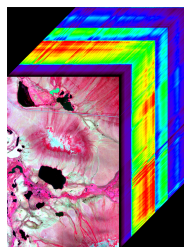


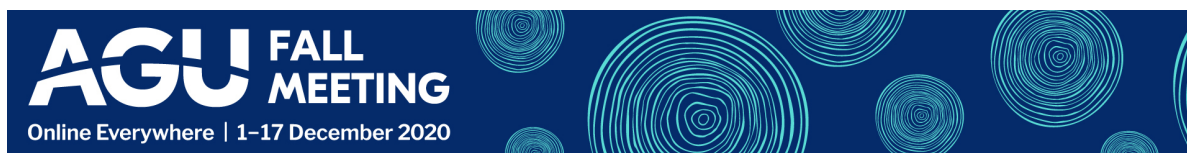
Evaluation of sensor characteristics on the retrieval of vegetation surface reflectance in high-latitude ecosystems

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PRESENTED AT:



BACKGROUND

Over the last four-plus decades, passive optical visible (VIS), near-infrared (NIR), and shortwave infrared (SWIR), as well as thermal infrared (TIR) remote sensing data have played key roles in characterizing and monitoring the composition, structure, and functioning of terrestrial and aquatic ecosystems. For example, optical spectral vegetation indices (SVIs), including the normalized-difference vegetation index (NDVI) using the ratio of visible red and NIR reflectance, have been used to monitoring broad-scale patterns in terrestrial vegetation seasonality, composition, to detect vegetation stress and track changes in primary productivity (Serbin and Townsend, 2020). Similarly, TIR platforms have enabled the regular tracking of plant stress, changes in surface energy balance, evapotranspiration, and monitoring the fluxes of carbon, water, and energy from terrestrial ecosystems (Sobrino et al. 2016). Together, TIR and optical platforms provide invaluable tracking of vegetation composition, function, and stress across Earth's biomes.

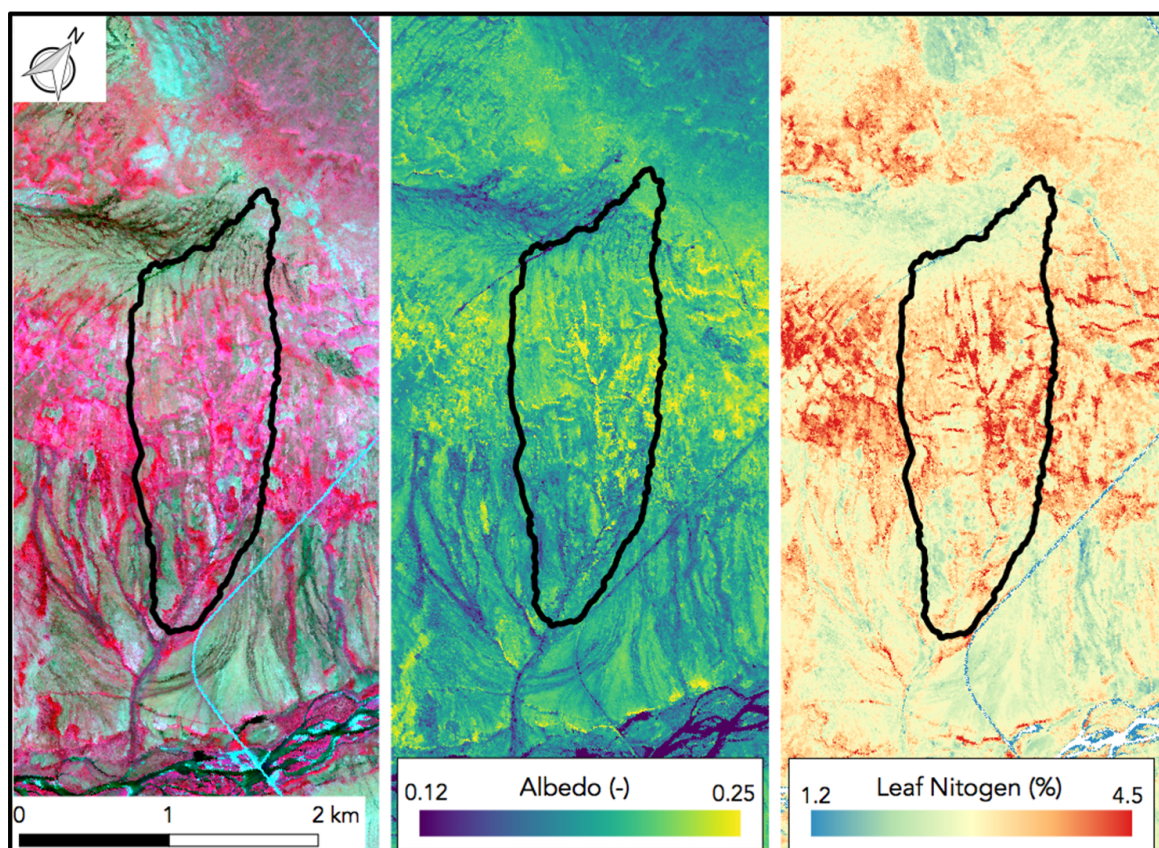


Figure 1. Example AVIRIS-ng image data from the Seward Peninsula, Alaska collected in support of the DOE Next-Generation Ecosystem Experiment (NGEE) in the Arctic and the NASA Arctic/Boreal Vulnerability Experiment (ABOVE). This example shows a near-infrared (NIR) composite (NIR-Red-Green image stack, left) where darker red is more dense vegetation, the average shortwave (0.4-2.5 micron) reflectivity (middle), and an estimated canopy nitrogen map derived using standard trait-mapping approaches (Serbin and Townsend, 2020).

Recently, there has been increased interest in the use of high spectral resolution optical data within the full SWIR region (i.e. 0.35 to 2.5 microns). These data have been identified as critical for monitoring global plant function and biodiversity of ecosystems (Cavender-Bares et al., 2020), given the more direct connection between remote sensing measurements and the underlying functional properties of plants and ecosystems (Serbin and Townsend, 2020). For example, airborne imaging spectroscopy (IS) data has been used to remotely estimate plant nutrition and nutrient cycling, functional traits, and carbon fluxes (Serbin and Townsend, 2020) as well as a means for improving process model representation of ecosystems through model-data integration approaches (Shiklomanov et al., 2020). As a result, a range of airborne IS platforms have been developed, providing high spectral resolution datasets across terrestrial ecosystems, ranging from the Arctic to the tropics. However, a lack of spaceborne Earth Observing (EO) IS platforms has led to a critical lack of consistent global coverage, particularly in critical habitats. In addition, most IS data has traditionally been collected during "peak greenness", biasing observations to a single

phenological stage. The previous spaceborne Hyperion platform (Middleton et al. 2013) addressed some of these challenges but had significant limitations given the small image swath width and poor signal-to-noise ratio (SNR). As a result, new global platforms are critically needed to improve the capacity to regularly monitor global biodiversity and plant function.

THE NASA SURFACE BIOLOGY AND GEOLOGY (SBG) MISSION & UNCERTAINTY QUANTIFICATION EFFORTS

Given the importance of consistent global IS observations, the recent NASA Decadal Survey (<https://science.nasa.gov/earth-science/decadal-sbg>) (National Academies of Sciences, 2018) identified the Surface Biology and Geology (SBG) Mission (Figure 2), a combined IS and TIR mission, as a critical Designated Observable for Earth Science. The NASA SBG mission (<https://sbg.jpl.nasa.gov/>) has specific architecture requirements (<https://sbg.jpl.nasa.gov/architecture>) to provide a high spectral resolution VSWIR image spectrometer capable of providing VNIRSWIR coverage of 10nm or better together with a 5-band TIR component with mid-infrared with TIR spectral channels. The platform(s) would have a revisit frequency of 2-16 and 1-7 days, for the IS and TIR components, respectively and a 30-45m IS and 40-60m TIR spatial resolution.

The SBG Mission Study has three objectives:

- Identify and characterize a diverse set of high-value SBG observing architectures
- Assess the performance and cost-effectiveness of architectures against SBG research and applications objectives
- Perform sufficient in-depth design of one or more candidate architectures to enable near-term science return

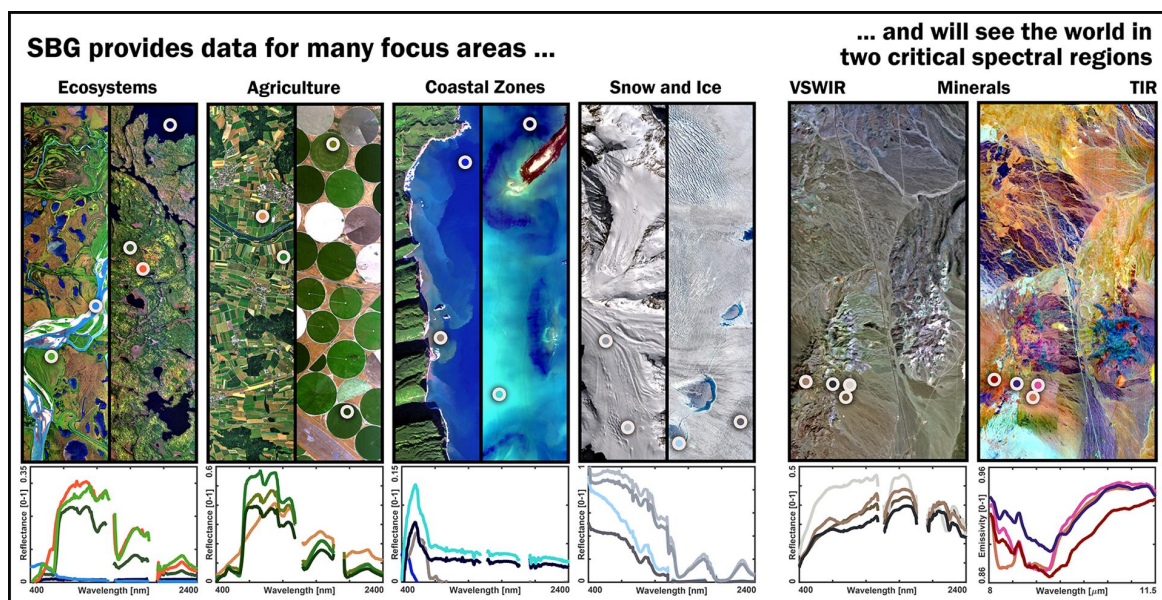


Figure 2. The NASA SBG platform is being designed to address critical challenges in the monitoring and mapping of critical terrestrial and aquatic habitats. The resulting rich spectral information, combined with the capacity for regular repeat Global coverage means that the SBG mission will provide an unprecedented opportunity for improving biodiversity monitoring, measuring ecosystem function in critical ecosystems, and informing process modeling efforts.

The NASA SBG VNIRSWIR Uncertainty Quantification (UQ) Effort

As part of the larger Modeling End-to-End Traceability (MEET) SBG effort within the SBG Mission Study, our team is conducting a range of UQ analyses to help guide the development of the SBG VNIRSWIR sensor and ensure that it meets the designated requirements (<https://sbg.jpl.nasa.gov/framework>) for the core focal areas (Figure 2). The MEET-SBG effort is providing a framework to quantify L2 uncertainty and propagation of errors from the surface to atmosphere to sensor, and the roles of retrieval methods to support end-to-end traceability of SBG. The modeling activity is a collaboration between JPL, ARC, GSFC, DOE-BNL industry, academic institutions, and non-profit organizations.

Here we report specifically on some of the preliminary results from the VNIRSWIR UQ synthesis. For this effort, we are utilizing existing observations (e.g. Figure 3) of high spectral resolution surface radiance and reflectance observations across a range of scales, platforms, locations, and focal areas.

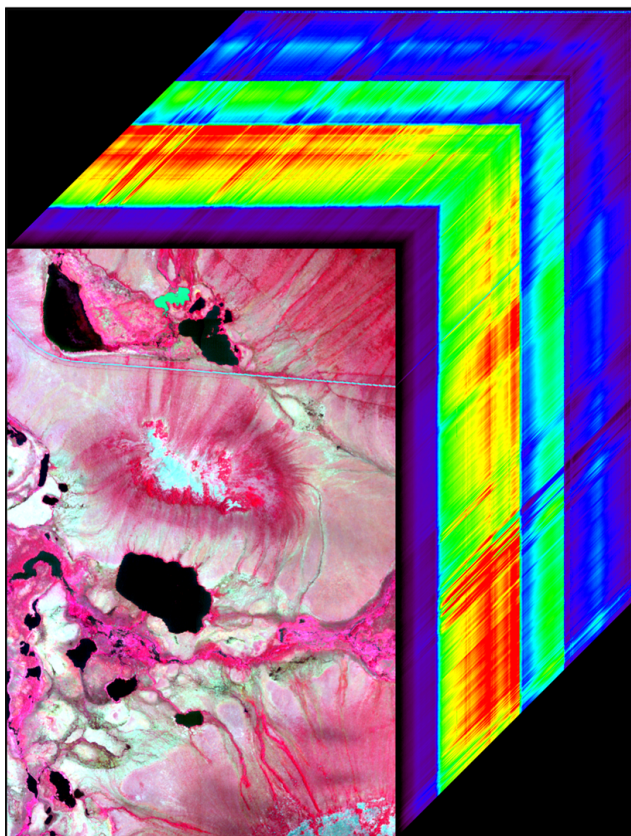


Figure 3. Example AVIRIS-NG image collected over the Kougarak watershed NGEA-Arctic Study site. This image was collected on 2018-08-15 as part of the NASA ABoVE Airborne Campaign.

With these existing datasets, MEET-SBG is exploring the retrieval performance of different proposed full-range, optical VNIRSWIR instrument designs (e.g. sensor properties, spectral resolution, band centers, FWHMs) and collection characteristics (sun-sensor geometries, atmospheric correction protocols, etc). These sensor design differences are represented by the use of different parametric noise descriptions (Figure 4) in our uncertainty quantification workflow (Figure 5). The overarching goal is to develop a set of metrics that can help guide the selection of architectures based on requirements and the value framework (<https://sbg.jpl.nasa.gov/framework>) used for final selection.

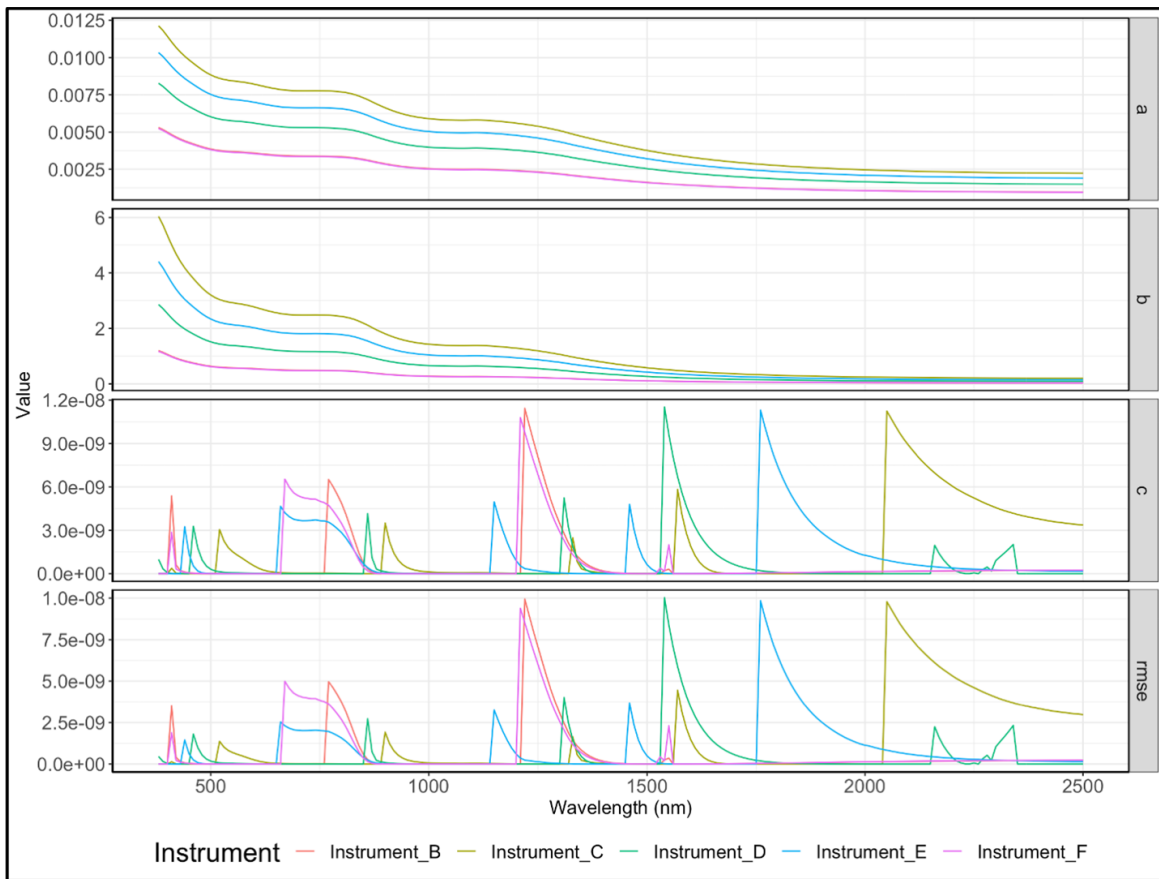


Figure 4. A visual depiction of different hypothetical instrument models that represent different design choices, instrument characteristics, band configurations, and signal-to-noise properties used in our SBG uncertainty quantification (UQ) analysis. These instrument models are based on a three-channel parametric noise description (https://isofit.readthedocs.io/en/latest/custom/best_practices.html?highlight=noise#instrument-models).

A core component of our VNIRSWIR UQ workflow (Figure 5) is the evaluation of proposed instrument models. For this, we are using parametric noise descriptions (e.g. Figure 4) which are then used in the forward simulation of top-of-atmosphere radiance and the inverse simulation of surface reflectance (Figure 5). These three-parameter noise models predict a noise-equivalent change in radiance as a function of L , the at-sensor radiance, described as:

$$L_{noisy} = a\sqrt{b + L} + c$$

where a , b , and c are the three parameters used to convert L to L_{noisy}

ISOFIT-HYPERTRACE WORKFLOW

ISOFIT-Hypertrace workflow for the MEET-SBG VNIRSWIR uncertainty quantification and instrument design analysis

As part of the SBG Mission Study and specifically the MEET-SBG effort, we have developed an open-source Python workflow, Py-Hypertrace (<https://github.com/isofit/isofit/tree/master/examples/py-hypertrace>), that acts as a wrapper for the core Imaging Spectrometer Optimal FITting (ISOFIT) (<https://github.com/isofit/isofit/engine>) (Thompson et al., 2018). ISOFIT provides the core functionality for fitting surface, atmosphere, and instrument models to imaging spectrometer data. ISOFIT can be used to simulate instrument characteristics, explore atmospheric correction procedures, and evaluate instrument assumptions and atmospheric conditions, through the use of different radiative transfer models (RTMs), on the retrieval of at-surface reflectance over the different surface and aquatic targets. ISOFIT supports the use of multiple RTMs, including MODTRAN (<http://modtran.spectral.com/>), LibRadTran (<http://www.libradtran.org/doku.php>), and SixS ([https://en.wikipedia.org/wiki/6S_\(radiative_transfer_code\)](https://en.wikipedia.org/wiki/6S_(radiative_transfer_code)))

Py-Hypertrace provides a wrapper to these core ISOFIT functionality as a workflow (Figure 5) to automate the forward simulation, atmospheric modeling, inversion to surface reflectance, and the evaluation of retrieval characteristics under different data, instrument model, and atmospheric conditions using existing or simulated observations as the benchmark.

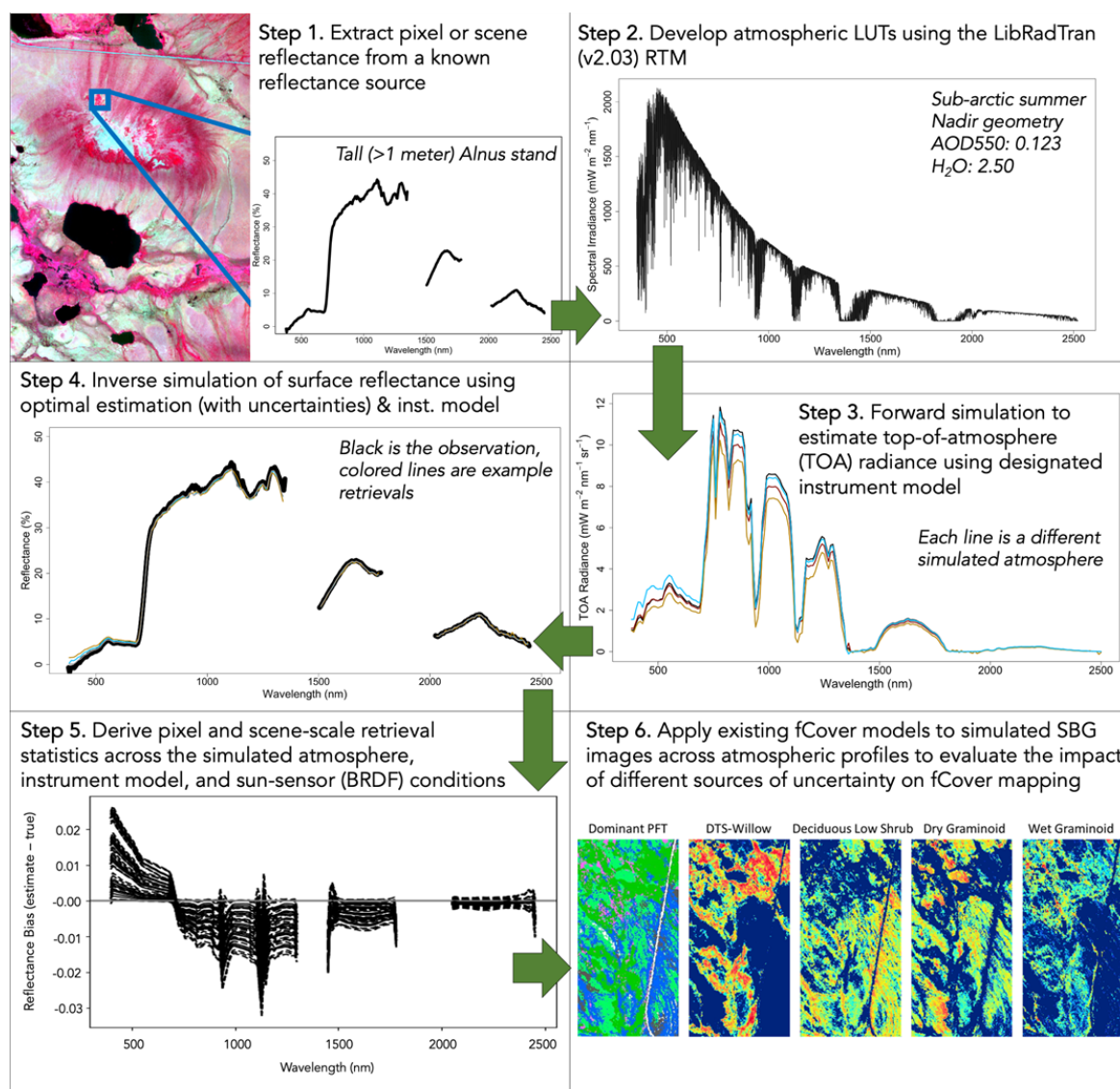


Figure 5. Schematic diagram depicting the overall ISOFIT-Hypertrace workflow used in this study

Using the ISOFIT-Hypertrace, it's possible to generate simulated surface reflectance retrievals using a range of input observations, from single pixels, whole images, as well as field-measured spectral datasets. The output from the ISOFIT-Hypertrace workflow can also be used in subsequent analyses to explore design choice, atmospheric conditions, RTM choice, and inversion approach on algorithms leveraging standard L2 surface reflectance.

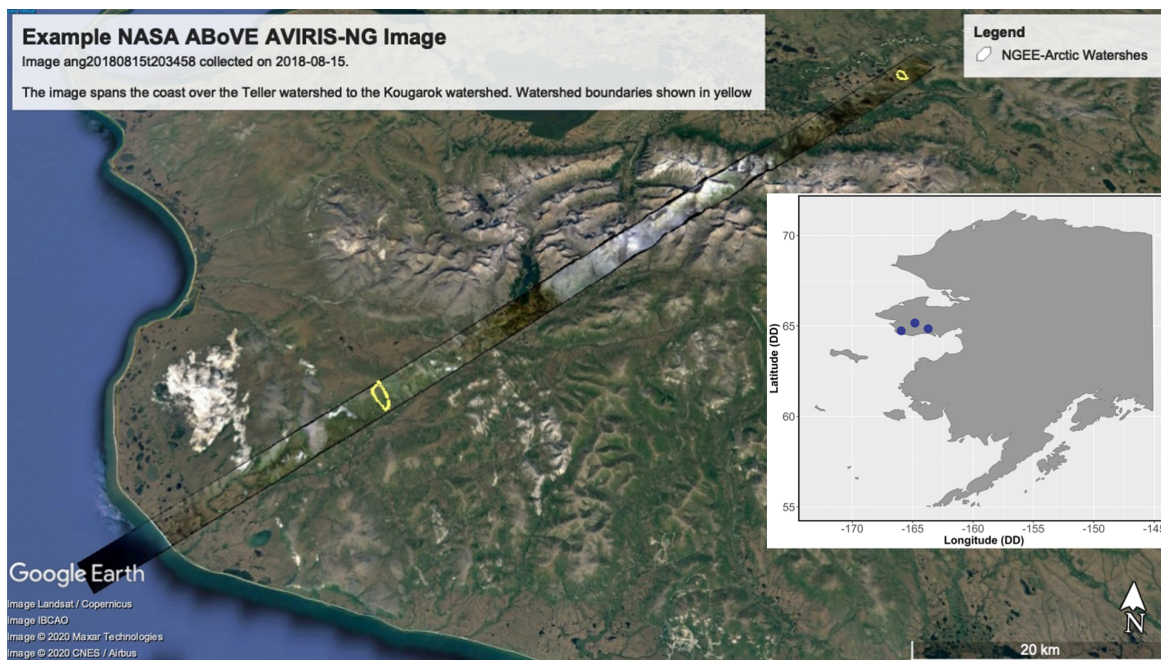


Figure 6. For this study, we focused on running the ISOFIT-Hypertrace workflow at two sites on the Seward Peninsula, Alaska, that are part of the DOE NGEE-Arctic (<https://ngee-arctic.ornl.gov/>) study and which has had NASA AVIRIS-NG imagery collected as part of the ABoVE Airborne Campaign (<https://iopscience.iop.org/article/10.1088/1748-9326/ab0d44/meta>). The two study areas (of the three NGEE sites, blue dots) included here are the Teller and Kougarak watersheds (yellow polygons) where in-situ and UAS-based high spectral resolution data has been collected since 2017.

In this study, we focused our ISOFIT-Hypertrace modeling efforts on two sites located in the Seward Peninsula, Alaska (Figure 6). These are two of the DOE NGEE-Arctic (<https://ngee-arctic.ornl.gov/>) core watersheds located in this region. These sites have a wealth of in-situ and UAS spectral measurements (e.g. Yang et al., 2020a (<https://www.mdpi.com/2072-4292/12/16/2638>)), as well as detailed information on vegetation composition and structure, useful for evaluating simulated surface reflectance from the workflow, as well as the impacts of canopy structure and BRDF on retrieval characteristics. In addition, these sites have multiple years of peak-season AVIRIS-NG data provided through the collaboration with the NASA ABoVE (<https://above.nasa.gov/>) Airborne Campaign. In addition, as part of the NGEE-ABoVE collaboration, various vegetation algorithms are being developed that leverage L2 reflectance observations, including fCover (Yang et al., 2020b (<https://astm6-agu.ipostersessions.com/Default.aspx?s=54-3B-0B-9D-DF-9A-8A-0F-F9-94-41-3A-6B-94-6F-86>))) and which we can use to evaluate the impact of instrument design and atmospheric conditions on mapping performance (Figure 5).

Atmospheric radiative transfer model (RTM)

The ISOFIT-Hypertrace workflow leverages look-up tables (LUTs) generated by an atmospheric RTM, such as MODTRAN, LibRadTran, or SixS. In this study, we leveraged the open-source LibRadTran (ver 2.0.3) model, specifically the *uvspec* function, to generate different atmospheric LUTs using a standard sub-arctic summer base atmosphere but varying aerosol optical depth (AOD), column water vapor (H₂O), and sun-sensor geometry (sun/sensor azimuth, zenith angles). Using these pre-populated LUTs the ISOFIT-Hypertrace workflow creates simulated top-of-atmosphere radiance (Figure 7) and then uses optimal estimation to derive estimated at-surface reflectance for each location or pixel. More details on how ISOFIT conducts its forward and inverse modeling can be found at the readthedocs (<https://isofit.readthedocs.io/en/latest/index.html>) site.

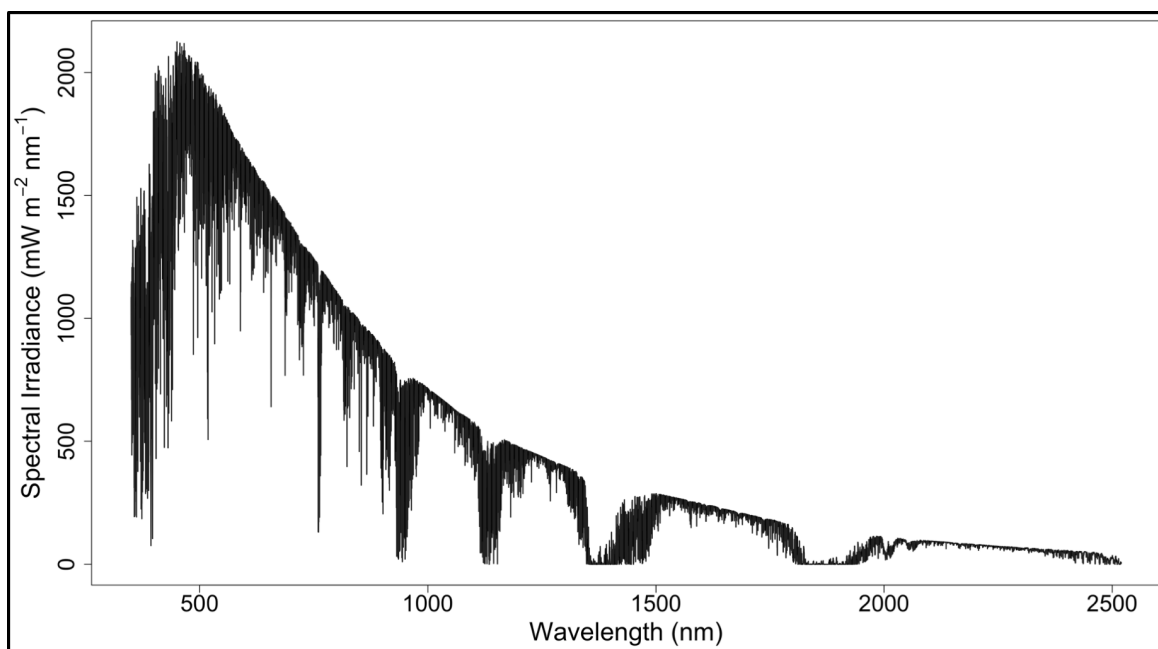


Figure 7. Example simulated TOA radiance using ISOFIT and the LibRadTran RTM.

The resulting at-surface reflectance generated by ISOFIT can then be compared with the input data to evaluate the overall retrieval uncertainties. For example, the workflow allows for the evaluation of retrieval bias by wavelength (Figure 8), which is dependent on the input noise model or SNR (Figure 4), the source image, selected atmospheric model, and the input simulation atmospheric conditions, including column water vapor and aerosol optical depth (AOD).

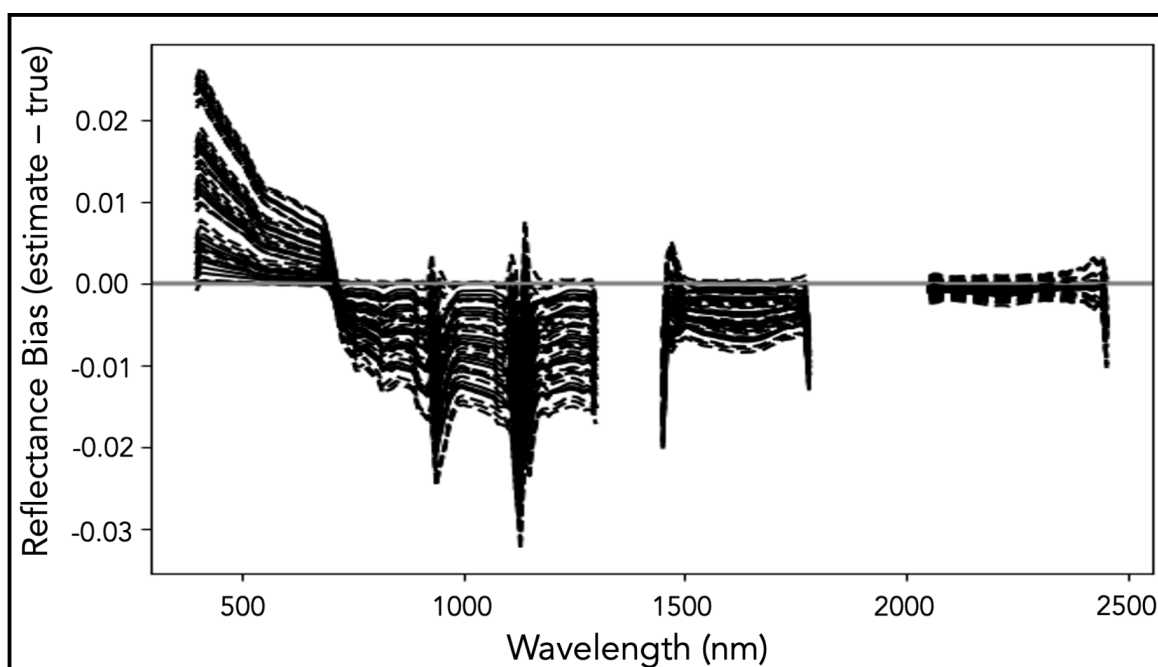


Figure 8. Example retrieval bias from the ISOFIT-Hypertrace workflow.

The ISOFIT and associated python Py-Hypertrace code base is open-source and available through GitHub:

ISOFIT-Hypertrace source code: ISOFIT (<https://github.com/isofit/isofit>) and Py-Hypertrace (<https://github.com/isofit/isofit/tree/master/examples/py-hypertrace>)

Example workflow performance characteristics:

The ISOFIT-Hypertrace workflow can be run on a range of machines, including Mac OSX and Linux. The easiest way to install and run the code is by using a conda environment on the host computer. For simulations reported here, we ran the workflow on both a Mac and Linux machine using conda. We evaluated the performance of the ISOFIT-Hypertrace (git hash c818055) workflow by reviewing the performance metrics provided by ISOFIT while the code is executing.

For example:

CentOS 8 Linux HPC running Intel(R) Xeon(R) CPU E5-2695 v4 @ 2.10GHz CPU we achieved an max inversion performance of:

93.677 spectra/s, 3.9032 spectra/s/core on 24 cores running in parallel via the python package *Ray*

MacPro running OSX 10.14.6 with a 6-core Intel(R) Xeon(R) E5:

4.7565 spectra/s, 0.4757 spectra/s/core on 10 cores running in parallel via the python package *Ray*

These simulations were all run on a single node on Linux, using SLURM, or on a MacPro desktop.

PRELIMINARY RESULTS

Evaluation of instrument design and atmospheric conditions on Arctic tundra surface reflectance retrievals

A suite of simulation experiments were run using the ISOFIT-Hypertrace workflow. These simulations were conducted using select AVIRIS-NG scenes collected over the Seward Peninsula, Alaska containing a variety of typical Arctic vegetation plant functional types (PFTs). In addition, the simulations were conducted over a range of atmospheric conditions, sun-sensor geometries, and theoretical instrument models representing different proposed SBG designs.

Preliminary results suggest a strong impact of instrument design on reflectance retrieval that scales with aerosol/atmospheric conditions, but also a clear dependence on PFT (Figure 9). In this example, we find that the reflectance retrieval bias increases with AOD, but that within a single AOD bin there is a difference in performance by instrument model. We also find that the within-AOD class variance is driven by impacts of geometry on reflectance estimation. Finally, we also find that moving from short-stature grass cover to tall deciduous shrub cover with more complex canopies tended to increase retrieval bias across all conditions, suggesting a strong BRDF effect.

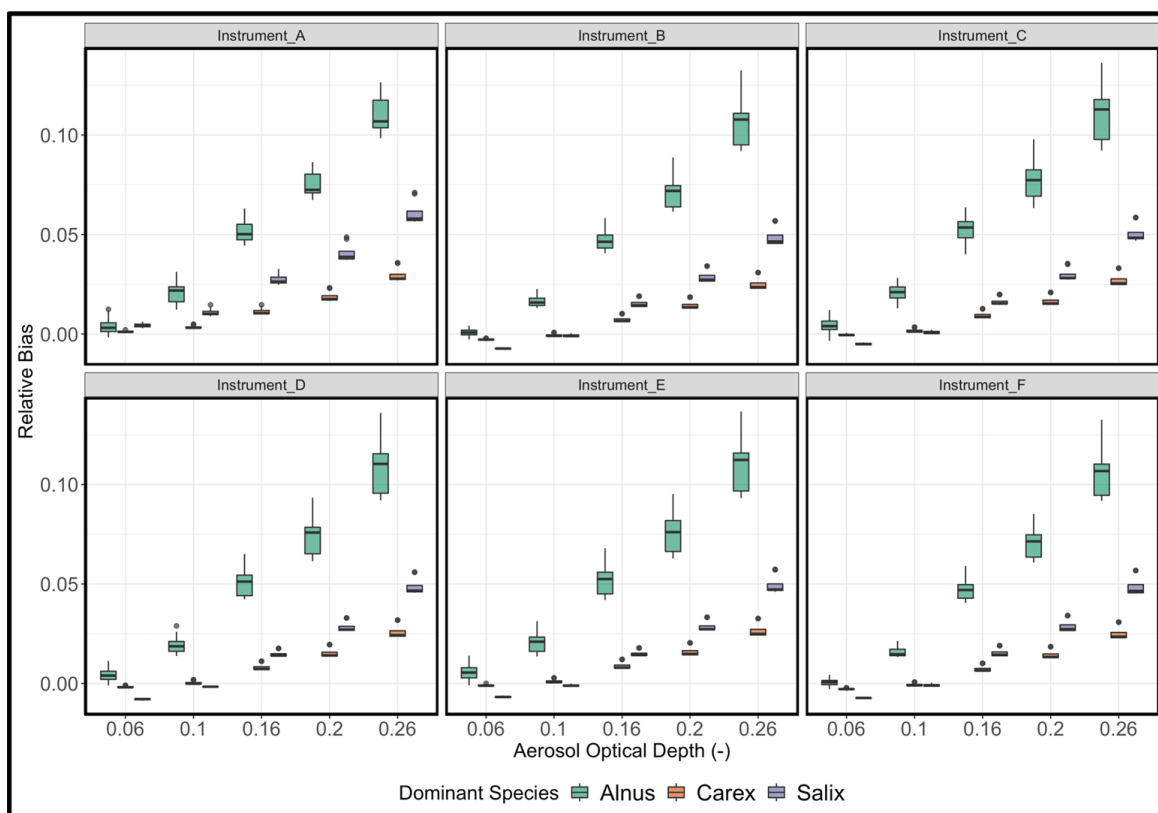


Figure 9. Example ISOFIT-Hypertrace retrieval bias across AOD, instrument model, and Arctic vegetation type. The variation within an AOD class is related to water vapor and sun-sensor geometry differences. In this example, we find that error increases moving from short-stature graminoid species to tall shrub pixels, suggesting that BRDF is another key consideration in the design of SBG.

Evaluation of instrument design and atmospheric conditions on vegetation fCover mapping in high latitudes

In addition, to explore the impacts on L2 surface reflectance, we also explored how retrieval performance would impact higher-level derived products. Here we explore the impacts on the mapping of vegetation fractional cover (fCover) using an existing set of algorithms derived for this region using the same AVIRIS-NG imagery (Figure 10; Yang et al., 2020b (<https://astm6-agu.ipostersessions.com/Default.aspx?s=54-3B-0B-9D-DF-9A-8A-0F-F9-94-41-3A-6B-94-6F-86>)). Overall we find that instrument design has a large impact on fCover performance (Figures 11-15), where atmospheric and geometry differences play a smaller role. In general, in these preliminary analyses, we find that the instrument model was the most important variable in determining the impact on fCover mapping (e.g. Figures 16 & 17).

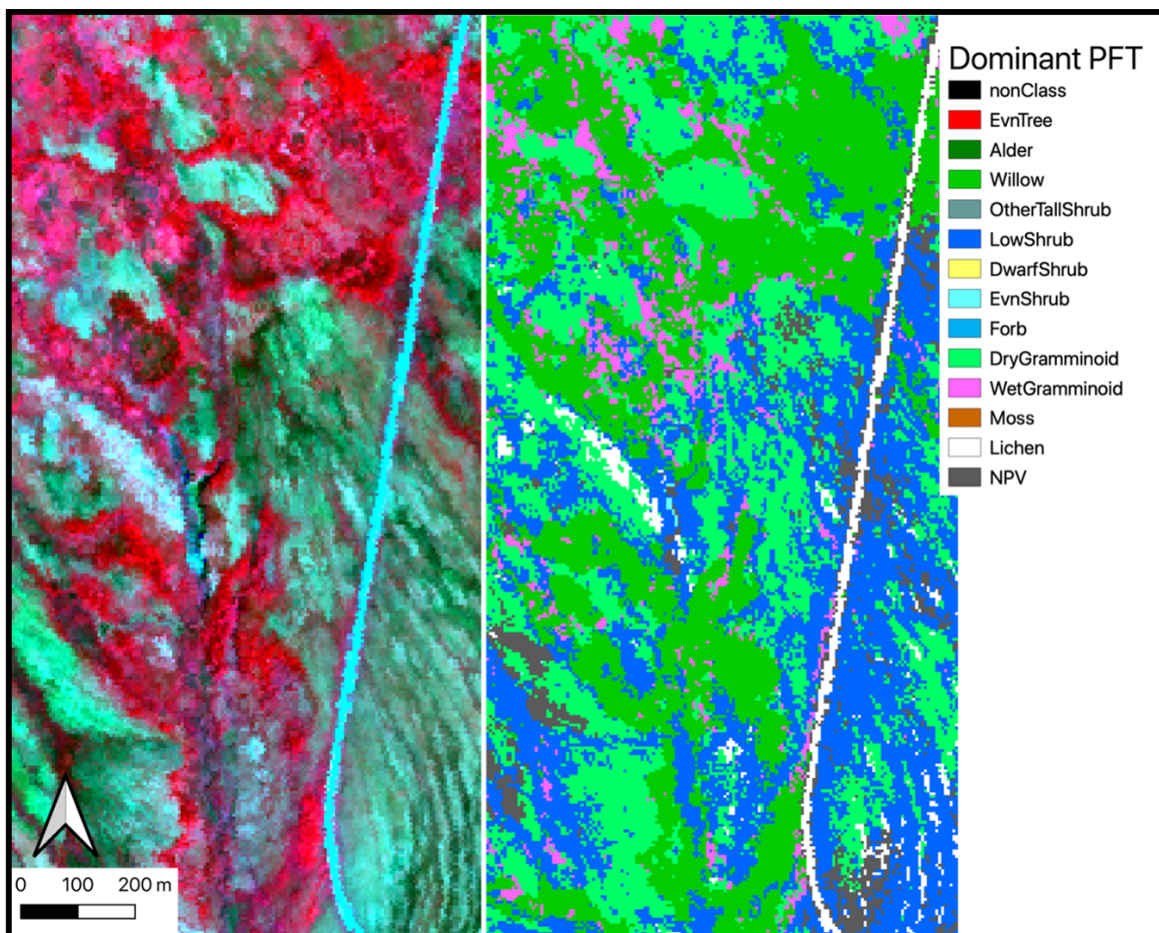


Figure 10. AVIRIS-NG VNIR composite (left) and dominant PFT map (right, Yang et al, 2020b (<https://astm6-agu.ipostersessions.com/Default.aspx?s=54-3B-0B-9D-DF-9A-8A-0F-F9-94-41-3A-6B-94-6F-86>)) of a select subset of the NGEE-Arctic Teller watershed used for exploring the impacts of instrument design, atmospheric conditions, and sun-sensor geometry on the retrieval of fractional vegetation cover. In the VNIR image, the deeper red areas represent areas of more dense and vigorous vegetation cover, including tall shrub cover such as Salix (Willow in the PFT map).

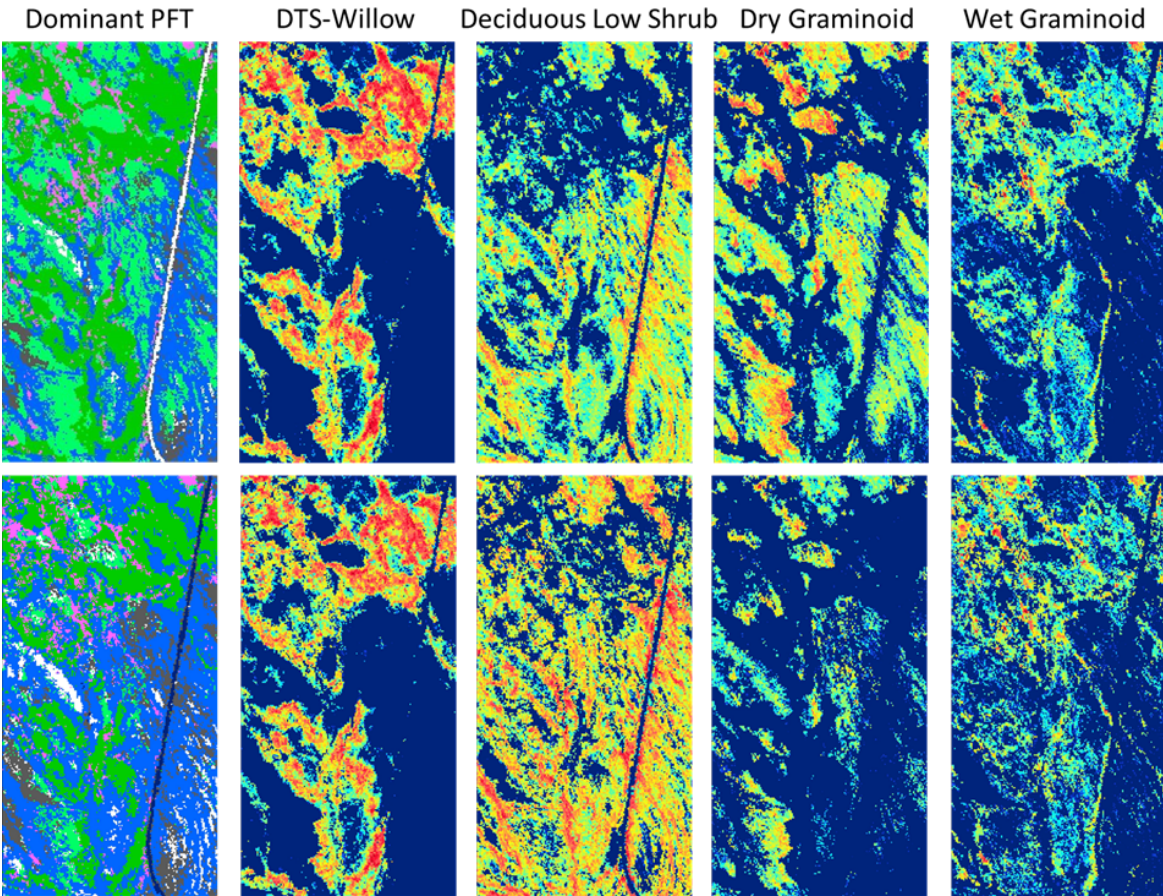


Figure 11. Example comparison of an original (top) and simulated SBG fCover fraction (bottom row) for select Arctic plant functional types (PFTs) using the ISOFIT-Hypertrace UQ workflow. The fCover model is based on an algorithm developed using AVIRIS-NG imagery (Yang et al. 2020b (<https://astm6-agu.ipostersessions.com/Default.aspx?s=54-3B-0B-9D-DF-9A-8A-0F-F9-94-41-3A-6B-94-6F-86>)) collected as part of the NASA ABoVE Airborne Campaign.

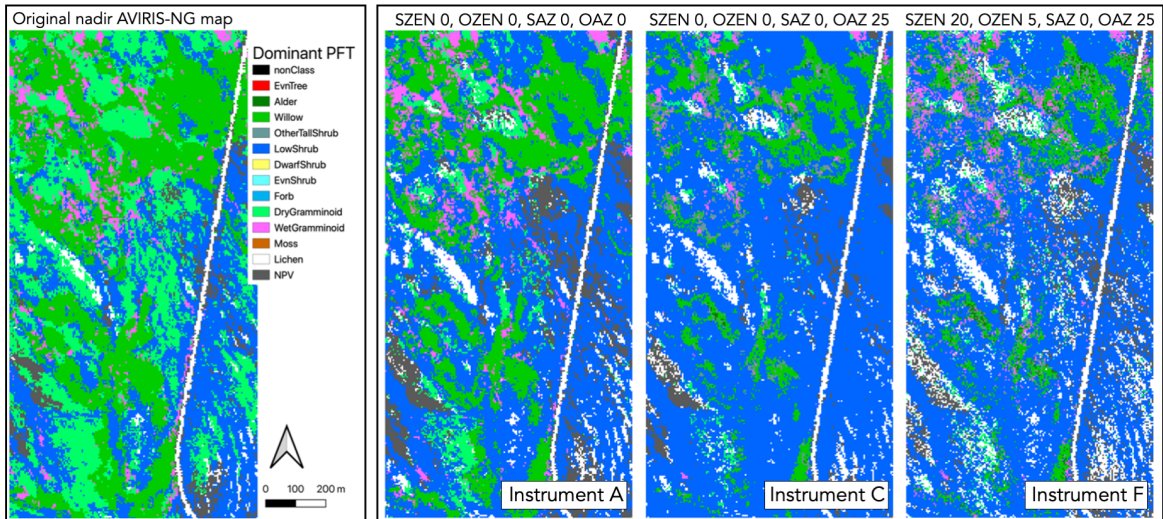


Figure 12. Comparison of dominant Arctic PFT classes based on the original AVIRIS fCover maps (left), as well as select instrument model and atmospheric conditions (right). This example clearly illustrates the change in mapped dominant vegetation composition across the Teller watershed given different proposed instrument models, sun-sensor, and atmospheric conditions, specifically AOD.

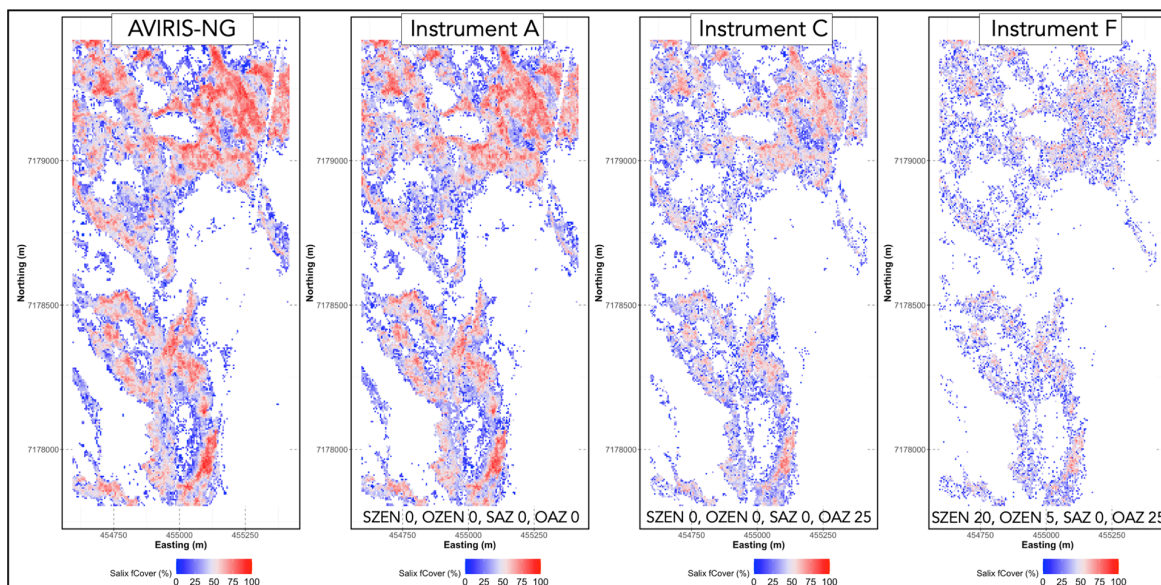


Figure 13. Similar to Figure 12, except showing the change in mapped *Salix spp* fCover across the same sets of the instrument and atmospheric conditions. In this example, the far left map is the original fCover map and the following three maps represent the different instrument models and atmospheric conditions.

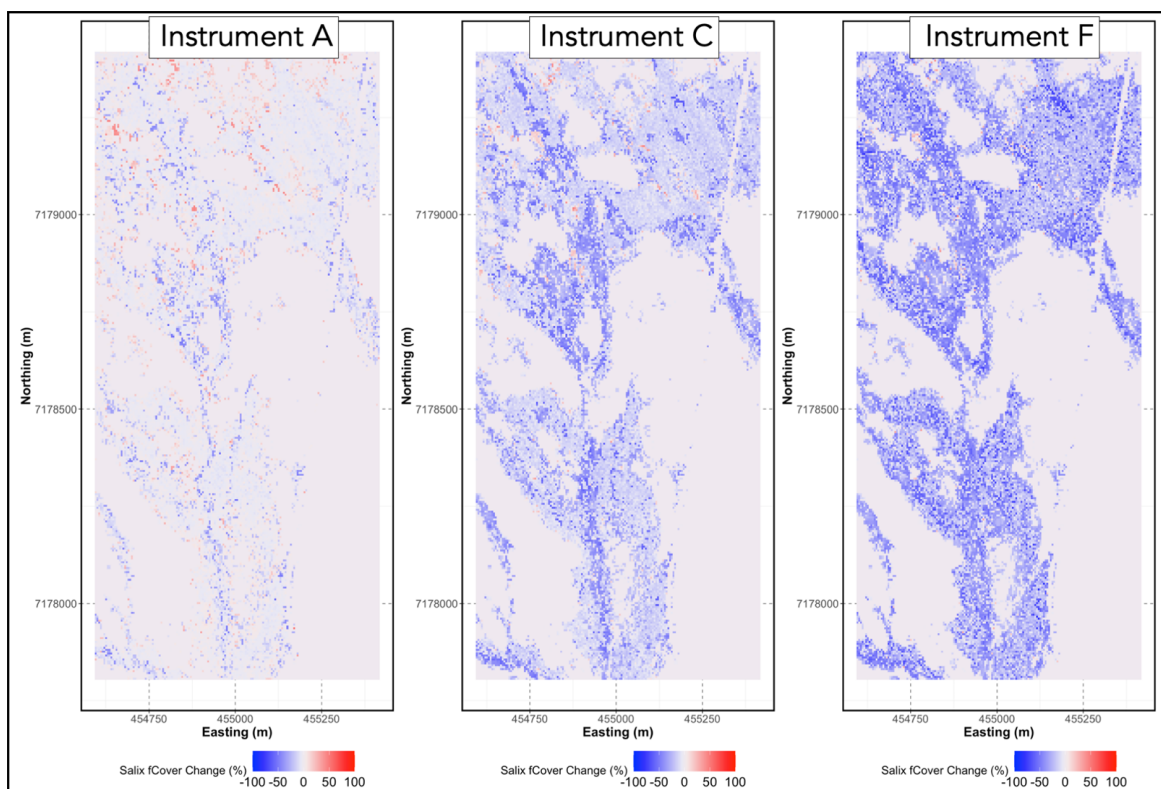


Figure 14. The change in *Salix spp* fCover fraction from the base image (Figure 13, left) across the same simulated conditions.

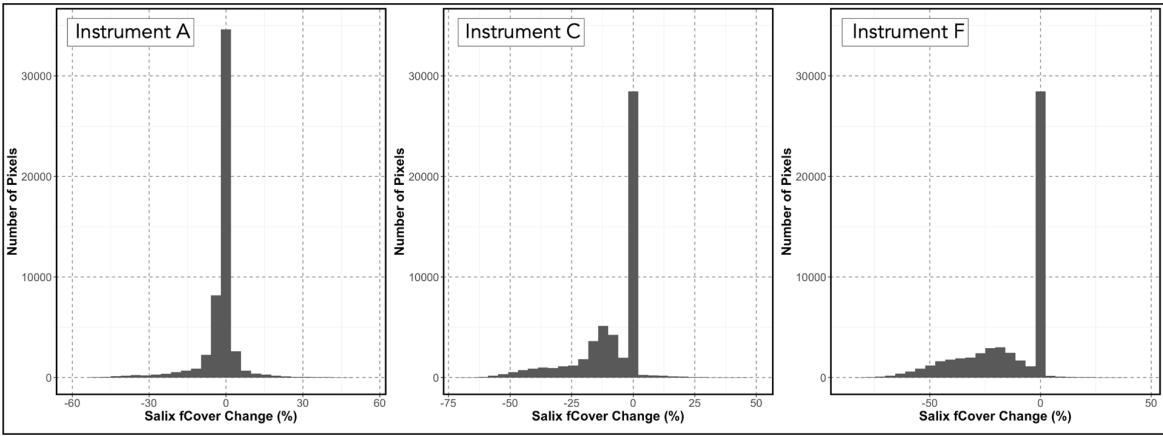


Figure 15. Histogram of the pixel value changes shown in Figure 14. In this specific example, the impact of the different instrument and atmospheric conditions results in an overall reduction in mapped *Salix spp* fCover fraction by an average of -13% including the no-change/zero pixels and 28% excluding those pixels.

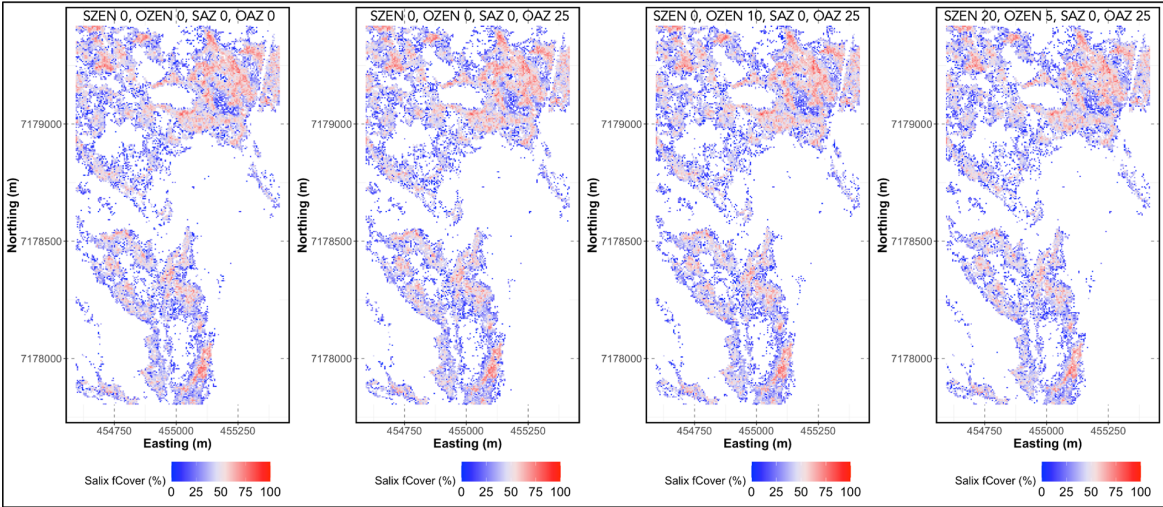


Figure 16. Comparison of the *Salix spp* fCover for the same instrument model across different atmospheric conditions.

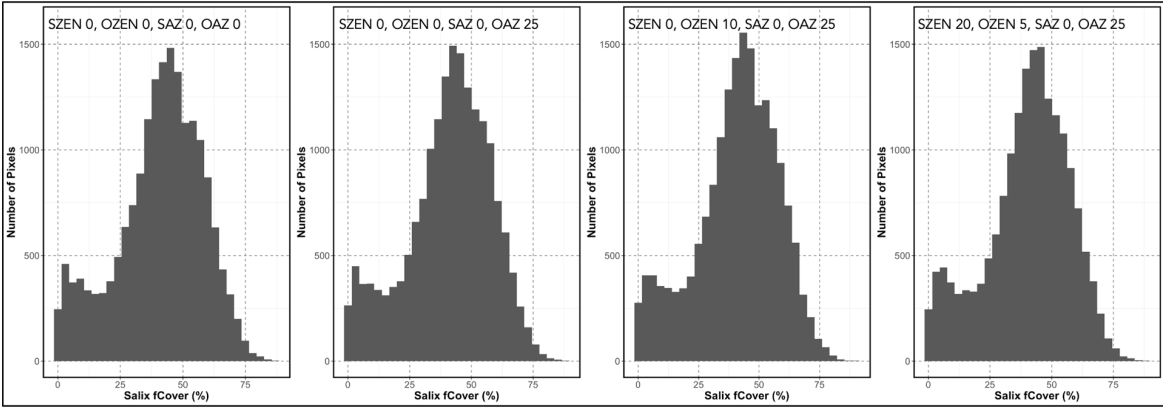


Figure 17. The pixel-level histograms from Figure 16

CONCLUSIONS & NEXT STEPS

Our ISOFIT-Hypertrace workflow provides an efficient way to meet the needs of the MEET-SBG effort by providing a consistent framework to simulate the impacts of instrument design, atmospheric conditions, retrieval approach, and other assumptions on L2 surface reflectance. This approach can be applied to the various focal areas (Figure 2) that are critical to a successful SBG mission. Applying this workflow to high-latitude vegetation contained within scenes from NASA ABoVE airborne campaign, we find that the instrument model is a key variable impacting L2 surface reflectance retrieval performance. In addition, we find a strong influence of vegetation type on simulated L2 reflectance across instrument models, suggesting that the analysis should be expanded to including more variation in factors that influence BRDF, such as additional vegetation types across more complex topographic gradients. The influence of these assumptions on L2 reflectance also had significant impacts on Arctic vegetation fCover mapping. This suggests that it will be important to not only evaluate L2 performance but also the down-stream impacts on L3 and L4 product performance when evaluating the proposed SBG instrument designs.

Next Steps

- Expand the current suite of simulations to a larger set of instrument design options, atmospheric conditions, and vegetation types, including mixed vegetation conditions
 - Include an evaluation of different channel configurations, such as variable bandwidths or FWHMs
- Run simulations across scenes from multiple years for the same locations to explore a temporal dependence on instrument performance
- Run the ISOFIT-Hypertrace simulations over larger scenes and explore any potential spatial patterns in error or performance
- Add additional sources of retrieval uncertainty not currently included:
 - e.g. Imperfect calibration, uncertain spectral response functions, and different atmospheric correction approaches
- Test the impact of the additional source of uncertainty on fCover mapping and other higher-level products
- Incorporate in-situ observations for exploring L2 cal/val approaches for SBG or to improve retrieval priors for Arctic vegetation in the ISOFIT inversion step

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ABSTRACT

Over the last nearly five decades, optical remote sensing has played a key role in monitoring and quantifying global change, plant diversity, and vegetation functioning across Earth's terrestrial biomes. As a key tool for researchers, land managers, and policy makers, optical remote sensing facilitates scaling, mapping, and characterizing surface properties over large areas and through time. In addition, steady technological improvements have led to transformational changes in our ability to understand ecosystem state and change, particularly through the expansion of high spectral resolution (i.e. spectroscopic) remote sensing platforms. Point and imaging spectroscopy systems have been used across a range of scales, vegetation types, and biomes to infer plant diversity, leaf traits, and ecosystem functioning. However, despite the acknowledged utility of spectroscopic systems, data availability has been limited to smaller geographic regions given a number of technical challenges, including issues related to data volume and limited spatial coverage by previous Earth Observing (EO) missions (i.e. Hyperion). The NASA Surface Biology and Geology (SBG) mission is designed to fill this gap in ecosystem monitoring. As part of the Space-based Imaging Spectroscopy and Thermal pathfinder (SISTER) and Modeling end-to-end traceability (MEET) SBG efforts, we used field, unoccupied aerial system (UAS), and airborne imagery (from NASA's AVIRIS-NG platform) to evaluate the impacts of proposed and theoretical sensor instrument properties on the retrieval of vegetation reflectance across tundra, shrub, and treeline ecosystems in Alaska. Existing observations and open-source tools are used for the simulation of surface reflectance under a range of atmospheric conditions, vegetation types, and different sensor properties. We find that retrieval uncertainty is reduced across all surface types with increasing detector signal-to-noise (SNR) but also key differences across different plant types. Results were also strongly tied to sun-sensor geometry and atmospheric state. Through this exercise we highlight key outcomes to consider for the SBG mission to optimize surface reflectance retrieval in high latitudes that will help to minimize errors in down-stream algorithms, such as functional trait retrievals.

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