# Comparison of ARTS and JPL MLS models for the 118.75-GHz Zeeman-split $O_2$ line

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# Motivation

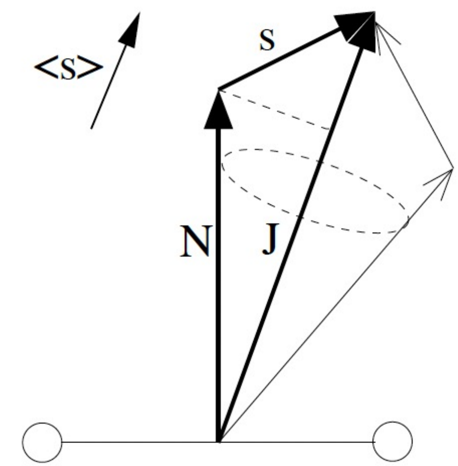


- I work with data from three satellite instruments for which processing requires radiative transfer models capable of modeling polarized signals from atmospheric emission from Zeeman-split molecular oxygen lines:
  - The Microwave Limb Sounder on the EOS Aura satellite (EMLS)
    - Custom Zeeman-aware forward model in mlsl2 provides radiances and Jacobians
  - The Microwave Limb Sounder on the Upper Atmosphere Research Satellite (UMLS)
    - 1991-1997. UMLS has been reprocessed using EMLS algorithms to retrieve temperature.
    - This is about as "general purpose" as mlsl2 gets
  - The Electrojet Zeeman Imaging Explorer (EZIE)
    - Small-sat constellation scheduled for **launch as early as October 2024**
    - A custom RT module based upon the ARTS Zeeman algorithms (Larsson et al. 2014) is integrated into the production software
- ARTS is a general-purpose radiative transfer package
  - Publicly available, community supported, with active development
- I would like to understand how ARTS compares to the both the EMLS and EZIE models, and whether it would be advantageous to use ARTS in future production software (possibly including a rushed reworking of EZIE production software.)

# Molecular O2 mm-wave spectrum



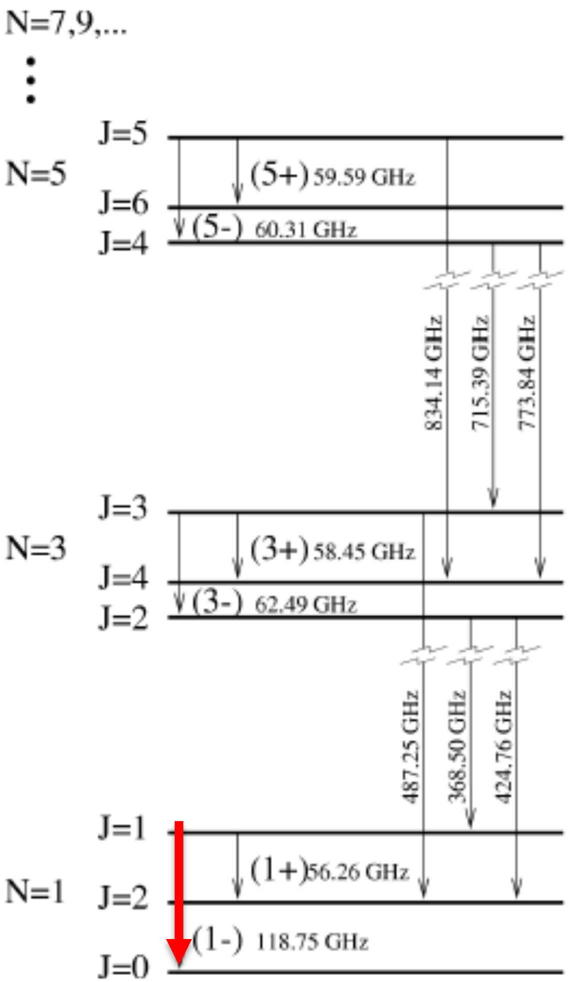
- O2 is essentially a rigid rotator at Earth atmospheric temperatures
- It is "frozen" in its electronic ground state
- It is "frozen" in its vibrational ground state
- The last two electrons of the electronic ground state have aligned spins, so it is spin=1
- This spin 1 adds to the rotational angular momentum to give total angular momentum, J (roughly Hund's case B, where **N**+**s**=**J**). For $^{16}O_2$ , only odd N values of are allowed.

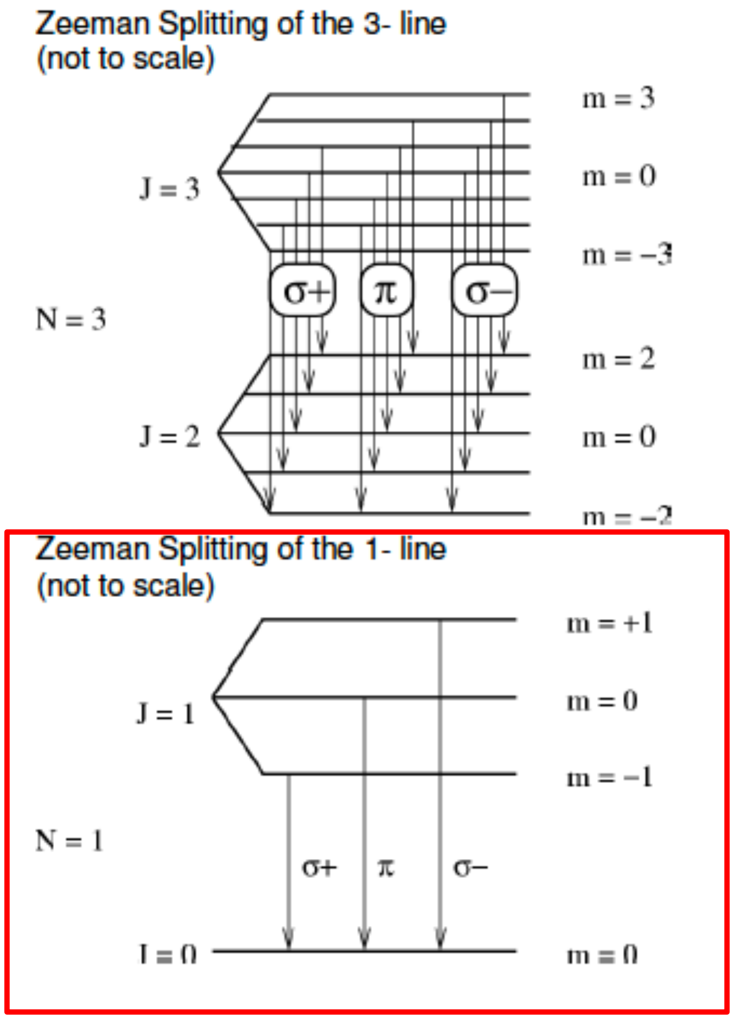



- Magnetic dipole transitions change J by +1, 0 or -1 and m by +1, 0 or -1
- Magnetic dipole transitions at 118 GHz and in the 60-GHz band are between states with the same rotational quantum number, N, but with the electronic spin (s) alignment changing: J=N → J= N+1 or J= N → J=N-1.
- The magnetic dipole moment associated with the spin 1 interacts with an external magnetic field (like the Earth's magnetic field) to give Zeeman splitting

# Diatomic Oxygen Spin-Rotation Spectrum





# The Microwave Limb Sounder on EOS Aura

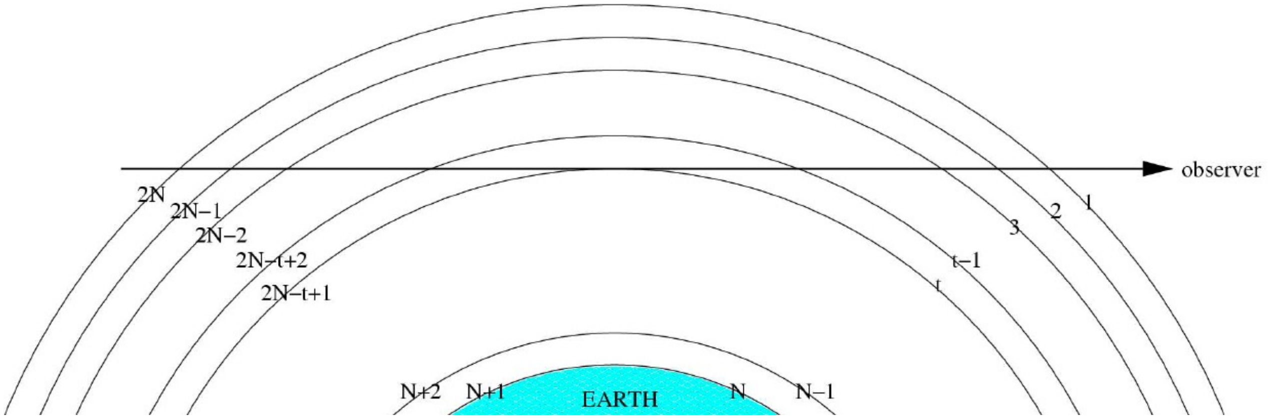


- The EOS Microwave Limb Sounder (EMLS) was launched on the NASA Aura satellite in August, 2004 and since that time has provided near-continuous, 3500 daily sets of atmospheric composition and temperature profiles from 8–90 km along the suborbital track.
- The Aura orbit has been sun synchronous (83 S–83 N) with 1:30 and13:30 equator crossings since launch. It is beginning to drift a bit.
- MLS scans the atmospheric limb along-track, 240 times per orbit and successive MLS along-track limb scans overlap. A 2-D optimal-estimation is used to retrieve 1.5° uniformly-spaced suborbital profiles, using blocks of limb scans to retrieve blocks of profiles.
- Design life was 5 years, but almost most of the system is still operating after nearly 20 years. Dwindling supplies of propellant are necessitating changes in orbital maintenance. Over the next two years the orbit will have an accelerating drift, which will eventually result in lack of illumination of the solar panels and the end of the science mission.
- Data is highly used by the community (~1700 publications). It has provided a 20-year, well-sampled record providing a de facto standard for stratospheric and UT $H_2O$, stratospheric $O_3$, etc.

# Limb Sounding Viewing Geometry



- In limb sounding, the atmosphere is viewed through the horizon (limb) giving long ($\sim 500$ km) pathlengths near the tangent point.
- Long paths provide appreciable emission signals from many otherwise-unobservable trace gases.
- Large antennae ($\lambda/D$ of order $10^{-3}$) provide vertical resolution. At $\sim 700$ km orbital height, the tangent point is $\sim 3000$ km distant.
- Along-track horizontal resolution is poor.

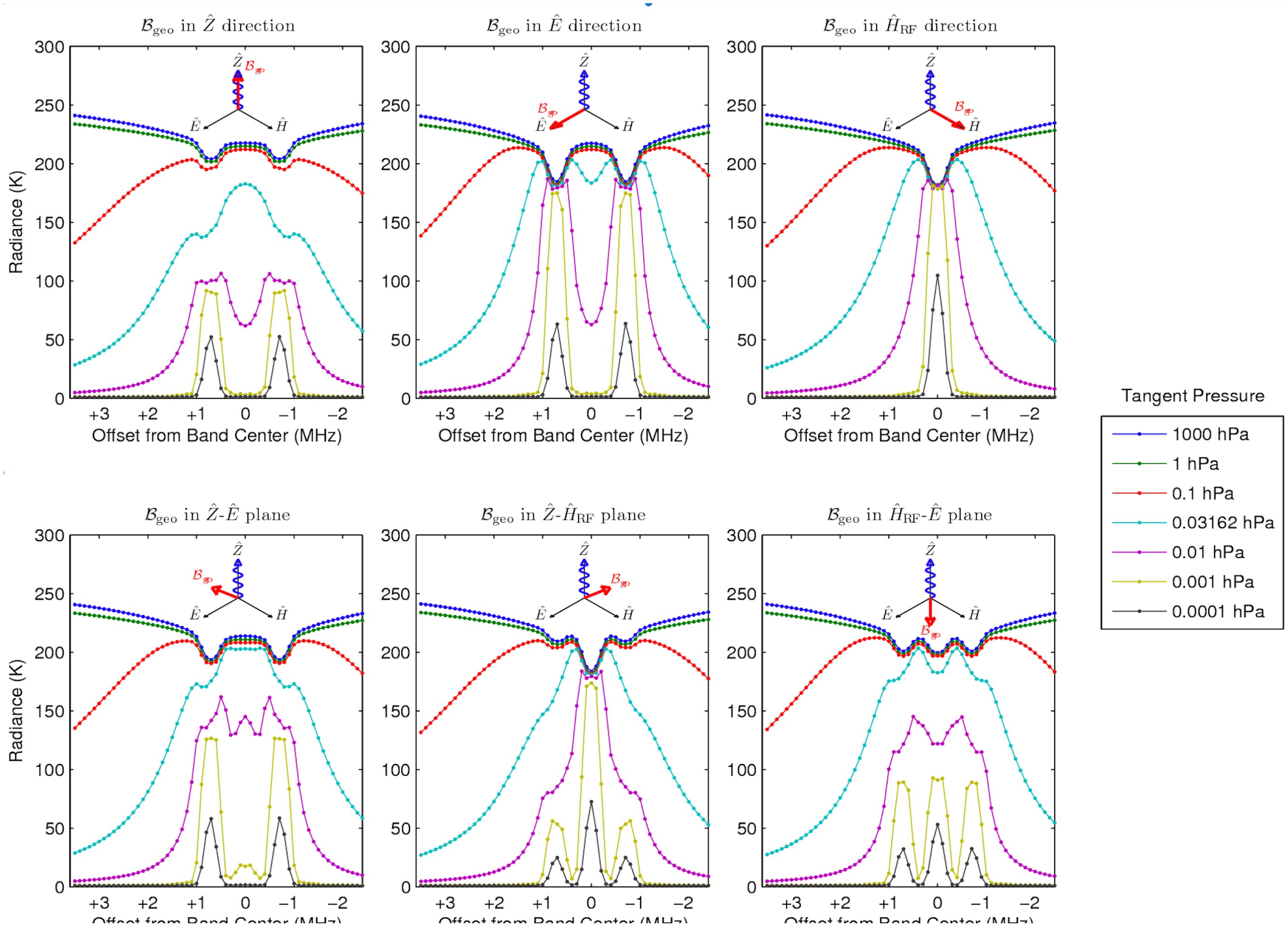


# EMLS



- EMLS provides daily, global, day and night profiles of ~19 atmospheric constituents over atmospheric levels ranging the upper troposphere (~8 km, 300 hPa) through the mesosphere (~90 km, 0.001 hPa), depending on species. These include:
  - Ozone and species involved in ozone destruction chemistry (ClO, HNO3, H2O, CH3Cl, HOCl)
  - H2O, Ozone Important greenhouse gases in the upper troposphere and stratosphere
  - CO, CH3CN, N2O useful in studies of transport, including pollution transport
  - Temperature and Geopotential Height: Dynamics, waves, geostrophic wind, etc.
- Temperature and tangent-pressure and GPH are primarily obtained from emission from molecular oxygen, which has a known mixing ratio, and radiance is a function only of atmospheric temperature.
- Line emission of other species need this temperature to retrieve species mixing ratios.
- Above ~80 km (~0.01 hPa) tangent height, Zeeman-splitting of the O2 118.75-GHz line center is significant relative to line widths.

- For EMLS, Zeeman splitting of the 118.75-GHz O2 line is an annoyance, (unlike for EZIE, where inference of Geomagnetic perturbations is the goal.)
- It must be modeled because, at low pressures (~<0.01 hPa), radiances become VERY strongly dependent upon magnetic field orientation and strength
- These figure show MLS-like, limb radiance variability due to changes only in the orientation of the imposed magnetic field, with field strength and temperature profile held fixed.



# MLS Forward Model



- The MLS optimal-estimation retrieval system (Livesey,et al. TGARS 2006) includes a forward model (Read, et al. TGARS 2006) that produces radiances and Jacobians for composition retrievals. Its polarized, Zeeman forward model (Schwartz, et al. TGARS 2006) is specific to the temperature/ptan retrieval from the 118-GHz line.
- MLS routinely measures only one polarization at 118 GHz (vertical), because spectrometer backends are timeshared with other bands. Even when both linear polarizations are measured by spectrometers, phase between them is not measured, so at most we get the first two Stokes components.
- The mlsl2 polarized forward model is based upon the coherency-matrix formulation of Lenoir. It models all four Stokes components, but in the form of a complex, 2x2 intensity matrix. The power transmittance matrix $\tau_i$ (power from the $i_{th}$ layer boundary to the observer) is built up of sandwiched layer "field" transmittance matrices, with successive layers' propagation matrices operating on both ends of the stack. Order is important because these matrices generally do not commute.
- In each layer, the polarization of the layer transmittance in complex 2x2 matrices is common to all O2 Zeeman components with the same $\Delta m$ = $\{\pm 1,0\}$, but the imposed geomagnetic field generally changes from layer to layer. Matrices are rotated from the natural frame-of-reference defined by the propagation direction and the geomagnetic field direction to that of the antenna's linear polarization.

# Radiative Transfer Equation



$$\boldsymbol{I} = \sum_{i=0}^{N} \boldsymbol{\mathcal{T}}_i \Delta B_i$$

where $\boldsymbol{\mathcal{T}}_i$ is built out of layer transmittance matrices, $\boldsymbol{E}_j$,

$$\boldsymbol{\mathcal{T}}_i = \boldsymbol{E}_1 \boldsymbol{E}_2 \ldots \boldsymbol{E}_i \boldsymbol{E}_i^{\dagger} \ldots \boldsymbol{E}_2^{\dagger} \boldsymbol{E}_1^{\dagger}.$$

Layer Field Transmittance:

$$\boldsymbol{E}_i = \exp\left( - \int_{s_i}^{s_{i-1}} \frac{\imath \pi \nu}{c} \boldsymbol{\chi} \, \mathrm{d}s \right)$$

Magnetic susceptibility matrix:

$$\boldsymbol{\chi} = \chi_{+} \boldsymbol{\rho}_{+} + \chi_0 \boldsymbol{\rho}_0 + \chi_{-} \boldsymbol{\rho}_{-} \ ,$$

where

$$\boldsymbol{\rho}_{\pm} = \boldsymbol{R}_{\phi} \begin{bmatrix} 1 & \mp \imath \cos\theta \\ \pm \imath \cos\theta & cos^2\theta \end{bmatrix} \boldsymbol{R}_{\phi}^{\dagger} \ ,$$

$$\boldsymbol{\rho}_0 = \boldsymbol{R}_{\phi} \begin{bmatrix} 0 & 0 \\ 0 & \sin^2\theta \end{bmatrix} \boldsymbol{R}_{\phi}^{\dagger} \ ,$$

and the $\phi$ rotation is

$$\boldsymbol{R}_{\phi} = \begin{bmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{bmatrix} \ .$$

# MLS Forward Model Optimizatons



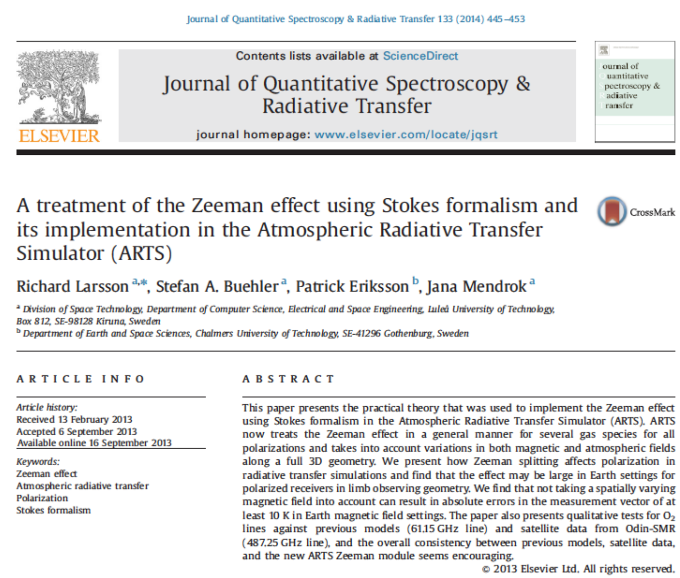
- Model is implemented in Fortran and optimized for MLS.
- Spectral convolution has been optimized for speed/accuracy.
- Antenna convolution uses Fourier methods.
- Digital autocorrelation spectrometers (DACS) sinc spectral response convolution is done in Fourier space.
- Matrix exponentiation of complex, 2x2 matrices in the Zeeman code is done with Cayley Hamilton.
- Limb-geometry quadrature and methods for dealing with the singularity at the tangent point are baked in.
- First-order line mixing (Rosenkranz) is included in complex line shape (modified Faddeeva) in the polarized calculations, but doesn’t really matter much for MLS simulations both because MLS doesn’t see deep into the  atmosphere and the 118-GHz line is isolated.

- Some of these optimizations present challenges in model comparisons.

# The ARTS Zeeman model



- The capability in ARTS to model Zeeman-split lines, including the 118.75-GHz O2 line observed by both EMLS and EZIE, is based upon algorithms in Larsson et al., JQSRT 2014
- The EZIE production forward model is also based upon algorithms in this paper, but implemented by EZIE PI, Sam Yee, rather than Richard and the ARTS team.
- These algorithms use 4x4, real matrices to propagate power and Stokes vectors give the radiances.
- In the appendix of his paper, Richard shows the equivalence of this 4x4 real matrix formalism and the complex coherency matrix formalisms, although some “messy algebra” has been omitted.
- Analytic and numeric Jacobians can be calculated, and composition, T, wind and magnetic field can be optimally estimated.
- I would still like to do compare some two-layer cases where lack of commutation of layer field transmittance matrices is an issue in the coherency matrix formalism.



Journal of Quantitative Spectroscopy & Radiative Transfer 133 (2014) 445–453

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

A treatment of the Zeeman effect using Stokes formalism and its implementation in the Atmospheric Radiative Transfer Simulator (ARTS)

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ARTICLE INFO

*Article history:*
Received 13 February 2013
Accepted 6 September 2013
Available online 16 September 2013

*Keywords:*
Zeeman effect
Atmospheric radiative transfer
Polarization
Stokes formalism

ABSTRACT

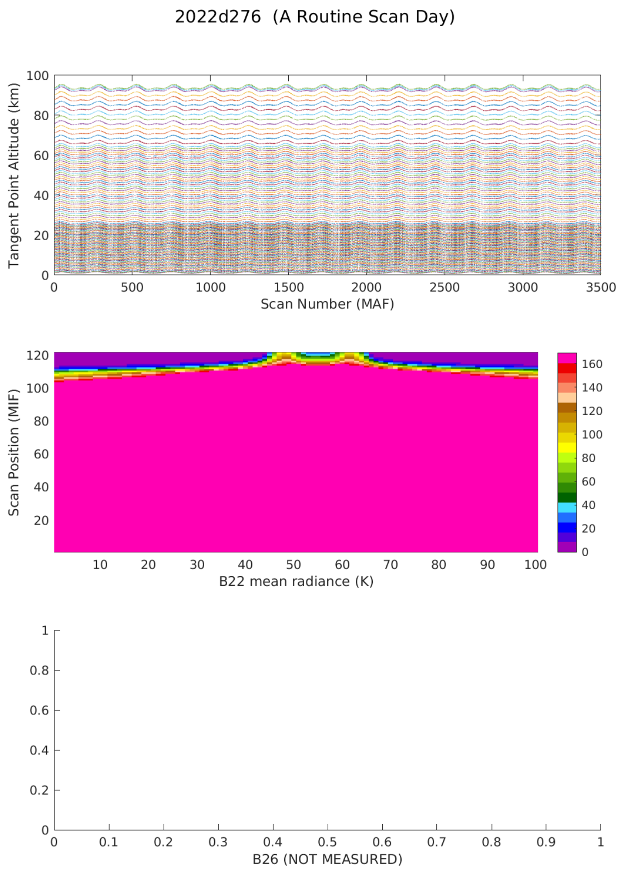
This paper presents the practical theory that was used to implement the Zeeman effect using Stokes formalism in the Atmospheric Radiative Transfer Simulator (ARTS). ARTS now treats the Zeeman effect in a general manner for several gas species for all polarizations and takes into account variations in both magnetic and atmospheric fields along a full 3D geometry. We present how Zeeman splitting affects polarization in radiative transfer simulations and find that the effect may be large in Earth settings for polarized receivers in limb observing geometry. We find that not taking a spatially varying magnetic field into account can result in absolute errors in the measurement vector of at least 10 K in Earth magnetic field settings. The paper also presents qualitative tests for $O_2$ lines against previous models (61.15 GHz line) and satellite data from Odin-SMR (487.25 GHz line), and the overall consistency between previous models, satellite data, and the new ARTS Zeeman module seems encouraging.

# Special EMLS high-altitude scan to Facilitate Zeeman FWM Intercomparisons



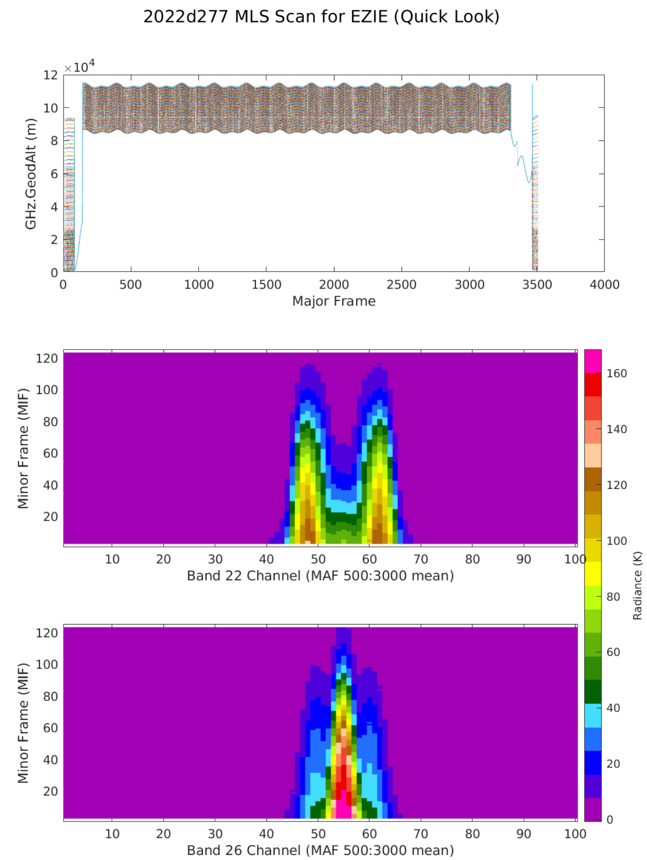
## MLS Typical Scan

This is the day before the high-scan. B26 (H-pol) is not measured with a DACS
0-93 km scan




## MLS High-Scan Day

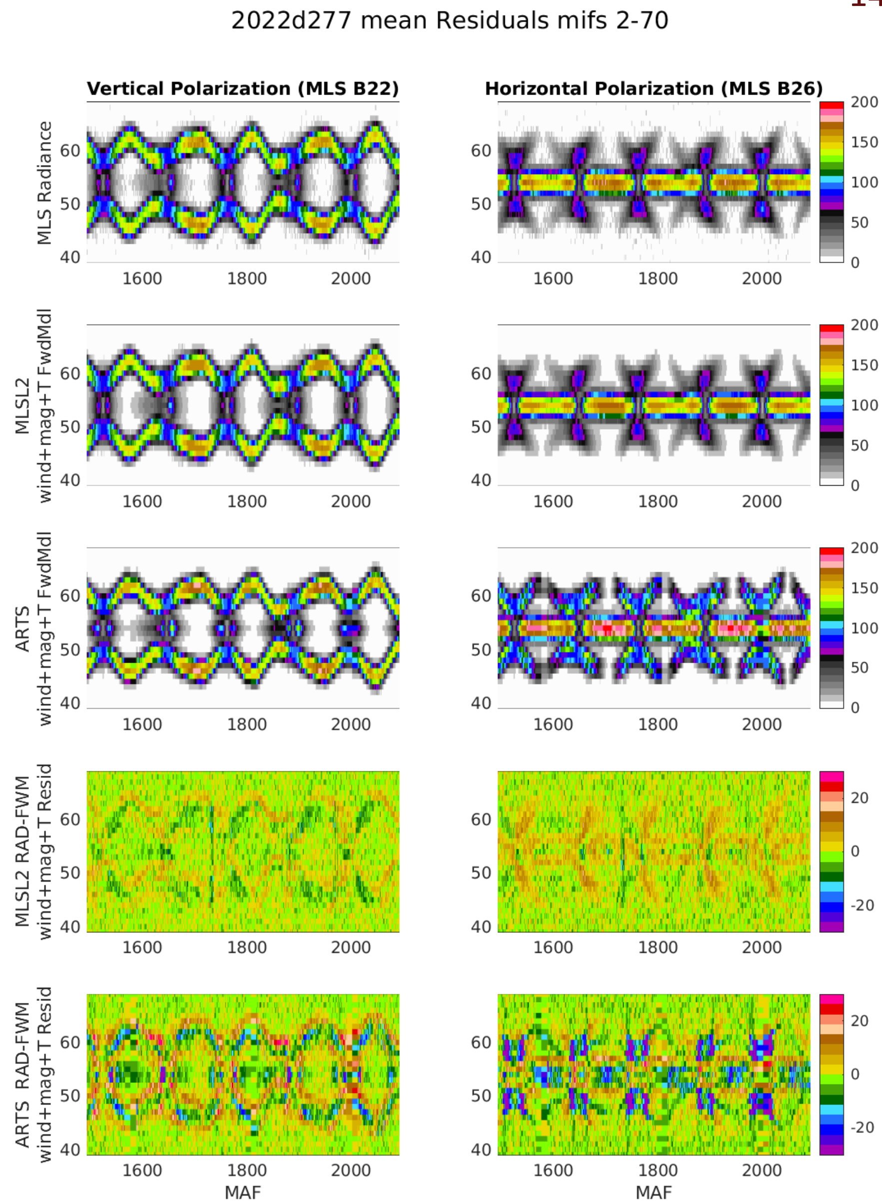
Most of 2022d277 scans 90-115 km
Both polarizations of the 118 GHz line are sent
to high-resolution digital autocorrelation spectrometers (DACS)



# Comparison of MLS and ARTS models of MLS High Scan



- Columns are V and H linear polarizations, respectively.
- Rows are
  - MLS radiances,
  - mlsl2  fwm with wind and |B|
  - ARTS fwm with wind and |B|
  - mlsl2 residual  (rad-fwm)
  - ARTS residual  (rad-fwm)
- Significant effort was expended to make sure all of the inputs are the same.  It is not as easy as it sounds. There is still work to be done.
- Near each equator crossing, $\sigma$ lines pull in (weaker field) and  $\pi$ lines disappear (looking along magnetic field).
- ARTS $\pi$ looks stronger
- ARTS residual "features" are not yet well understood

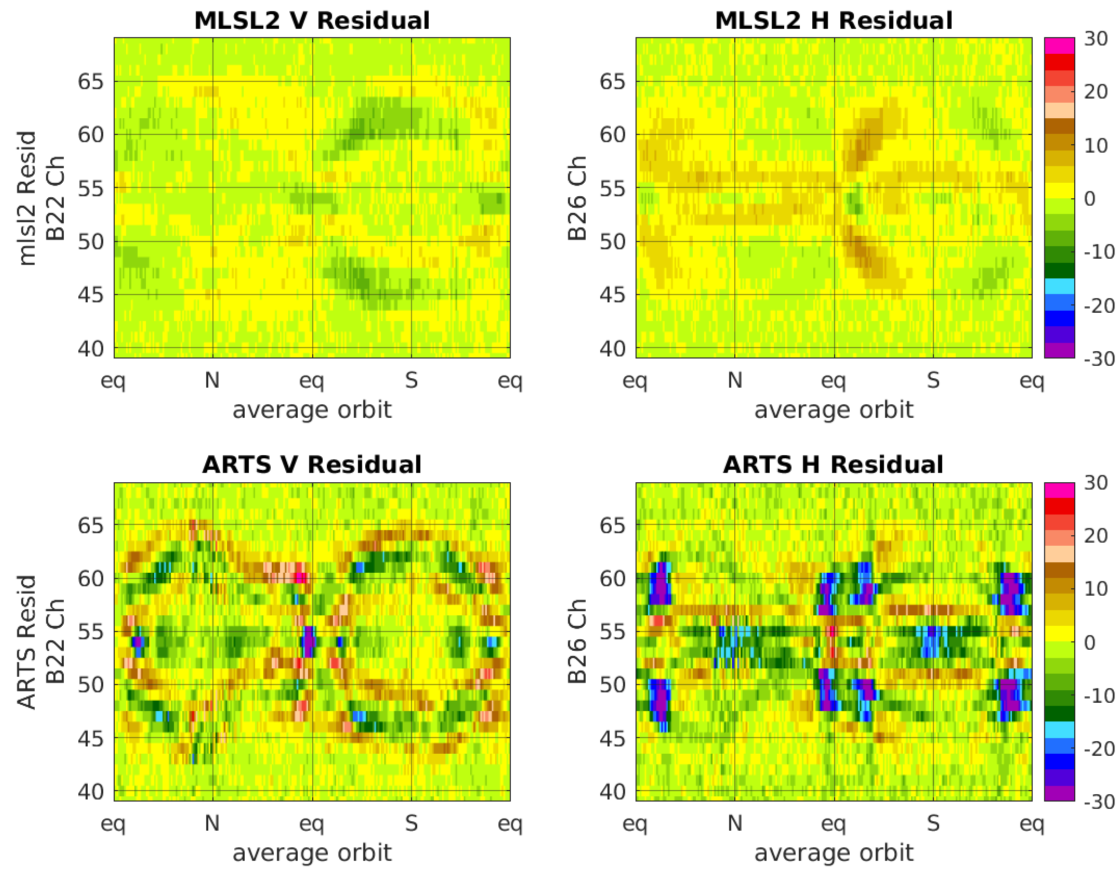


# Orbit-Averaged MLS high-scan residuals from mlsl2 and ARTS Retrievals



- These are average residuals around an orbit, showing MLSL2 residuals above, and ARTS residuals below..
- Note: ARTS Residual colorbars are saturated.
- mlsl2 closes residuals to ~<5K.

- Both models are 1D and retrieve line shift (along-track wind) and magnetic field magnitude from the split of the sigma lines.
- The field magnitude and wind retrievals were added to an offline version of mlsl2 developed by Bill Read specifically for this exercise.

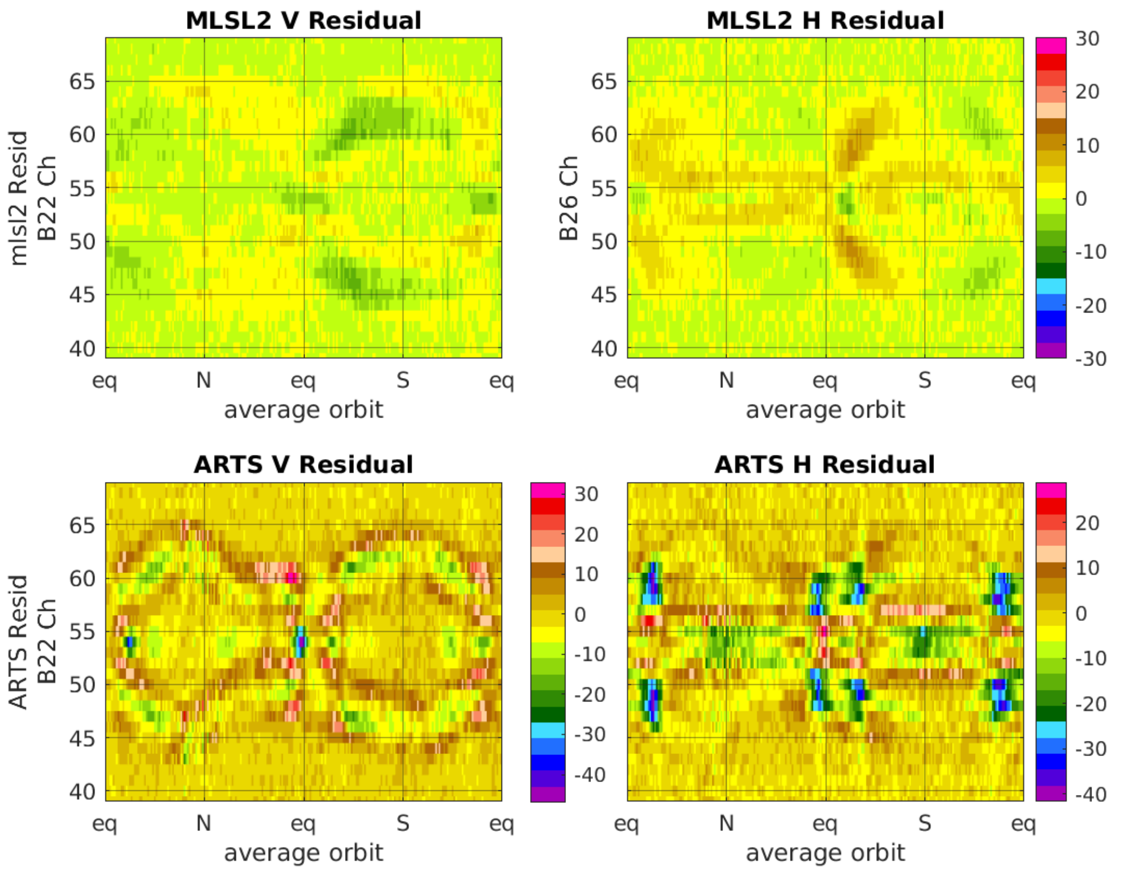


# Average MLS high-scan residuals from mlsl2 and ARTS Retrievals



- Same data as the previous slide, but ARTS Residual colorbars are not saturated, and colorbars have their own ranges.
- mlsl2 closes residuals to ~<5K.

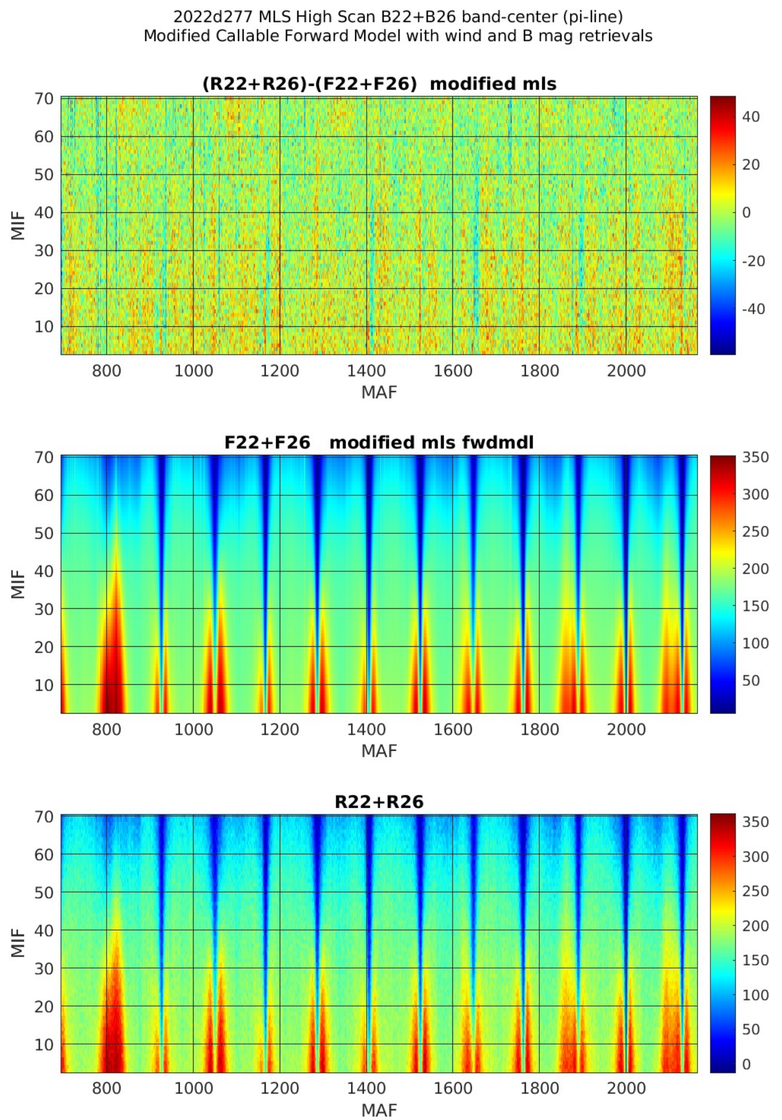
- ARTS sigma lines appear to be too broad.
- This comparison is a work in progress.



# Sharp Features in band center (pi line)



- These are curtains of the center three channels for V+H (1st Stokes) for mlsl2+w+|B|.
- Since these aren't vertically averaged, the residual noise is larger.
- Near each equator crossing EMLS looks along the magnetic field, the sigma lines become circularly polarized and the pi line disappears.
- We see (emperically) that these features are very sharp (blue line coming down into red.)



# Persistent Pi Line Center Residual

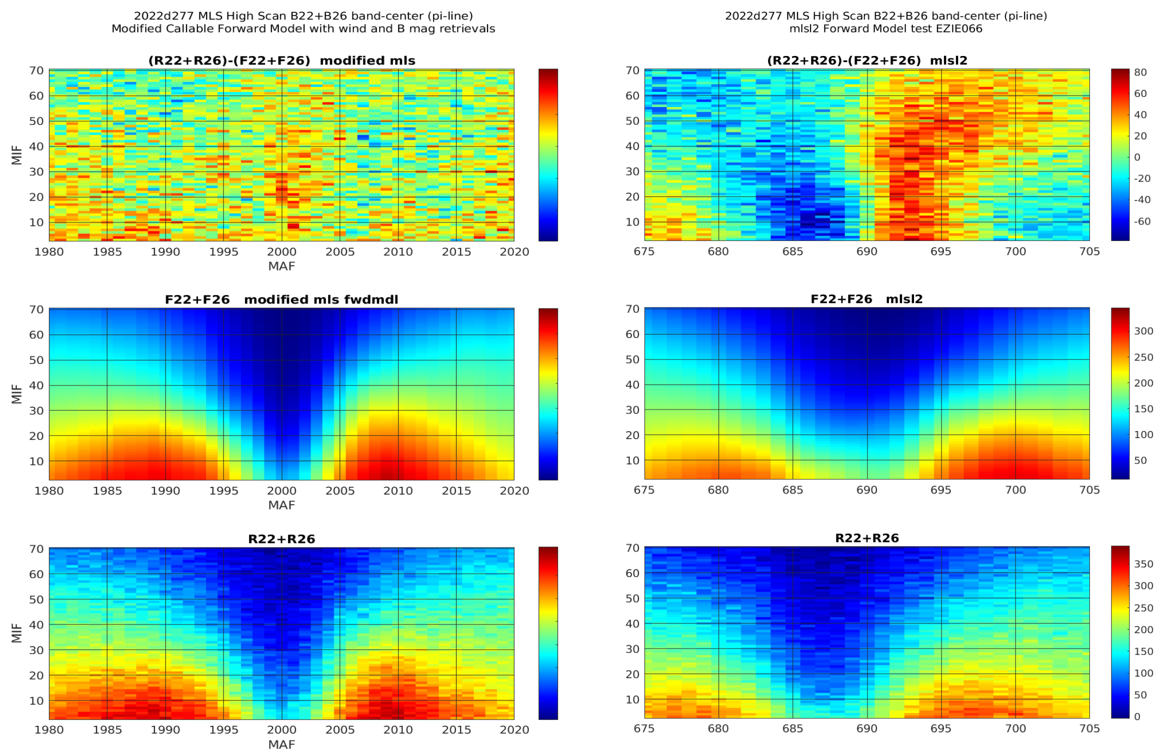


- Along-track location of the transition from strong pi line to no pi line has been a persistent problem in MLS retrievals, requiring a 2+ profile shift to match fwm & rad  in the line center. Such a shift gives worse residuals off of line center.
- The 1D (with wind and |B|) does a much better job than the standard 2D processing, even though 2D should capture B variability along track.

- It may be that getting along-track B only matters in for the most-opaque line centers, where radiances saturate on the spacecraft side of the tangent point.
- It may be that we are putting magnetic field on the path incorrectly.
- I may have discovered a 20+ year old bug!

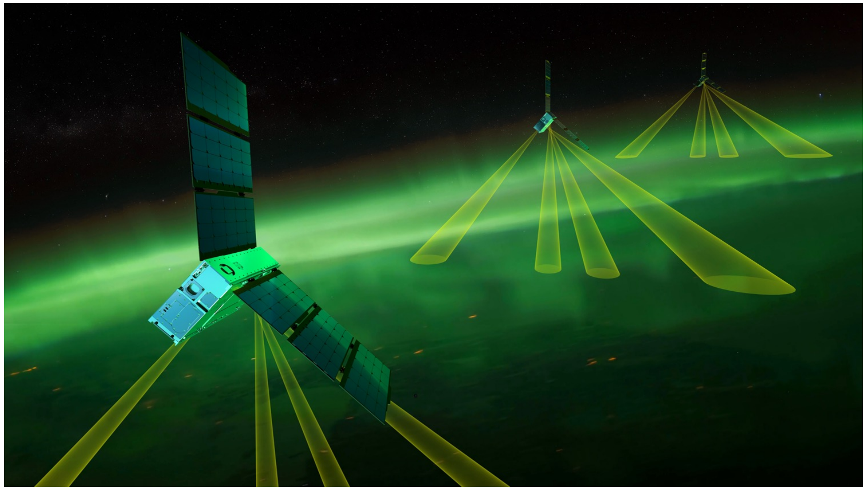
1D +W+|B mlsl2|

2D mlsl2



# EZIE: The Electrojet Zeeman Imaging Explorer

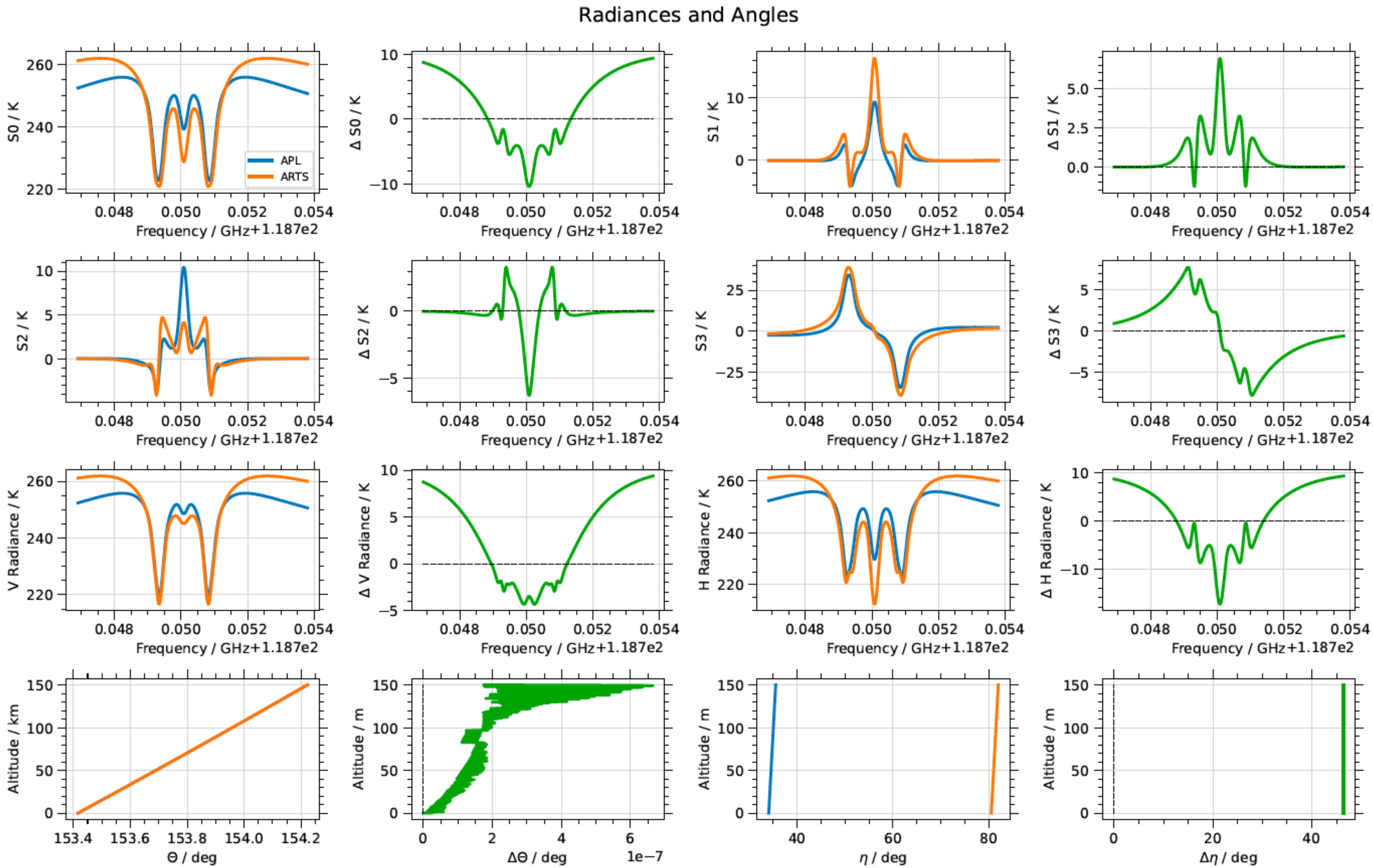




- JHU APL-led Mission to understand auroral electrojet current system. Sam Yee is PI.
- Geomagnetic field perturbations at ~80 km are inferred from spectra of the Zeeman-split, 118-GHz O2 line.
- Zeeman-split line centers saturate at ~80 km and are viewed against a typically warmer background at that saturates at ~50 km near the stratopause.
- Remotely-sensed magnetic field perturbations at 80 km should provide for inference of more fine structure the currents at ~100-110km than would in situ magnetic field measurements from satellite altitudes or from the ground.
- Three small sats each have four fully-polarimetric, JPL-built radiometers with spectrometers resolving spectra at 48 kHz resolution.
- Magnetic perturbations from Electrojet currents are typically <<2% of IGRF a priori.
- There are no calibration targets, but will roll to view cold sky and use stratopause T.
- EZIE retrievals are based upon code adapted by Sam Yee from Richard's 2014 JQSRT paper (idl->python->production pipeline->attempted speed-up).
- EZIE launch may be as soon as October 2024
- We are still finding bugs in the code.

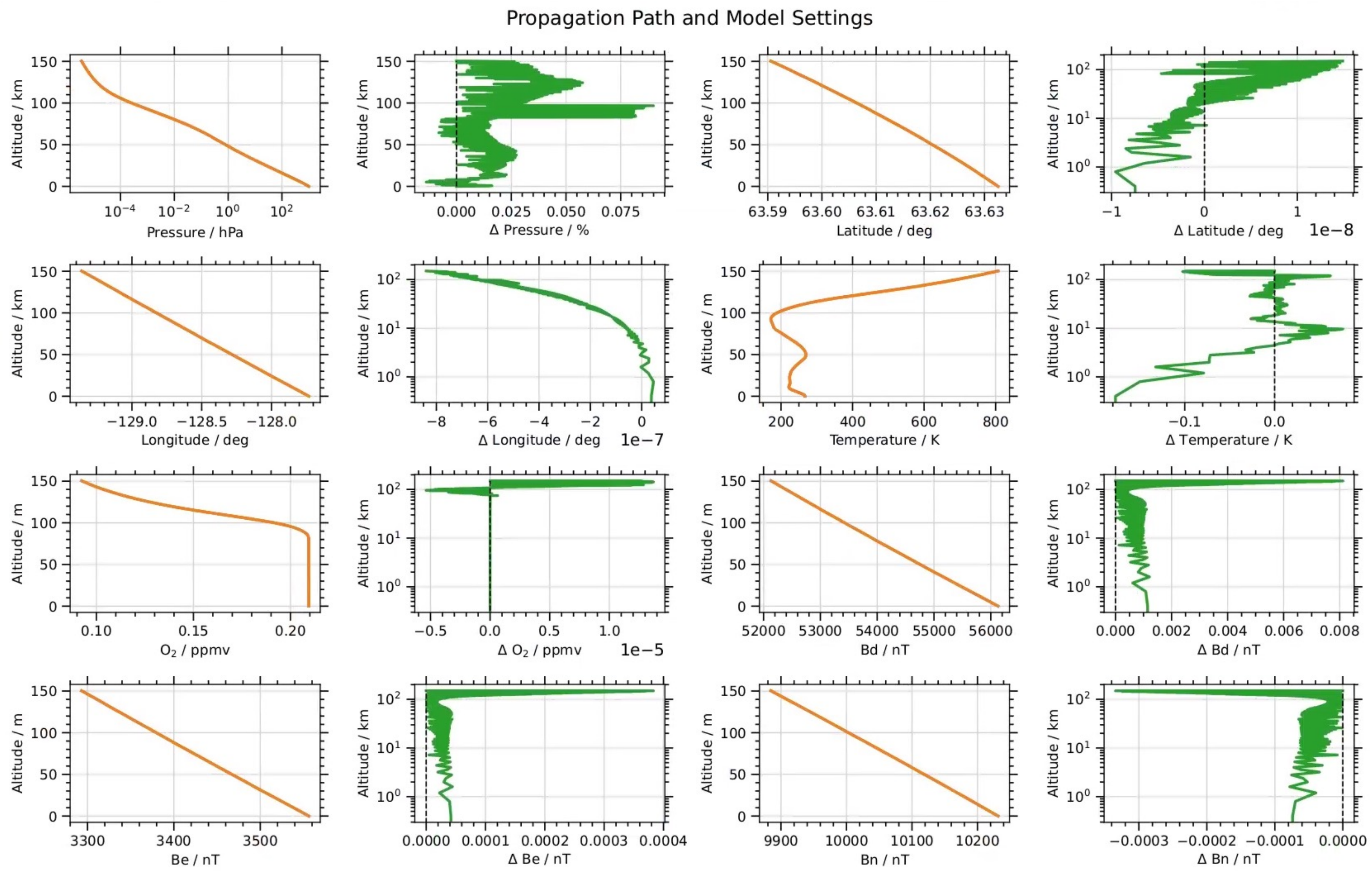
# Comparison of ARTS and EZIE Radiances and Angles





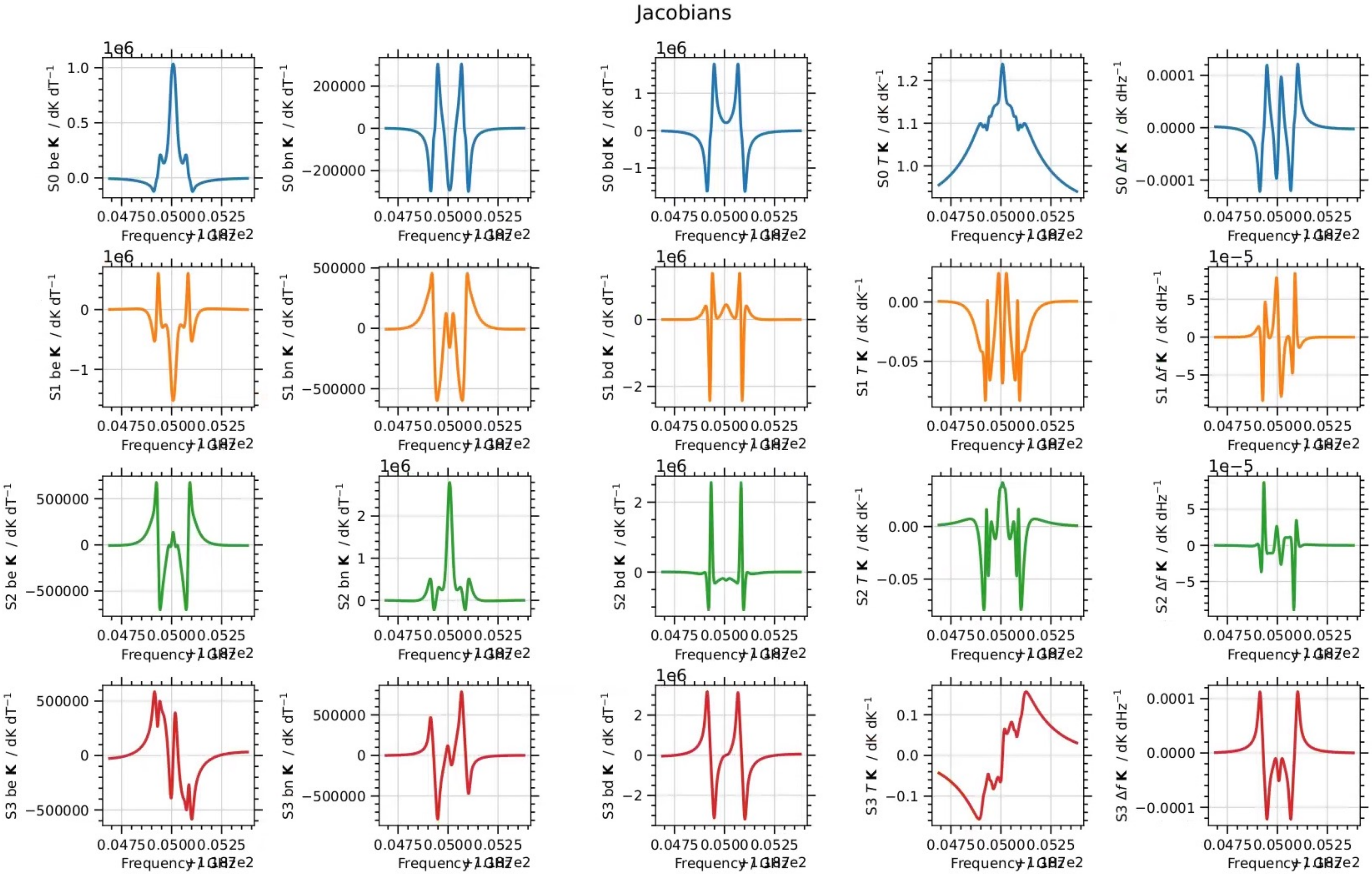
# ARTS and EZIE Geolocation Inputs





# ARTS Jacobians  (Be, Bn, Bd, T, Δfreq)





# Conclusions



- Inter-model comparisons are harder than it seems they should be.
- Inflexible models, like those bound to mlsl2 or the EZIE retrieval code present particular problems.
- Bill Read’s new, offline mlsl2 that retrieves wind magnetic field magnitude does a really nice job, but declining funding makes its implementation in production code unlikely.
- This forward model intercomparison exercise is a work in progress