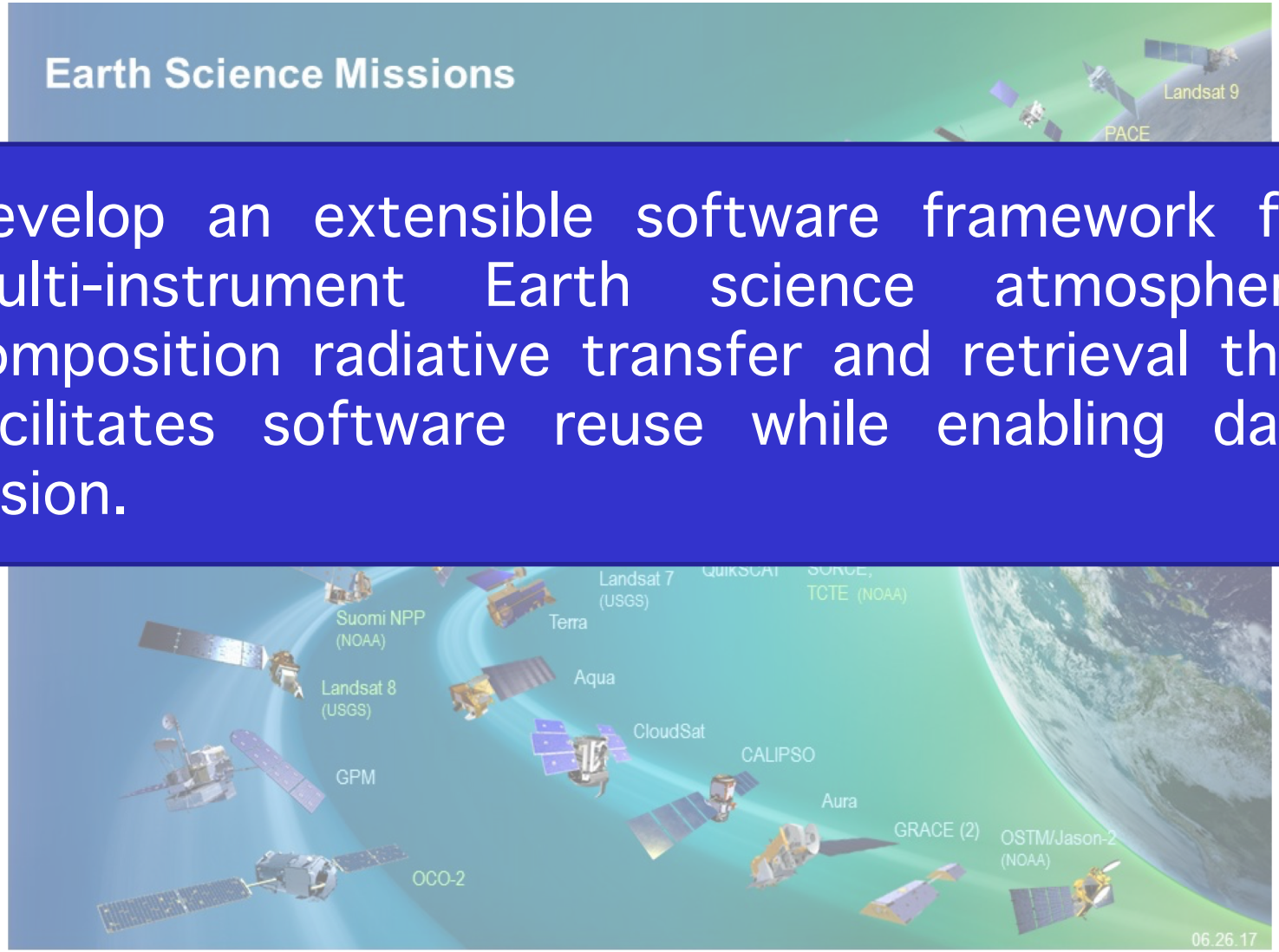
Team Members

Team Member	Responsibilities
James McDuffie	PI / Software engineering
Kevin Bowman	Co-I / Science
Jonathan Hobbs	Co-I / Uncertainty quantification
Vijay Natraj	Co-I / Radiative transfer
Edwin Sarkissian	Retrieval implementation
Mike Smyth	Software engineering
Matthew Thill	Signal processing
Sebastian Val	Software engineering

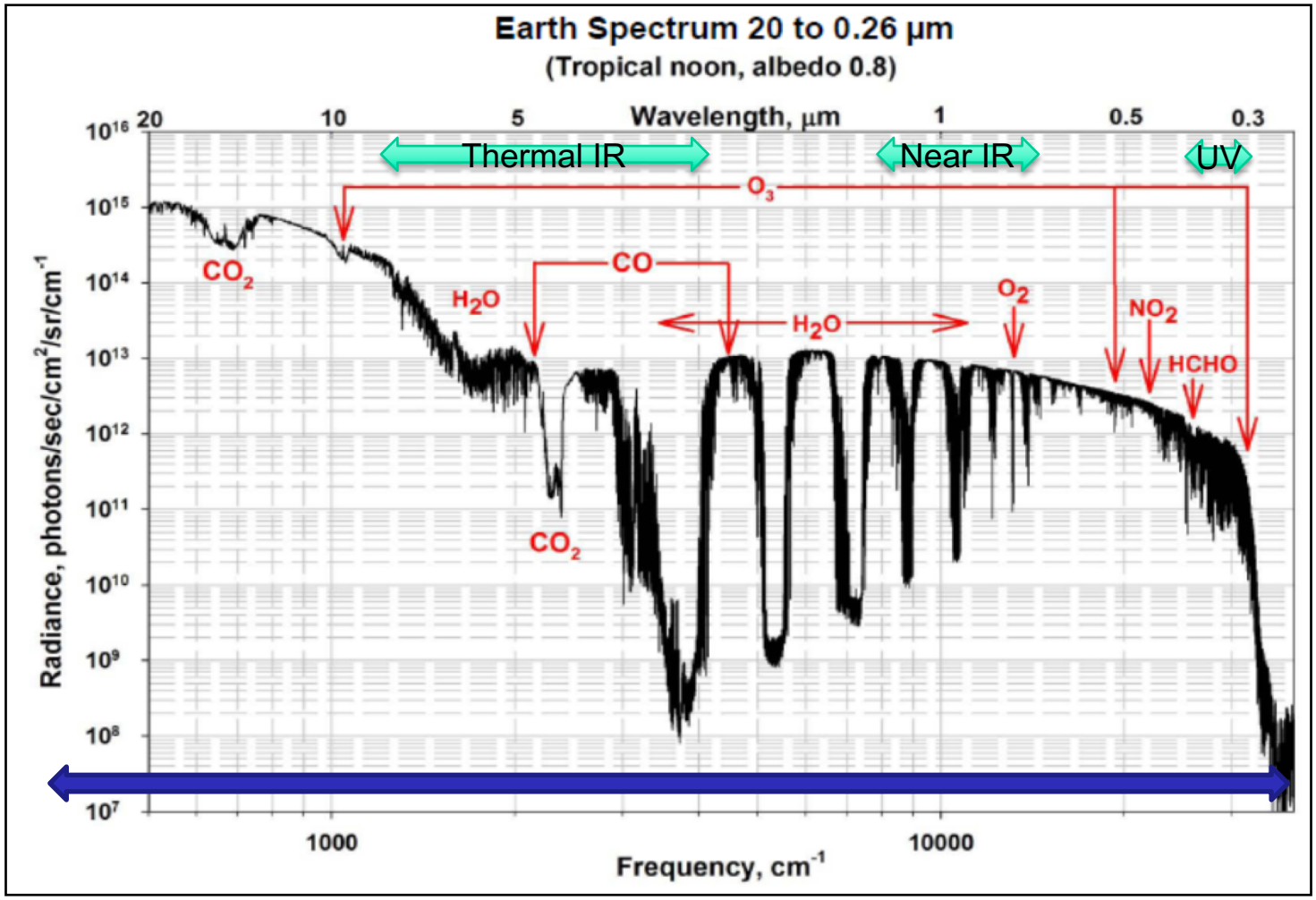
All team members are affiliated with Jet Propulsion Laboratory, California Institute of Technology.

Objective



Develop an extensible software framework for multi-instrument Earth science atmospheric composition radiative transfer and retrieval that facilitates software reuse while enabling data fusion.

Area of Technical Advancement



Target spectral modeling region capabilities: 0.2 µm to 100 µm

Approximate spectral range of targeted instrument implementations

Reusability

- Reusable and extensible allowing different instrument teams to use the same code base
  - New instrument missions can start with a framework that has tested and verified algorithms
  - New missions can focus on the novel algorithmic pieces unique to their instrument

- Help reduce the cost and risk of L2 development for new atmospheric composition Earth science missions
  - Eliminates duplication, and lowers costs while providing critical capabilities that support missions

Data Fusion

- Support data fusion of radiance measurements from multiple instruments through joint retrievals

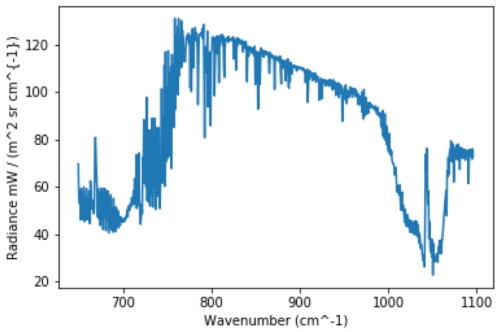
- Multi-instrument not only in the sense that different instruments can use the same software, but also in the sense that data products can be enhanced from multiple instruments through joint retrievals

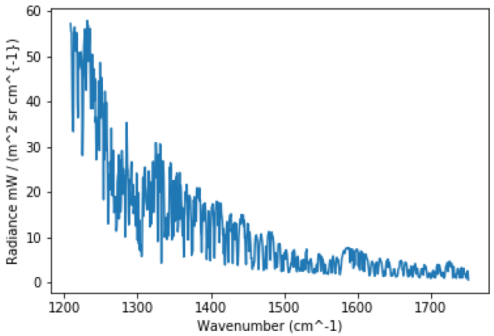
CrIS + OMPS NM

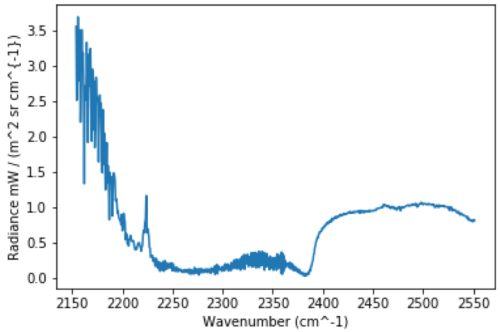
- Ultimate milestone is a CrIS + OMPS Nadir Mapper proof of concept joint Ozone retrieval
- Information from different spectral bands provides better sensitivity to the vertical stratification of atmospheric constituents
- Overlapping spatial and temporal information reduces measurement uncertainty
- Eliminates need to do bias correction between instruments done with multiple models

Multi-Instrument Atmospheric Composition Retrievals

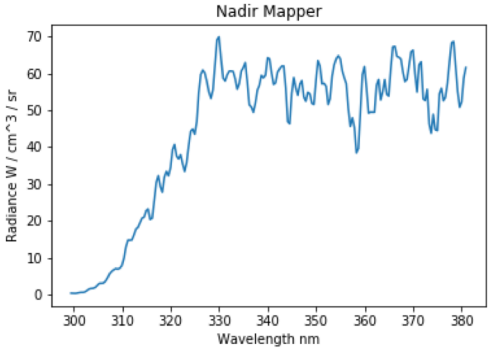
CrIS

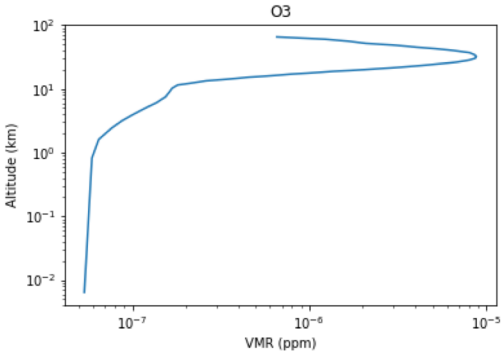






OMPS





Software Methodology

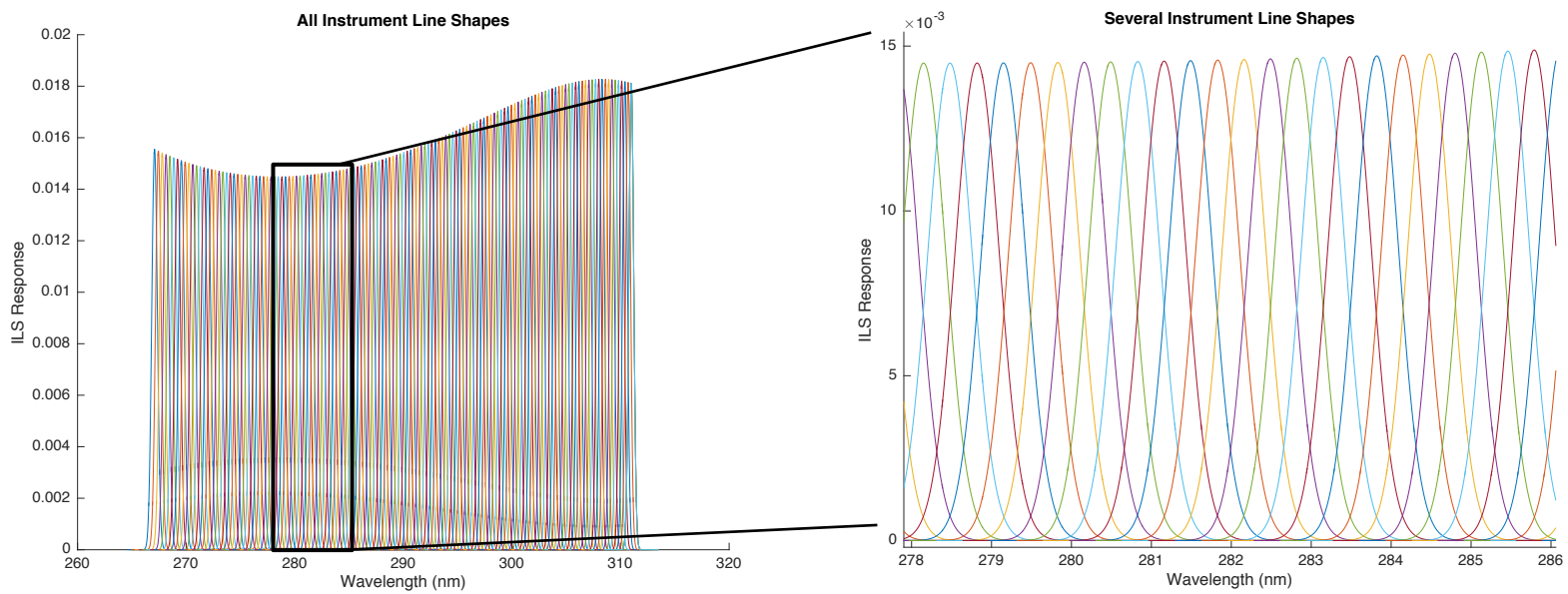
- Strive to hide complexity from user until they need to know about it
- Provide working examples that can be copied and adapted
- Facilitate the addition of new algorithms to work with existing code

Data Pairing

- Allows querying for closest observations temporally and spatially
- Used to create pairs of observations between instruments
- Only minimal extra code required per instrument implementation
- Class hierarchy that works in concert with existing L1B readers to provide overview information of L1B files

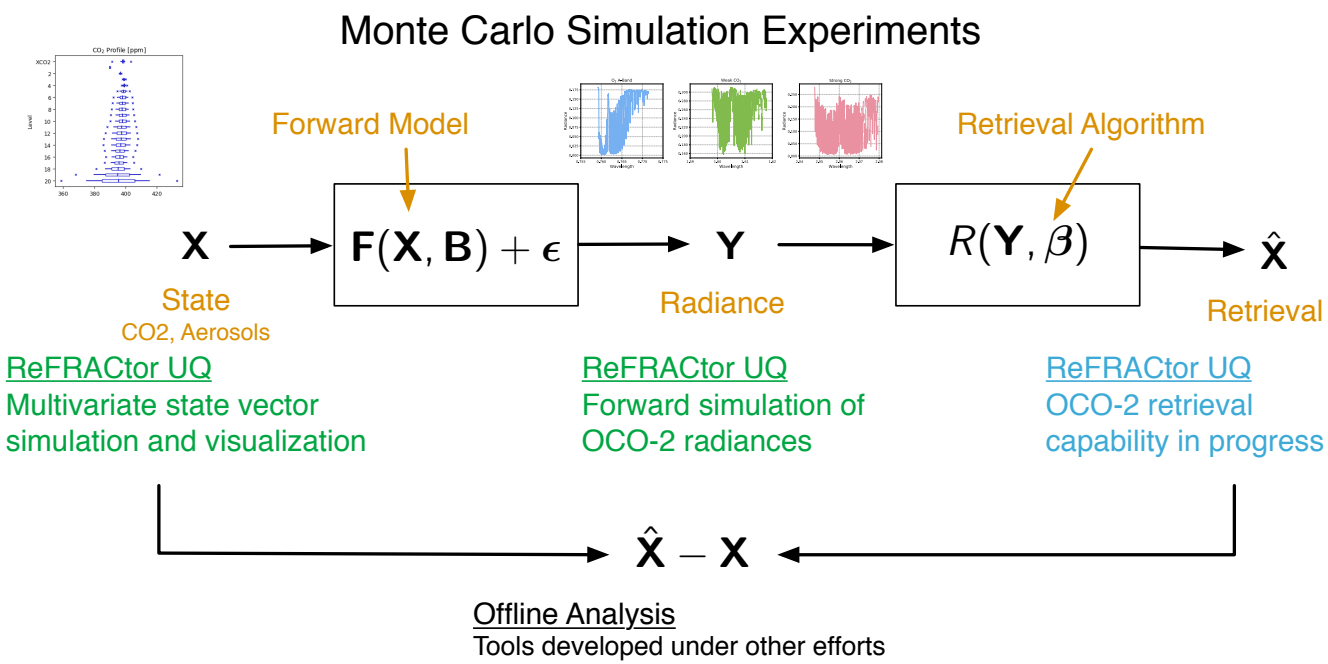
Instrument Model

- CrIS specific CCAST instrument implementation
  - Version using existing framework convolution method
  - Fast version using Fourier transforms
- Fast arbitrary ILS convolution computation
  - Utilizes commonality in spectral response functions to precompute part of the work needed



Uncertainty Quantification

- UQ Objective: Develop tools to execute probabilistic simulations of retrieval systems within ReFRACtor



Multi-Step Strategy

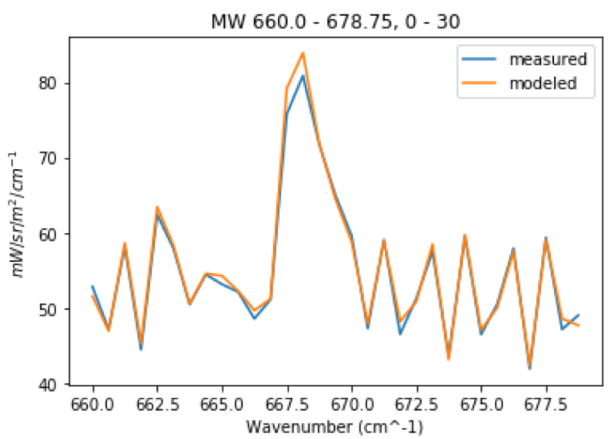
- Overall retrieval consists of multiple steps using small spectral regions known as “micro-windows”
- Retrieval quantities vary between steps and feed into subsequent steps
- Allows fine tuning certain quantities based on where information is present in the spectra
- Improved our code to reuse the atmospheric state between subsequent steps
- Added mechanisms for defining steps in terms of micro-windows and retrieval components
- Built reader to use climatological inputs from the MUSES project

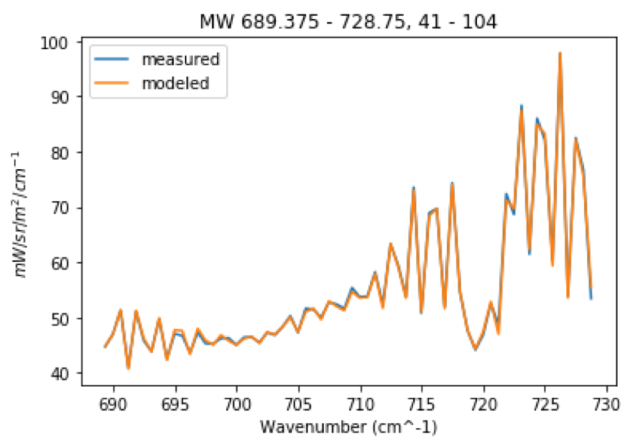
Multi-Platform Building

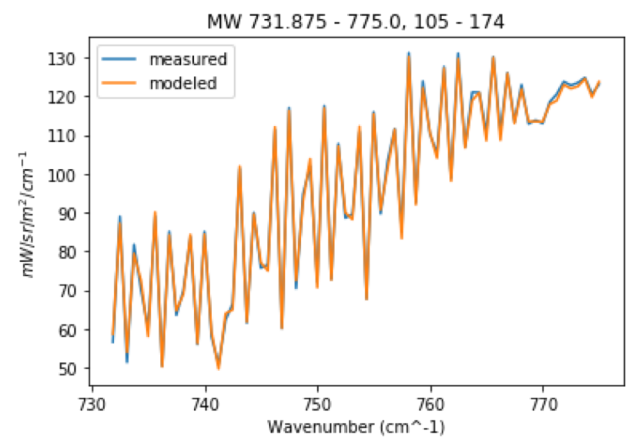
- Utilizing Conda package management system with dependency handling to simplify building and deploying across supported architectures
- Conda is an open source package management system for Windows, macOS and Linux
- Simplifies installation and use by end users who are not necessarily developers
- Supports developers by setting up required packages necessary for building

CrIS

- Initial retrieval working and being fine tuned
  - Utilizing multi-step approach along with micro-windows of spectra where information content of target species is highest
  - Adapting earlier research to focus on ozone
- Ongoing work to validate against other models

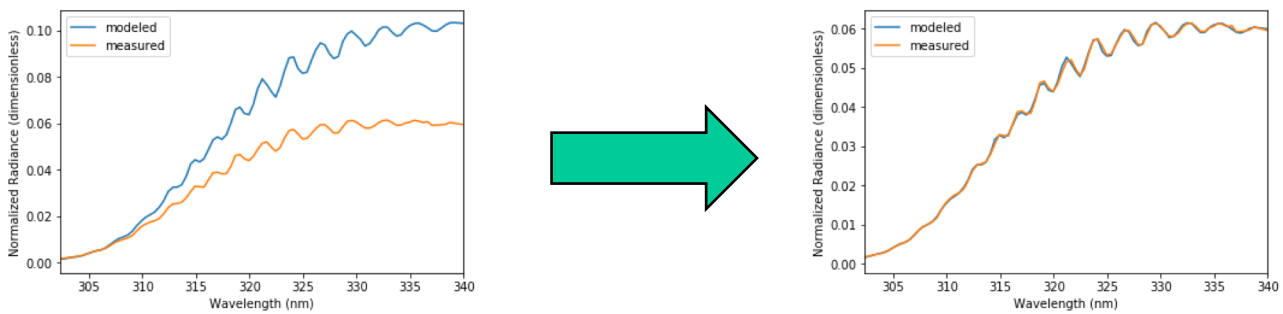


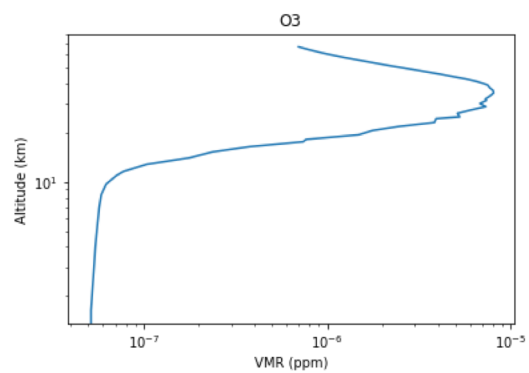




OMPS

- Initial retrieval working
- Still needs Raman scattering integration so results are not accounting for all atmospheric effects





Impact and Engagements

- Environment Climate Change Canada
  - Investigating issues with CO_2 retrievals that were measured over snow using existing algorithms
- University of Toronto
  - Atmospheric Imaging Mission for Northern Regions concept study
- JPL
  - Research into retrieving cloud thickness and height from sounder data in the A-band
  - Research into increasing the accuracy of XCO_2 using spatial correlations
  - Interest in use for future missions by science and technical sections

Ongoing Work

- Radiative transfer speed up using Principal Component Analysis techniques
- Generic mapping of forward model properties into subsets suitable for use retrieval
- Further refinements to instrument models and investigations into empirical approaches to help automatically compute certain key forward model parameters that are tied to the instrument model
- Working to integrate the forward model of two different instruments in one retrieval
- Making retrieval multi-step approach more turn-key

Backup

Acronyms

List of Acronyms

Acronym	Meaning
AER	Atmospheric and Environmental Research
CARBO	Carbon Balance Observatory
CRIS	Cross-track Infrared Sounder
FP	Full Physics
GeoCARB	Geostationary Carbon Observatory
ILS	Instrument Line Shape
MUSES	MUlti-SpEctra, MUlti-SpEcies, Multi-SEnsors
NLLS	Non Linear Least Squares
OCO-2	Orbiting Carbon Observatory 2
OMPS NM	Ozone Mapping Profiler Suite Nadir Mapper
OTS	Ozone Trend Science
RT	Radiative Transfer
TES	Tropospheric Emission Spectrometer
UQ	Uncertainty Quantification

Physical Modeling Approach

- Full Physics (FP) atmospheric composition modeling and retrieval approach
- Simulate the transfer of energy from the sun to the instrument using a sophisticated model of the atmosphere and the surface of the Earth
- Uses radiative transfer versus statistical methods
- Trades off accuracy for speed, but can optimize with approximations later

Impact and Engagements - Research

- Sébastien Roche - Ensemble of spectra was generated over a range of different geometric and geophysical conditions, and for two instrument types: dispersive and Fourier transform spectrometers
  - The column-average dry-air mole fraction of CH4 (XCH4) and CO (XCO) has been retrieved from those spectra.
  - The Level 2 (XCH4, XCO) accuracy and precision requirements will be traced to Level 1 data (spectra) requirements and provide constraints on instrument requirements.

Impact and Engagements - Research

- Joseph Mendonca - Environment Climate Change Canada
  - Investigating issues with CO_2 retrievals that were measured over snow using existing algorithms
  - Determining if optimizations to bidirectional reflectance distribution function (BRDF) will improve retrievals

"The modular nature of the code along with python wrappers make it easy to investigate the impact of factors such as different surface models, aerosol types, and the use of empirical orthogonal functions on these retrievals. The code is written in a way that enables users to implement python classes to test new functions with the existing framework in order to see if the retrievals can be improved."

Impact and Engagements - Research

- Mark Richardson at JPL to use ReFRACtor code for operational cloud retrieval code based on his previously published research using older versions of our software
- Previous research:
  - Richardson, M., Leinonen, J., Cronk, H. Q., McDuffie, J., Lebsock, M. D., & Stephens, G. L. (2019). Marine liquid cloud geometric thickness retrieved from OCO-2's oxygen A-band spectrometer. Atmospheric Measurement Techniques, 12(3), 1717–1737. https://doi.org/10.5194/amt-12-1717-2019
  - Richardson, M., McDuffie, J., Stephens, G. L., Cronk, H. Q., & Taylor, T. E. (2017). The OCO-2 oxygen A-band response to liquid marine cloud properties from CALIPSO and MODIS. Journal of Geophysical Research: Atmospheres, 122(15), 8255–8275. https://doi.org/10.1002/2017jd026561

Impact and Engagements – Line Management

- Working with JPL section 398 to make ReFRACtor a part of the section's "product lines" available to be used by projects for atmospheric composition retrievals
- Section would lean on projects using our personnel to use section core capabilities

Virtual Sounder Project

- “Virtual” project looking into the impact of ReFRACtor for future work
- Led by John Worden involving science and data systems sections
- Identified several use cases for future work

VSP – Use Cases –Sounders

- Multi-Sounding XCO_2 retrievals
  - Take CO_2 accuracy from 1 ppm down to 0.5 ppm
  - Introduce spatial correlations to improve retrieval
- Ozone Trending Science
  - Use ReFRACtor for completing multi-year / mult-instrument Ozone record
  - Retrievals of ozone, CH_4, CO, PAN, H_2O, HDO
- AIRS + OMI
- OSSES for known future projects (CARBO, SBG)

VSP – Use Cases - Imaging Instruments

- AVIRIS NG (leads potentially to SBG)
  - OE joint spectral surface reflectance / atmosphere retrievals plus multi-scene retrievals

- SBG
  - Use optimal estimation atmosphere / joint spectral surface reflectance SBG retrievals