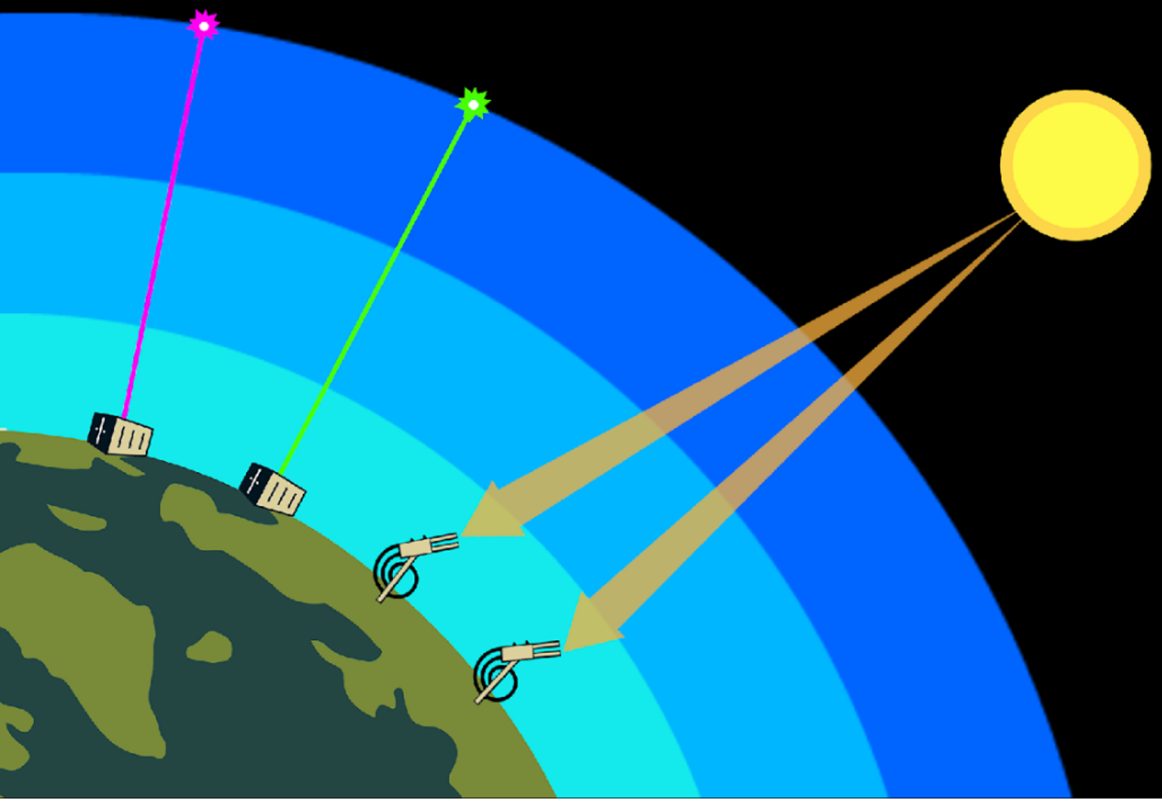
National Aeronautics and Space Administration



NASA Atmospheric Composition Ground Networks Supporting Air Quality and Climate Applications

Part 3: Introduction to Pandora Instrument and the Pandonia Global Network

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August 15, 2024

Part 3 – Trainers

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Job Title

NASA GSFC

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NASA GSFC

Part 3 – Trainers

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Assistant Research Engineer

University of Maryland Baltimore County

Dr. Bryan Place

Atmospheric Scientist

SciGlob

Part 3 Objectives

By the end of Part 3, participants will be able to:

- Identify the basic characteristics of the Pandora instruments used by NASA for ground-based passive remote sensing of trace gases.
- Recognize how the Pandonia Global Network sustains global long-term observations, supports air quality and climate applications, and complements satellite observations.
- Access relevant Pandora and Pandonia Global Network data for a given location and application purpose.

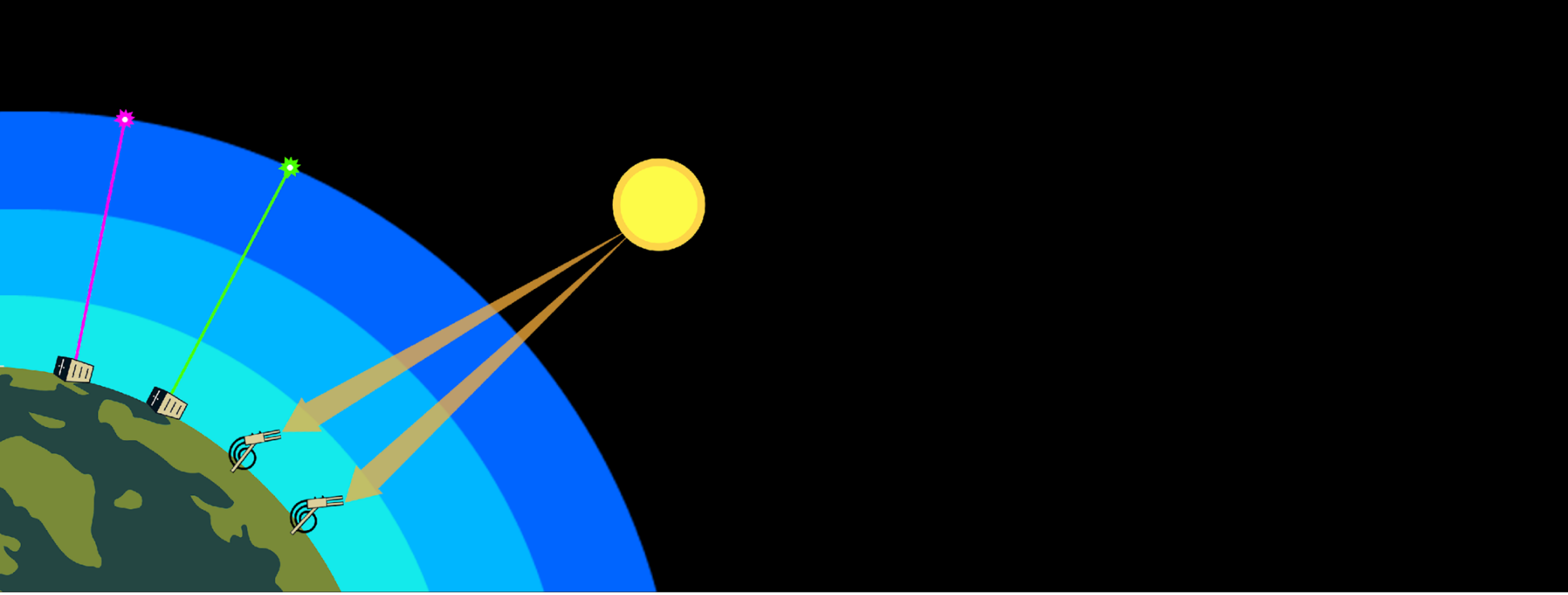
Review of Prior Knowledge

Network	Type	Primary Measurands	Number of Sites	Vertical Coverage
AERONET	Passive	Aerosols (Optical, Microphysical, Radiative)	~600 Active	Total Column

- Trace gases such as nitrogen dioxide, formaldehyde, and ozone are present in small amounts, yet have major impacts on air quality and climate.
- Detection of atmospheric trace gases requires remote sensing instruments with a high spectral resolution, called hyperspectral instruments.
- Examples of hyperspectral remote sensing instruments on satellites providing trace gas data are:
  - OMI on the Aura satellite
  - TROPOMI on the European Sentinel-5P satellite
  - The newly launched TEMPO geostationary instrument

How to Ask Questions

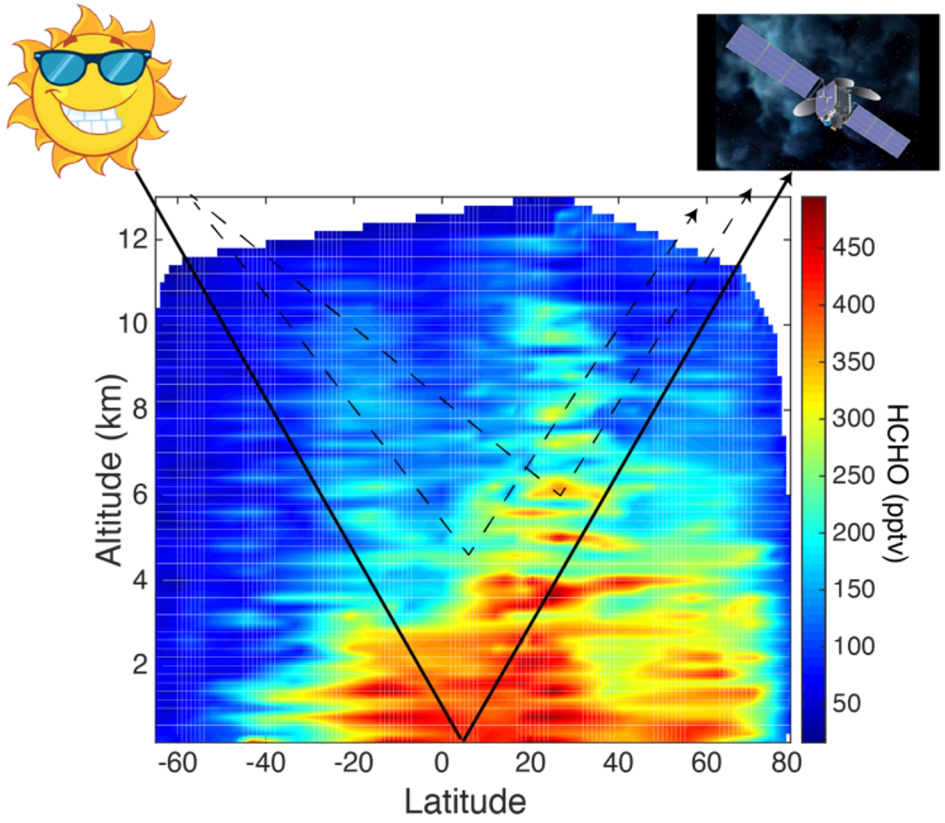
- Please put your questions in the Questions box and we will address them at the end of the webinar.
- Feel free to enter your questions as we go. We will try to get to all of the questions during the Q&A session after the webinar.
- The remainder of the questions will be answered in the Q&A document, which will be posted to the training website about a week after the training.



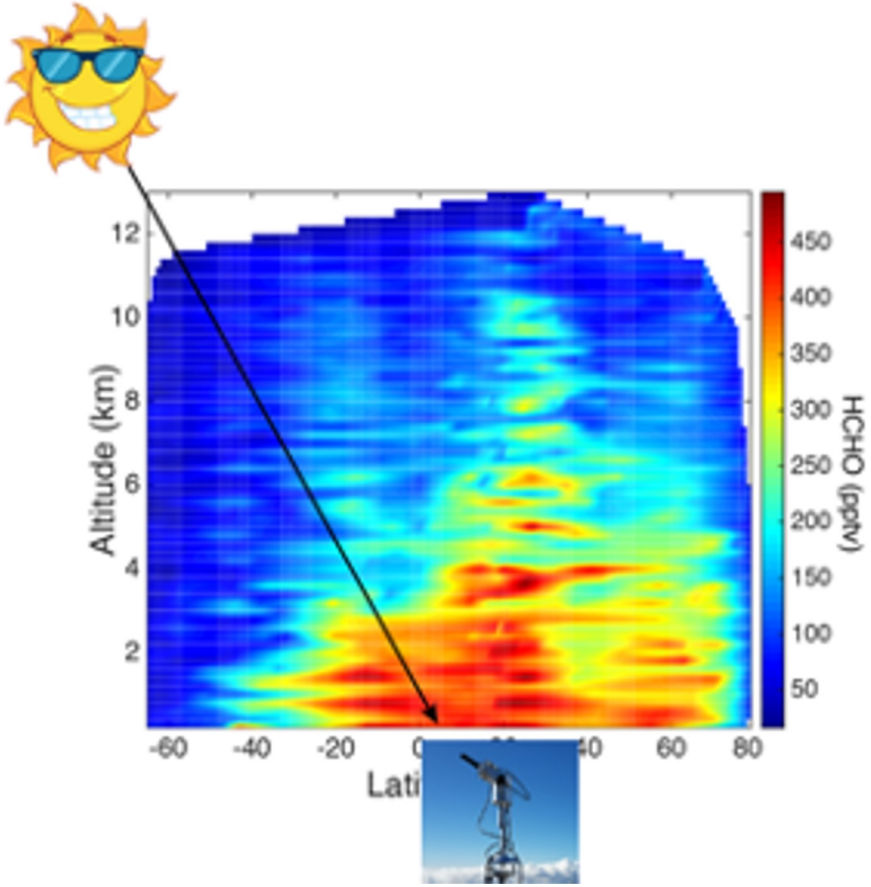
Part 3:

Overview of the Pandora Instrument and Pandonia Global Network (PGN)

Motivation



Satellites measure sunlight reflected from the Earth's surface and scattered from the atmosphere. This is complicated and requires assumptions that are not always correct.



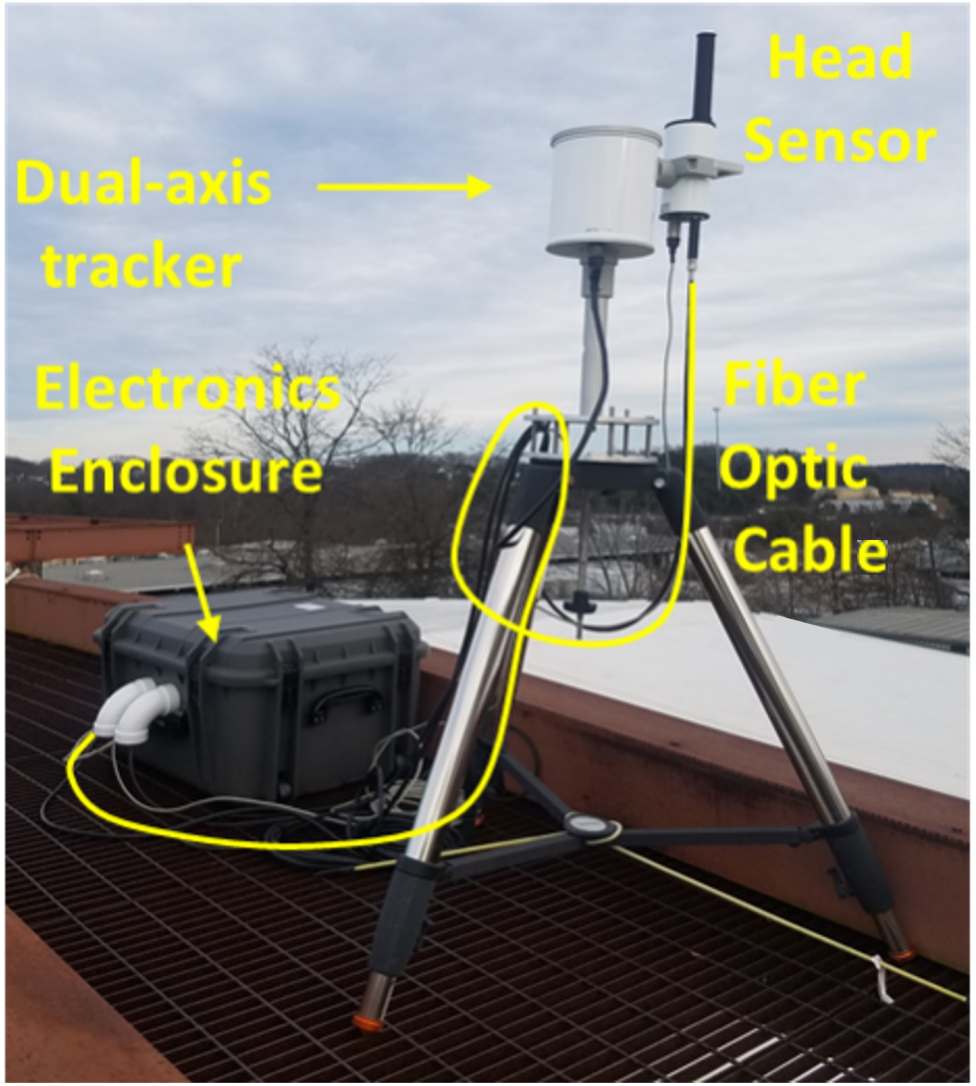
Ground-based remote sensing instruments have better signal-to-noise and can probe different parts of the atmosphere by tracking the sun or measuring sky-scattered light.

The Pandonia Global Network: Reference Measurements of O_3, NO_2, SO_2, and HCHO

- The NASA Pandora Project works within a framework called the Pandonia Global Network (PGN).
- The PGN operates a global network of Pandora Instruments.
- Our partners are the European Space Agency (ESA) and two firms, SciGlob and LuftBlick.

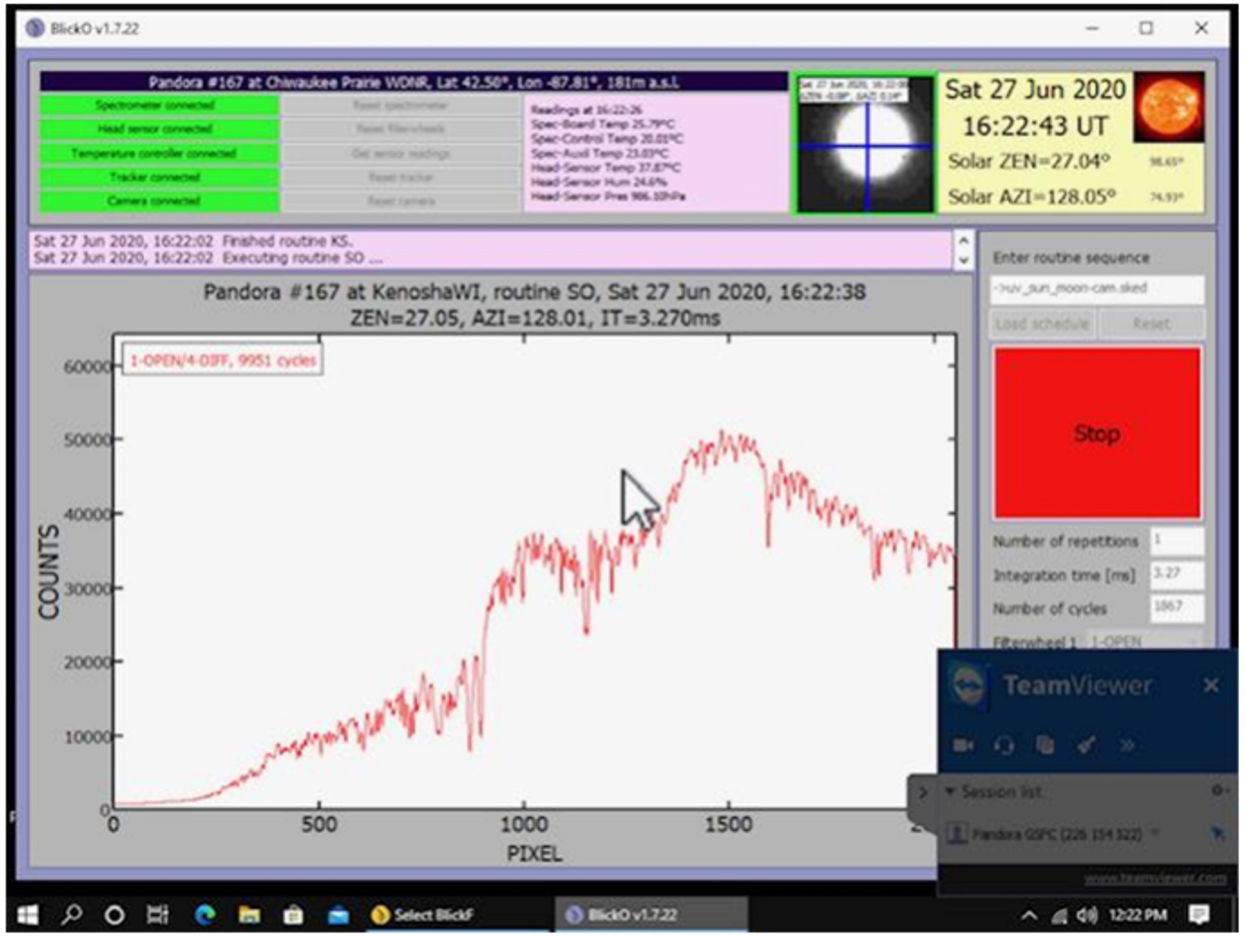
Instrumentation

- Pandora is a ground-based sun/sky/moon viewing spectrometer system.
- The sensor head (light collector) is mounted on a dual-axis tracker.
- The sun/sky/moon-light is directed to the input of a Charge-Coupled Device (CCD) spectrometer with a fiber optic cable.

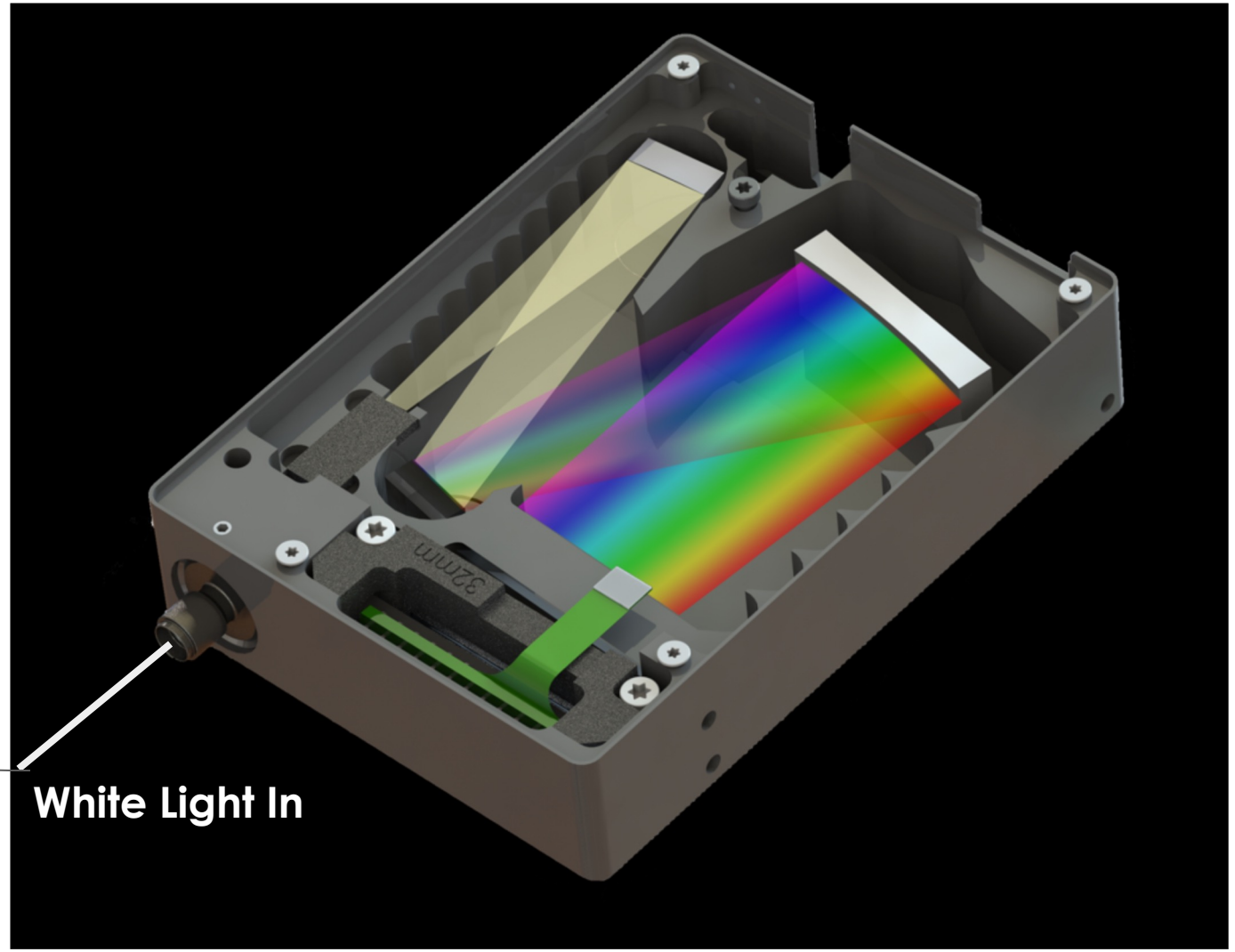


Control and Interface

- Control electronics allow for semi-autonomous operation in all-weather conditions.
- **Pixels** (wavelength) and **counts** (intensity) are used to derive trace gas abundance.



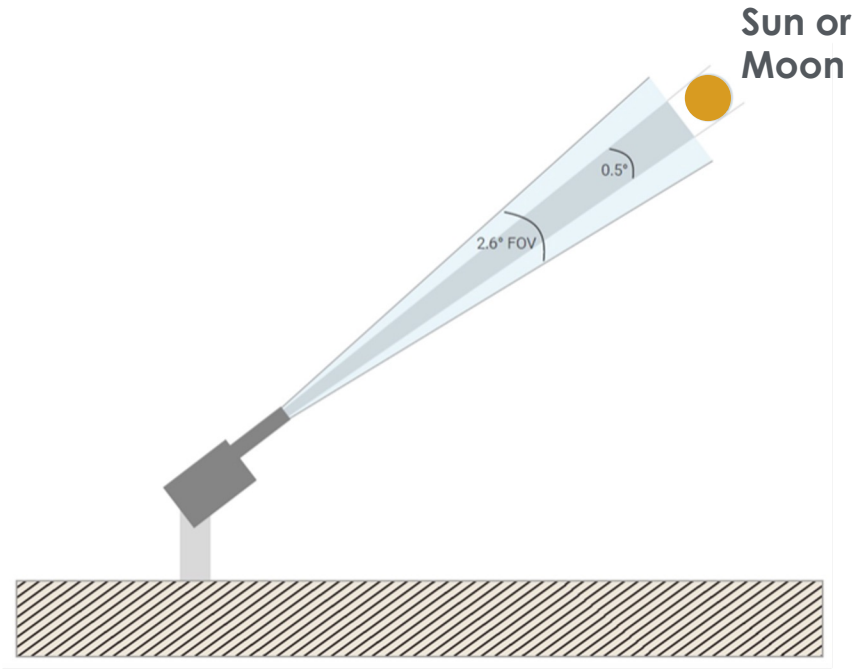
Pandora: Hyperspectral Measurement Basics

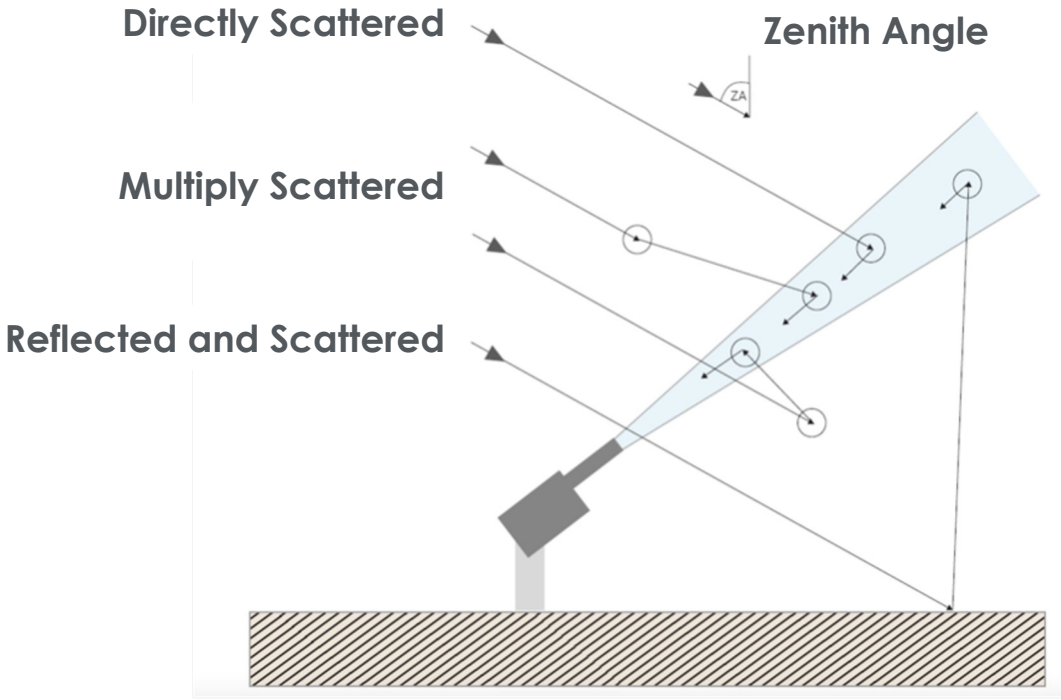


Hyperspectral Measurements = Intensity of Light as a Function of Wavelength.

- Pandora spectrometers operate in the UV-visible range.
- When compared to a reference, measured spectra contain information about light absorption by trace gases.
- What we observe is a function of the spectrometer, fiber, and head sensor optics.

Pandora Measurements





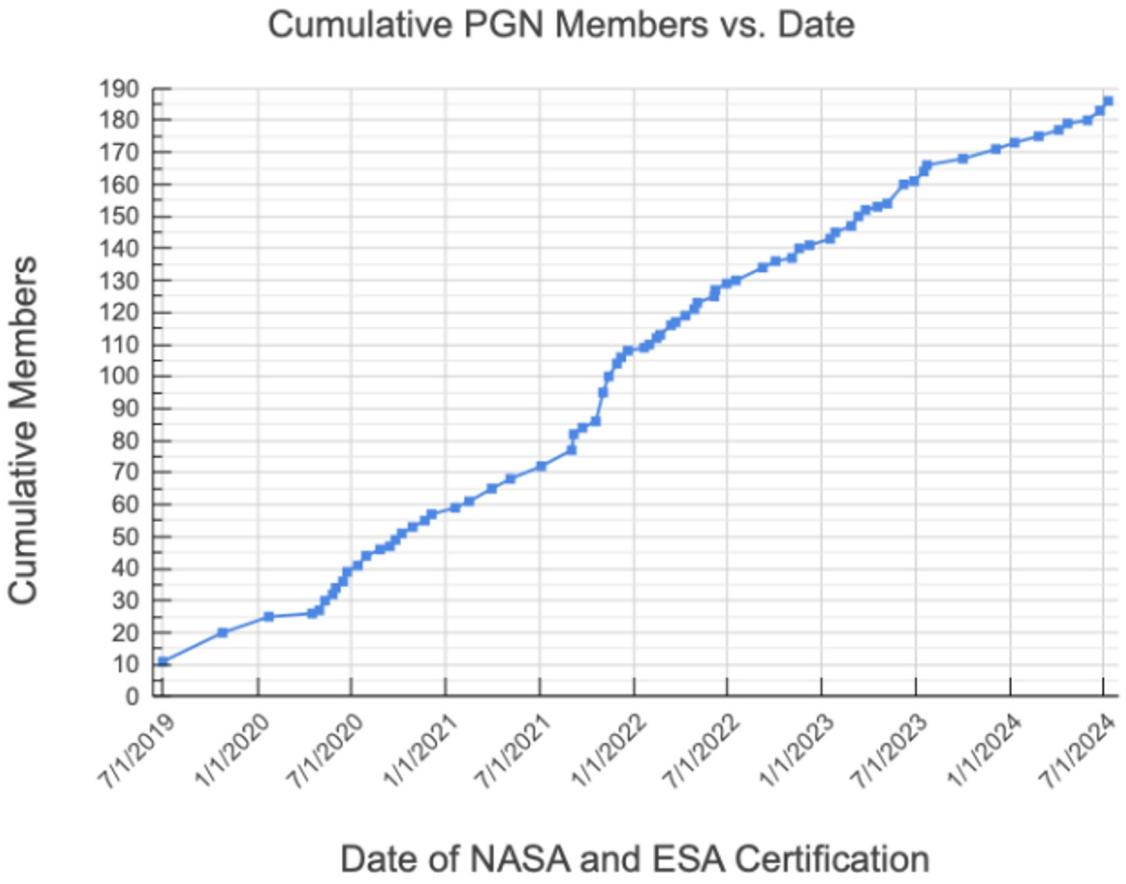
Direct Sun or Moon

- Mostly described by BEER's Law
- Total absorption used to derive column abundance between instrument and top of atmosphere

MAX-DOAS

- Multi-Axis Differential Optical Absorption Spectroscopy
- Multiple angle BEER's Law
- Differential measurements used to derive abundance at multiple elevations

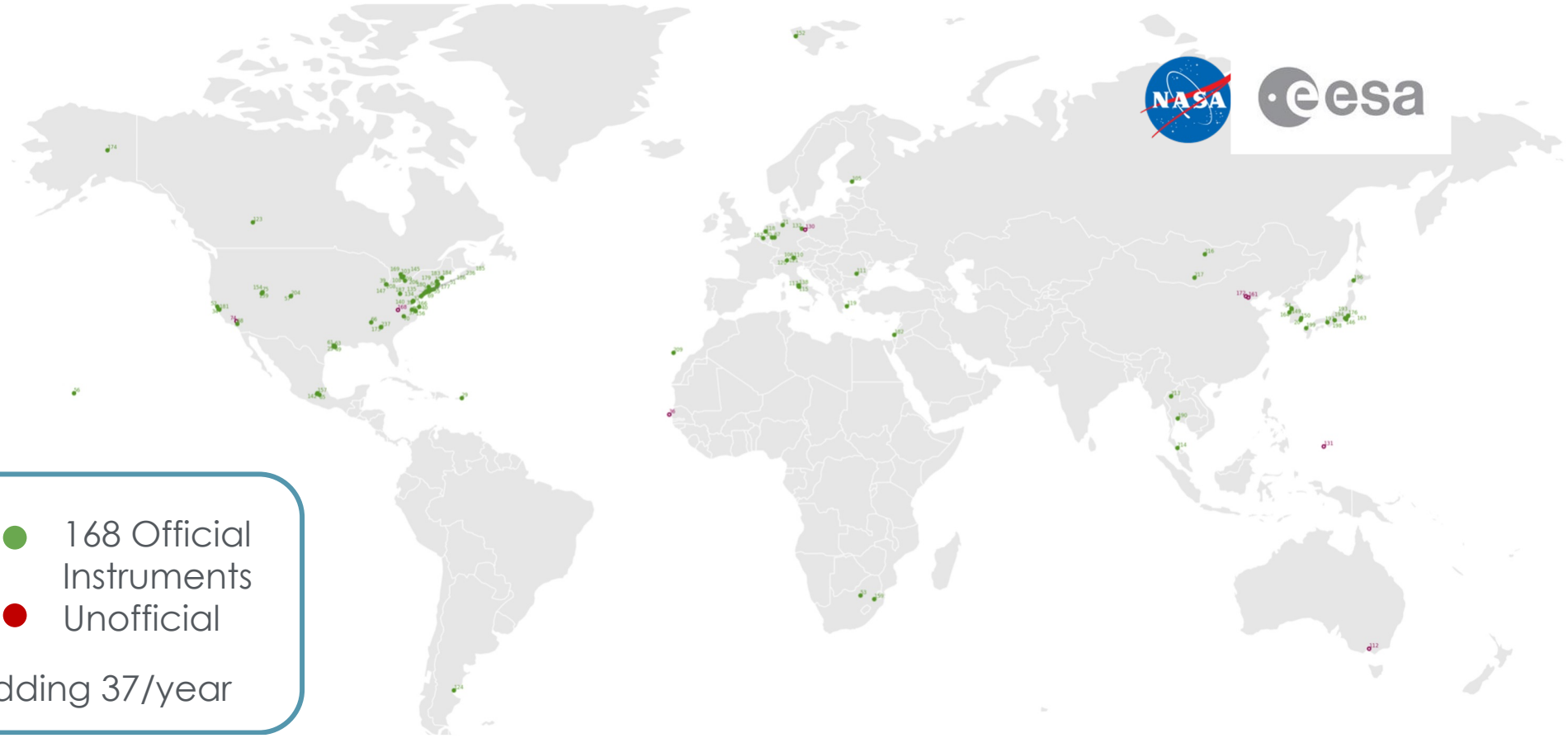
Growth of the ESA/NASA Pandonia Global Network



Owner/Funding Source	Number
University/Other*	50
NASA	50
EPA	25
ESA	21
KOICA	20

*Other includes NIER (S. Korea) JAMSTEC (Japan) and ECCC (Canada)

ESA/NASA Pandonia Global Network

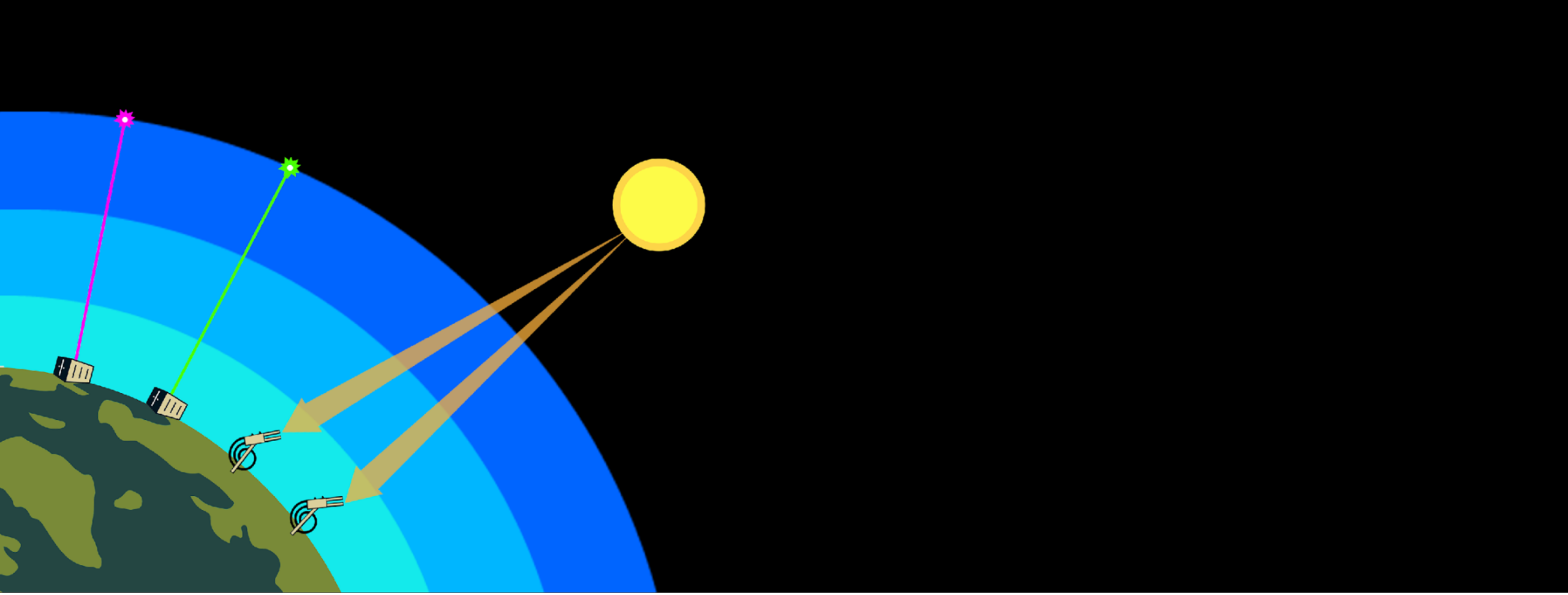


- 168 Official Instruments
- Unofficial

Adding 37/year

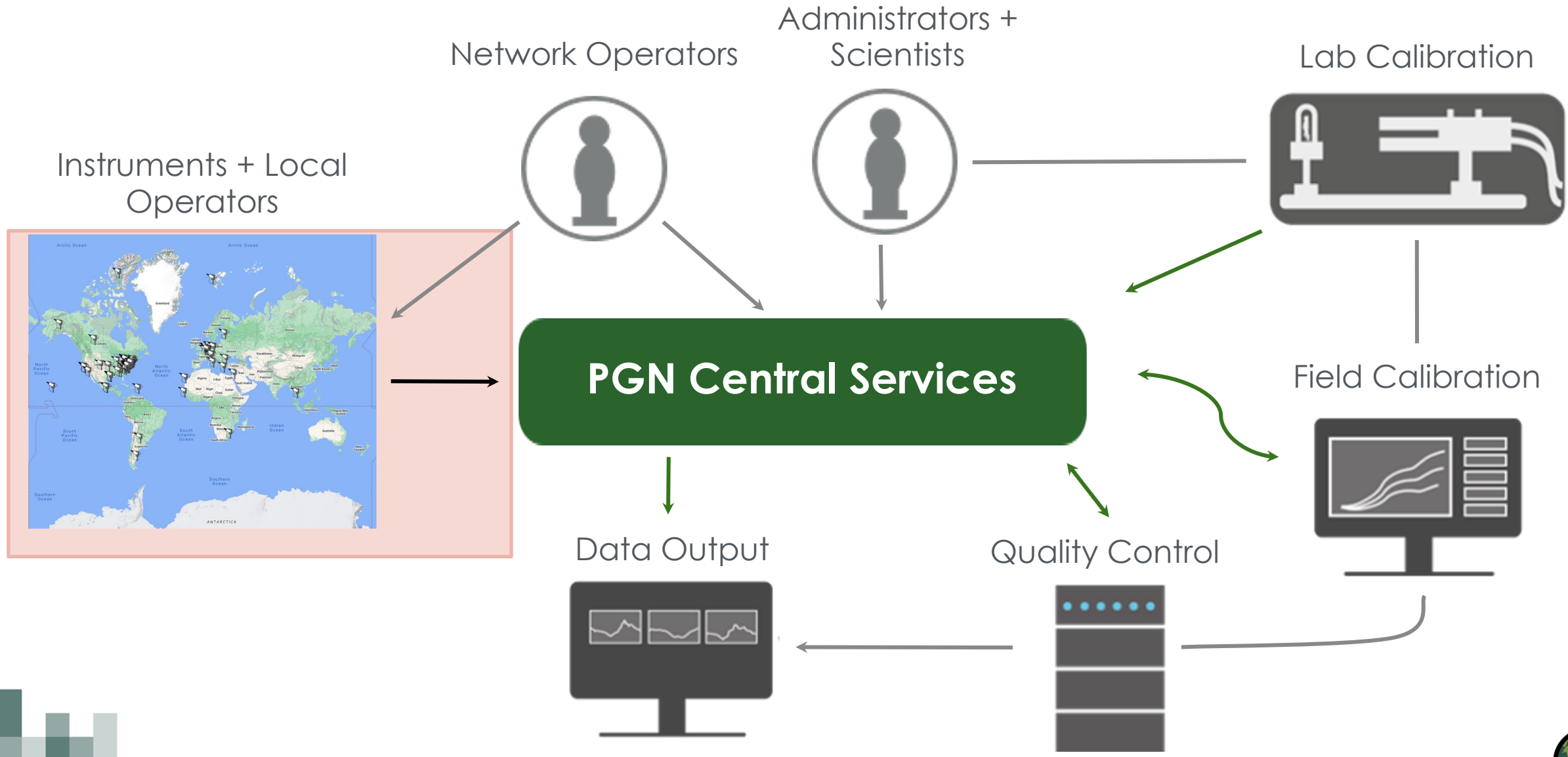
61 AldineTX
168 BlacksburgVA*
206 BuffaloNY
179 CornwallCT
29 Fajardo*
209 Izana
142 MexicoCity-UNAM
166 PhiladelphiaPA
75 SaltLakeCityUT-Hawthorne
182 Tel-Aviv
40 WallopsIslandVA
65 Altzomoni
155 BostonMA
20 Busan
36 Dakar
199 Fukuoka
30 Juelich
157 MexicoCity-Vallejo
187 PittsburghPA
181 SanJoseCA
194 Tokyo-TMU
140 WashingtonDC
119 Athens-NOA
57 BoulderCO
118 Cabauw
217 Dalanzadgad
32 GreenbeltMD*
198 Kobe
34 MountainViewCA
53 Potchefstroom
196 Sapporo
145 Toronto-Scarborough
177 WestportCT
173 AtlantaGA*
204 BoulderCO-NCAR
184 CapeElizabethME
120 Davos
37 HamptonVA
63 LaPorteTX
197 Nagoya
55 QueensNY
164 Seosan
108 Toronto-West
208 Windsor-West
237 AtlantaGA-SouthDeKalb
21 Bremen
70 ChapelHillNC
39 DearbornMI
156 HamptonVA-HU
110 LabLuftBlick
69 NewBrunswickNJ
52 RichmondCA
54 Seoul
193 Tsukuba
68 WrightwoodCA
190 Bangkok
134 BristolPA
31 CharlesCityVA
103 Downsview*
105 Helsinki
130 Lindenberg
64 NewHavenCT
138 Rome-IIA
149 Seoul-SNU
176 Tsukuba-NIES
161 Xianghe
38 BayonneNJ
112 Broadmeadows
213 ChiangMai
185 EastProvidenceRI
25 HoustonTX
183 LondonderryNH
236 NewLondonCT
115 Rome-ISAC
214 Songkhla
163 Tsukuba-NIES-West
146 Yokosuka
172 Beijing
180 BronxNY
49 ClearLakeShoresTX
74 EdwardsCA
66 HuntsvilleAL
186 MadisonCT
152 NyAlesund
117 Rome-SAP
139 SouthJordanUT
216 Ulaanbaatar
80 BeltsvilleMD
162 Brussels-Uccle
67 Cologne
169 Egbert
106 Innsbruck
135 ManhattanNY-CCNY
51 OldFieldNY
147 SWDetroitMI
109 StGeorge
150 Ulsan
132 Berlin
111 Bucharest
124 ComodoroRivadavia
174 FairbanksAK
121 Innsbruck-FKS
56 MaunaLoaHI
131 Palau
154 SaltLakeCityUT
123 StonyPlain
159 Wakkerstroom

* more than one instrument

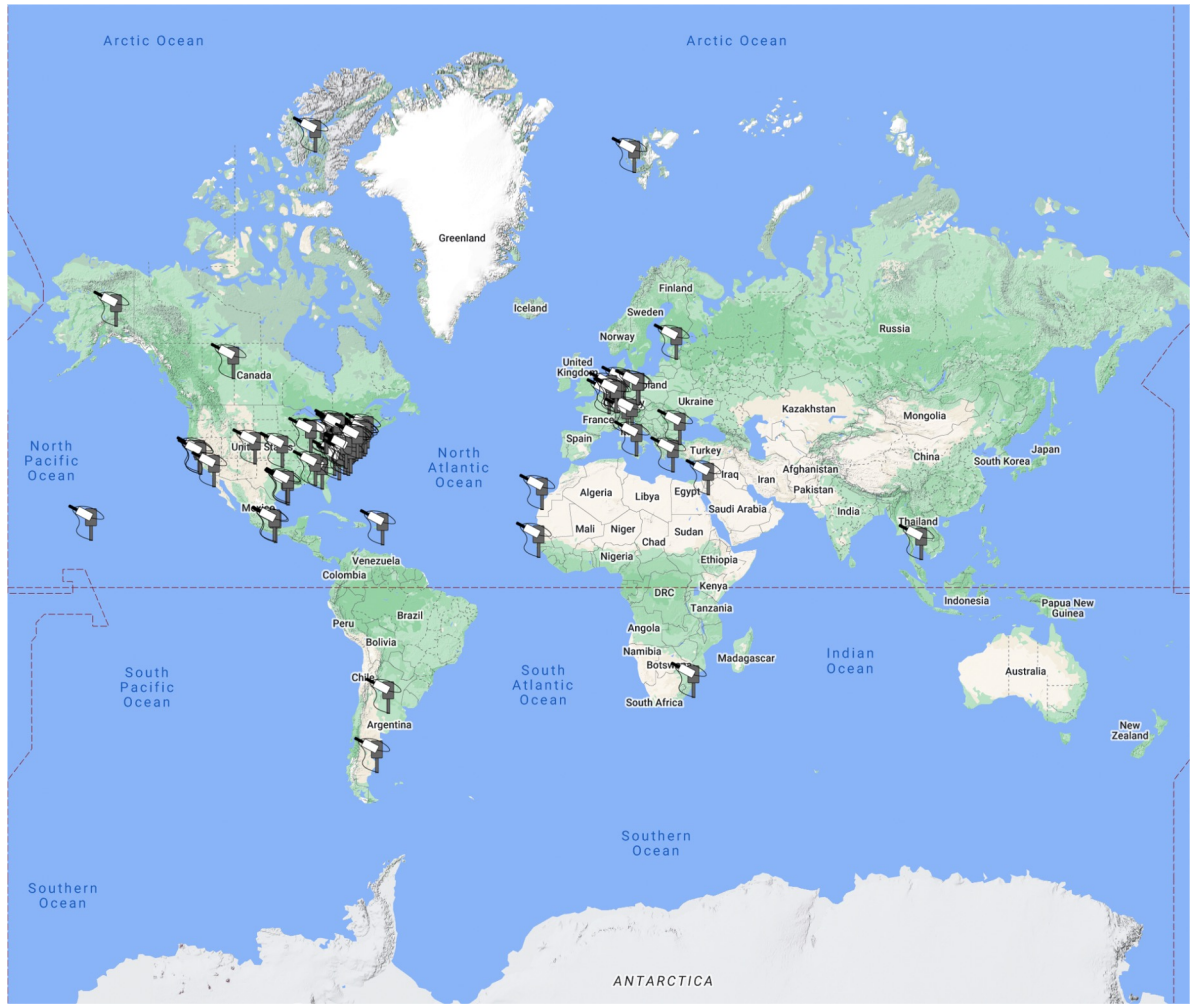


PGN Structure and Calibration

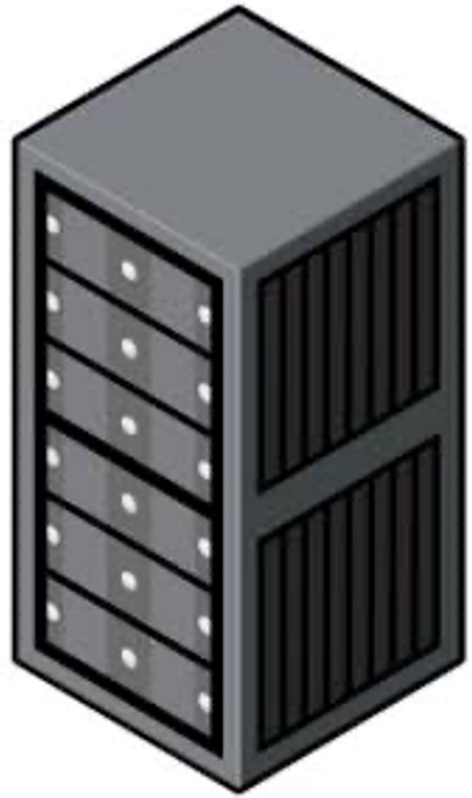
Network Structure



Remote Data Pushing

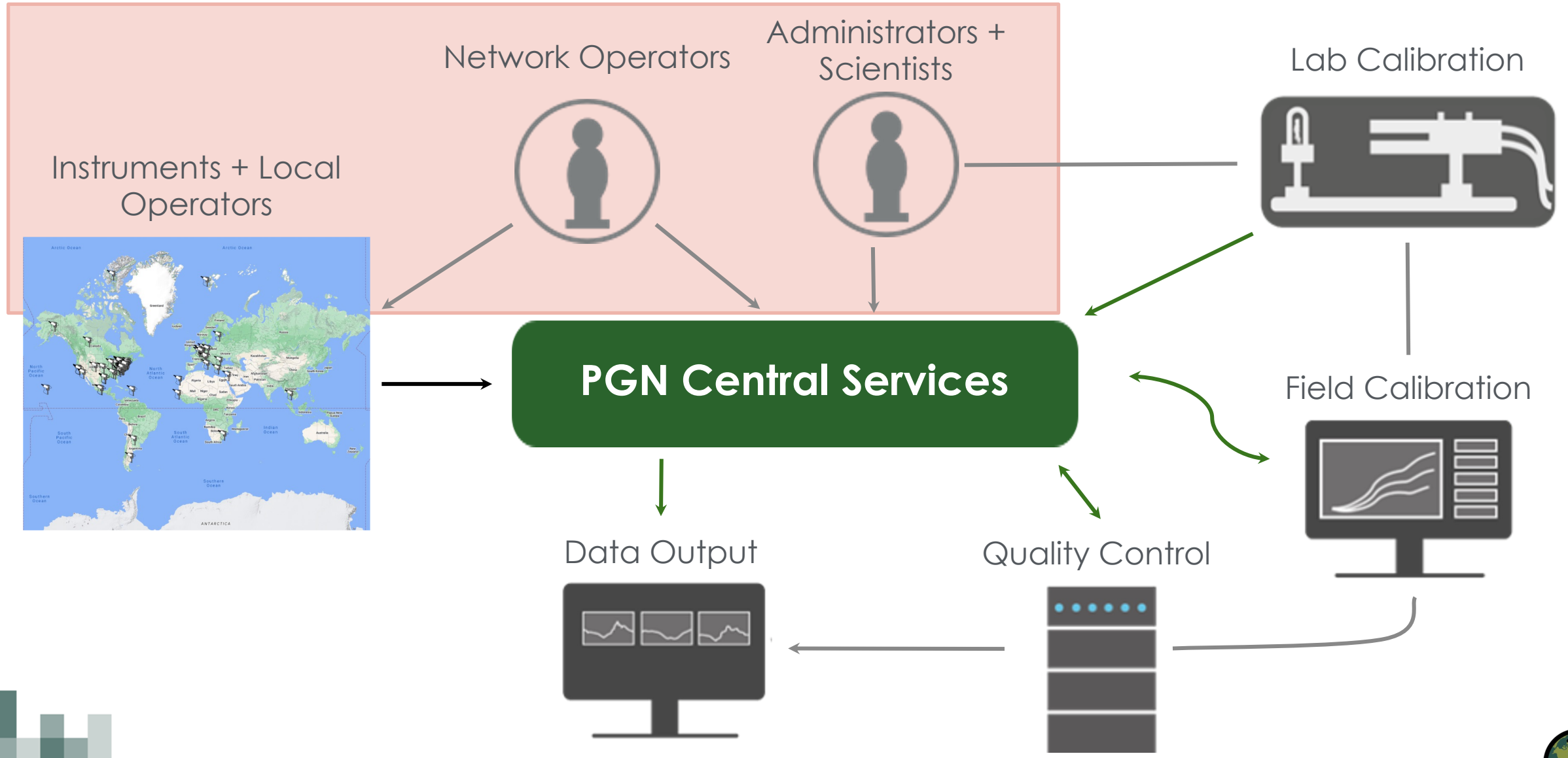


PGN Central Services



Data Processing + Quality Assurance

Monitoring the health of the network



Operator Roles

Local Operators

- Perform regular inspections of instruments
- Communicate with network operators to diagnose any issues
- Work with the PGN team to coordinate instrument repairs and upgrades

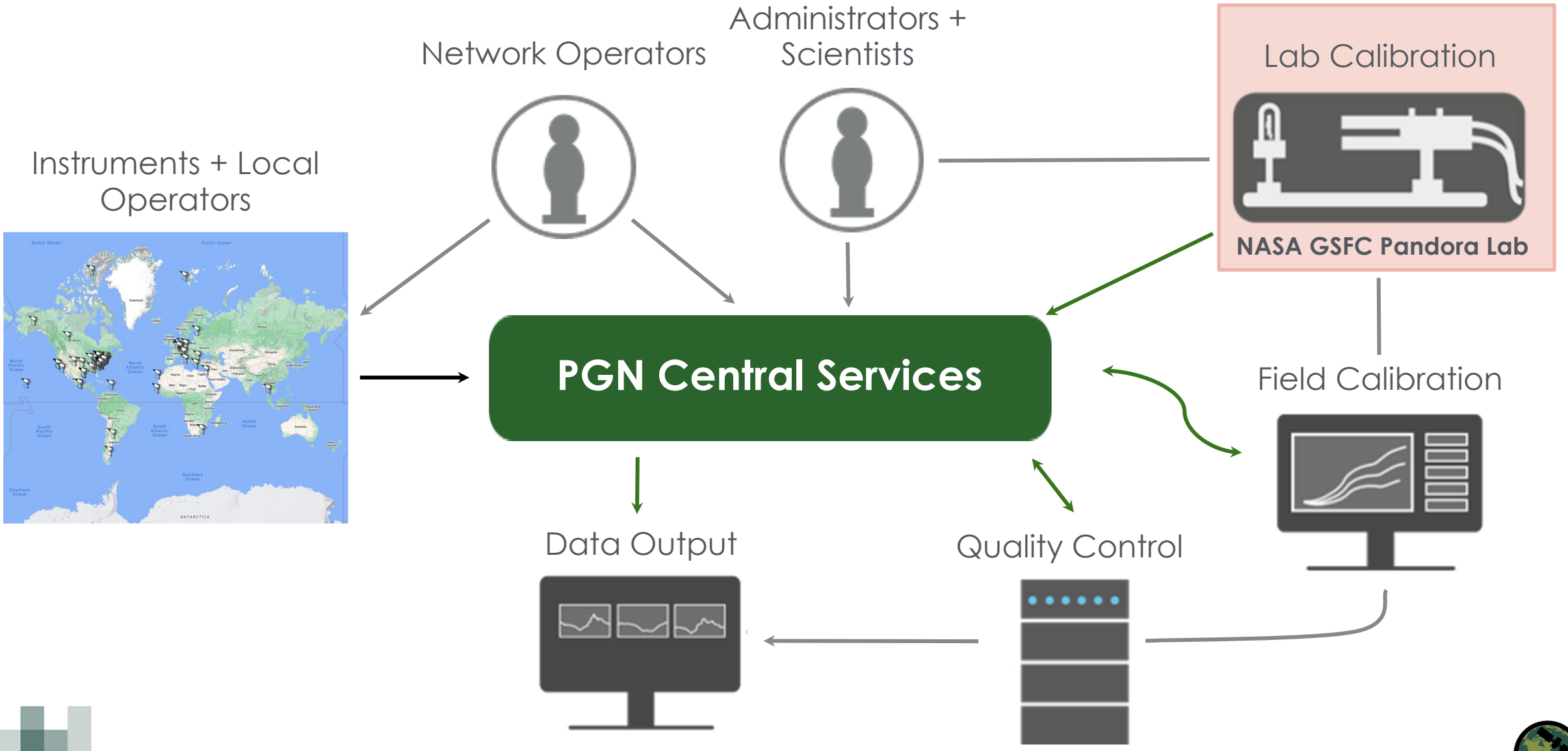
Network Operators

- Perform weekly diagnostic checks of each instrument remotely
- Communicate with local operators to diagnose any issues
- Coordinate repairs and shipments

Administrators + Scientists

- Perform laboratory/field calibrations and analysis
- Regularly check data quality
- R&D into hardware & software improvements and development of new products

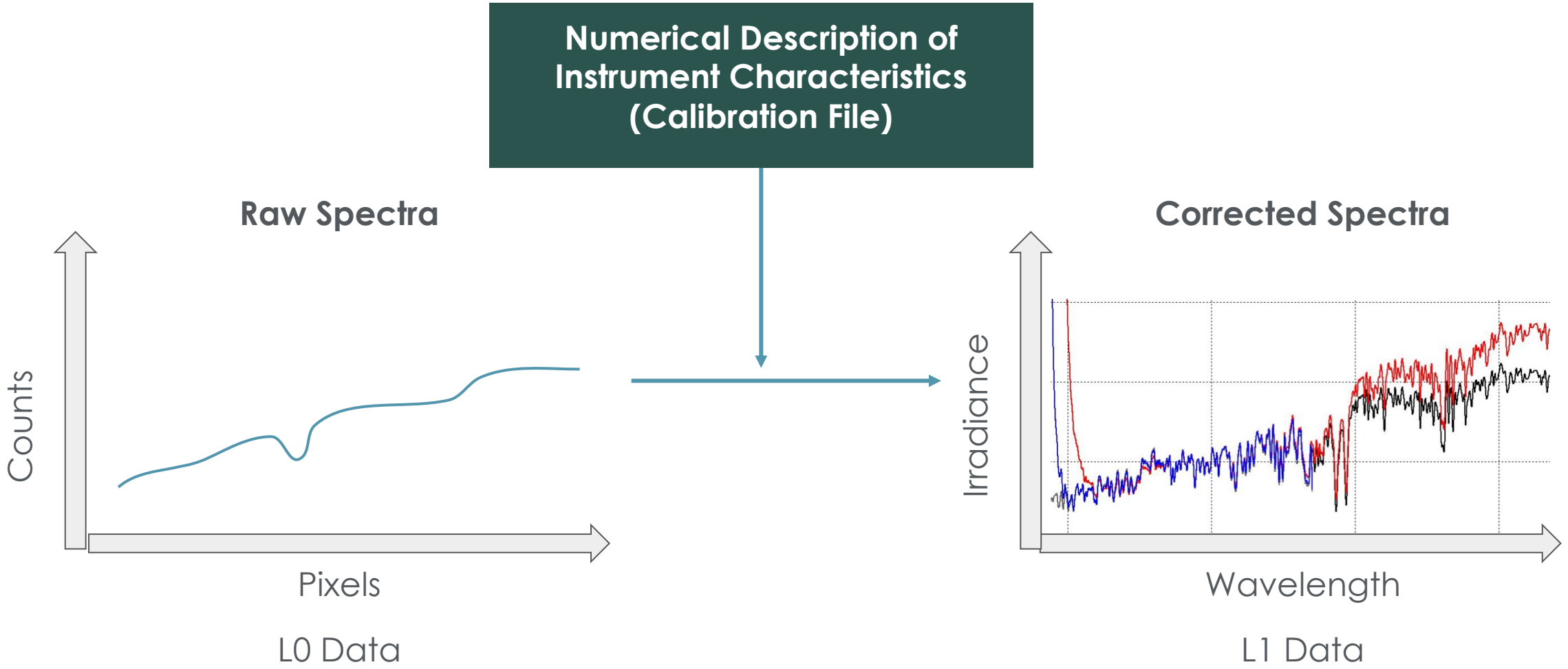
Laboratory Instrument Calibrations



Lab Calibration: Goals

- Use laboratory measurements to generate an initial calibration file that converts Level 0 (raw data) to Level 1 (lab-corrected) processed data
- Determine and record additional instrument characteristics needed for the processing of final Level 2 data retrievals
- **Begin processing of out-of-the-box Pandora data products using the initial calibration file and either reference spectrum**
  - Out-of-the-box data include **O_3 total columns**, and MAX-DOAS data products — **tropospheric columns, surface concentration and profiles — for NO_2 and HCHO**.
  - Other data products need field calibration in addition to the lab characterization.

Lab Calibration: Raw to Corrected Spectra



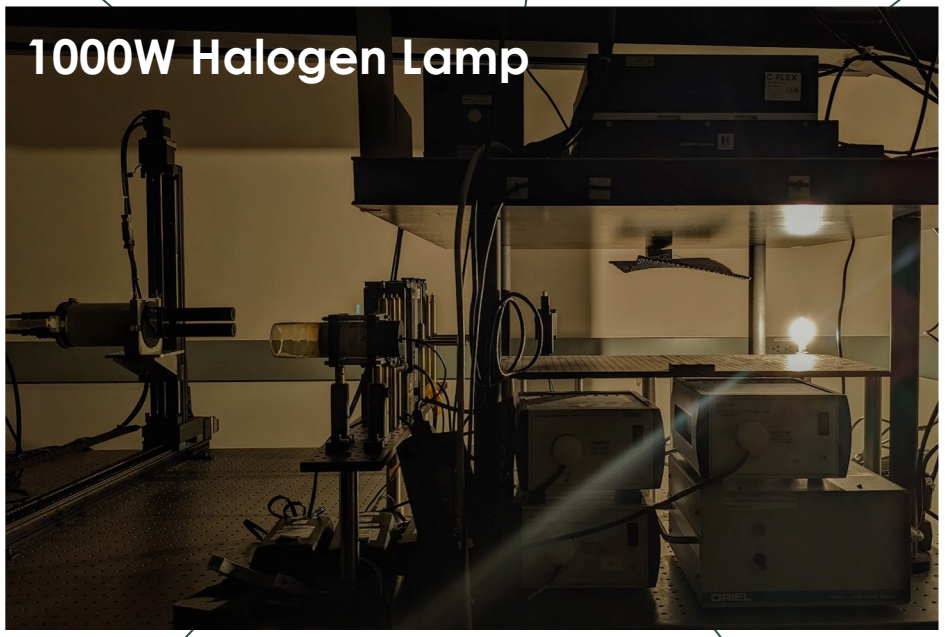
Lab Calibration: Equipment

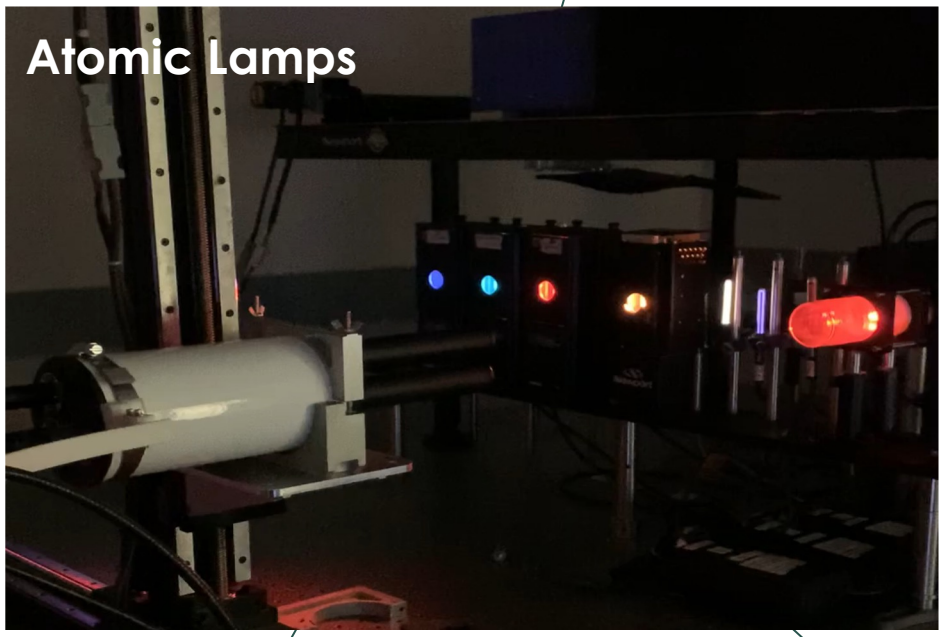
Pixel Non-Uniformity

Sensitivity

Signal to Noise

Wavelength Dispersion





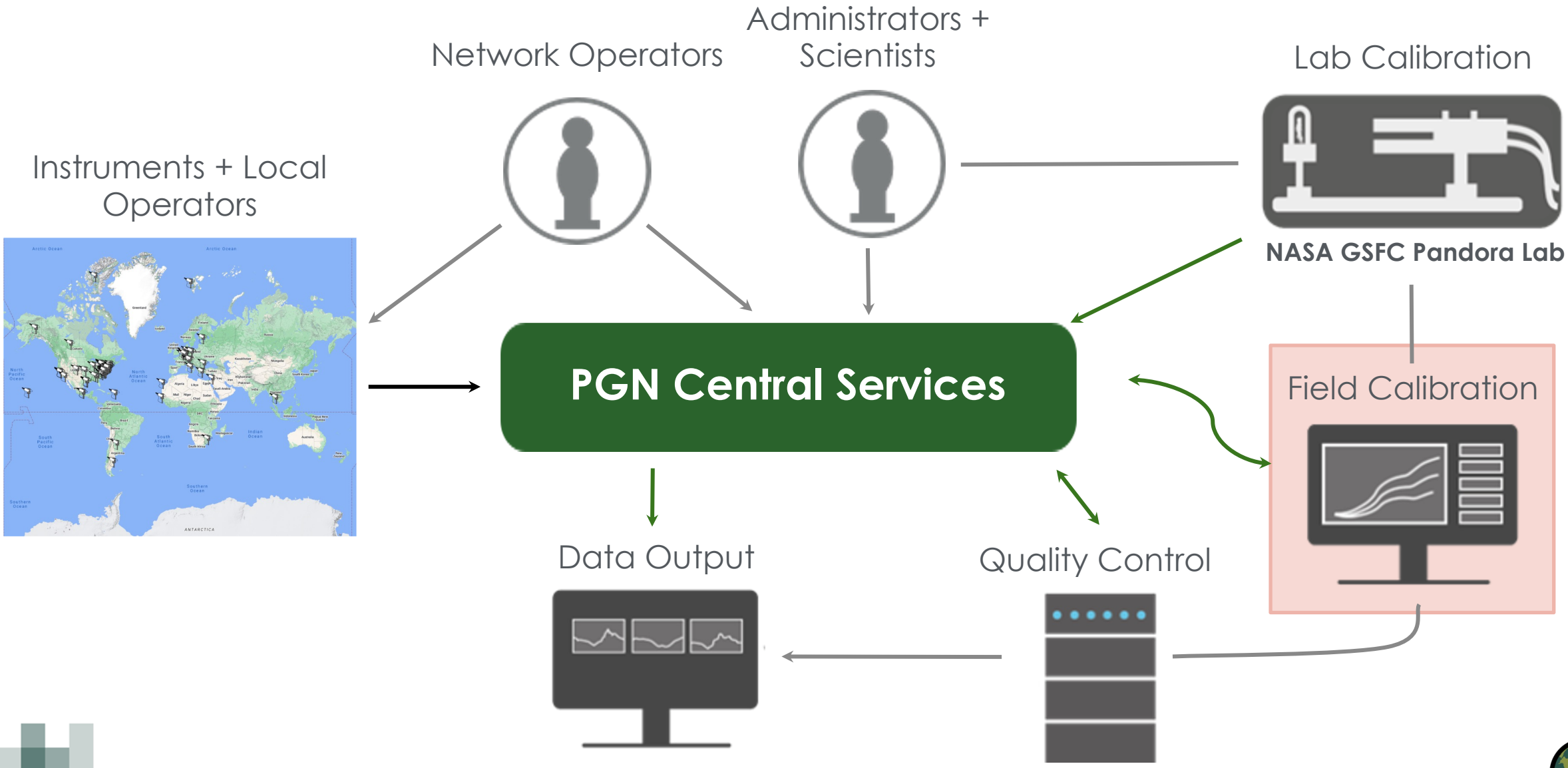
Bright Non-Linearity

Filter Transmissions

Slit Function

Temperature Effects

Field Calibration of Deployed Instruments



Field Calibration: Goals

- Generate an absorption-free synthetic reference spectrum for the retrieval of several PGN trace gas products (**NO_2, HCHO, and SO_2 total columns**)
  - The reference is based on measurements around local noon on a clear day.
  - Typically, one month of field data is needed to fully describe the reference.
- Verify the quality and usability of each trace gas product
- If needed, produce multiple reference spectra for time periods when instrument characteristics shift or drift

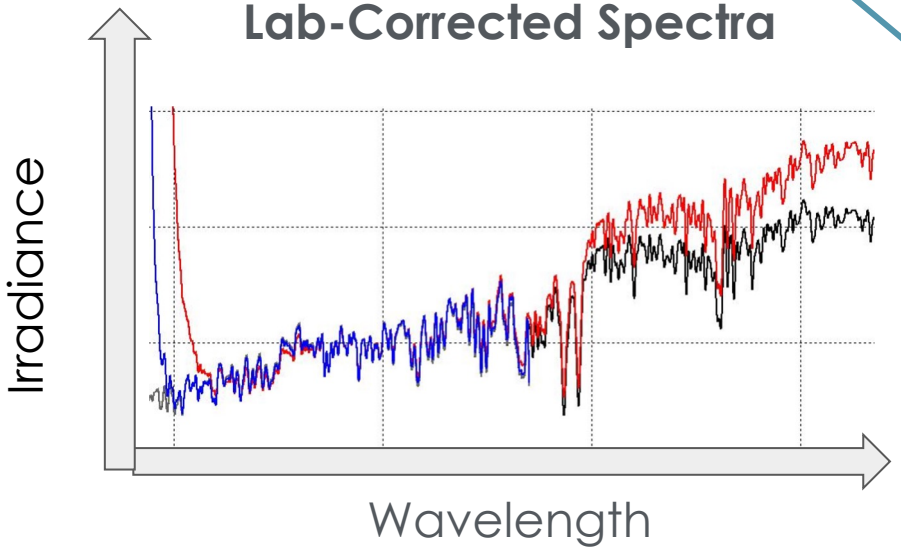
Fitted Slant Columns from Calibrated Measurements

Measured or Literature Reference (out-of-the-box data)

or

Calibration File Containing Absorption-Free Synthetic Reference from Field Calibration

Lab-Corrected Spectra



L1 Data

Lambert-Beer's Law Fitting

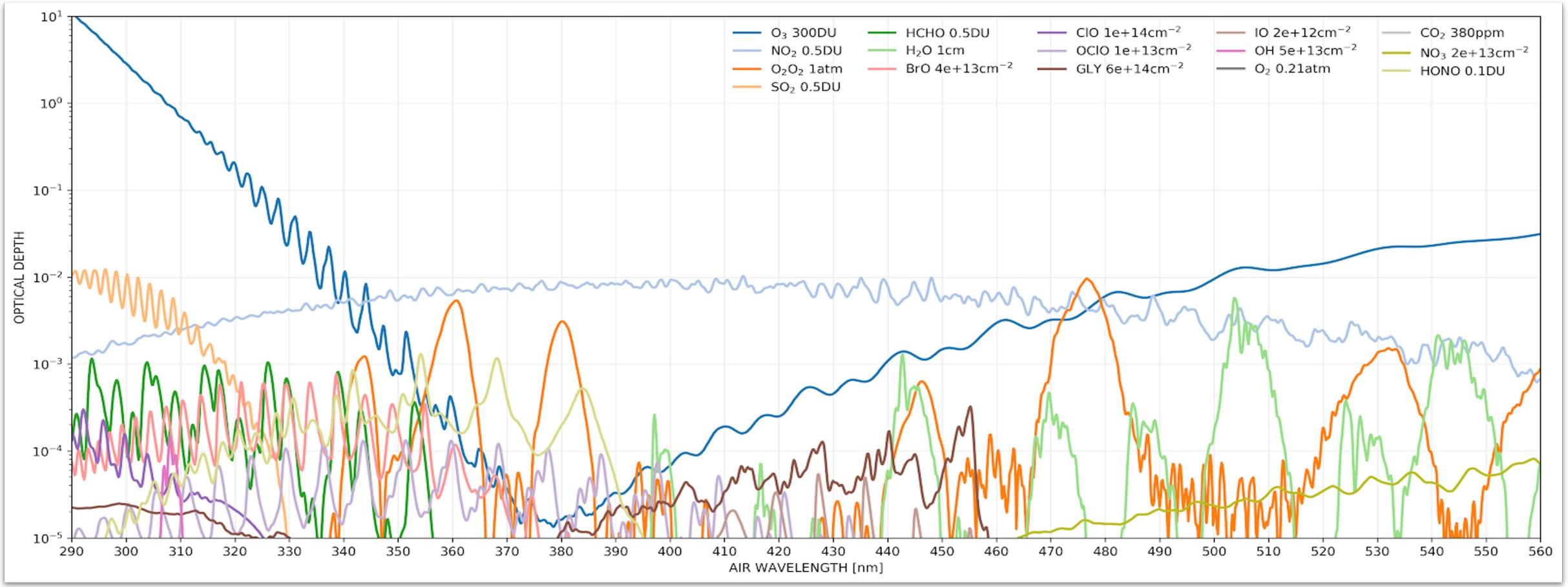
$$slant\ column \times \sigma_{abs} = \ln\left(\frac{I_0}{I}\right)$$

σ_{abs} = Absorption Cross Section
I_0 = Reference Spectrum
I = Measured Spectrum Being Fitted

L2Fit Data

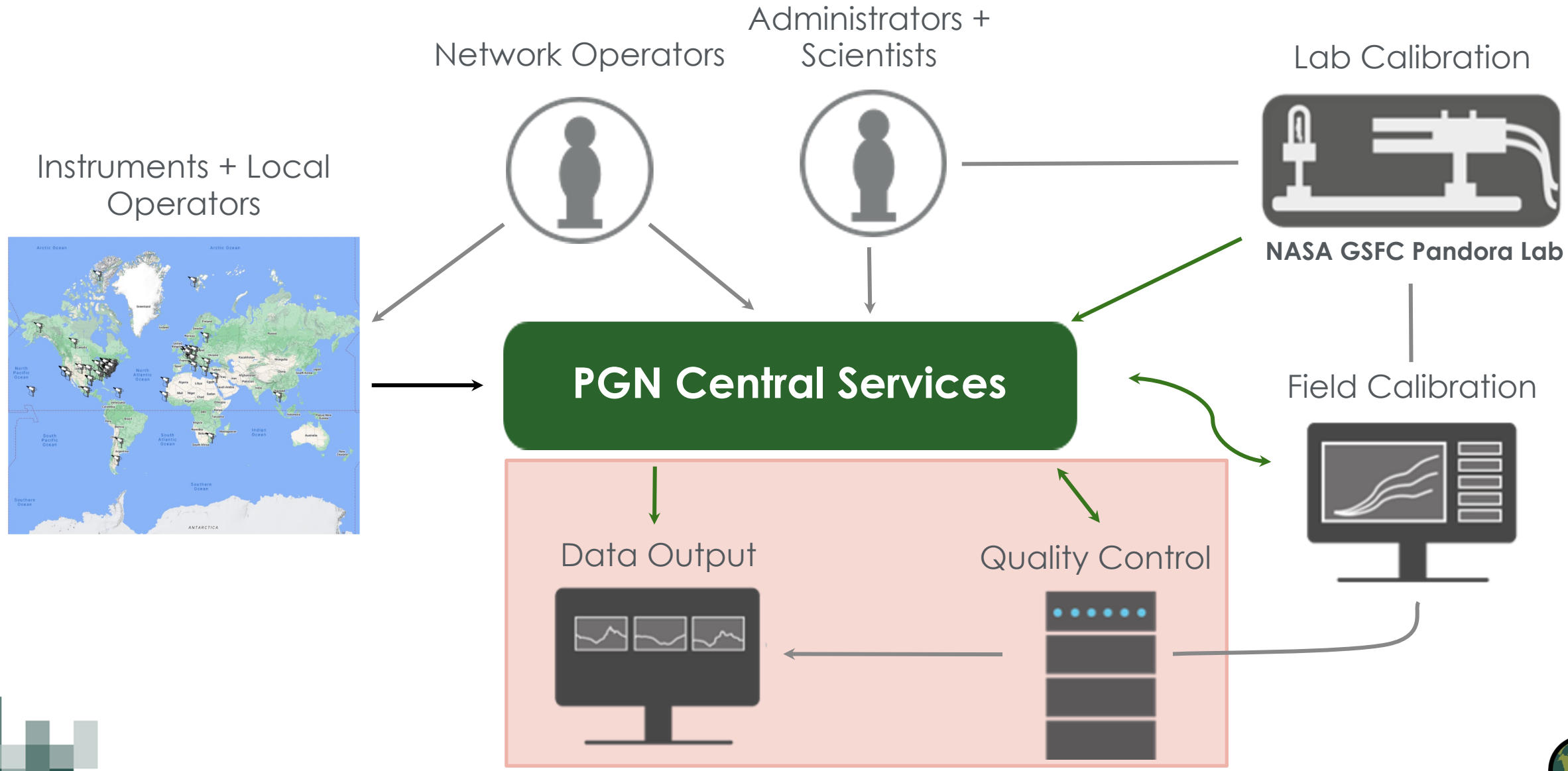
Slant Columns of Trace Gases

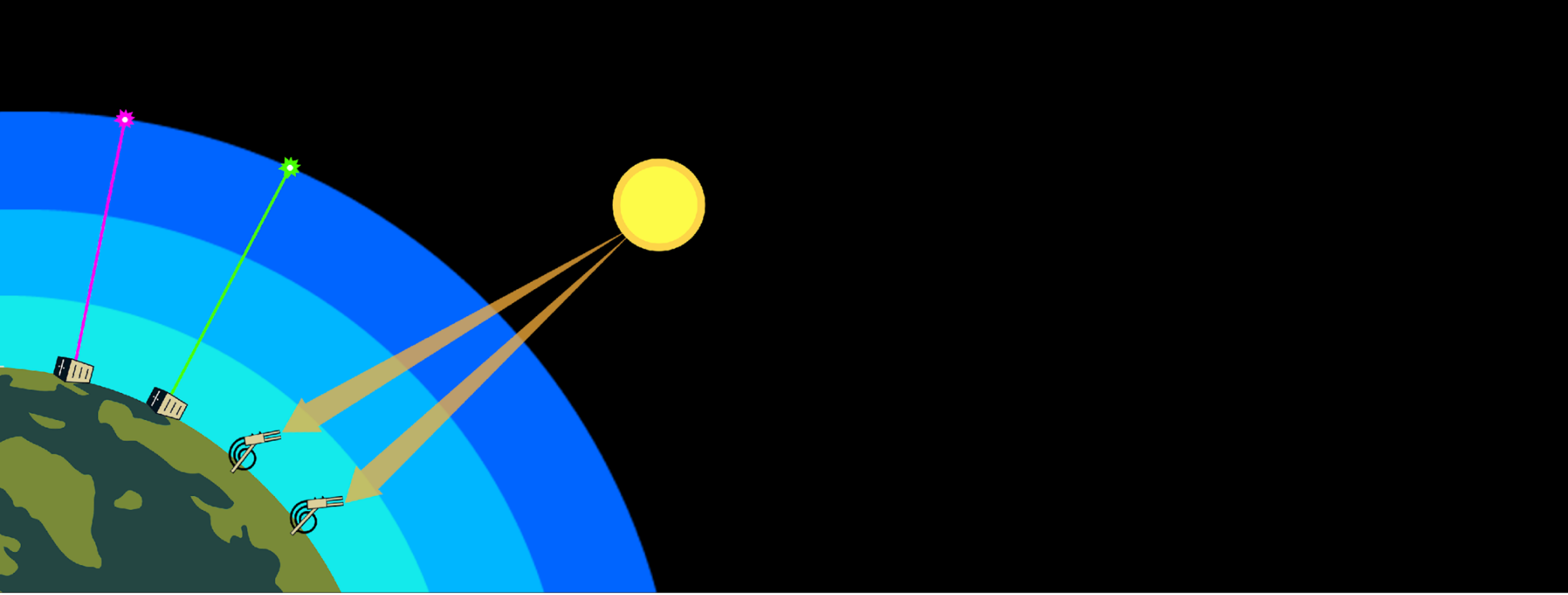
Intermediate Production of L2Fit Data



- Trace gas absorption cross-sections are inputs to spectral fitting.
- Each fitted trace gas has its associated wavelength window where its absorption signature is distinctive.

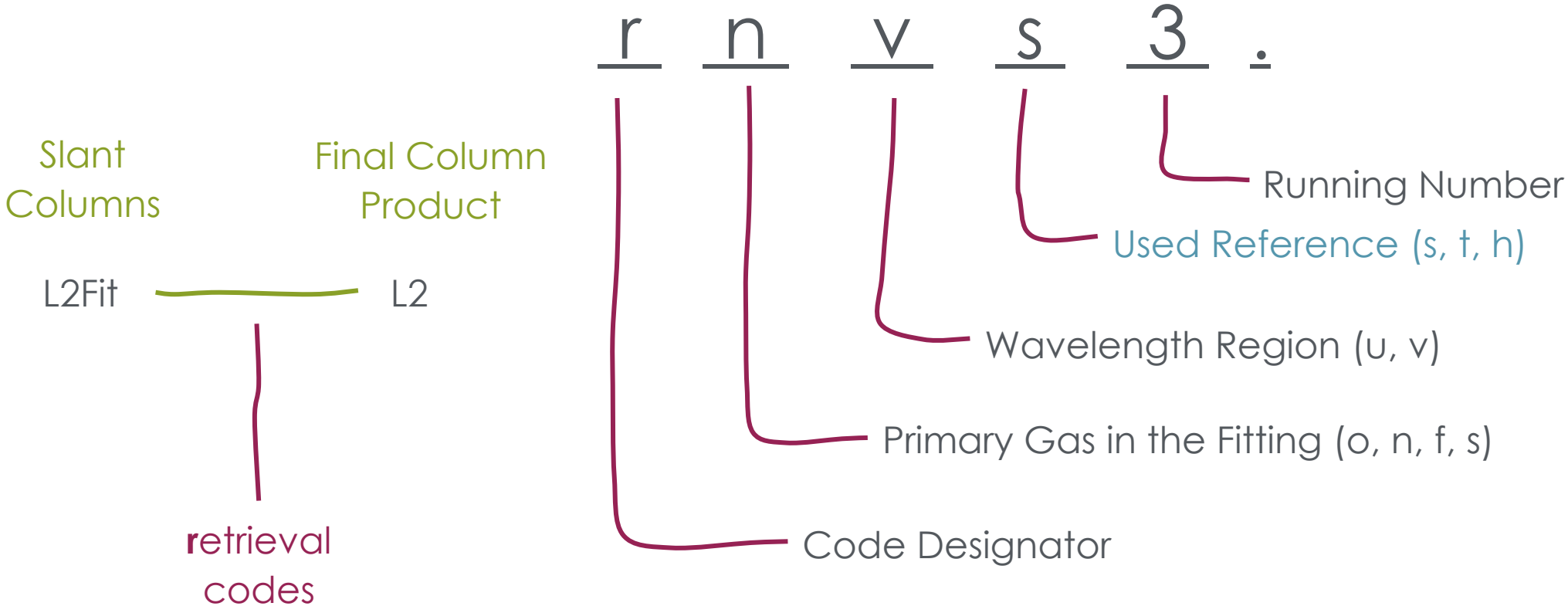
Network Structure





Data Products

Final Data for End Users: L2



What 'r-codes' Do

Direct Sun

Vertical Column

Slant Column

I_0 (Reference) is
- Synthetic for NO_2, SO_2, HCHO
- From Literature for O_3

Multi-Axis

Several Elevation Angles are Scanned
I_0 (Reference) is from Horizon Scan

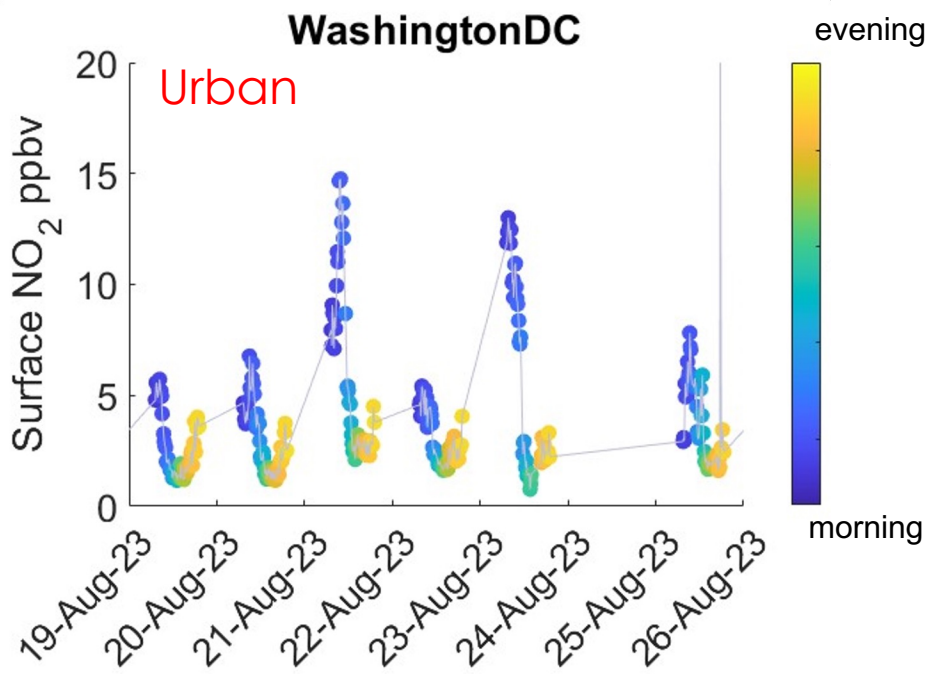
Partial Column

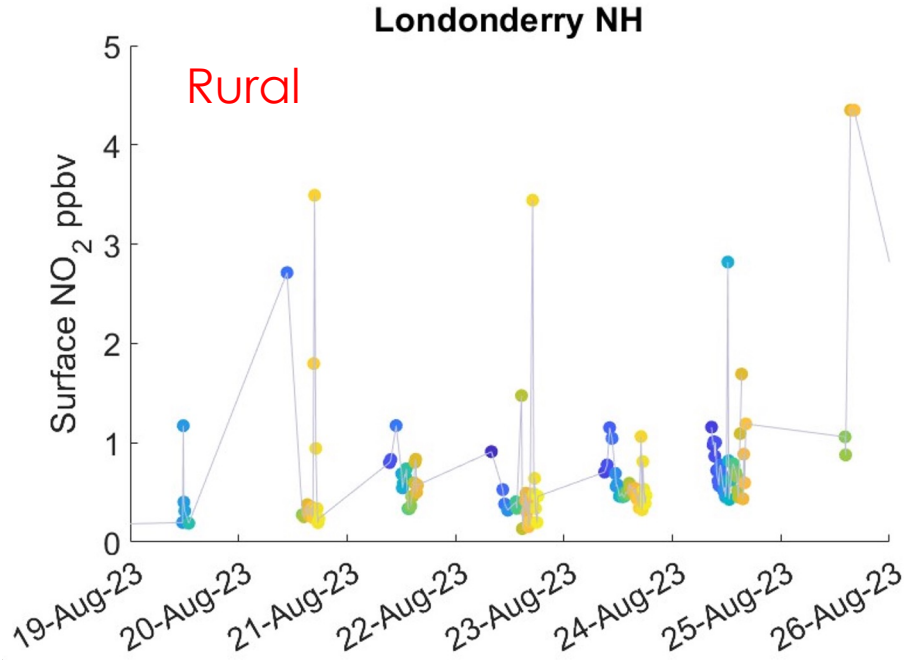
Elevation Angle

How much of the atmosphere did light pass through?

Near-Surface Concentrations

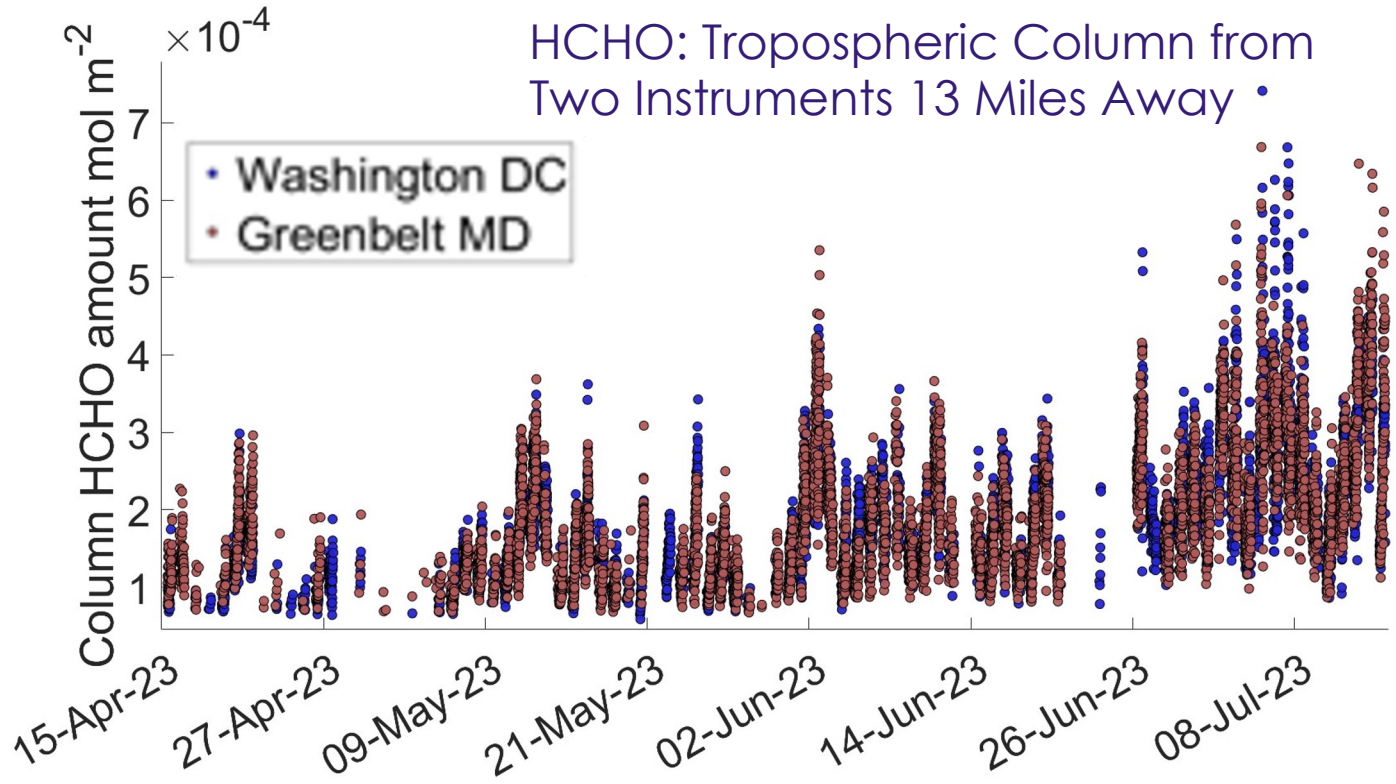
- Available for HCHO, NO_2: Out-of-the-Box Data
- Near-horizon measurements (typically 1 degree elevation from the ground) extrapolated to horizon
- Units: mol/m^3, conversion to typical concentration units (ppb/ppt) requires temperature and pressure
- Not a concentration value at any point in space: horizontally "smudged"



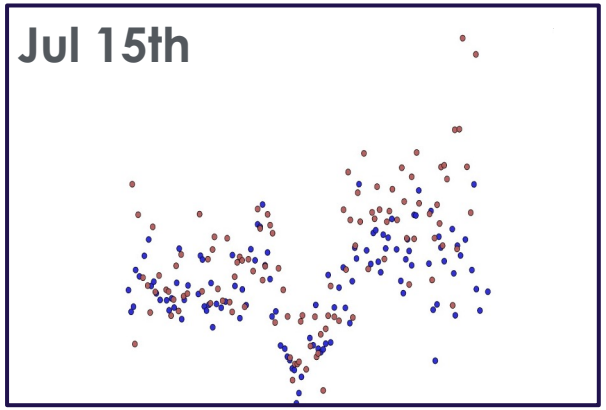


(Lower) Tropospheric Columns

- Available for HCHO, NO_2: Out-of-the-Box Data
- Estimated from 75° and 60° zenith angle observations
- "Sees" the lowermost ~ 3 km of the atmosphere

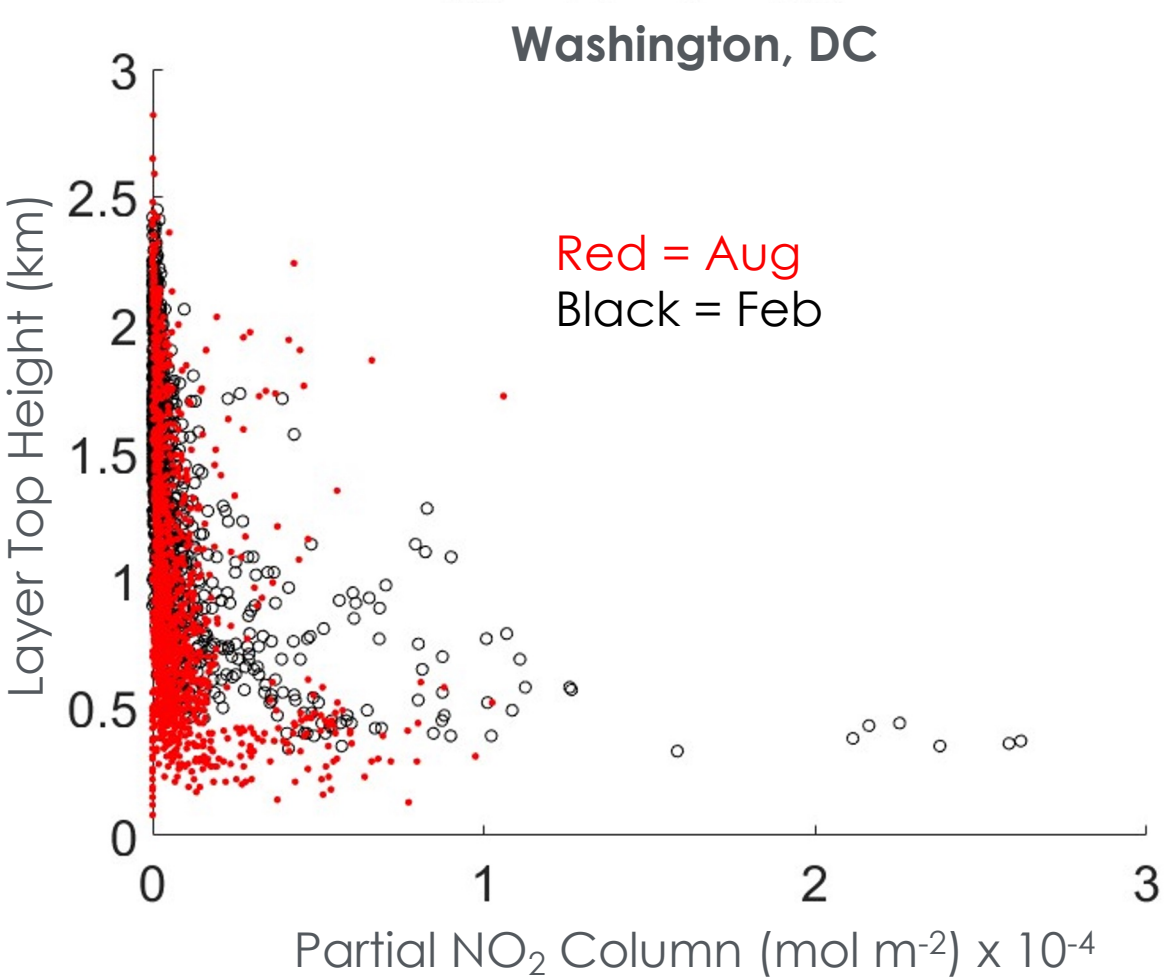


Zoomed in on a Single Day



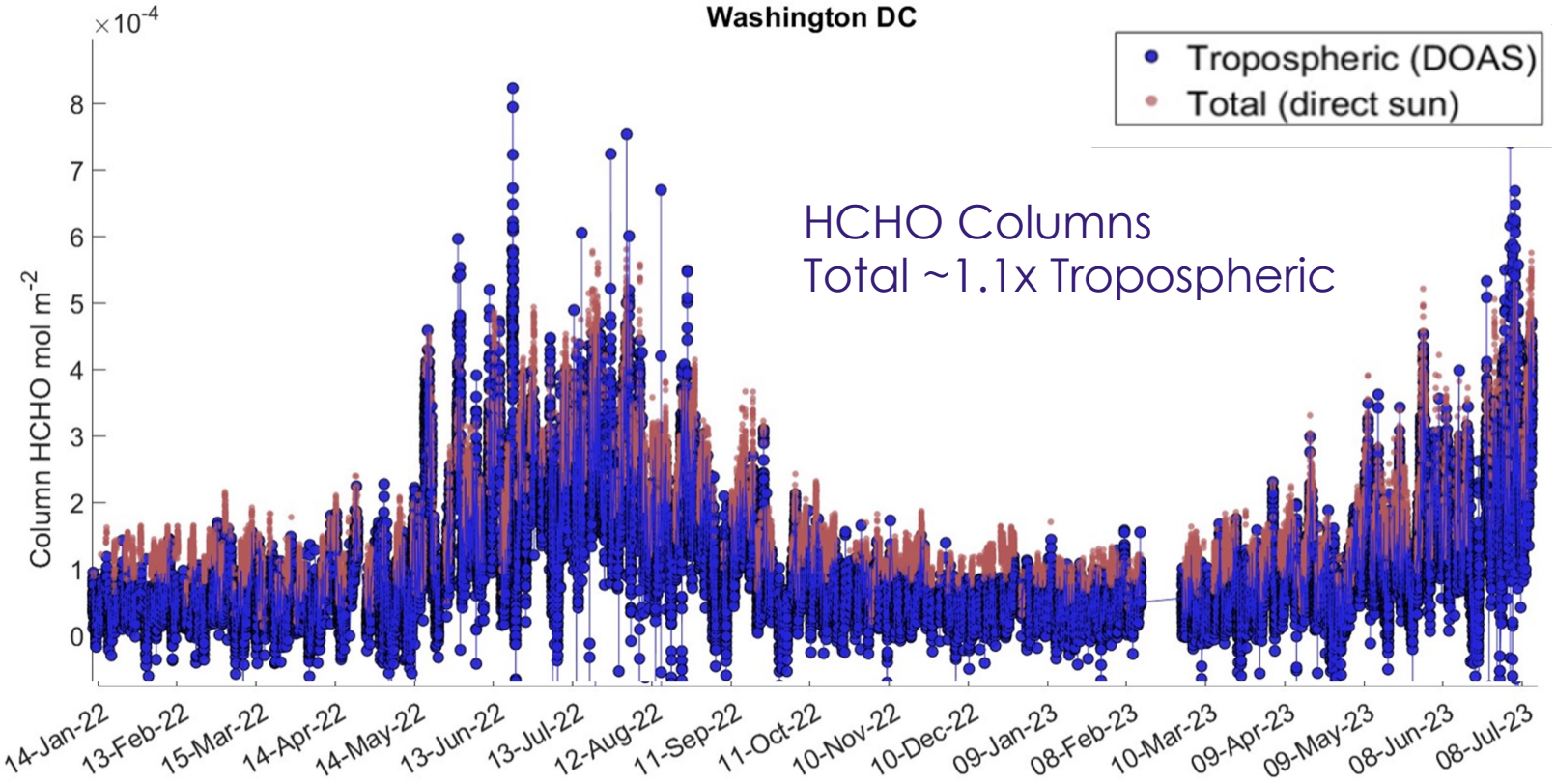
Vertical Profiles: Partial Columns

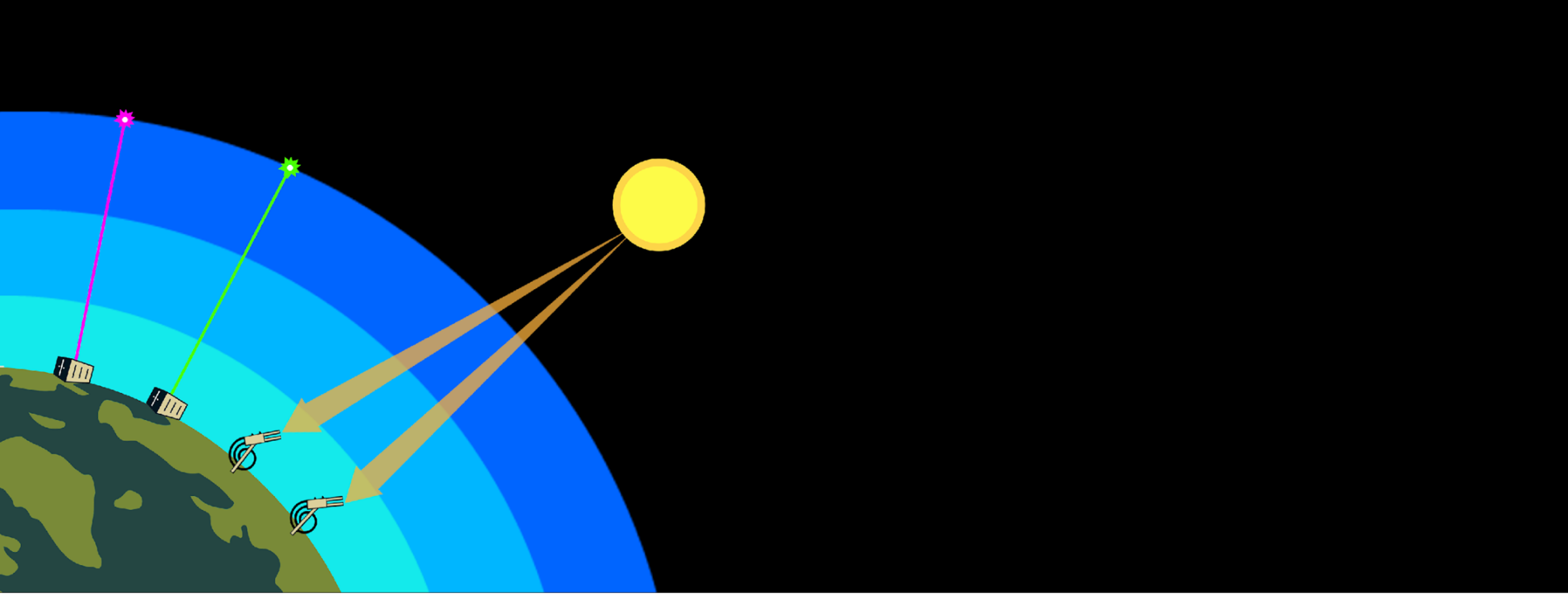
- Available for HCHO, NO_2: Out-of-the-Box Data
- Measurements made at 11-13 zenith angles
- Profile data contain top height of first layer above the surface, followed by partial column in the first
- Same for the second layer and so on…



Total Vertical Column

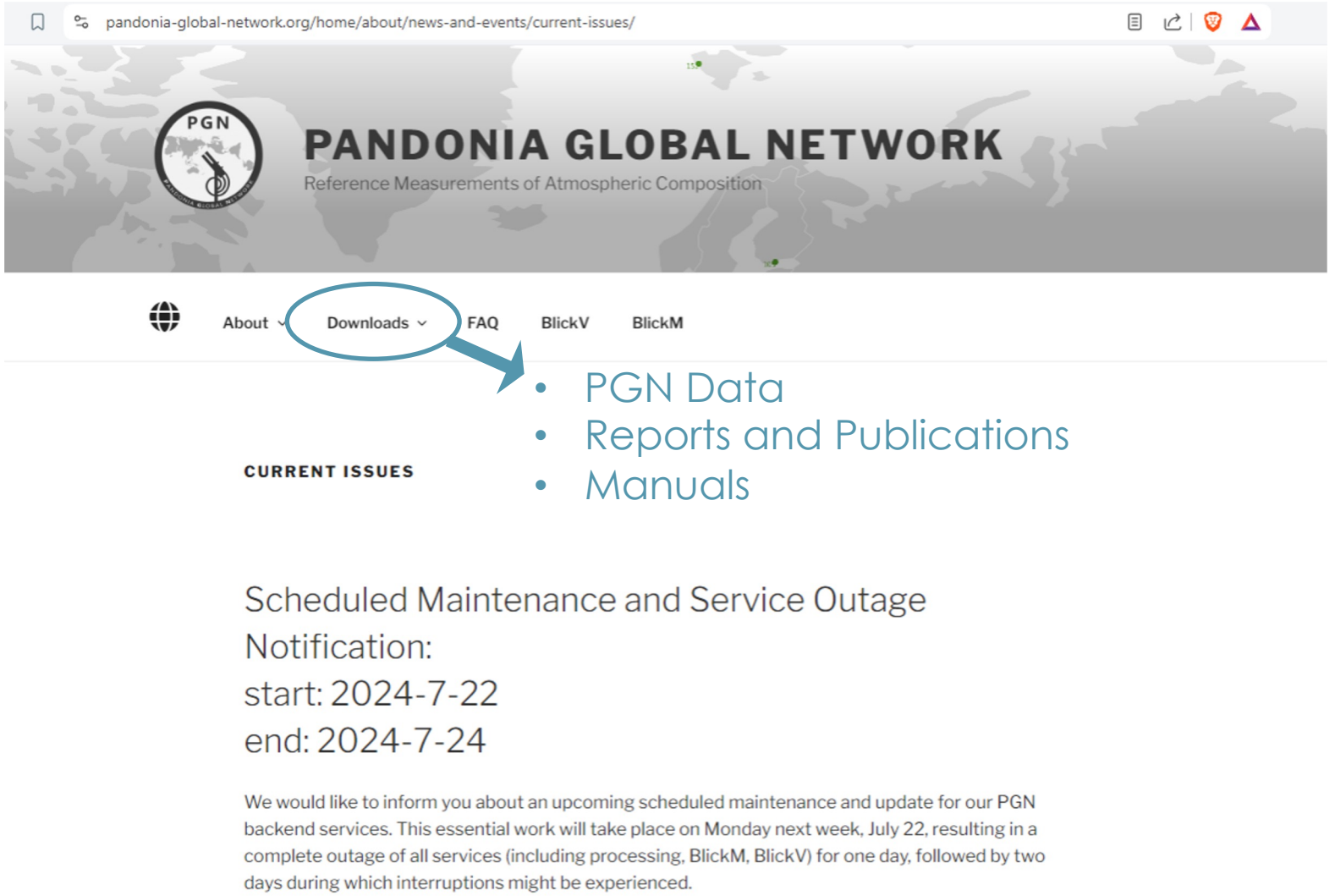
- Fitted for all gases from direct sun measurements
- This retrieval needs a synthetic reference spectrum and field calibration
- High signal-to-noise measurement but sensitive to instrument changes over time





Working with PGN Data Files

Where to Find PGN Data



- PGN Data
- Reports and Publications
- Manuals

https://www.pandonia-global-network.org/home/about/news-and-events/current-issues/

Reference for all L2 Data

2.10 nvs3

nvs3 is as nvs2, but uses updated quality flag thresholds based on *Gebetsberger et al.* [4]. It has replaced nvs2 as official PGN total column NO_2 product code on 21 May 2021.

- Pandonia Global Network Data Products Readme Document

- What do the data represent?
- Which part of the atmosphere is samples?
- How should the data be used?
- What shortcomings might the data have?

r-code	nvs3
Code creator	Alexander Cede & Martin Tiefengraber, 20 Nov 2020
DQ limits creator	Manuel Gebetsberger, 21 May 2021
Output product	NO2 TotCol [mol/m^2]
Processor requirement	1.8 and higher
Product status	official
Observation mode	Direct sun
Filters used	OPEN
Effective heights	BL+NO2s
Number of fitting windows	2
Reference	Synthetic reference spectrum
Wavelength window	400.0 nm - 470.0 nm
Order of polynomials	SMO 4, OFFS 0, WLC 0, RSC 0
Fitted gases	O3-2 (O3-clim), NO2-1 (BL-clim), O2O2-1 (O2O2-clim), H2O-1 (BL-clim), OIO-1 (BL-clim), I2-1 (BL-clim); *O3-2 (O3-clim), NO2-1 (NO2s-clim), O2O2-1 (O2O2-clim), H2O-1 (BL-clim), OIO-1 (BL-clim), I2-1 (BL-clim)*
Ring	Not fitted
Molecular scattering	Subtracted
Uncertainty	INSTR
AMF limits	7, 14
AtmVar limits	36, 42
Wavelength shift limits	0.05, 0.1
wrms limits	9.7e-4, 1.52e-3

Data Archive Contents

Pandonia Global Network Data Navigate to Location → Pandora ID → L2

Retrieval Code	Fitted Gas	Fitting Wavelengths (UV/Visible)	Measurement Type
fuh5	HCHO	UV	**Sky Scan**
fus5			**Direct Sun**
nvh3	NO_2	Visible	**Sky Scan**
nvs3			**Direct Sun**
sus1	SO_2	UV	**Direct Sun**
wvt1	H_2O	Visible	**Direct Sun**
out2	O_3	UV	**Direct Sun**

Lower Tropospheric Column, Near-Surface Concentration, Profiles

Total Column Only

Pandora Data Files Basics

- File Names: Pandora###s1_*location*_L2_*RetrievalCode*p1-8.txt

- Files are space-delimited and contain all measurements for a given instrument-location combination to-date.

https://data.pandonia-global-network.org/WashingtonDC/Pandora140s1/L2/Pandora140s1_WashingtonDC_L2_rfuh5p1-8.txt

https://data.pandonia-global-network.org/WashingtonDC/Pandora140s1/L2/Pandora140s1_WashingtonDC_L2_rfus5p1-8.txt

Pandora Data Files: Header

Instrument Name and Location, PI, DOI

```
File name: Pandora61s1_AldineTX_L2_rnvh3p1-8.txt
File generation date: 20240722T064203.3Z
Data description: Level 2 file (columns and more)
Data file version: rnvh3p1-8
Data product status: Nitrogen dioxide data are official, Water vapor data are unvalidated
Local principal investigator: Tom Hanisco
Network principal investigator: Alexander Cede
DOI: 10.48596/pgn.rnvh3p1-8.AldineTX.P61s1
Instrument type: Pandora
Instrument number: 61
Spectrometer number: 1
Processing software version used: BlickP v1.8.17
Full location name: University Of Houston Trailer
Short location name: AldineTX
Country of location: United States
Location latitude [deg]: 29.9011
Location longitude [deg]: -95.3262
Location altitude [m]: 8
Data start time: 20210527T140322.
Data end time: NONE
Data caveats: None
```

Pandora Data Files: Column Headers

Measurement Settings (Duration, Pointing Zenith and Azimuth Angles, etc.), Fitting, and Diagnostic Information for Advanced Users

```
--------------------------------------------------------------------------------
Column 1: UT date and time for measurement center, yyyymmddThhmmssZ (ISO 8601)
Column 2: Fractional days since 1-Jan-2000 UT midnight for measurement center
Column 3: Effective duration of measurement [s]
Column 4: Solar zenith angle for measurement center [deg]
Column 5: Solar azimuth for measurement center [deg], 0=north, increases clockwise
Column 6: Lunar zenith angle for measurement center [deg]
Column 7: Lunar azimuth for measurement center [deg], 0=north, increases clockwise
Column 8: Pointing zenith angle for measurement center [deg]
Column 9: Pointing azimuth for measurement center [deg], 0=north, increases clockwise
Column 10: rms of unweighted fitting residuals, -9=fitting not successful
Column 11: Normalized rms of fitting residuals weighted with independent uncertainty, -9=fitting not successful or no uncertainty given
Column 12: Expected rms of unweighted fitting residuals based on independent uncertainty, -9=fitting not successful or no uncertainty given
Column 13: Expected normalized rms of weighted fitting residuals based on independent uncertainty, -9=fitting not successful or no uncertainty given
Column 14: Climatological station pressure [mbar]
Column 15: Climatological station temperature [K]
Column 16: Climatological effective O2 height [km]
Column 17: Climatological effective O2O2 height [km]
Column 18: Climatological surface O2 concentration [mol/m3]
Column 19: Climatological surface O2O2 concentration [mol2/m6]
Column 20: Climatological total O2 column [mol/m2]
Column 21: Climatological total O2O2 column [mol2/m5]
Column 22: Data processing type index
Column 23: Calibration file version
Column 24: Calibration file validity starting date
Column 25: Mean value of measured data inside fitting window [same units as measurements]
Column 26: Wavelength effective temperature [°C], 999=no effective temperature given
Column 27: Estimated average residual stray light level [%] (only valid for stray light correction methods 2 and higher)
Column 28: Retrieved wavelength shift from L1 data [nm], -9=no wavelength change determination
Column 29: Retrieved total wavelength shift [nm], -9=no wavelength change fitting
Column 30: Retrieved resolution change [%], -999=no resolution change fitting
```

Where was the instrument looking?

Pandora Data Files: Sky Scan Data Headers

- **Surface Concentration (mol/m^3)**
- **Tropospheric Vertical Column Amount (mol/m^2)**
- **Profiles (Layer-by-Layer Partial Vertical Column Amounts, mol/m^2):**
  - Top Height of Layer 1, Partial Layer 1 Column, Layer 2, Layer 3,...

```
Column 56: Nitrogen dioxide surface concentration [mol/m3], -9e99=retrieval not successful
Column 57: Independent uncertainty of nitrogen dioxide surface concentration [mol/m3], -6=no surface concentration was retrieved since the r
missing
Column 58: Nitrogen dioxide surface concentration index, 1=Fully mixed case from extrapolation to horizon, 2=Fully mixed case from largest p
angle, -6=no surface concentration was retrieved since the maximum viewing zenith angle was below 87deg
Column 59: Nitrogen dioxide heterogeneity flag, 0=well mixed conditions, 1=heterogeneous conditions, -6=no surface concentration was retriev
Column 60: Climatological nitrogen dioxide stratospheric column amount [moles per square meter]
Column 61: Uncertainty of climatological nitrogen dioxide stratospheric column amount [moles per square meter]
Column 62: Nitrogen dioxide tropospheric vertical column amount [moles per square meter], -9e99=retrieval not successful
Column 63: Independent uncertainty of nitrogen dioxide tropospheric vertical column amount [moles per square meter], -4=tropospheric column
measurements using stratospheric climatology, -7=uncertainty could not be retrieved since slant column uncertainties were missing
Column 64: Maximum horizontal distance for nitrogen dioxide tropospheric column [km]
Column 65: Maximum vertical distance for nitrogen dioxide tropospheric column [km]
Column 66: Top height of water vapor layer 1 [km], -6=no profile was retrieved since the maximum viewing zenith angle was below 87deg
Column 67: Partial water vapor vertical column amount in layer 1 [moles per square meter], -9e99=retrieval not successful
Column 68: Top height of nitrogen dioxide layer 1 [km], -6=no profile was retrieved since the maximum viewing zenith angle was below 87deg
Column 69: Partial nitrogen dioxide vertical column amount in layer 1 [moles per square meter], -9e99=retrieval not successful
From Column 70: Optional results for higher layers in the same sequence as for layer 1 (4 columns per layer)
```

Pandora Data Files: Direct Sun Data Headers

Total Vertical Column Amount (mol/m^2)

```
Column 36: L2 data quality flag for nitrogen dioxide, 0=assured high quality, 1=assured medium quality, 2=assured low quality, 10=not-assured high quality,
quality, 22=unusable low quality
Column 37: Sum over 2^i using those i, for which the corresponding L2 data quality parameter for nitrogen dioxide exceeds the DQ1 limit, 0=L2Fit data qualit
Column 38: Sum over 2^i using those i, for which the corresponding L2 data quality parameter for nitrogen dioxide exceeds the DQ2 limit (same parameters as
Column 39: Nitrogen dioxide total vertical column amount [moles per square meter], -9e99=retrieval not successful
Column 40: Independent uncertainty of nitrogen dioxide total vertical column amount [moles per square meter], -1=cross section is zero in this wavelength ra
uncertainty input was given, -9=spectral fitting was not successful
Column 41: Structured uncertainty of nitrogen dioxide total vertical column amount [moles per square meter], -1=cross section is zero in this wavelength ran
Column 42: Common uncertainty of nitrogen dioxide total vertical column amount [moles per square meter], -1=cross section is zero in this wavelength range,
was not successful
Column 43: Total uncertainty of nitrogen dioxide total vertical column amount [moles per square meter], -1=cross section is zero in this wavelength range, -
uncertainty input was given, -6=no common uncertainty input was given, -7=not given since method "MEAS" was chosen, -8=not given, since not all components a
Column 44: rms-based uncertainty of nitrogen dioxide total vertical column amount [moles per square meter], -1=cross section is zero in this wavelength rang
not successful
Column 45: Nitrogen dioxide effective temperature [K]
```

Data Quality Flags

Digit 1

From Manual QA/QC

0 = Quality Assured
1 = Not Assured
2 = Unusable ✖

Routine QA Procedures are Performed
10-12 Flags: No QA Yet
20-22 Flags: Indicated Instrument Problems

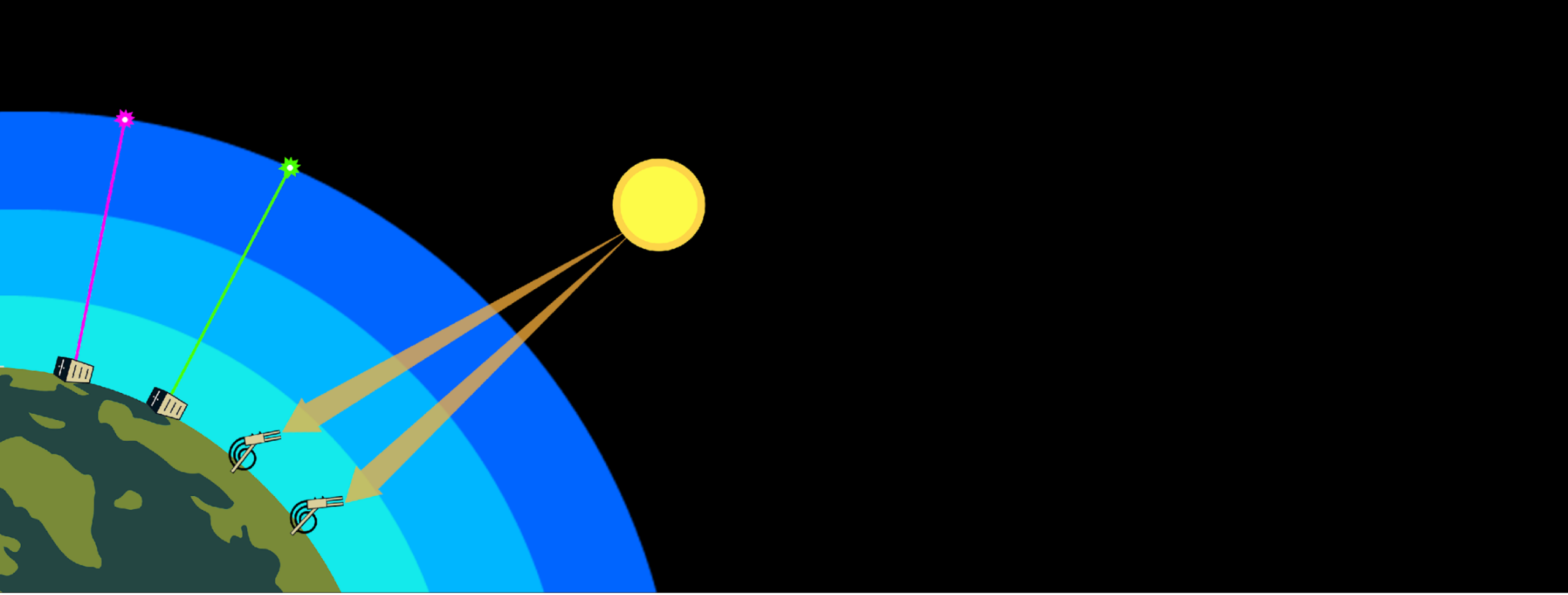
Digit 2

Automatically Generated from Fitting

0 = High Quality
1 = Medium Quality
2 = Low Quality

Based on Preset Thresholds of Root-Mean-Square Fitting Residuals and Wavelength Shift
Low Quality: Use with Caution, Investigate

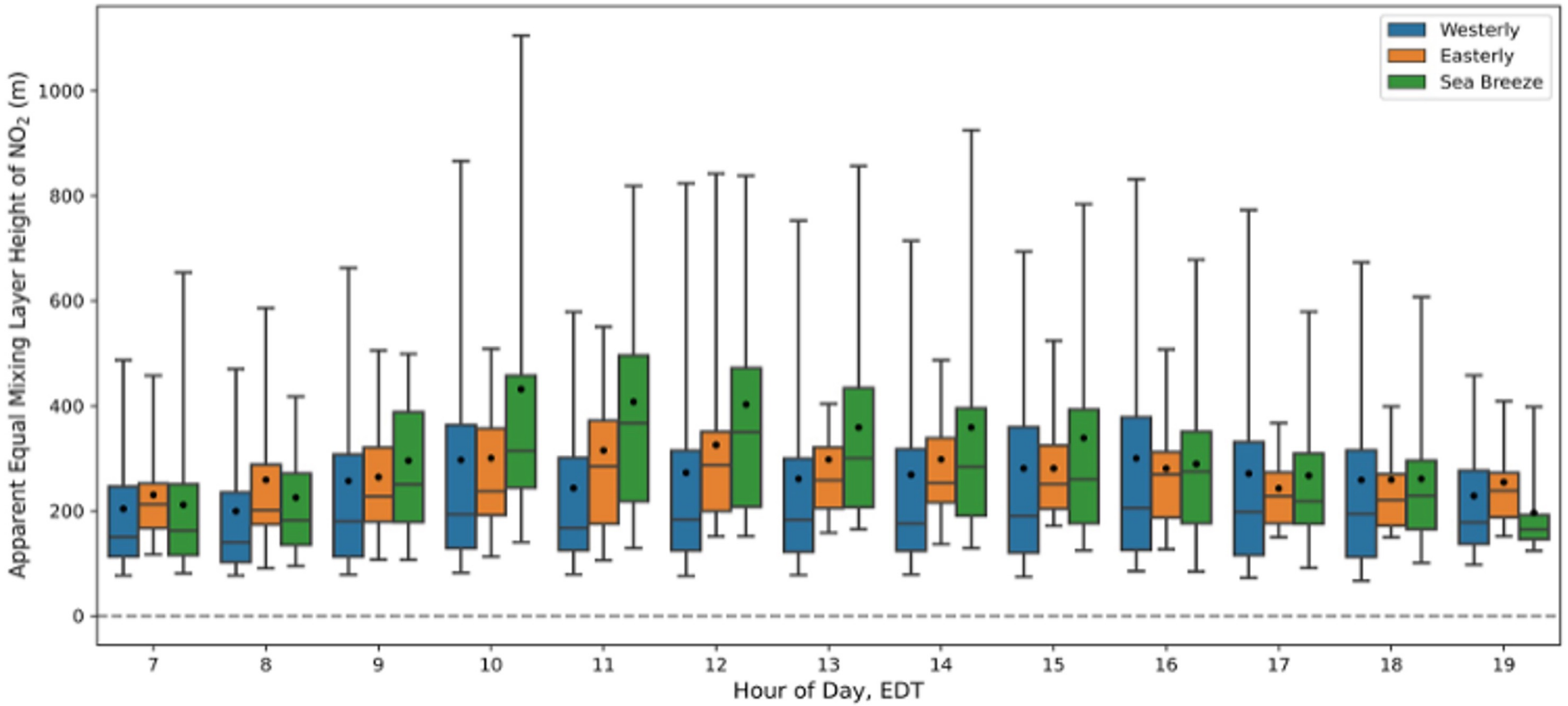
- Some "low quality" data are expected (weather, alignment).
- Persistent "low quality" or data flagged unusable = needs investigation



PGN Data Applications

Mixing Layer Heights

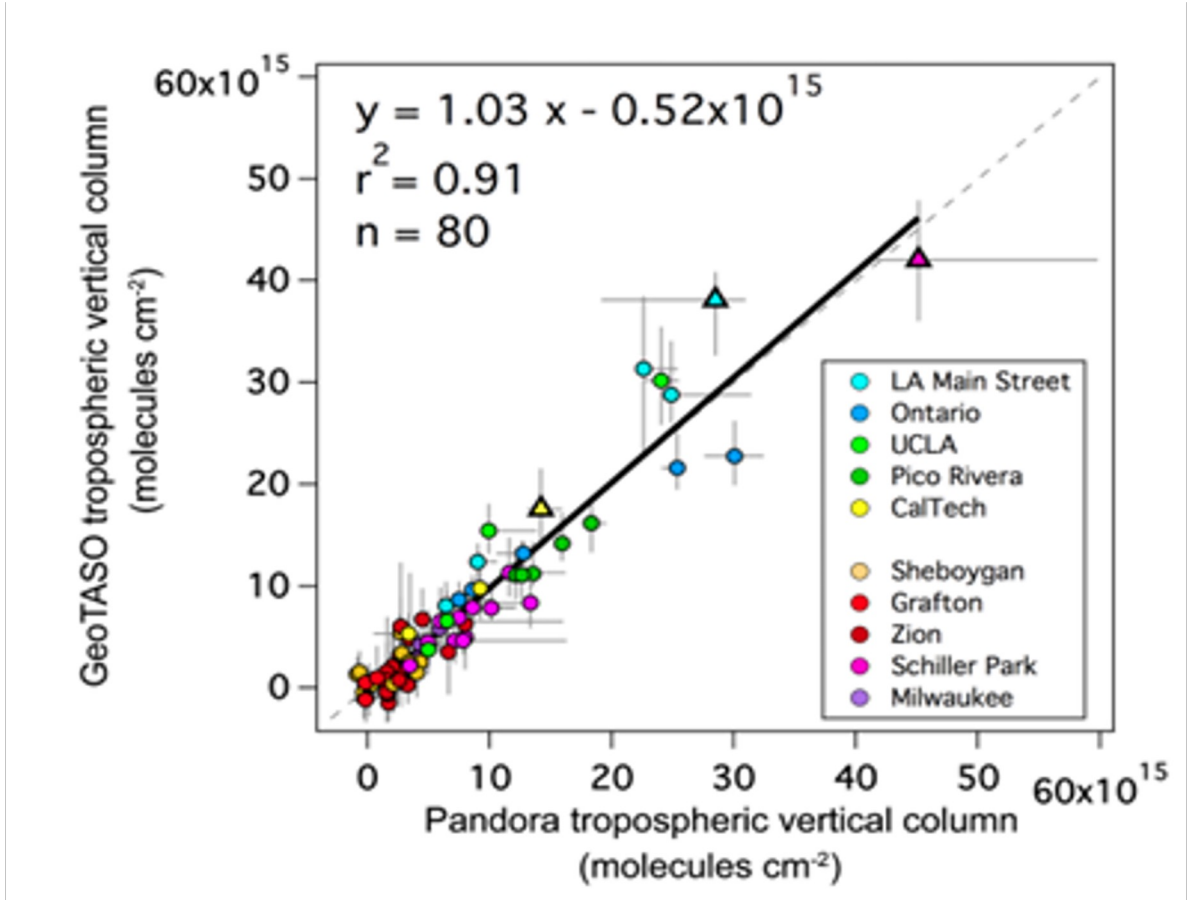
Adams et. al, 2023: Surface and column measurements of NO_2 were used to study mixing layer heights.



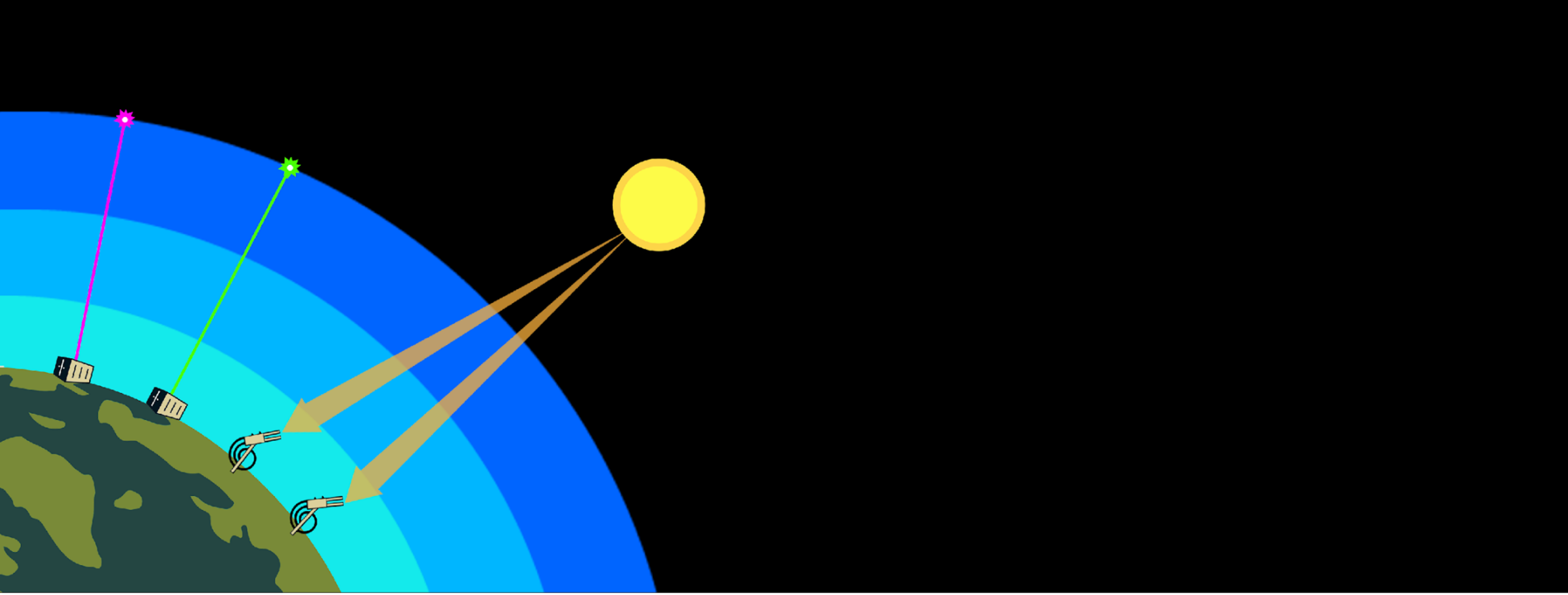
Adams et al. (2023). New insights into the role of atmospheric transport and mixing on column and surface concentrations of NO_2 at a coastal urban site. *JGR: Atmospheres*.

Satellite Instrument Validation

Judd et. al, 2019: Pandora NO_2 columns were compared with a new satellite instrument (validation).



Judd et al. (2019). Evaluating the impact of spatial resolution on tropospheric NO_2 column comparisons within urban areas using high-resolution airborne data. *AMT.*



Part 3:
Summary

Summary

Network	Type	Primary Measurands	Number of Sites	Vertical Coverage
AERONET	Passive	Aerosols (Optical, Microphysical, Radiative)	~600 Active	Total Column
Pandora (PGN)	Passive	Trace Gases (Ozone, NO_2, Formaldehyde)	168 Official	Total Column, Near-Surface, Lower Tropospheric Profiles

Looking Ahead to Part 4

- We will learn about the Tropospheric Ozone LiDAR Network (TOLNet)
- Unlike the networks we have covered so far, TOLNet uses an active remote sensing system

Homework and Certificates

- **Homework:**
  - One homework assignment
  - Opens on 22/08/2024
  - Access from the training webpage
  - Answers must be submitted via Google Forms
  - **Due by 05/09/2024**

- **Certificate of Completion:**
  - Attend all five live webinars (attendance is recorded automatically)
  - Complete the homework assignment by the deadline
  - You will receive a certificate via email approximately two months after completion of the course.

Contact Information

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Resources

- AERONET Website
  - AERONET data synergy tool
  - AERONET map explorer
- Pandora Website
  - Pandonia Global Network
  - Pandonia Network Data


APPLIED REMOTE SENSING TRAINING PROGRAM
TRAIN - EMPOWER - ADVANCE

Thank You!