National Aeronautics and Space Administration

UV-VIS-NIR Aerosol Data Assimilation

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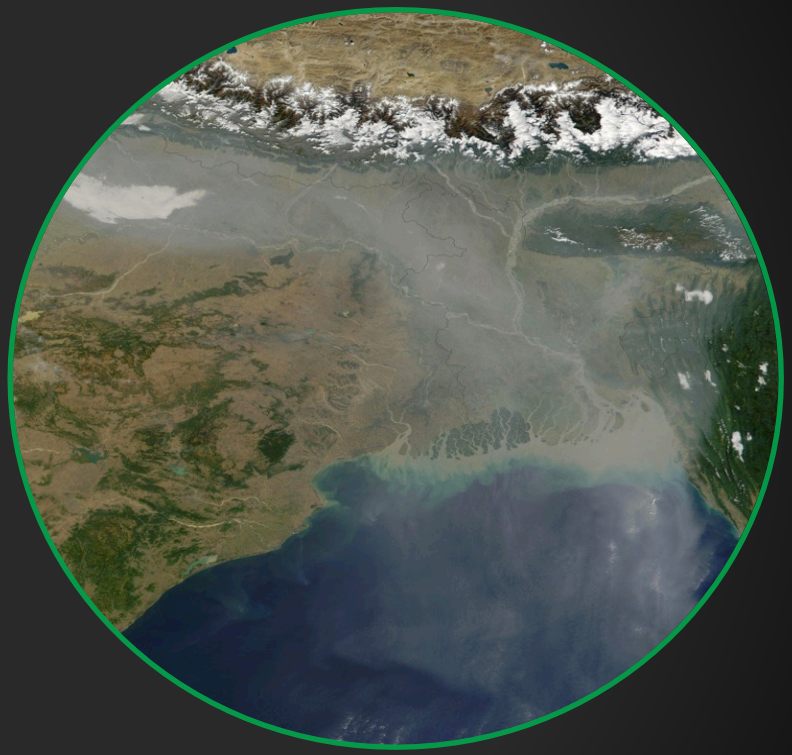
NOAA UV-VIS-NIR Workshop, 14-15 June 2022

** With contributions from Virginie Buchard, Patricia Castellanos, many others.*

Outline

- Challenges of Aerosol DA
- The Aerosol Observing System
  - Past, present, coming up
  - LEO, GEO
  - Passive, active
- Some examples
- Concluding Remarks



Challenges of Aerosol Data Assimilation

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- **State representation**
  - Multiple 3D concentrations
    - ✓ Mass
    - ✓ Number (modal schemes)
    - ✓ Bin sizes (sectional schemes)
  - Number of tracers: tens to hundreds
- **Emissions**
  - Dynamic: dust, marine, biogenic aerosols
  - Remotely sensed: biomass burning
  - Inventories: anthropogenic
  - *Emission estimation* is critical for producing an unbiased model needed for DA
- **Observation operators**
  - Proper OOs are critical
  - Intrinsic aerosol optical properties needed for assimilation of remotely sensed data
    - Mass extinction coefficient, single scattering albedo, phase matrix
  - These are often poorly known but assumed to be known due to identifiability issues:

$$\tau = \beta \bullet \mathbf{M}$$

  - Joint estimation of extensive and intensive properties will be necessary for reconciling a very diverse observing system (multi and hyper spectral, passive/active sensors)

Aerosol Observing System

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- **Aerosol Optical Depth (AOD)** is the most commonly available observable
  - Vertically integrated mass weighted by extinction coefficient, summed over multiple species: *low observability*
  - multi-spectral AOD measurements
- **Radiance assimilation**
  - Vector scattering calculations needed for UV-VIS measurements are not cheap
  - Surface BRDF characterization is a challenge
  - Multi-wavelength, multi-angle polarimeter brings much needed information content
- **Surface PM 2.5**
  - Single level
  - Often plagued by representativeness
- **Lidar measurements**
  - Provide vertical profile information
  - Spatially coverage is poor (pencil thin)
  - Attenuated backscatter entangles molecular and particulate scattering with
    - non-linear, non-local obs operator
  - New HSRL concept provides (calibrated) particulate backscatter
    - Linear & local obs operator

Aerosol Observing System in MERRA-2

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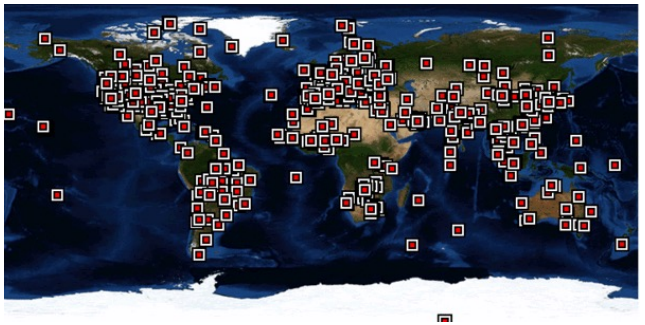
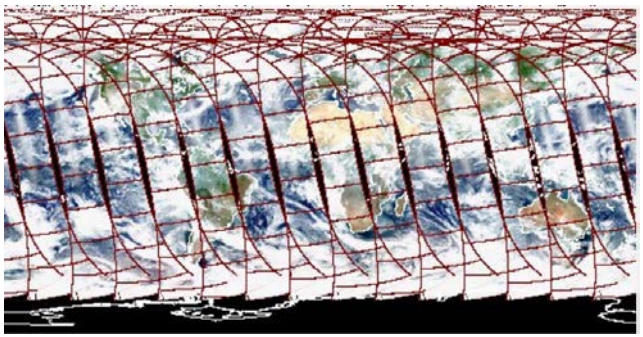
- **AVHRR for pre-EOS era**
- **MISR:** bright surfaces
- **AERONET**
  - Ground-based Sun photometers globally distributed
  - Direct measurements of multi-spectral Aerosol Optical Depth
  - AERONET measurements are considered the reference observation and are generally used to perform validation
- **MODIS Instruments on AQUA and TERRA satellites**
  - TERRA (20 years) and AQUA (18 years) may last until 2023
  - Temporal resolution: **Daily coverage of the globe**
  - Spatial Resolution: 250m, 500m, 1000m depending on bands
  - Level 2 Reflectances at ~10 km resolution:
    - ✓ Cloud-cleared Reflectances at 7 wavelengths
    - ✓ AOD at 550 nm and spectral AOD



https://aeronet.gsfc.nasa.gov/



https://modis.gsfc.nasa.gov/

Assimilation of Dark Target/Deep Blue Products in GEOS

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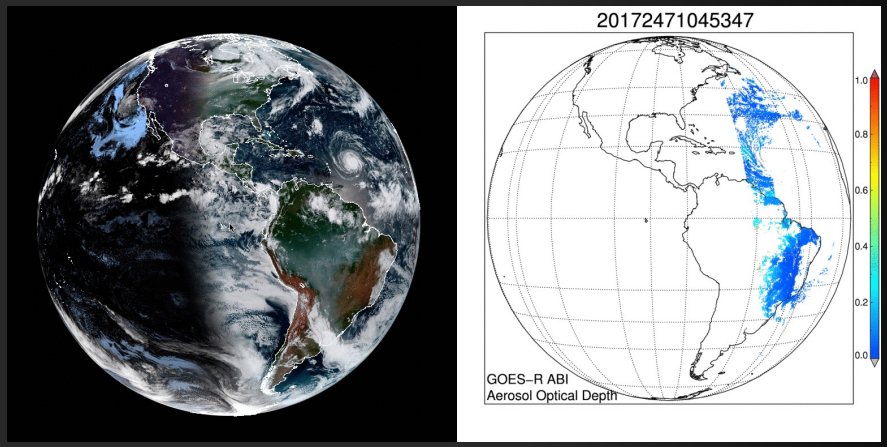
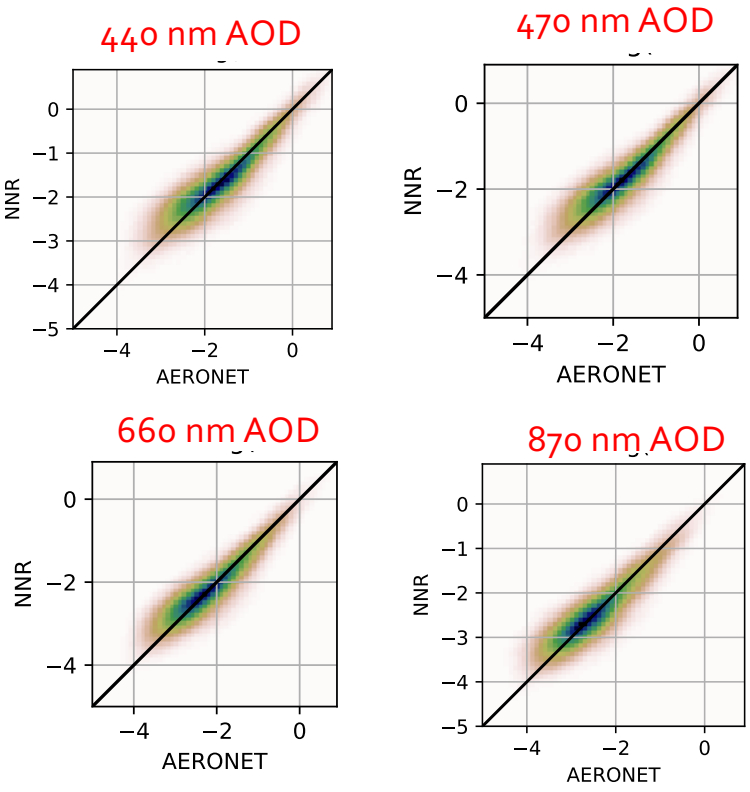
- MODIS DT/Deep Blue products are assimilated in GEOS NRT system and in the MERRA-2 reanalysis; VIIRS in progress
- DT/Deep Blue products are very convenient for assimilation in GEOS
  - Provides *cloud cleared/gas corrected* reflectances used for the retrieval (at ~10 km product resolution)
  - Product files are in NetCDF/HDF format
  - Variable names similar to MODIS
- Currently testing ABI on GOES-16/17, and AHI on Himawari-8 in 2019 during FIREX-AQ and CAMP²EX airborne campaigns
- Observations of diurnal aerosol!



Observing System Homogenization

- AERONET provides the calibration reference
- Originally developed Neural Net for bias correction of physical retrievals
- Currently, multi-channel Neural Net Retrieval (NNR) trained on AERONET
- Multi-channel AOD derived from multi-channel *Level 2 Reflectances*, no dependency on *aerosol model*



Estimating Obs Uncertainties with Evidential Deep Learning

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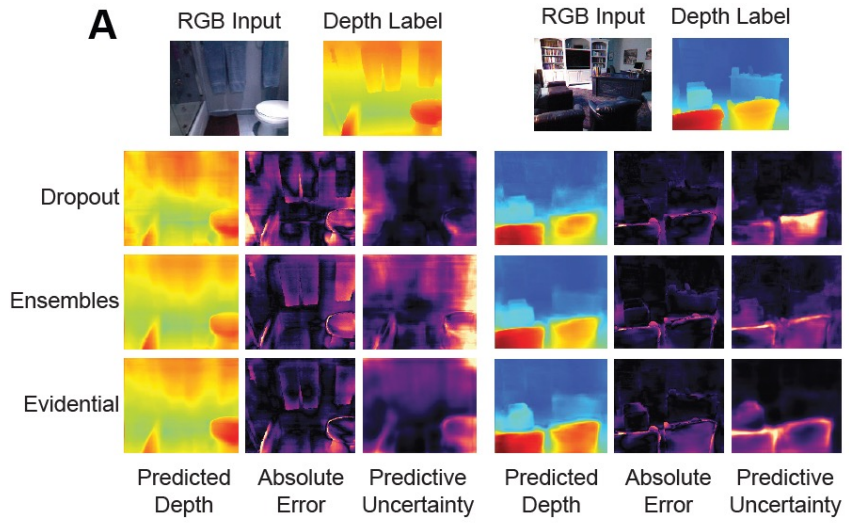
- Evidential regression simultaneously learns a target along with *epistemic* and *aleatoric* uncertainty
- Statistically robust and interpretable
- Provides much needed state-dependent observation errors for DA
- *Epistemic error* estimates are able to flag out-of-domain data
- Currently conducting OSSEs with UV-VIS-NIR polarimeter

Deep Evidential Regression

Alexander Amini[1], Wilko Schwarting[1], Ava Soleimany[2], Daniela Rus[1]
[1] Computer Science and Artificial Intelligence Lab (CSAIL), Massachusetts Institute of Technology (MIT)
[2] Harvard Graduate Program in Biophysics



Aerosol Data Available: LEO satellites

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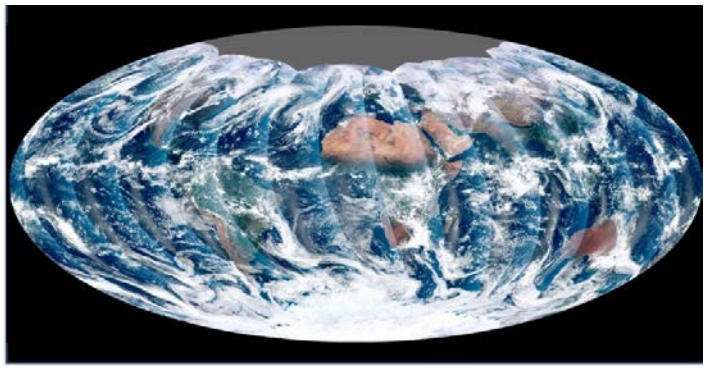
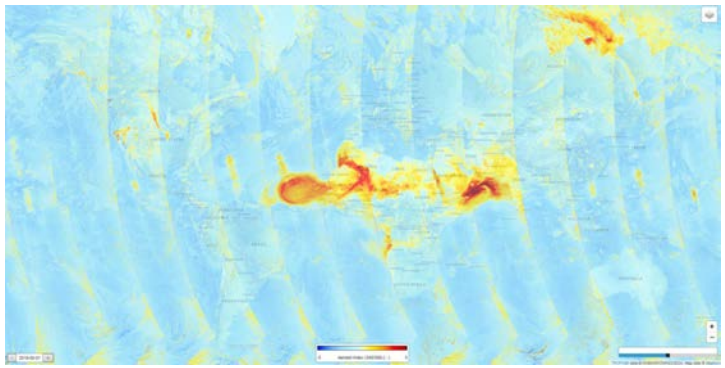
- **VIIRS onboard Suomi-NPP and N20 satellites:** replacement for Aqua MODIS
  - Available since 2011
  - Temporal resolution: **Daily coverage of the globe**
  - Spatial Resolution: ~750m for aerosol retrieval
  - Same retrievals algorithm as MODIS
  - NASA product "Level 2: cloud-cleared reflectance
- **OMP Limb** (Stratospheric Aerosols)
- **TROPOMI onboard SENTINEL-5P**
  - Launched in 2017
  - Temporal resolution: **Daily coverage of the globe**
  - Spatial Resolution: ~7km
  - Spatial resolution is a challenge, peaky about cloud clearing
  - Reflectance measurements over the UV-SWIR spectral range



https://ncc.nesdis.noaa.gov/VIIRS/



http://www.tropomi.eu/

Assimilation of UV AI at NRL

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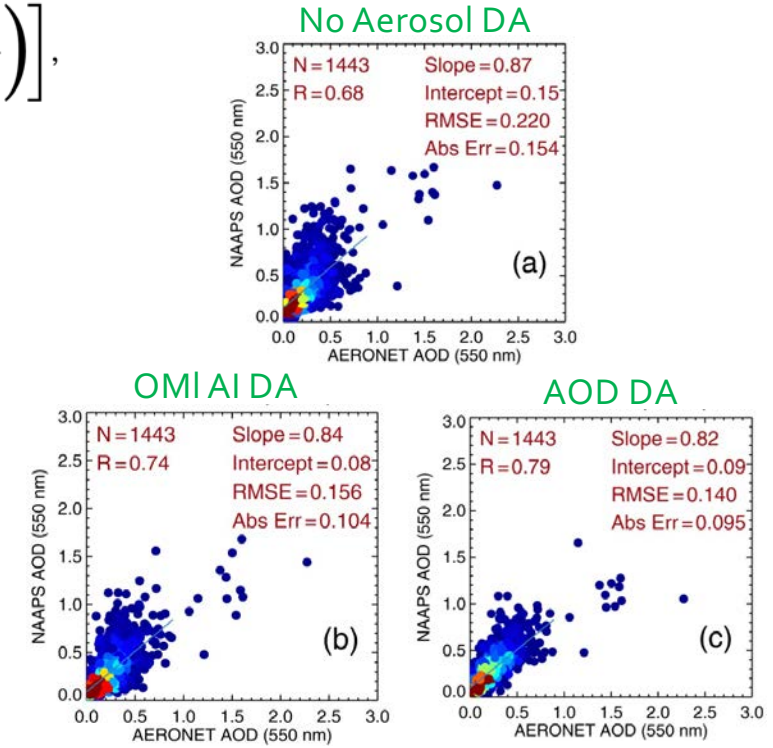
Development of an Ozone Monitoring Instrument (OMI) aerosol index (AI) data assimilation scheme for aerosol modeling over bright surfaces – a step toward direct radiance assimilation in the UV spectrum

Jianglong Zhang[1], Robert J. D. Spurr[2], Jeffrey S. Reid[3], Peng Xian[3], Peter R. Colarco[4], James R. Campbell[3], Edward J. Hyer[3], and Nancy L. Baker[3]

- The UV Aerosol Index $\mathrm{AI} = -100\left[\log_{10}\left(\frac{I_{354}^{\mathrm{Model}}}{I_{354}^{\mathrm{calc(Ray)}}(R_{388*}^{\mathrm{Model}})}\right)\right]$,
- Sensitive to differential aerosol absorption at 2 UV wavelengths
- Using the linearized VLIDORT Zhang *et al.* have developed this highly non-linear observation operator at NRL's NAAPS DA system.
- While the OMI UV AI improves the NAAPS assimilation when compared to no DA, it does not do as well as their control AOD assimilation.



Future Aerosol Data of Interest

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- **The GEO Ring and the Atmospheric Composition Virtual Constellation (AC-VC)**
- **Ocean Color Instrument and Multi-angle Polarimeters on PACE**
  - Launch planned in Fall 2023
  - A spectrometer and a pair of multi-wavelength, multi-angle polarimeters that will measure aerosol characterization from UV to SWIR -> UV channels allows retrieval of aerosol absorption
  - Global coverage every two days
  - Spatial resolution: 1 km
- **3MI on METOP-SG**
  - Launch planned in 2023
  - Multi-viewing Multi-channel Multi-polarisation Imager
  - Spatial resolution: 4km at nadir
- **EarthCARE**
  - Launch planned 2023
  - HSRL Lidar and a Multi-Spectral Imager (MSI)
    → Vertical profiles of UV aerosol extinction
- **AOS**
  - Date planned: 2028
  - Polarimeter and a lidar

Earthcare

ATMOSPHERE

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https://aos.gsfc.nasa.gov

EARTH SYSTEM OBSERVATORY

The AOS Constellation

- Science objectives addressed by the *constellation*
- Polar orbit essential for meeting almost all objectives
- Inclined orbit targets important processes tied to sub-daily variability
- Suborbital component addresses science not achievable from space
- AOS explores how interconnections between aerosols, clouds and precipitation impact public health, weather and climate

KDP-A planned for September 2022
Launches NET: 2028 (AOS-I), 2030 (AOS-P)

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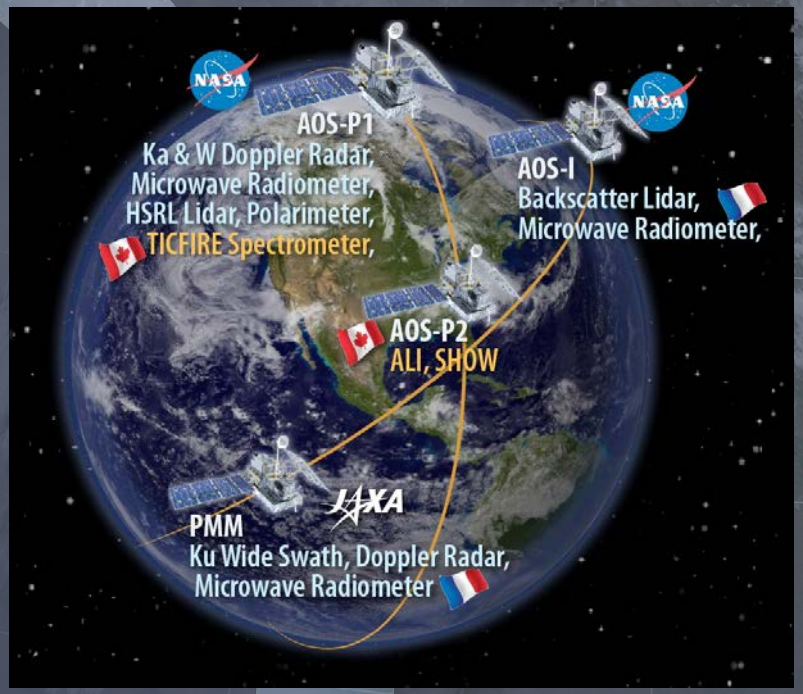
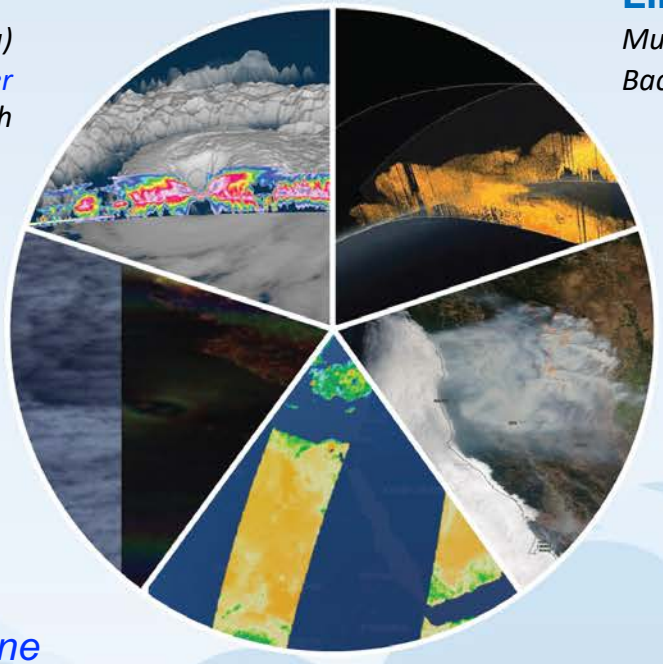


KDP-A planned for September 2022
Launches NET: 2028 (AOS-I), 2030 (AOS-P)

Key AOS INSTRUMENTS

RADAR
Multi-wavelength (W, Ku)
Doppler
Ku radar may have swath

LIDAR
Multi-wavelength (532 and 1064 nm)
Backscatter and HSRL (532 nm)



POLARIMETER
Multi-wavelength (UV-VNIR-SWIR)
Multi-angle, 500m or 1 km footprint
Swath: 600 km or 1,100 km

SPECTROMETER
Multi-wavelength (UV-VIS-NIR-SWIR-LWIR-FIR)
reflectances and brightness temperatures

AOS requires a suite of spaceborne instruments to measure and characterize the complexity of hydrometeors and aerosols.*

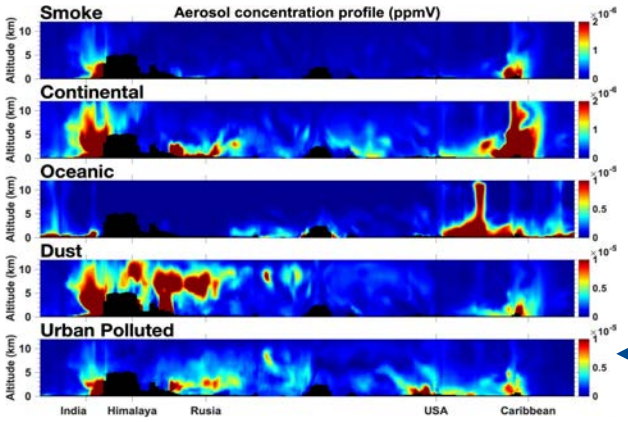
RADIOMETER
Multi-wavelength Microwave (~100-900 GHz)

**To also include as, or more capable, airborne in-situ and remote sensing instruments, deployed in synergistic/complementary suborbital campaigns.*

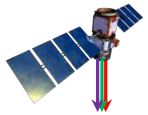
Slide Credit: Juan Cuesta

Impact of Lidar UV-VIS-NIR for improved retrievals of intensive properties and aiding aerosol speciation.

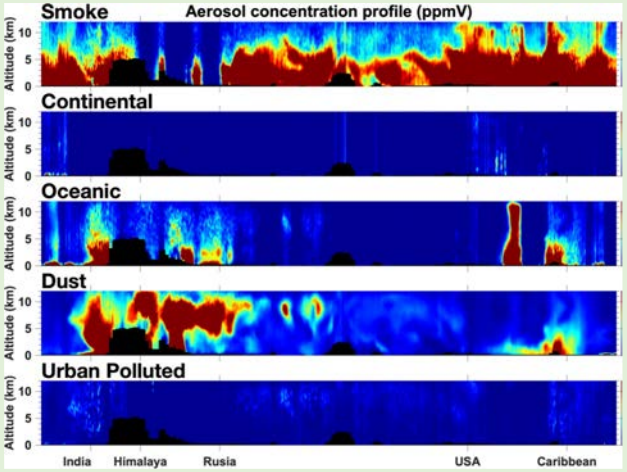
Retrieval Simulations



Prescribed "Truth":
Transects of profiles of 5 aerosol types, with noise and variability of aerosol properties

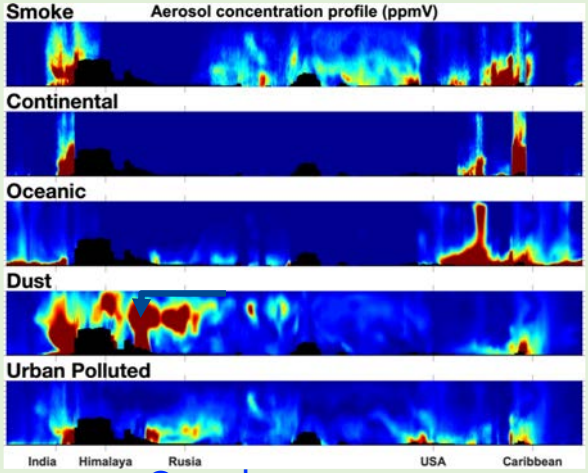


Backscatter Lidar (VIS-NIR)



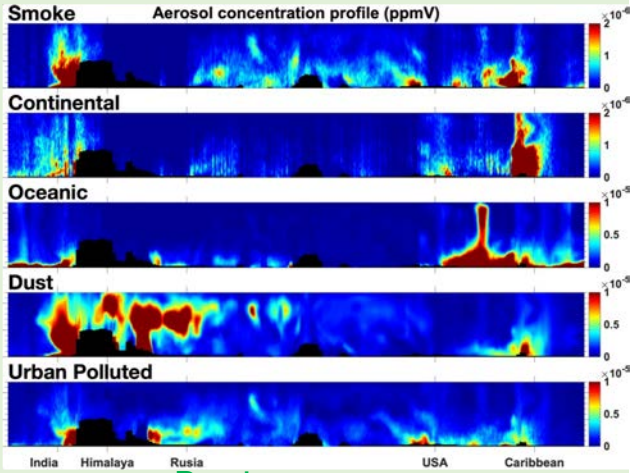
Unable to speciate, except for dust

HSRL Lidar (VIS-NIR)



Good performance

HSRL Lidar (UV-VIS-NIR)



Best performance

Concluding Remarks

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- Compared to trace gases, Aerosol Data Assimilation present some additional challenges:
  - Diversity in the way the aerosol state is represented
  - Observation operators depend on particle intrinsic properties as well as size and shape
  - While aerosol optical properties are typically prescribed, there remains a need for joint parameter-state estimation (identifiability issues)
- Progress will likely require
  - Aerosol models with microphysics for better representation of the mixing state
  - Multi-angle, multi-wavelength *UV-VIS-NIR passive measurements*, even better with polarization
  - Multi-wavelength vertical profiles of aerosol properties from lidars.

Extra Slides

EarthCARE Satellite

Orbit:

- 393 km mean altitude
- Sun Synchronous frozen orbit
- 97° Inclination
- 14h00 DSN MLST
- 25-days repeat cycle

Lifetime:

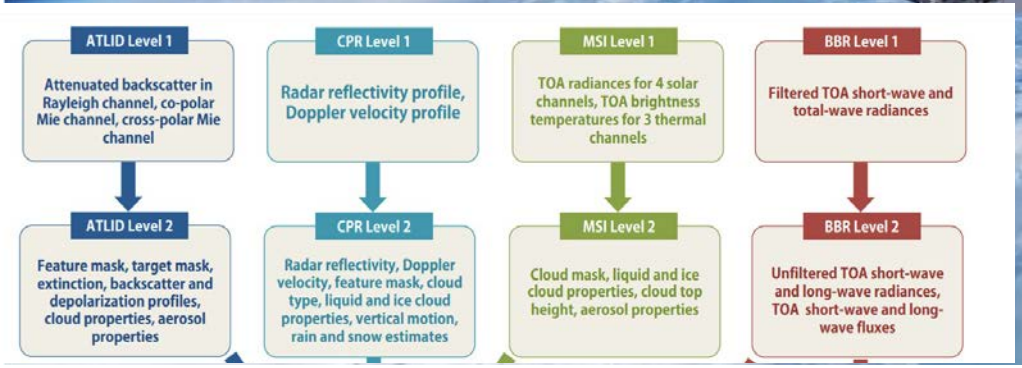
- 3 years + 1
  (incl. 6-months commissioning)

Launch: 2023

Satellite:

- 2350 kg (incl. 313 kg propellant)
- 3-axis stabilized / yaw-steering
- 1700W
- On-board data rates average:
  <15 kbps (HKTM)
  <2.5 Mbps (science)

Payload:
2 active instruments (ATLID & CPR)
2 passive instruments (BBR & MSI)

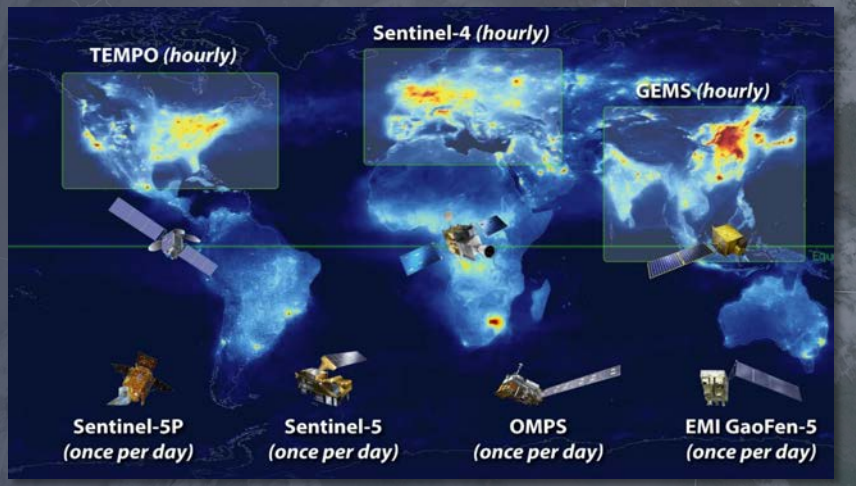


ATMOSPHERE

The Atmospheric Composition Virtual Constellation (AC-VC)

EARTH SYSTEM OBSERVATORY

- Geostationary Air Quality (Geo-AQ) constellation consists of geostationary satellite sensors with a strong focus on air quality.
  - ➢ hourly observations of key air pollutants over Asia, Europe, and North America.
- GEO-AQ missions:
  - GEMS (launched in 2020)
  - TEMPO (to launched in 2022)
  - Sentinel-4 (to launched 2023)
- Complemented by LEO-AQ missions providing daily global atmospheric composition observations.



The Geo-AQ constellation is relevant for

- Providing measurements of aerosol precursor gases
- Providing UV and O2-band channels for further constraining geostationary aerosol retrievals from the operational Geo Ring.

NNR

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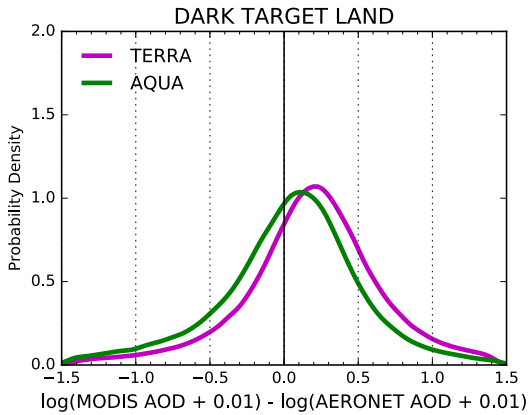
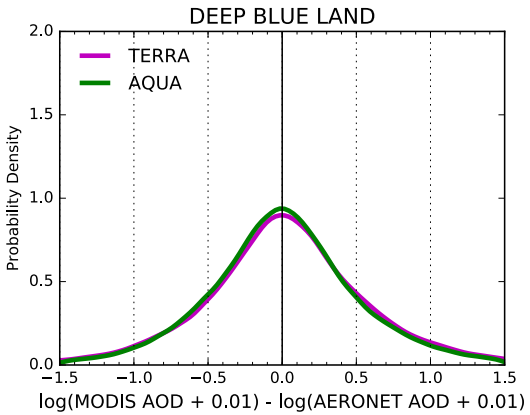
LAND - Dark Surface

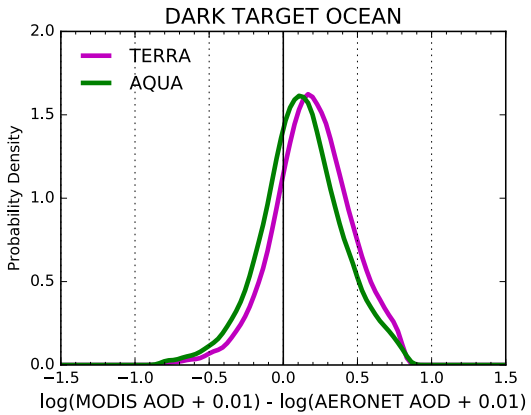
LAND - Bright Surface

OCEAN

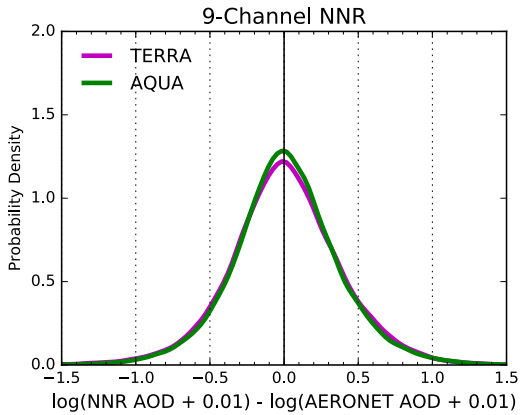
MODIS Standard Retrievals →

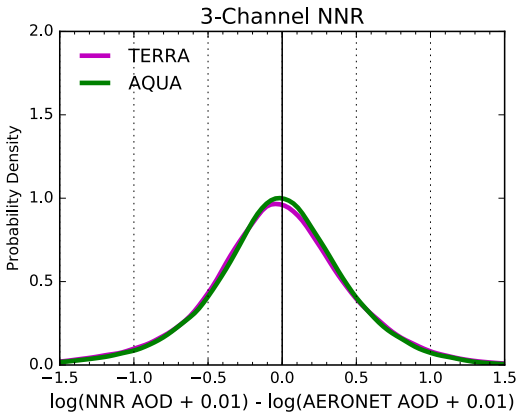


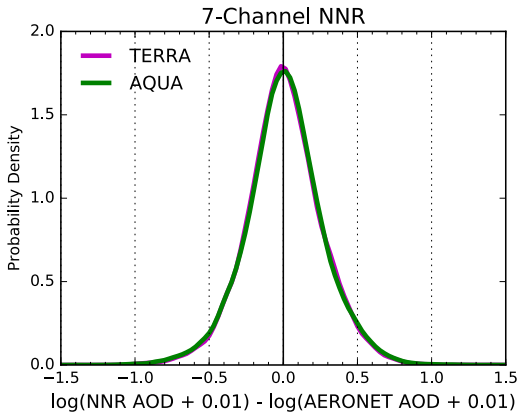




Neural Network Retrievals →







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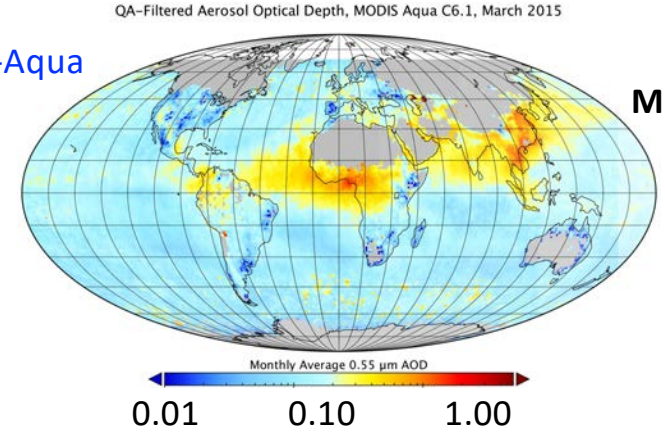
The Dark Target/Deep Blue Algorithms

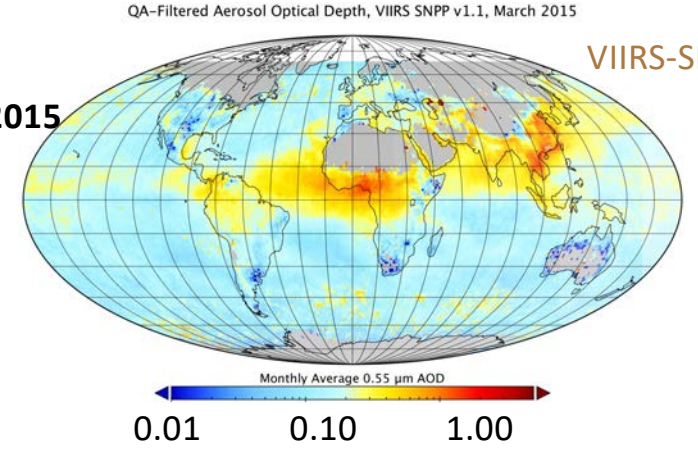
MODIS-heritage Algorithms

MODIS + VIIRS --> Long term climate

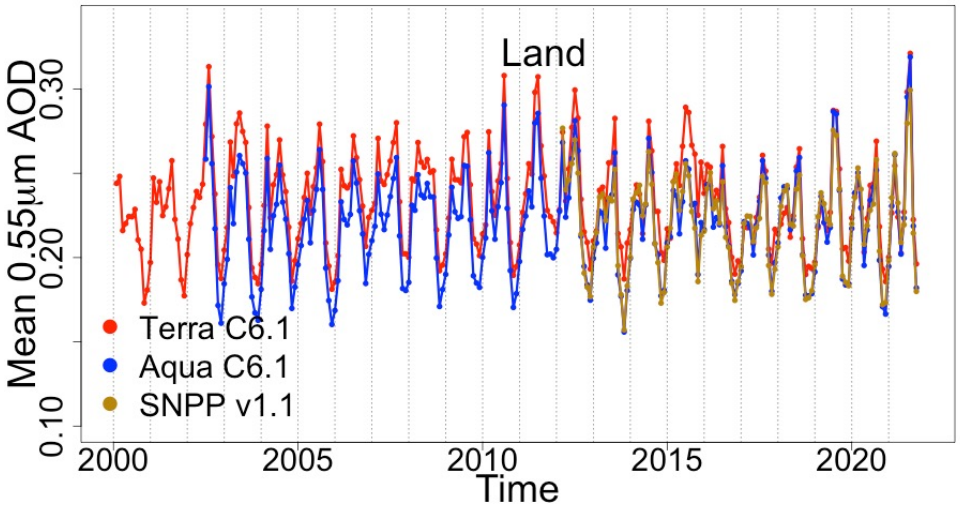
MODIS-Aqua



March 2015



VIIRS-SNPP



VIIRS-SNPP

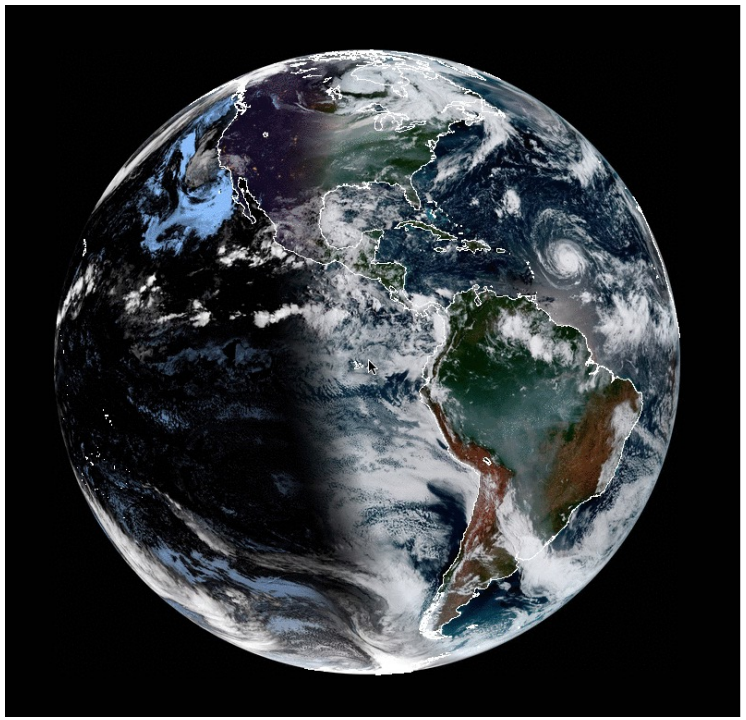
MODIS-Aqua

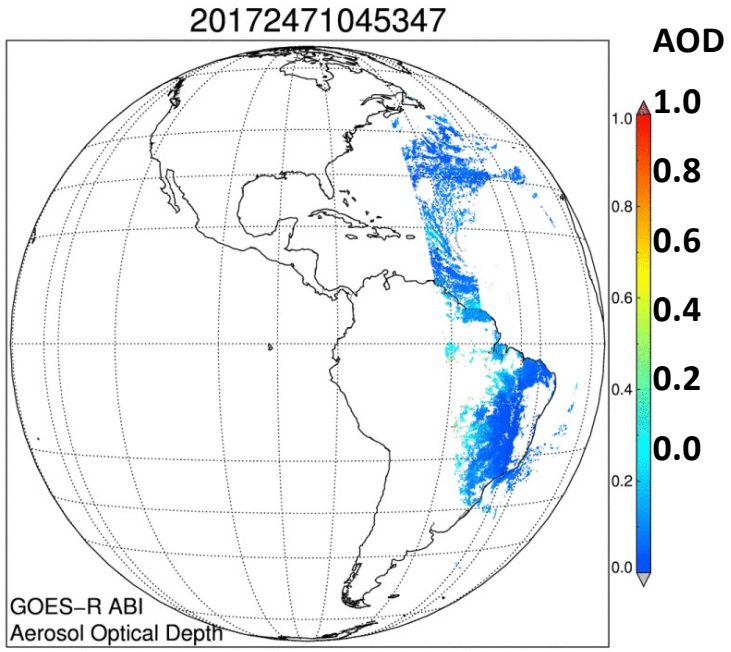
"funded" to continue on VIIRS-JPSS-1/NOAA20 (≥2021)

Slide credit: Rob Levy

Expanding to retrieve from GEO-Imager data!

RGB and AOD from ABI for Sep 4, 2017 (animation)
Canada/Washington fires and smoke mega-event



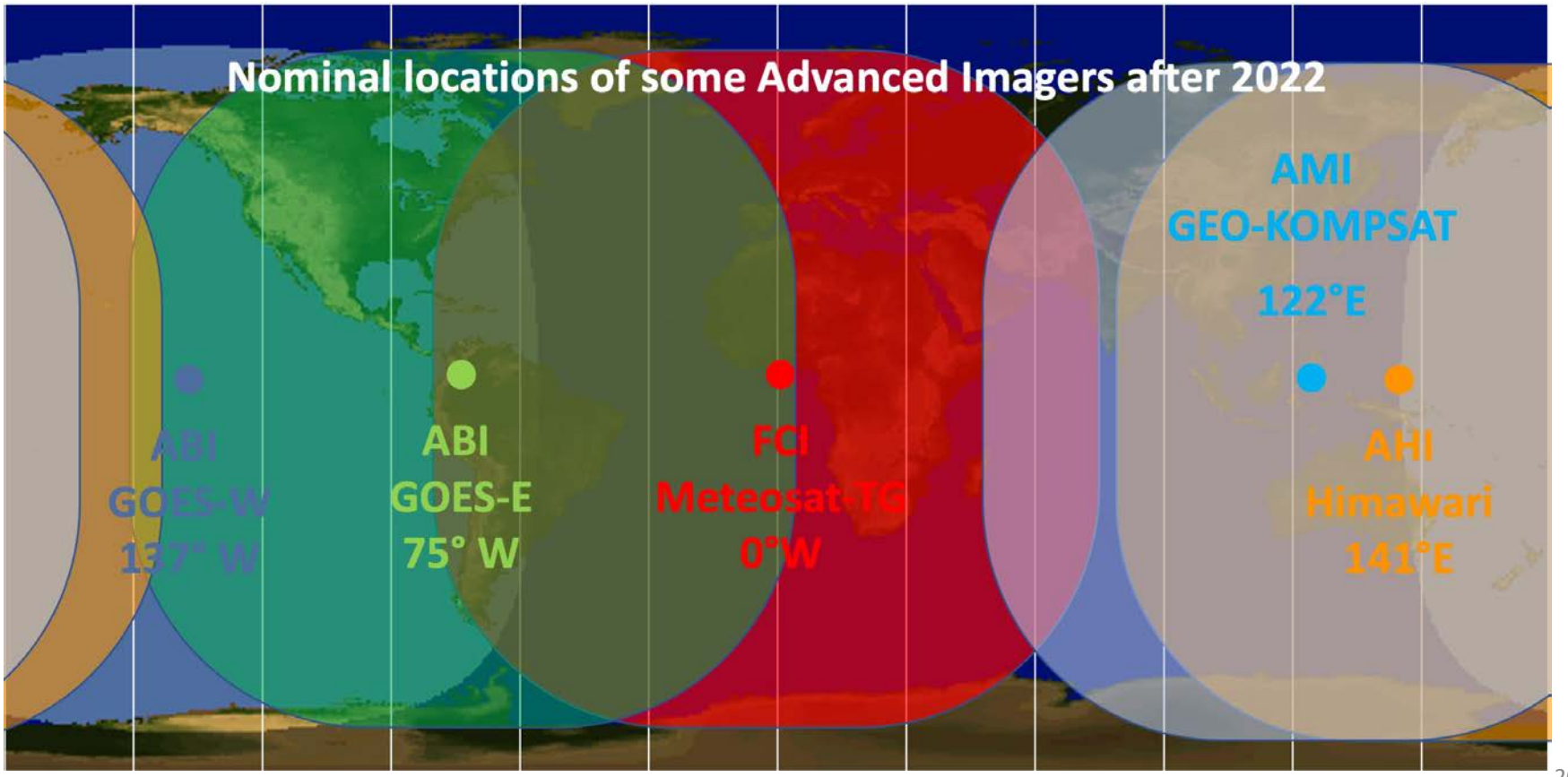


ABI = Advanced Baseline Imager

- Polar Orbiting Satellites: 1-3 observations per day, per sensor, cannot resolve diurnal cycle
- Current Geostationary Satellites: Every 10 min (Full Disk). Can resolve time

Slide credit: Rob Levy

With options for adding even more sensors!



Status of Dark Target/Deep Blue Aerosol Products

- **MODIS Collection 6.1 ('MxD04_L2' and 'MxD04_3K')**
  - Data (2000-present) available in HDF4 format.
  - Includes Dark-Target / Deep Blue (DT/DB) merge product
  - **Includes 3 km resolution product (MxD04_3K)**
- **VIIRS Version 1.1 Dark-Target ('AERDT_VIIRS_SNPP')**
  - DT Data available in NetCDF4. Most output parameters same as MODIS
  - Deep Blue already ('AERDB') available since early 2019, and no current merge
  - Funded development for retrievals on NOAA-20 ('AERDT_VIIRS_N20')
- **Geostationary Beta product ('AERDT_ABI_G16', 'AERDT_ABI_G17', 'AERDT_AHI_H08')**
  - Data are being processed 2019-present (and some earlier data).
  - DT Data available in NetCDF4. Most output parameters same as VIIRS
  - Deep Blue already ('AERDB') in funded development and plans for merge

- MODIS + VIIRS Data currently available on LAADS.
  - https://ladsweb.modaps.eosdis.nasa.gov/missions-and-measurements/science-domain/aerosol/
- GEO Beta available by asking Rob Levy! (Open to public on LAADS after 2022)