



GEOS Overview

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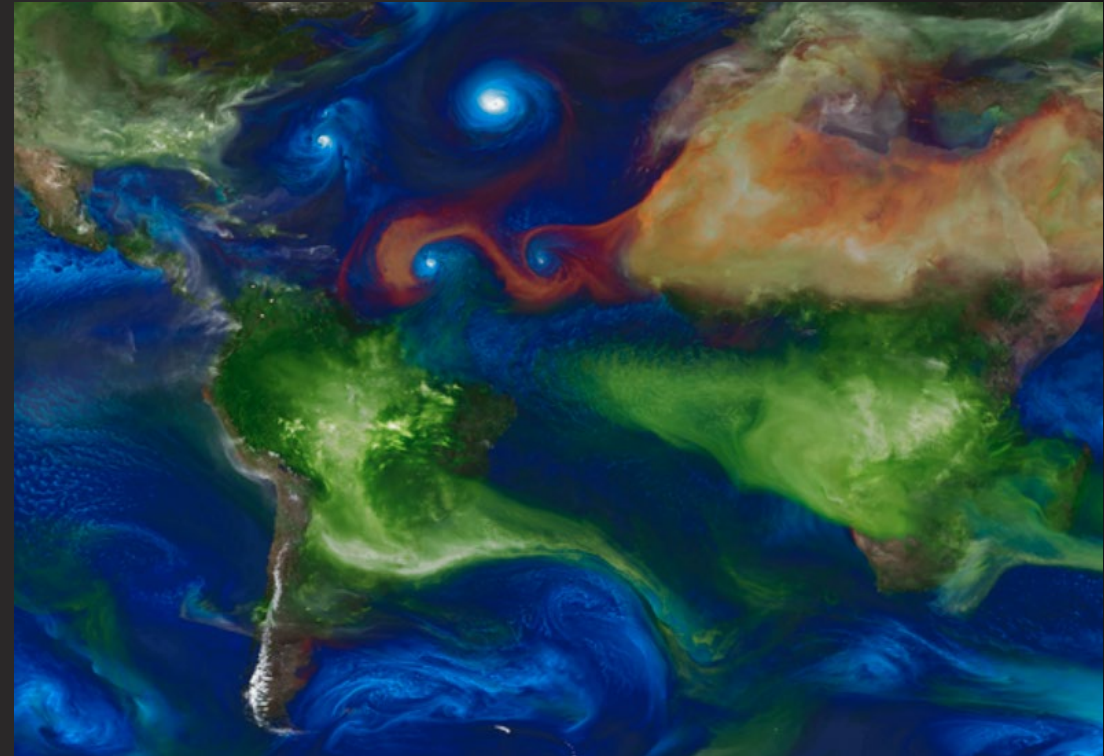
18-20 October 2022

** With contributions from P. Colarco, A. Darmenov, V. Buchard, P. Castellanos, A. Collow, S. Das, H. Bian et al.*



Outline

- GEOS Overview
- GOCART-2G Refactoring
- GOCART Science Updates since ICAP 2019
- GEOS Aerosol DA: Status
 - Observing System updates
 - JEDI-based Aerosol analysis
- Summary



GEOS ESM Architecture



GEOS is a hierarchy of ESMF components

An infrastructure for building GEOS applications:

- Standardized component interfaces
- Low level data containers for data sharing
- Grid classes for the physical domain
- Parallel communication
- Others: Regridding, Logging, Calendar

The MAPL layer interface to ESMF

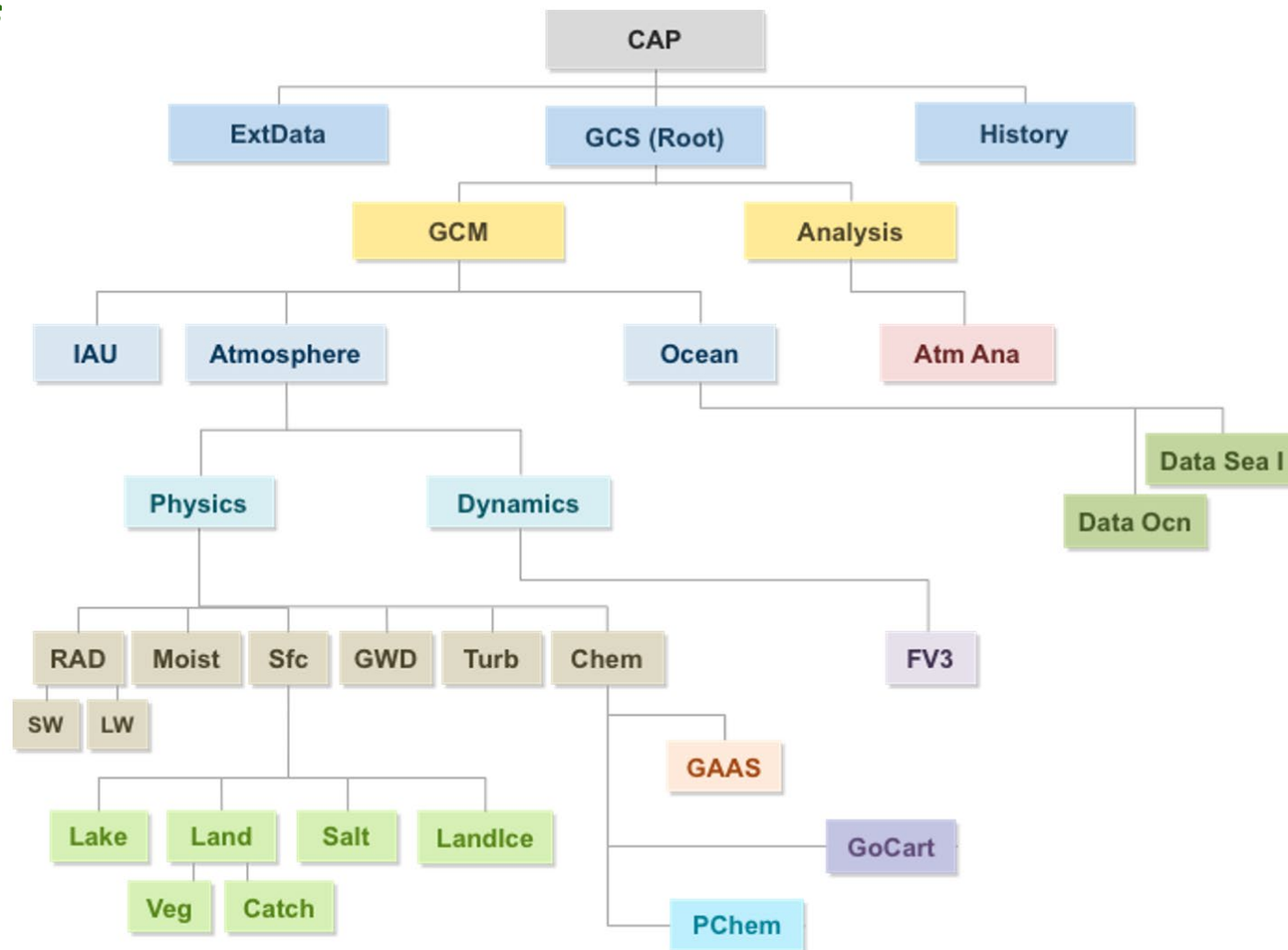
Provides an abstraction of software issues including:

- Generic Initialize/Finalize/Run
- Simplified hierarchy (creation of child components)
- IO Layers (Asynchronous file server output)
- Regridding transforms (grids and tiles)
- Profiling (Performance and Memory)
- Input (ExtData) / Output (History)

Architecture permits flexibility

- NWP configuration
- S2S configuration (seasonal, w/coupled ocean)
- CCM configuration (advanced chemistry)
- CF configuration (full chemistry NRT forecasting)
- NR configuration (high resolution for OSSEs)
- CTM configuration (offline met fields)

All these use the same core model components





GEOS Main Products

GEOS Products	Purpose	Nominal Res.	Aerosol DRE	Cloud Microphysics		Aerosol DA
				1M	2M	
GEOS-IT	N.R.T. analysis system for Instrument Teams	50 km	√	√		√
GEOS-FP	Wx/Aerosols 5-20 Forecasts (in ICAP MME)	12 km	√	√		√
GEOS-S2S	Coupled system for S2S predictions	50 km	√		√	(√)
GEOS-CF	Composition Forecast, full reactive gas chemistry (GEOSchem mechanisms) ▷ Being coupled to GOCART	50 km	√	√		(√)
MERRA-2	Current reanalysis	50 km	√	(√)		√



GEOS Reanalysis with Aerosols

GEOS Products	Purpose	Resolution	Production Start
MERRA-2	Current reanalysis	50 km	2012
GEOS-IT	N.R.T. analysis system for Instrument Teams Newer than MERRA-2 but uses Legacy GOCART	50 km	2022
R21C	Interim Reanalysis of the 21 st Century	25 km	2022
MERRA-3	Coupled Ocean-Atmosphere reanalysis with aerosols	12 km	2024?



GEOS Model Update

Status



Model Changes since ICAP 2019

GEOS Atmosphere (2022)

- FV3 dynamical core on cubed-sphere grid
- ~12.5 km horizontal resolution with 72 vertical levels
- Grell-Freitas deep convection
- Bretherton-Park shallow convection
- Lock turbulence
- Catchment land model
- P-L Chemistry (ozone)
- RRTMG (SW & LW) radiation
- Aerosol-aware single moment cloud microphysics for dynamic cloud and ice effective radii, freezing temperatures
- Other features not yet in production:
 - GWD: convective + Ridge orography
 - EDMF and SHOC Turbulence
 - Grell-Freitas 2020
 - GFDL 1M cloud microphysics
 - MG v2/3 2M cloud microphysics

GEOS Atmosphere (2019)

- FV3 dynamical core on cubed-sphere grid
- ~12.5 km horizontal resolution with 72 vertical levels
- RAS convection
- Lock turbulence
- Catchment land model
- P-L Chemistry (ozone)
- Chou-Suarez (SW) and RRTMG (LW) radiation
- Aerosol-aware single moment cloud microphysics for dynamic cloud and ice effective radii



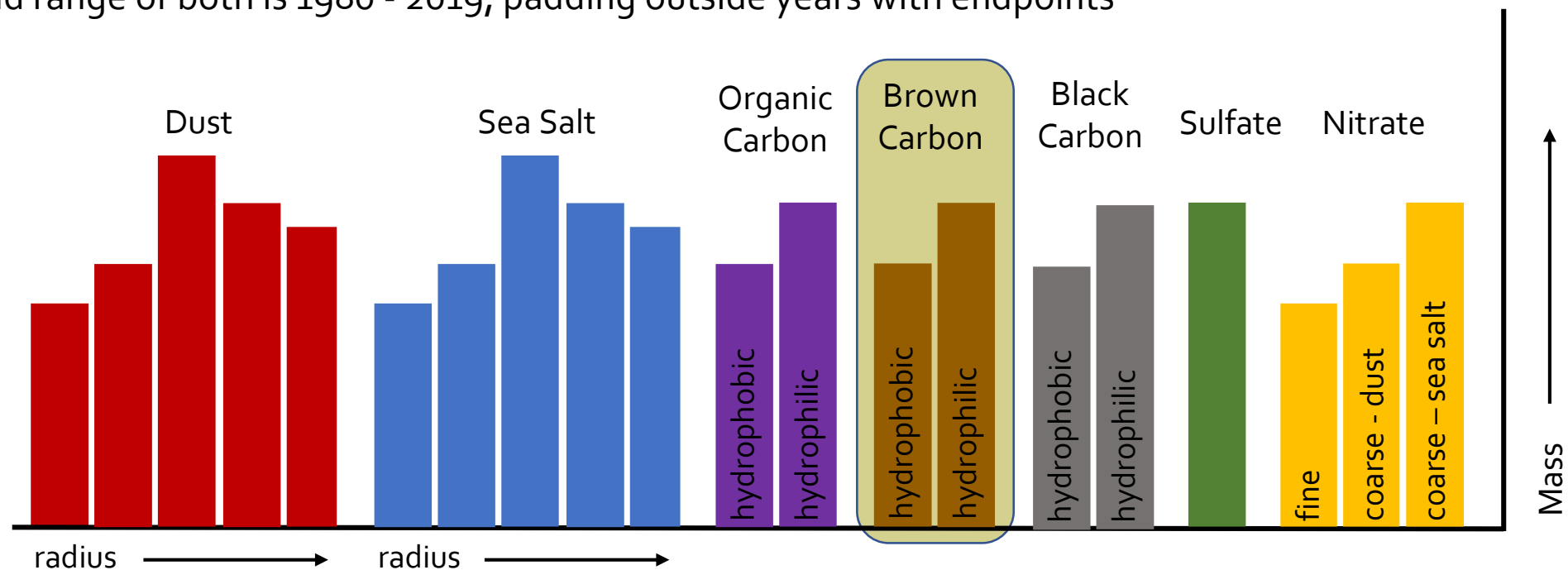
Refactoring of GOCART - Goals

- Better performance
 - Improved efficiency of settling and nitrate chemistry
 - Elimination of extraneous calculations (unknown performance impact)
 - Faster calculation of aerosol single scattering properties
- Elimination of (known) bugs
- **Improved flexibility** with introduction of active and passive instances of aerosol species and improved *Automatic Code Generator*.
- Several improvements for maintainability and extensibility
- Promote better sharing of code with external organizations that have different physics coupling frameworks (MAPL vs. CCPP)

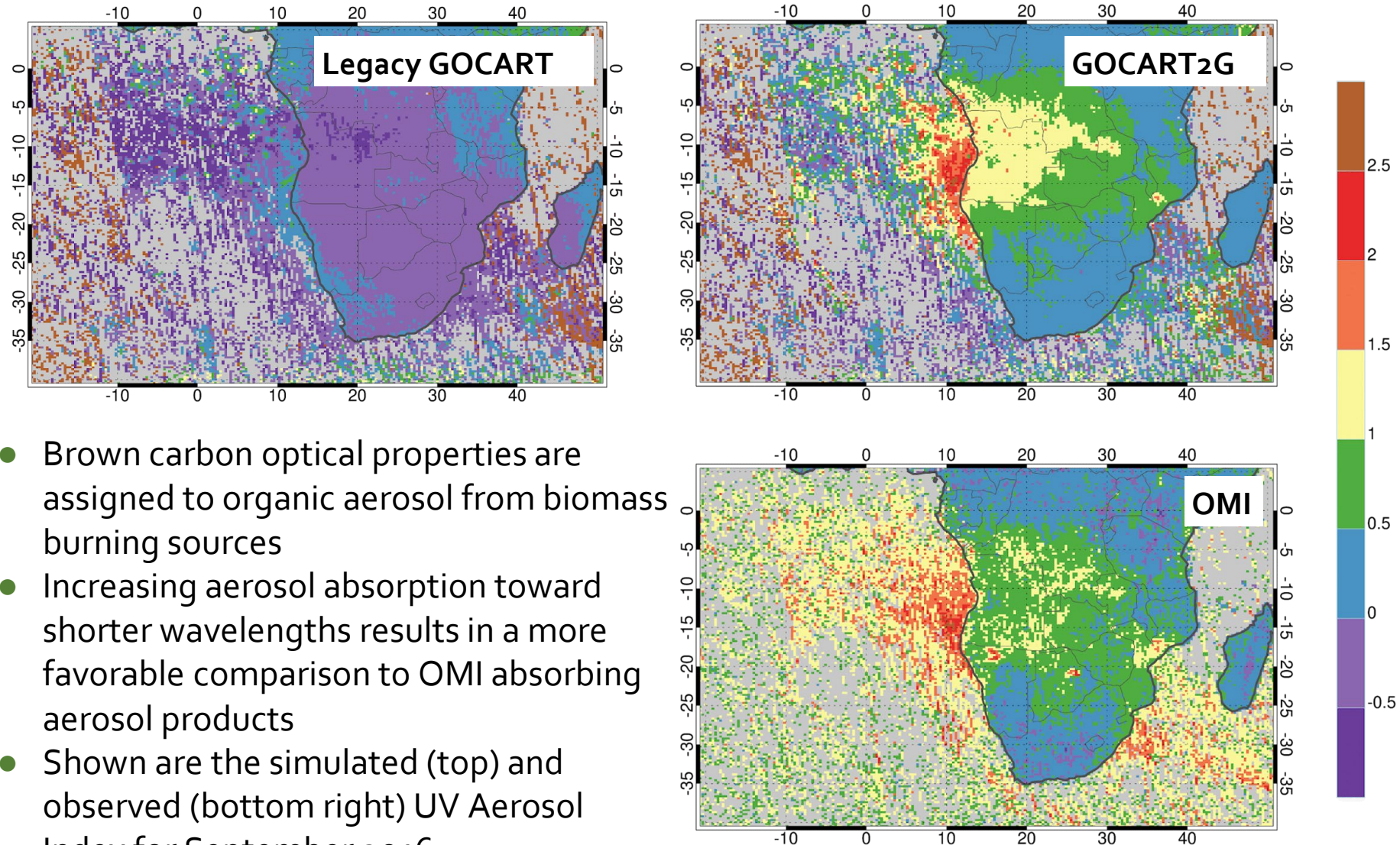
Science Changes Bundled with GOCART-2G



- Separation of organic aerosol into “white” (anthropogenic) and “brown” (biomass burning) components with distinct optical properties
- Increase OA:OC ratio in line with recent airborne measurements
- Inclusion of an AChem-driven SOA scheme for anthropogenic and biomass burning sources
- Inclusion of a HEMCO/MEGAN-driven biogenic SOA scheme
- Introduction of “point wise” source emissions for pyroCb inputs
- Update anthropogenic emissions to downscaled-CEDS emission inventory and input oxidant fields to MERRA-2 GMI (valid range of both is 1980 - 2019; padding outside years with endpoints)



Impact of Brown Carbon

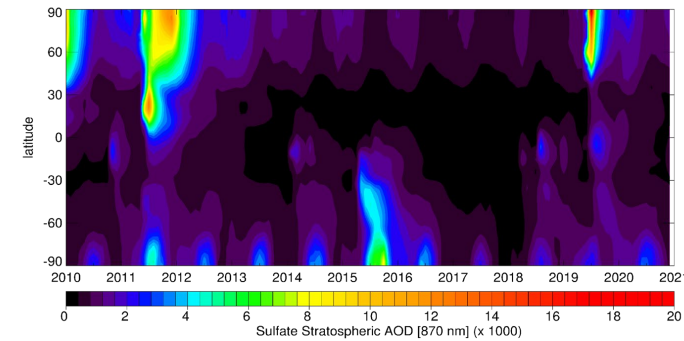
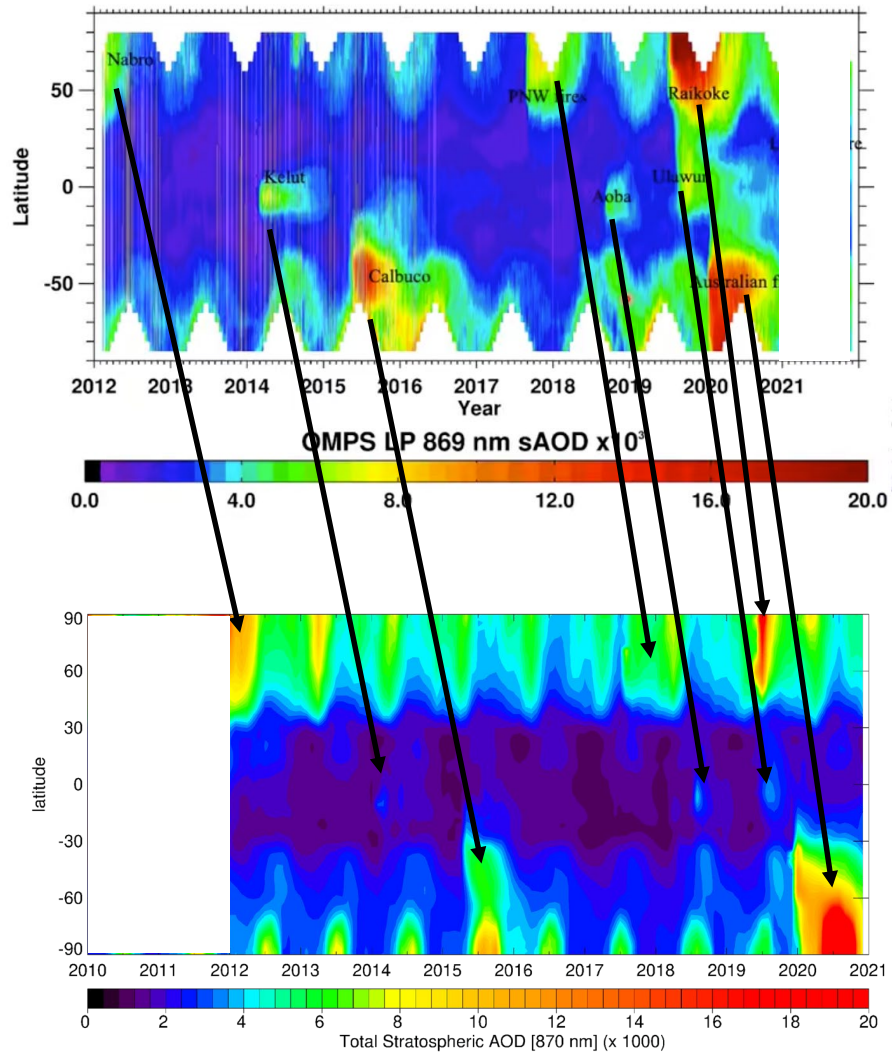


- Brown carbon optical properties are assigned to organic aerosol from biomass burning sources
- Increasing aerosol absorption toward shorter wavelengths results in a more favorable comparison to OMI absorbing aerosol products
- Shown are the simulated (top) and observed (bottom right) UV Aerosol Index for September 2016

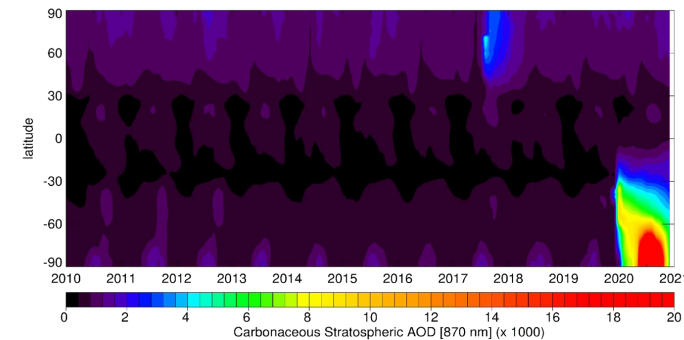
Stratospheric Optical Depth



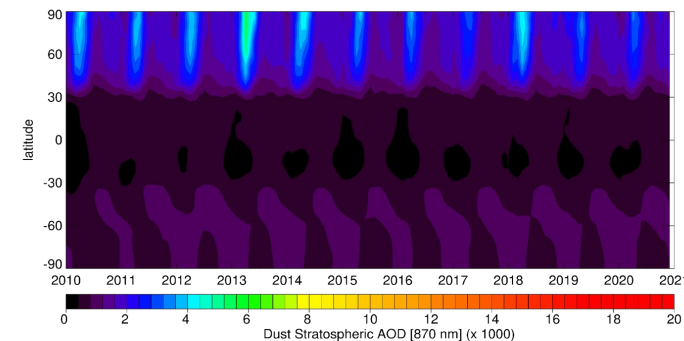
Zonal Mean Stratospheric AOD



Sulfate



Carbon

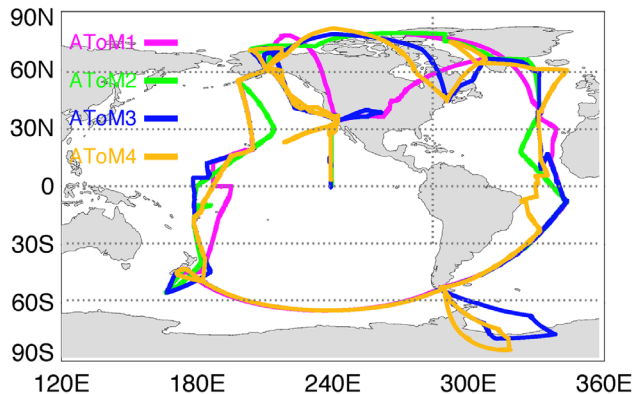


Dust

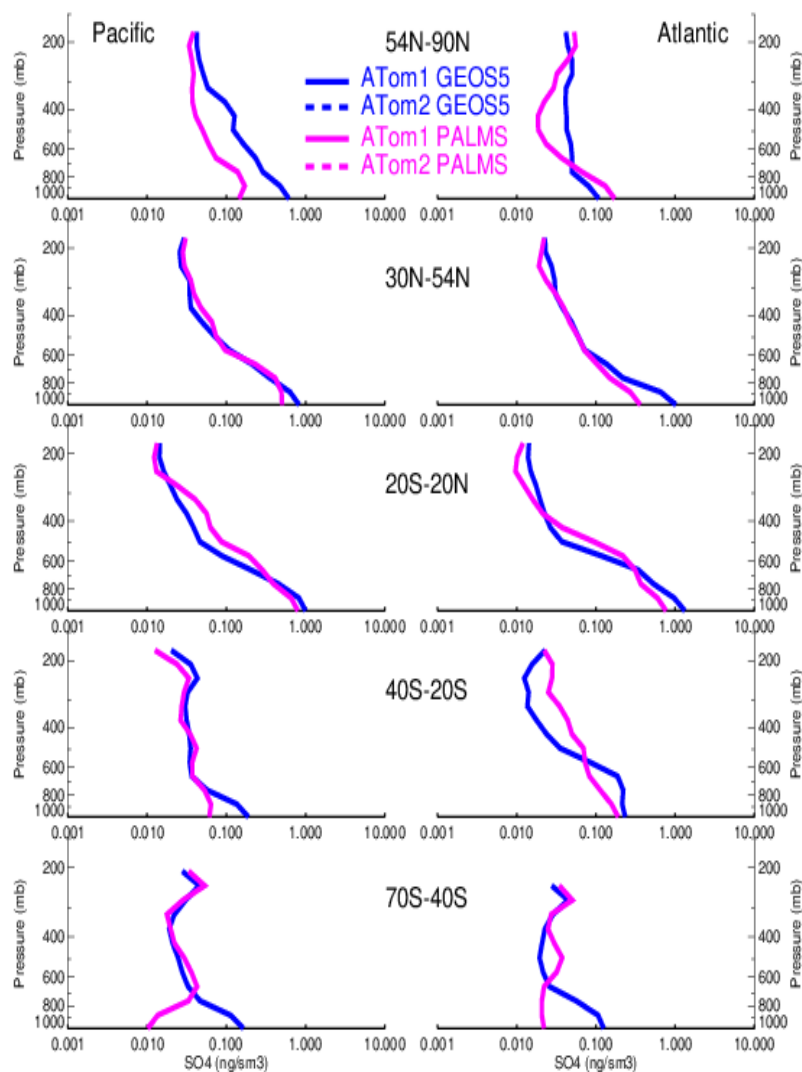
Comparison to ATom Vertical Profiles



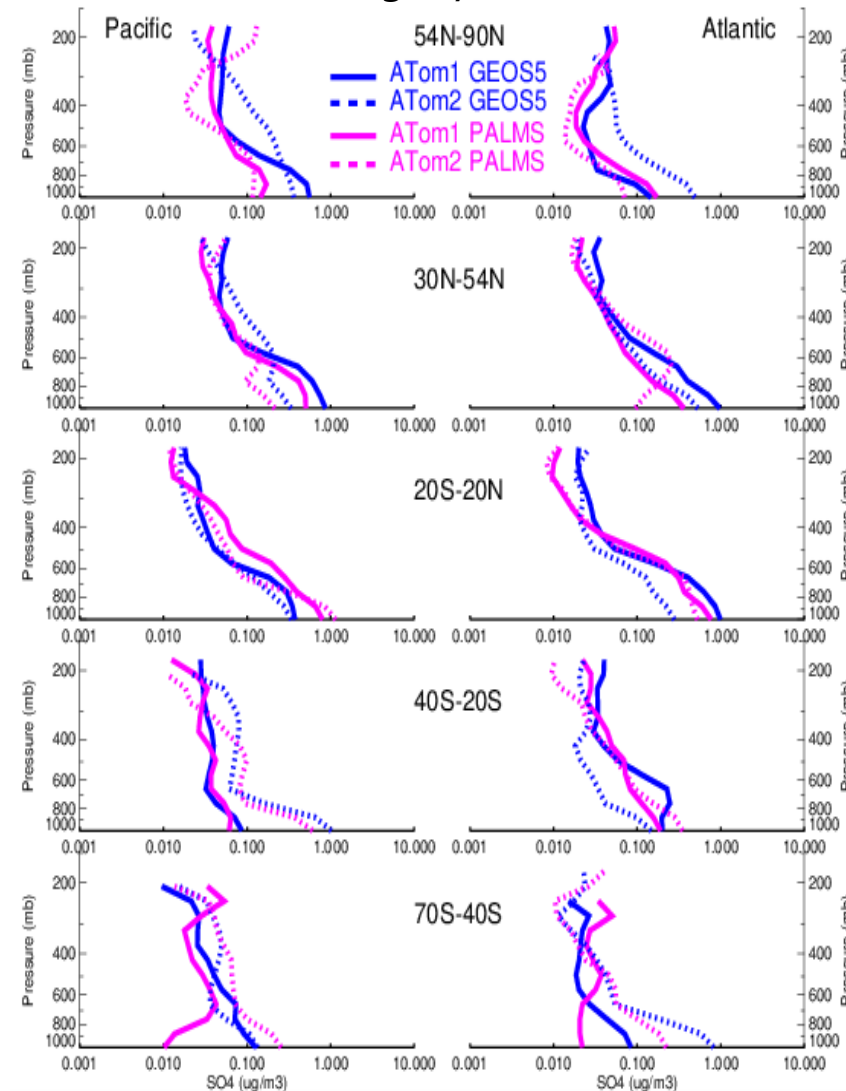
Sulfate



GOCART₂G



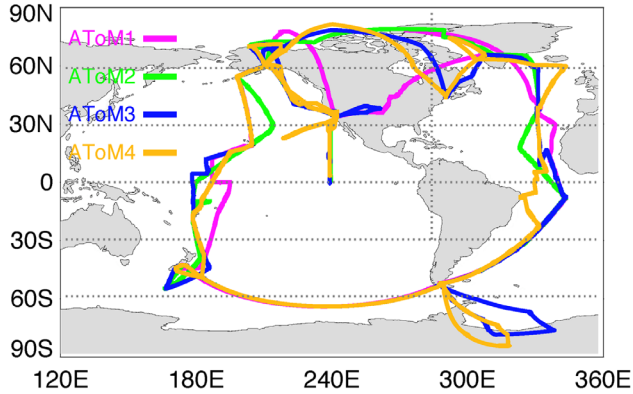
Icarus Legacy GOCART



Comparison to ATom Vertical Profiles

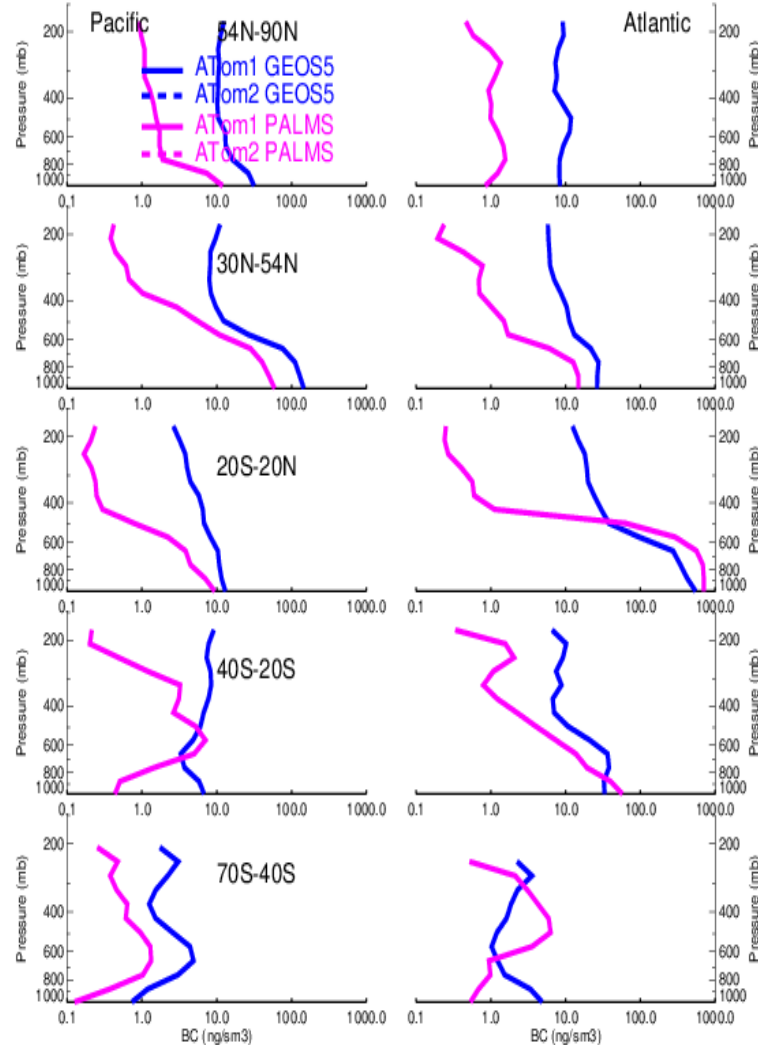


Black Carbon

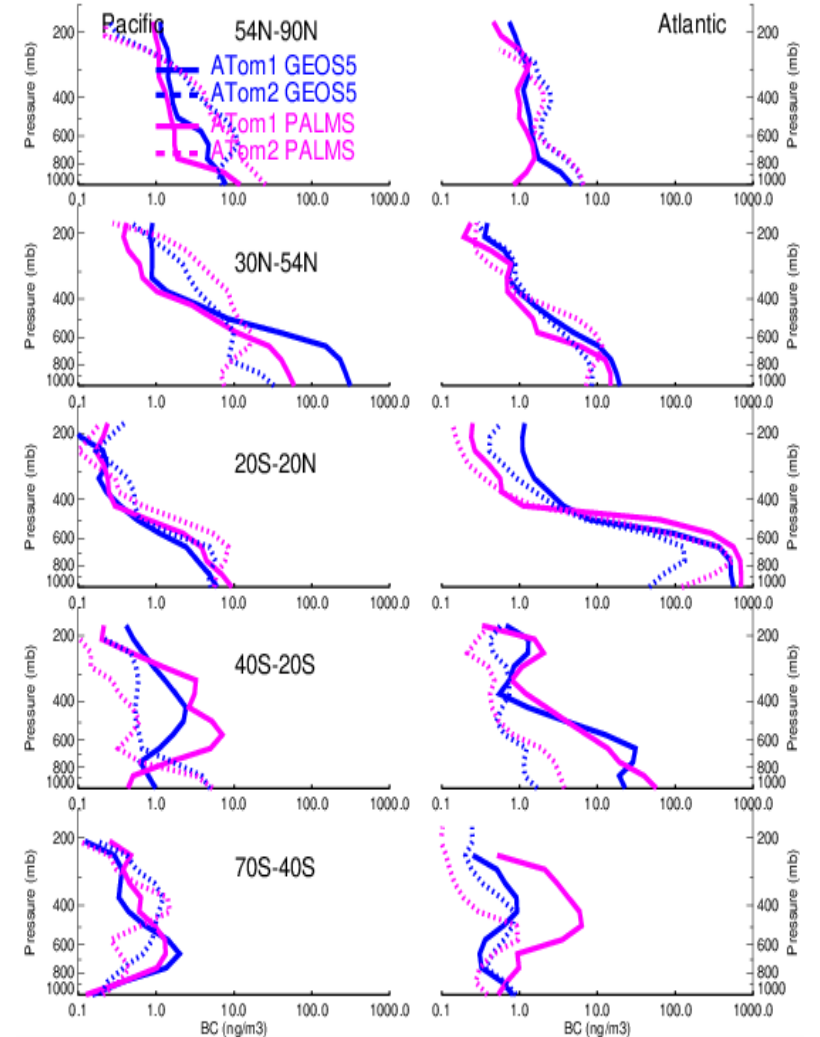


Bottom line: additional tuning of wet removal is warranted

GOCART2G

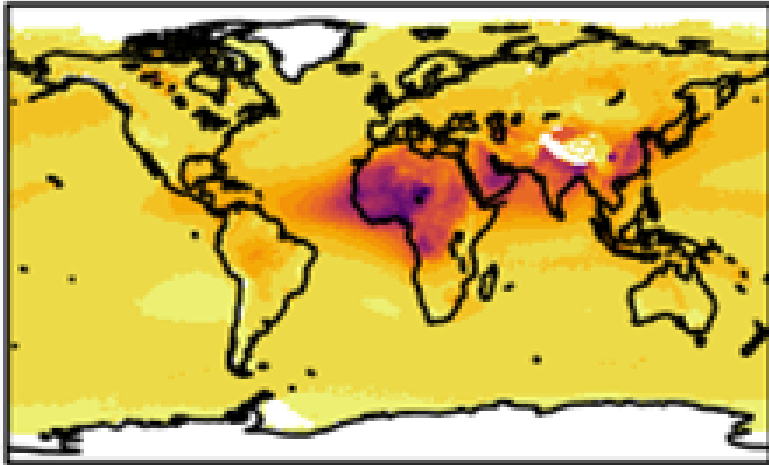


Icarus Legacy GOCART

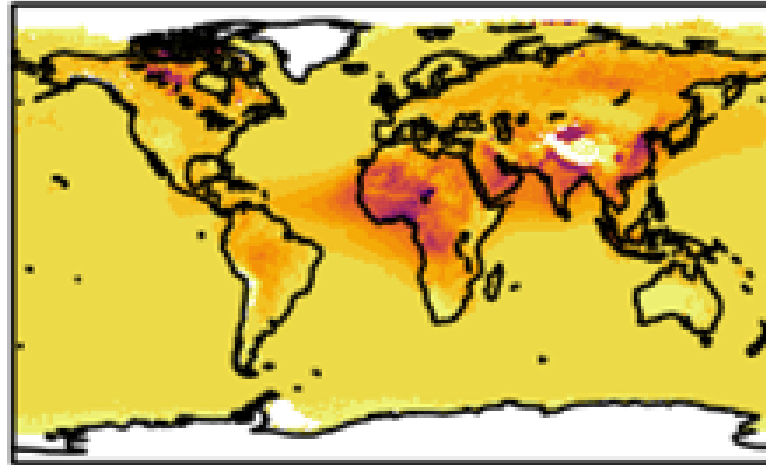


Benchmarking our Current Modeling

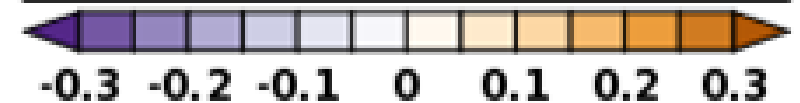
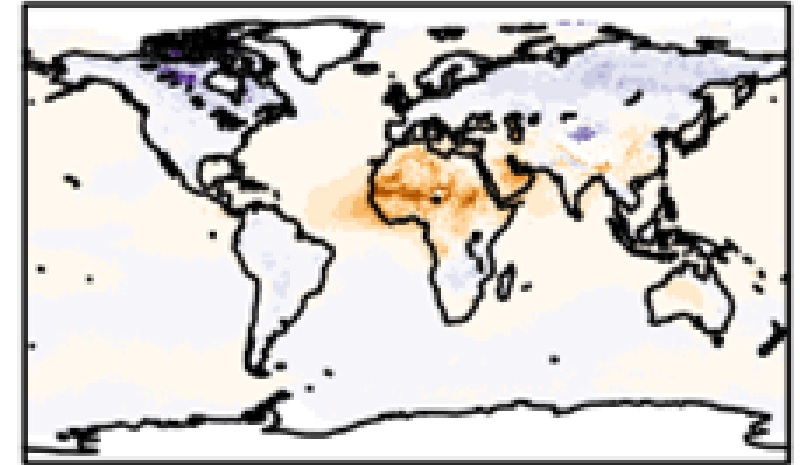
GEOS



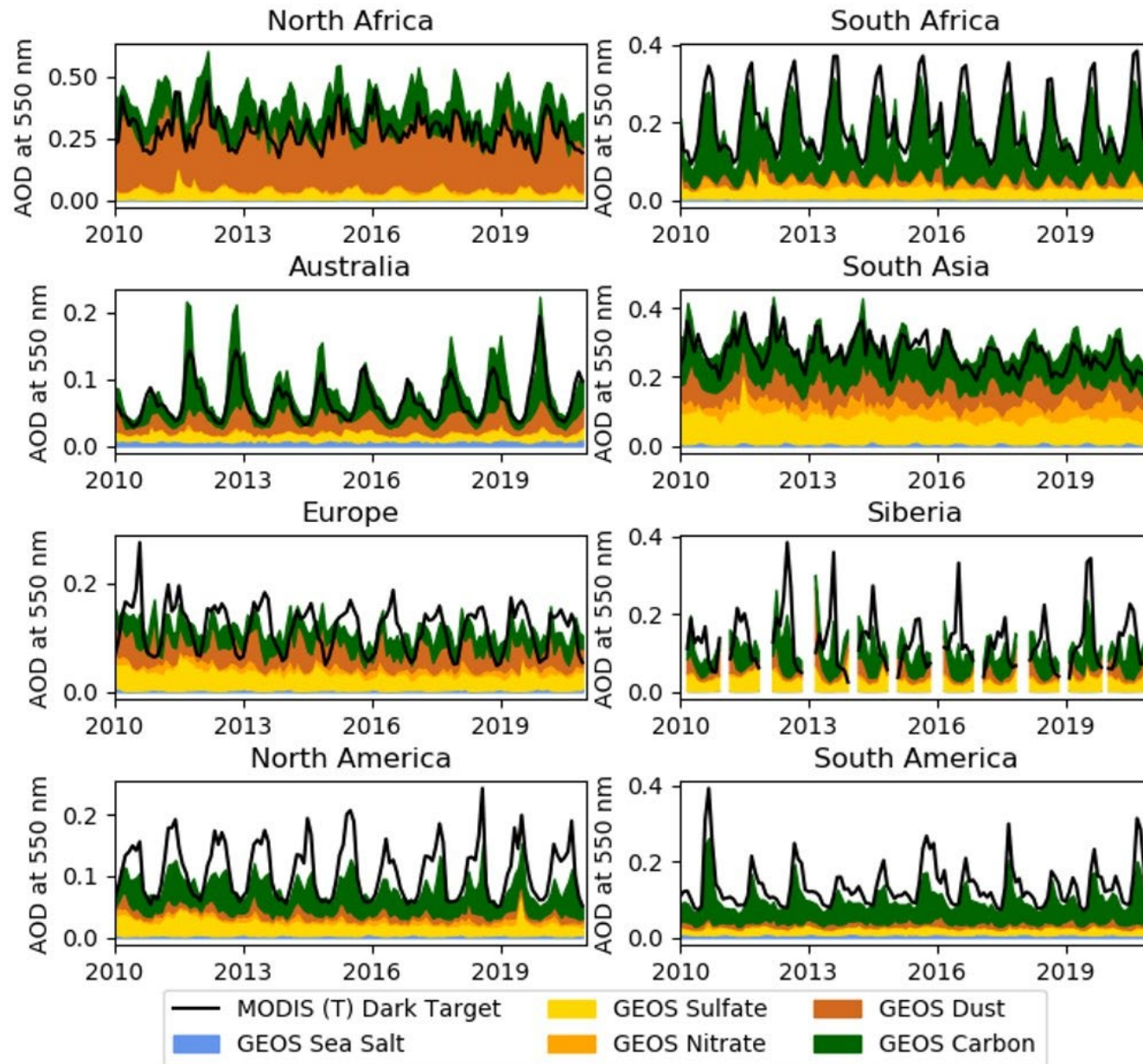
MODIS (Aqua)



GEOS - MODIS



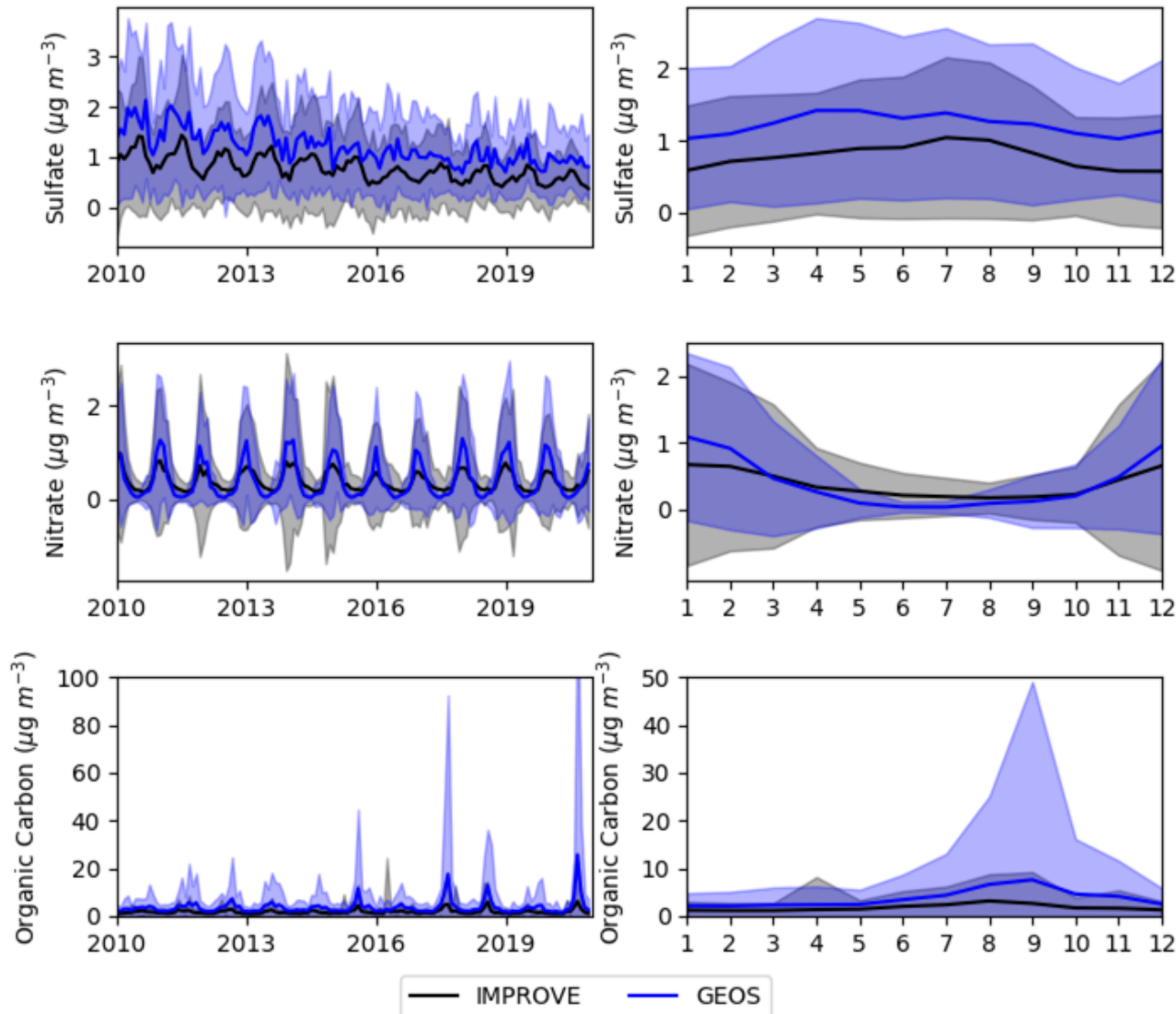
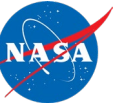
- 10+ year model run constrained to MERRA-2 meteorology *without* AOD assimilation
- MODIS (NMR) is an independent observation
- What should future development focus on?
- Overestimated AOD in North Africa linked to excessive dust (*recently retuned*)
- Seasonal underestimation in the Americas, Siberia due to deficiencies in carbon



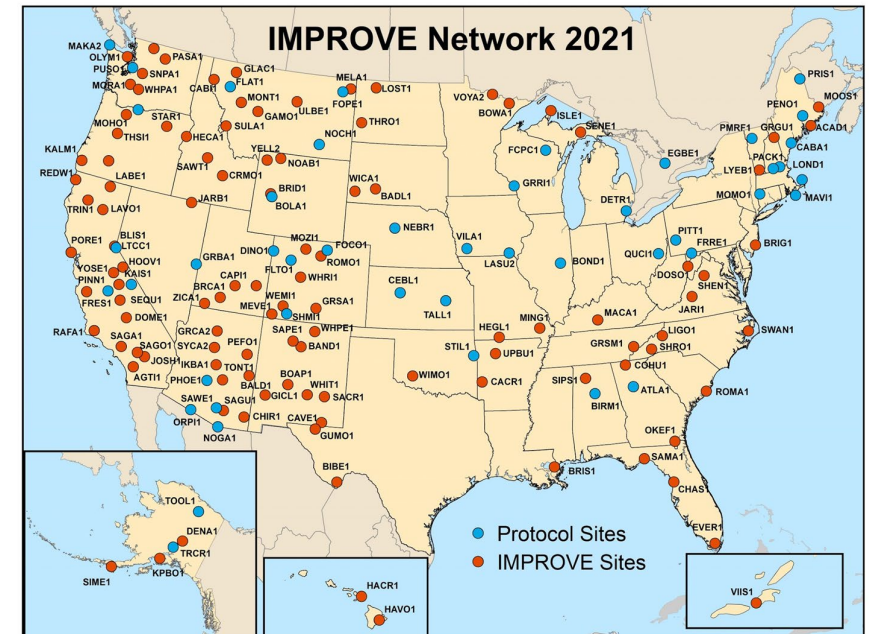
Timeseries of AOD

- GEOS generally captures the seasonal cycle of AOD around the globe
- Good agreement in South Africa, Australia, South Asia
- Overestimate of dust (North Africa) and underestimate of smoke (Siberia, Americas)
- Europe warrants further evaluation

Surface Aerosol Concentration in the United States

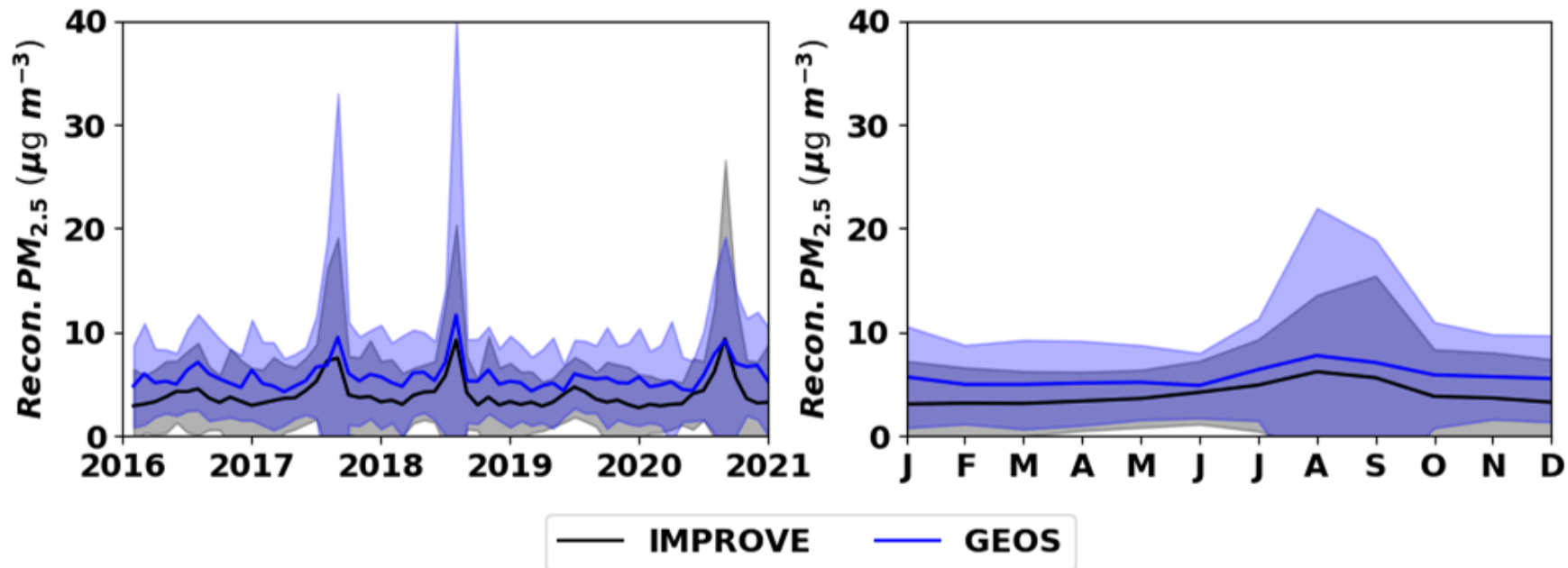


- Although AOD is constrained, aerosol mass is prognostic
- IMPROVE is a collection of air quality sites, typically located in National Parks
- Shading is +/- 1 standard deviation
- GEOS has too much aerosol mass, amplified seasonal cycle for nitrate



<http://vista.cira.colostate.edu/Improve/improve-program/>

Surface $PM_{2.5}$

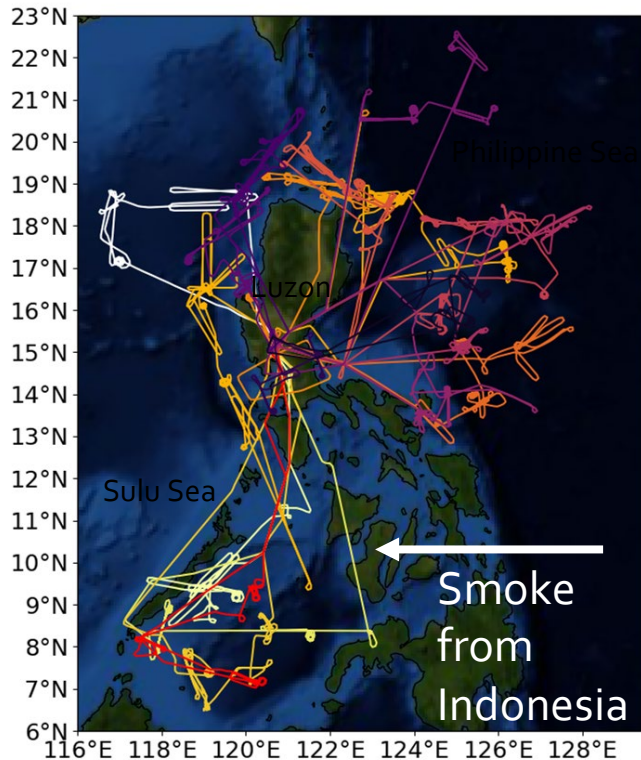


- Overestimate primarily due to sulfate and carbon as shown on previous slide
- Despite too much dust over Africa, GOCART-2G lacks enough dust over the U.S.

Field Campaign Observations for a Closer Look



- NASA P3 collected observations in the Philippines region before, during, and after the southwest monsoon transition
- In situ observations are needed to evaluate aerosol properties dictated by the optics tables and assumed by GEOS



Observations

LARGE = Langley Aerosol Research Group Experiment, in situ aerosol mass and optics (Luke Ziemba)

HSRL2 = High Spectral Resolution Lidar (Chris Hostetler)

FIMS = Fast Integrated Mobility Spectrometer, particle size distribution (Jian Wang)

GEOS

Modular earth system model from NASA's GMAO

GOCART Aerosol Module

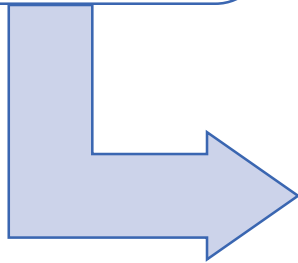
Assimilation of conventional and satellite observations + MODIS aerosol optical depth

GEOS Experiments Evaluated



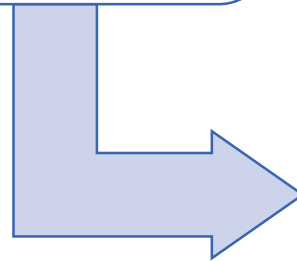
GEOS 5.22

- “Baseline”
- “Operational” in 2019 in NRT
- RAS Convection, Chou-Suarez Radiation
- Biomass burning emissions persisted from prior day



GEOS 5.25

- Currently “operational” model physics
- Grell-Freitas convection
- Introduction of shallow convection (UW)
- RRTM-G
- Retrospective biomass burning emissions



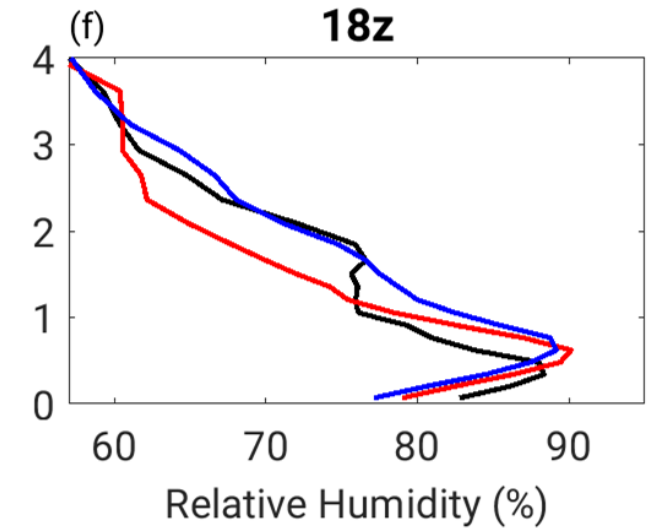
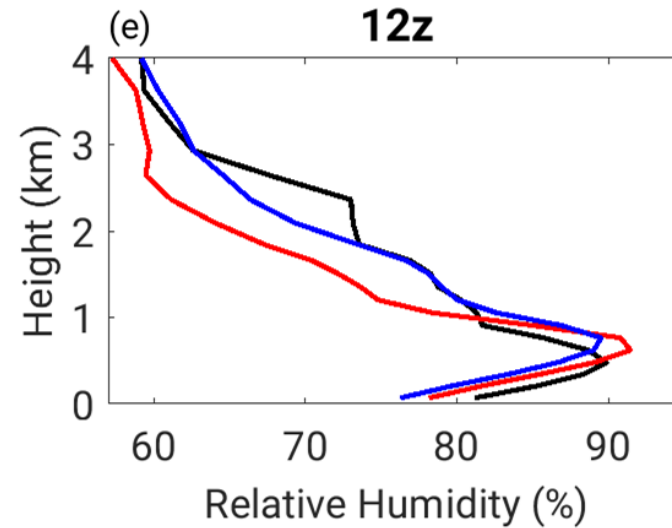
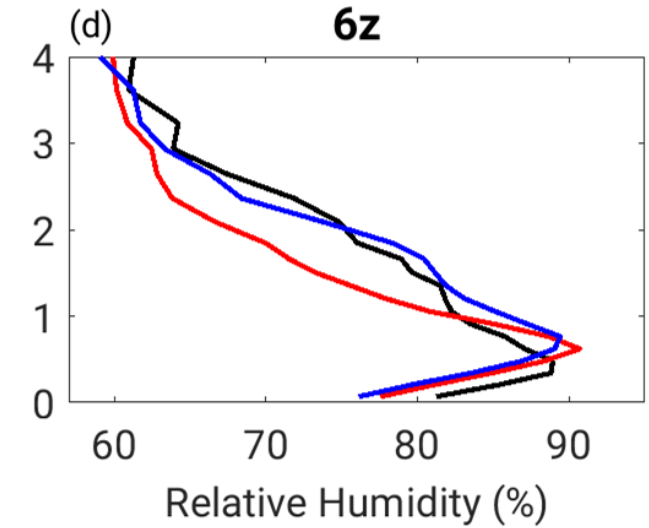
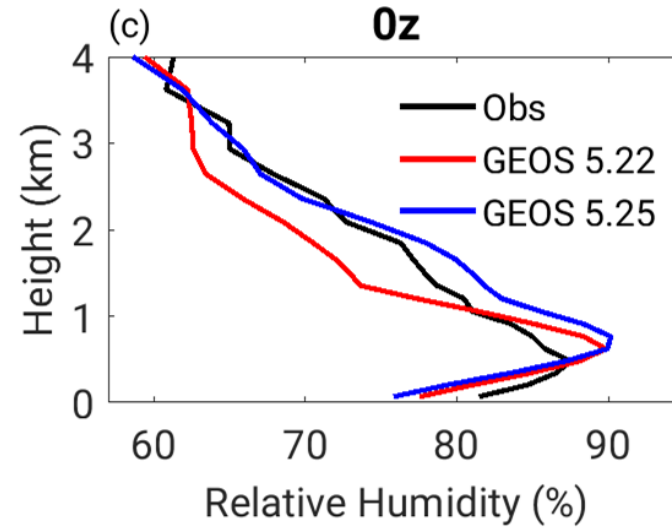
GOCART₂G

- “In development” aerosol model
- Introduction of brown carbon/SOA
- Organic carbon from biomass burning emissions as brown carbon
- Updated anthropogenic emissions and volcanic eruptions

Model Validation – All Dropsondes (RH)



Newest GEOS 5.25 has improved RH fields



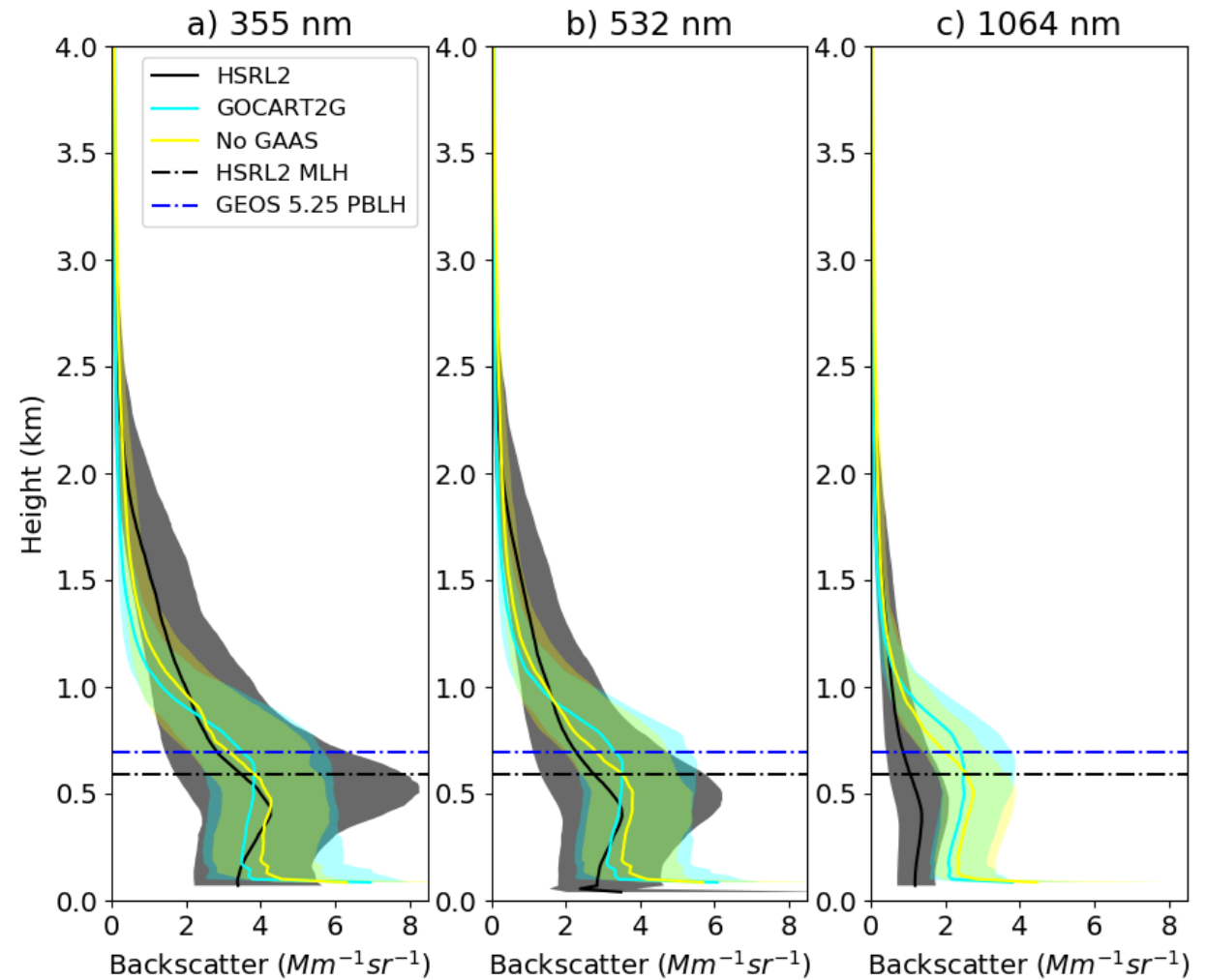


Aerosol Extensive Properties

Median backscatter at (a) 355 nm, (b) 532 nm, and 1064 nm during all research flights from the HSRL₂, GOCART₂G, and GOCART₂G without aerosol assimilation (No GAAS).

Mixed layer height (MLH) from the HSRL₂ and planetary boundary layer (PBL) height in GEOS are added for reference as dashed lines.

GEOS PBL higher than measurements

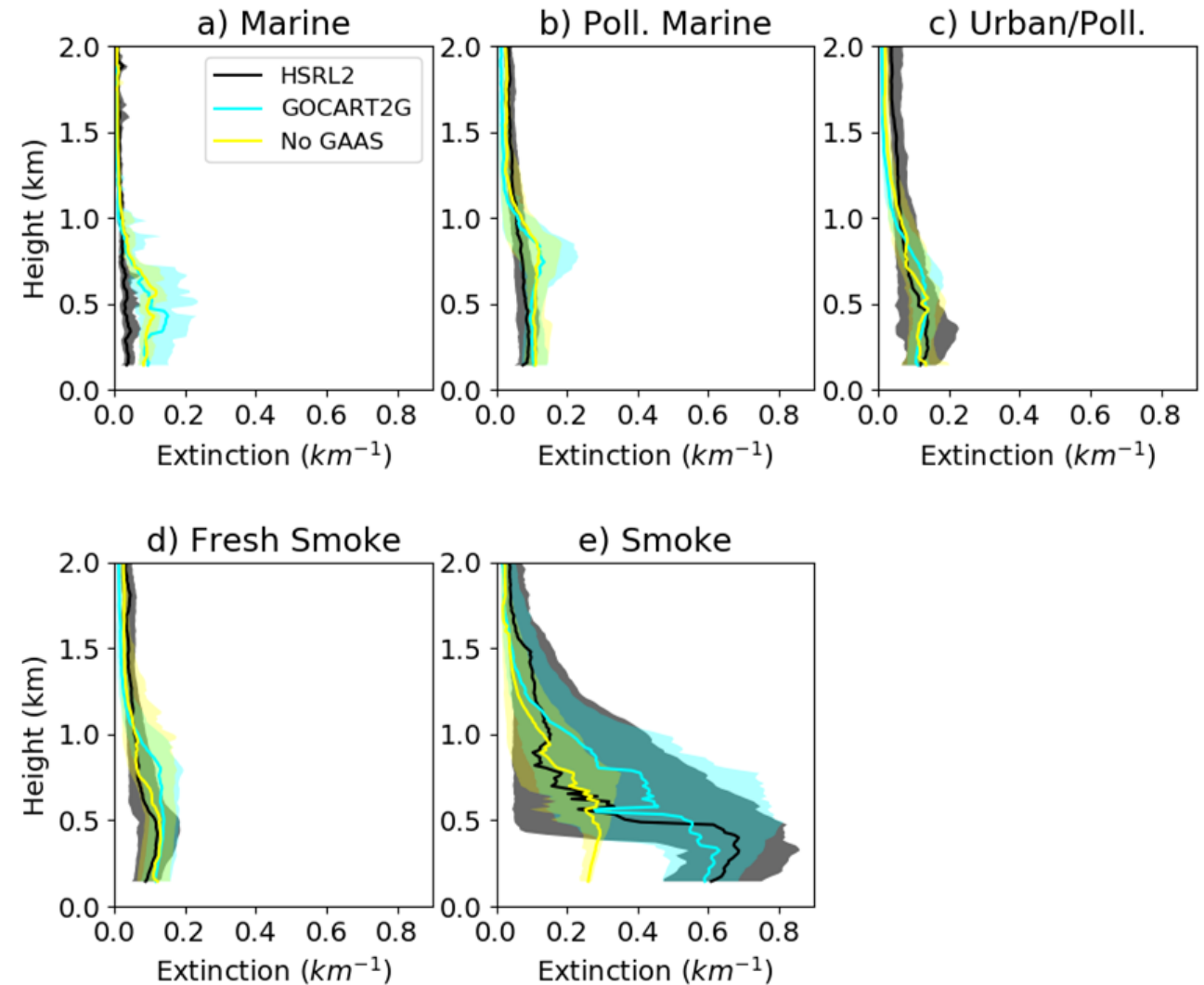


Speciated Extinction

Median extinction at 532 nm during all research flights from the HSRL2, GOCART2G, and GOCART2G without aerosol assimilation (No GAAS)

Filtered based on the HSRL2 aerosol *type labels* for (a) marine, (b) polluted marine, (c) urban pollution, (d) fresh smoke, and (e) smoke aerosols.

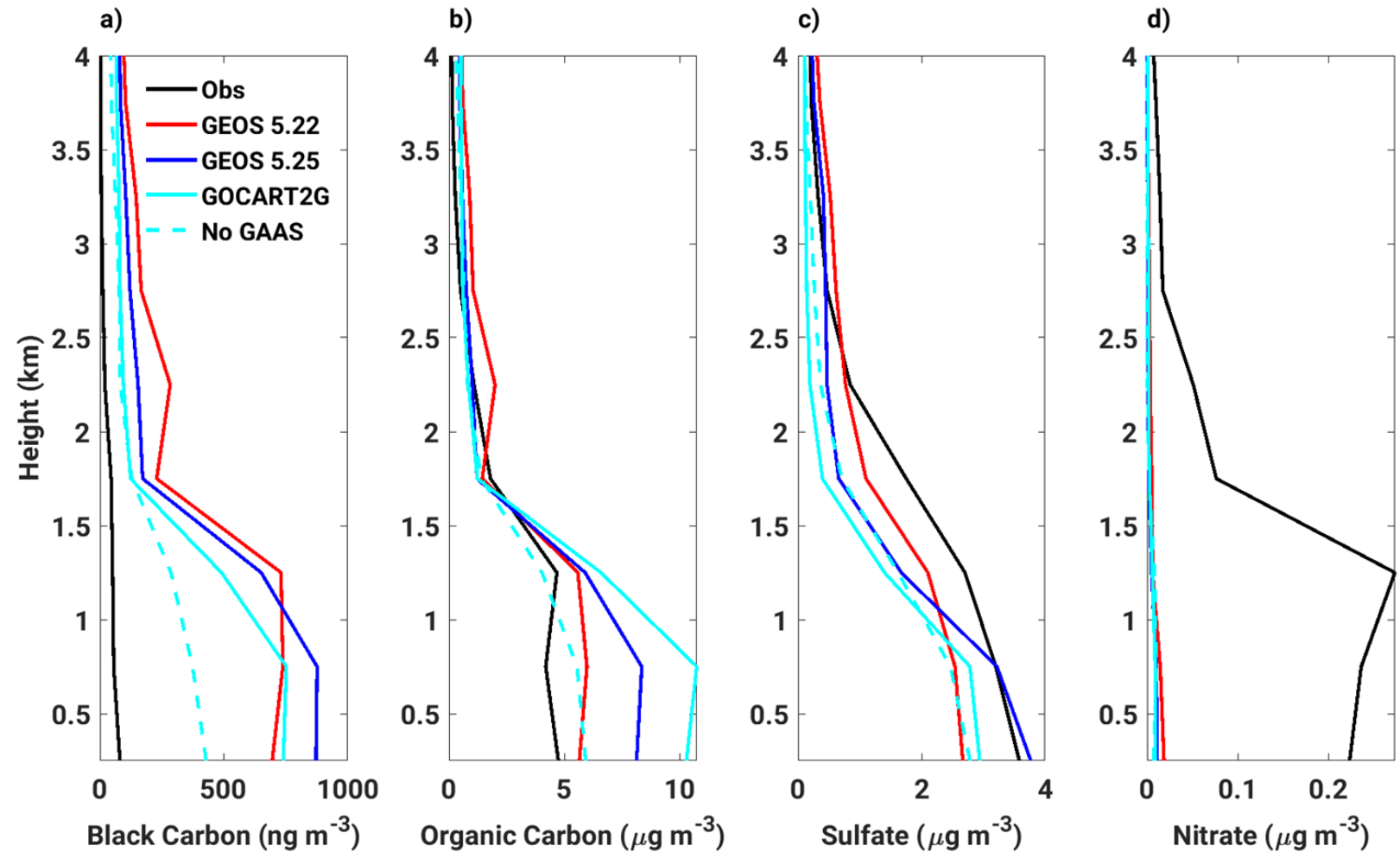
Without aerosol DA GOCART-2G
Has much lower smoke extinction
near the surface.



Mass Speciation

Mean vertical profile of aerosol mass concentration from the **LARGE** observations, GEOS 5.22, GEOS 5.25, GOCART2G, and GOCART2G without GAAS for (a) black carbon, (b) organic carbon, (c) sulphate, and (d) nitrate

- The situation is reversed for mass: more realistic OC concentration without aerosol DA
- Very small nitrate concentration



$f(\text{RH})$

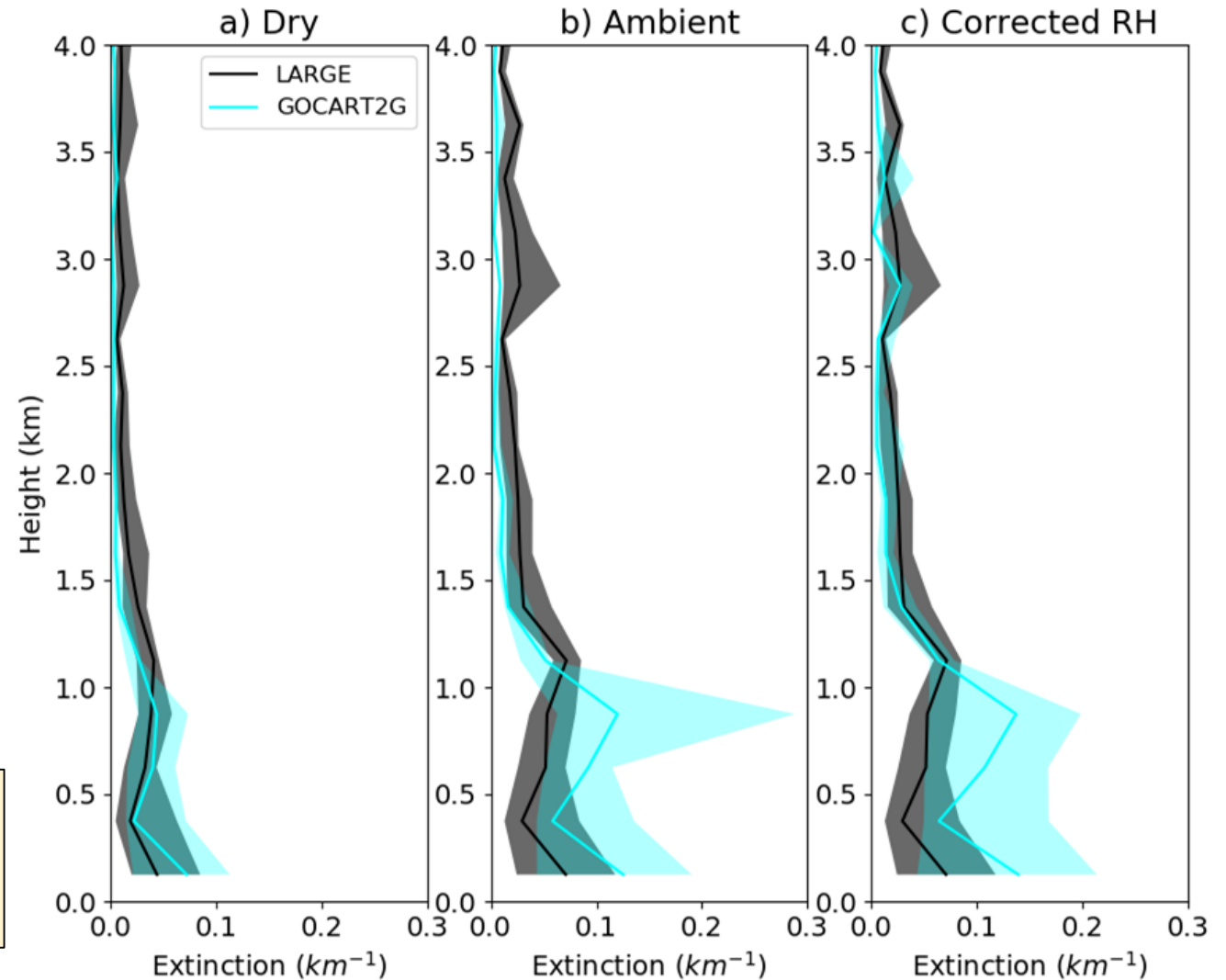
Median extinction at 532 nm
for all research flights from
LARGE and GOCART2G for

(a) ambient

(b) Dry

(c) observation corrected
relative humidity

Dry extinction compares better to
in-situ measurements than at ambient RH
➤ $f(\text{RH})$ is too high



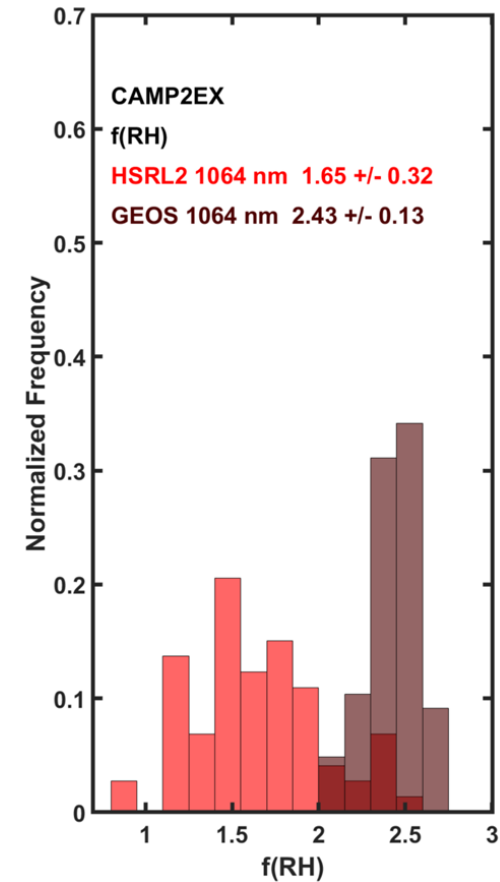
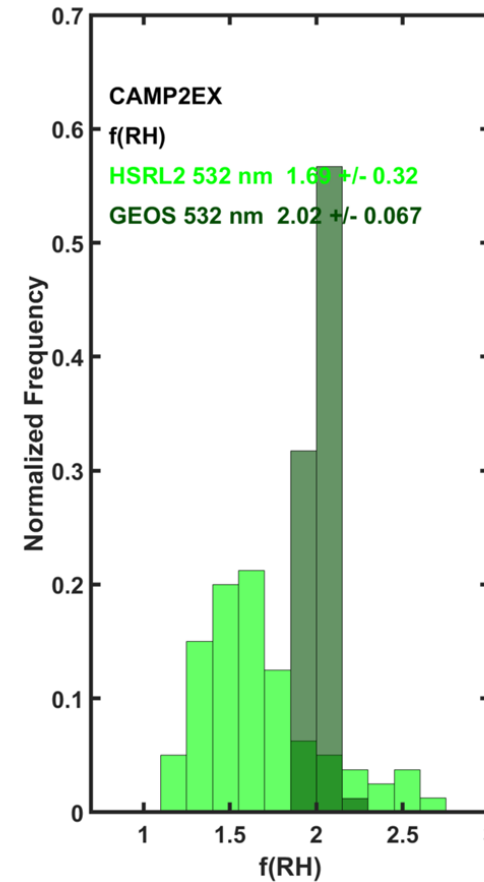
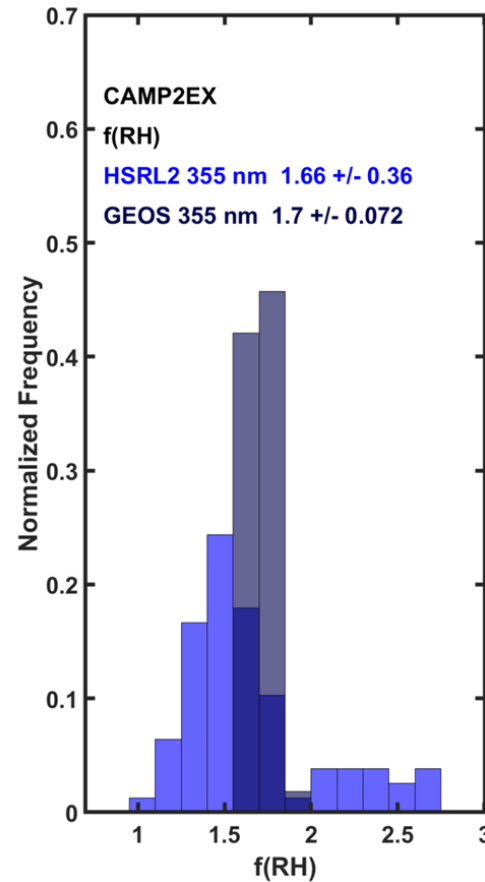


f(RH) – from HSRL2

HSRL-2 & Dropsonde f(RH) are more variable and, on average, show little change with wavelength

Courtesy: Rich Ferrare

GEOS f(RH) are less variable and increase with wavelength

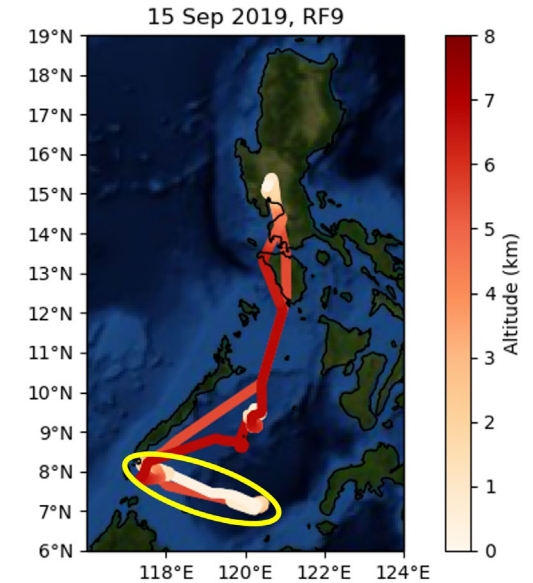
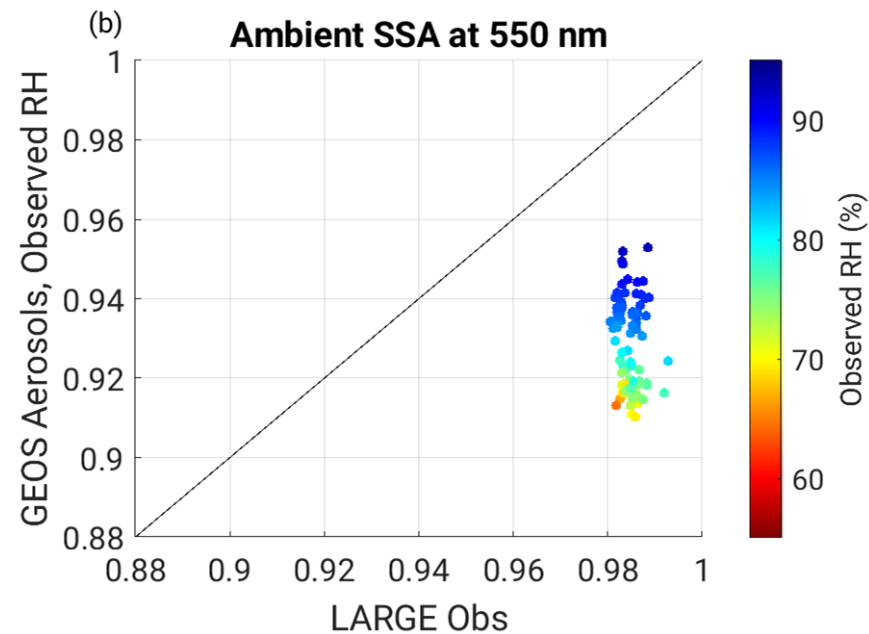
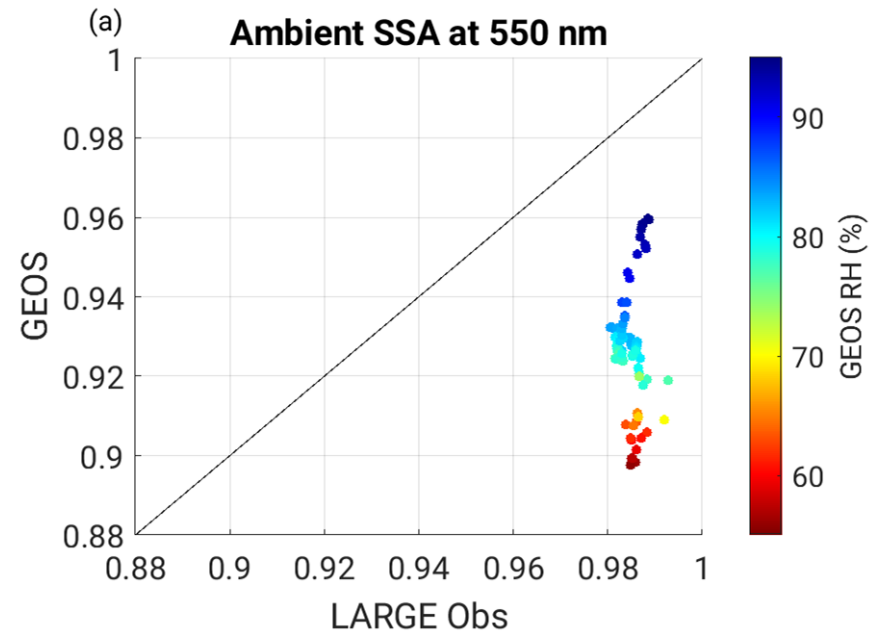


SSA

Ambient single scattering albedo at 550 nm computed using

- (a) the relative humidity from GEOS
- (b) observed relative humidity from the aircraft versus the observed single scattering albedo for the flight segment from RF9.

GEOS SSA is underestimated.



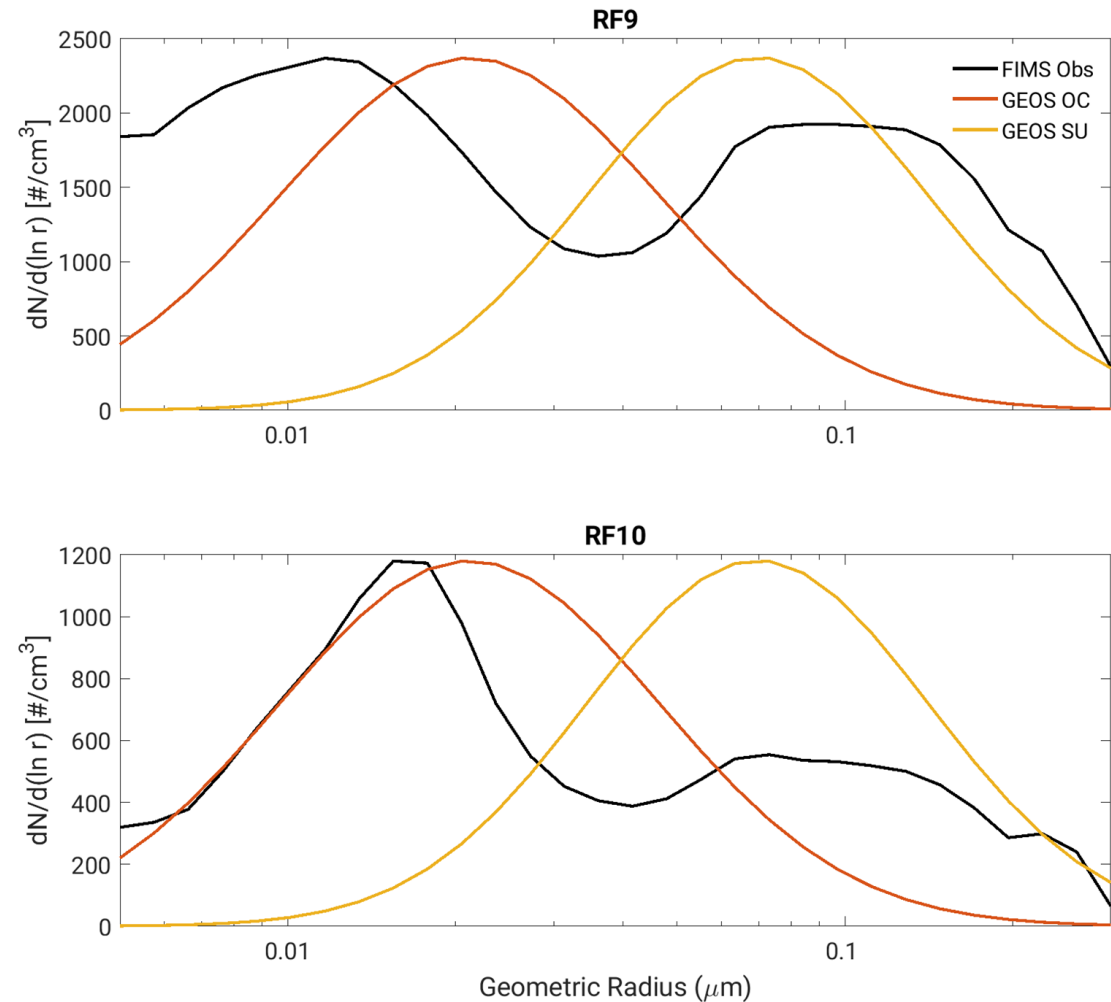


Size Distribution

Observed dry aerosol size distribution from FIMS for data points classified as a biomass burning regime from (a) RF9 and (b) RF10.

Assumed particle size distribution for organic carbon and sulphate in GEOS has been scaled to match the peak in the observed distributions.

GOCART-2G being a bulk model prescribes the size distribution for OC and SU and cannot properly Model the dynamic evolution of Aerosol size distributions.





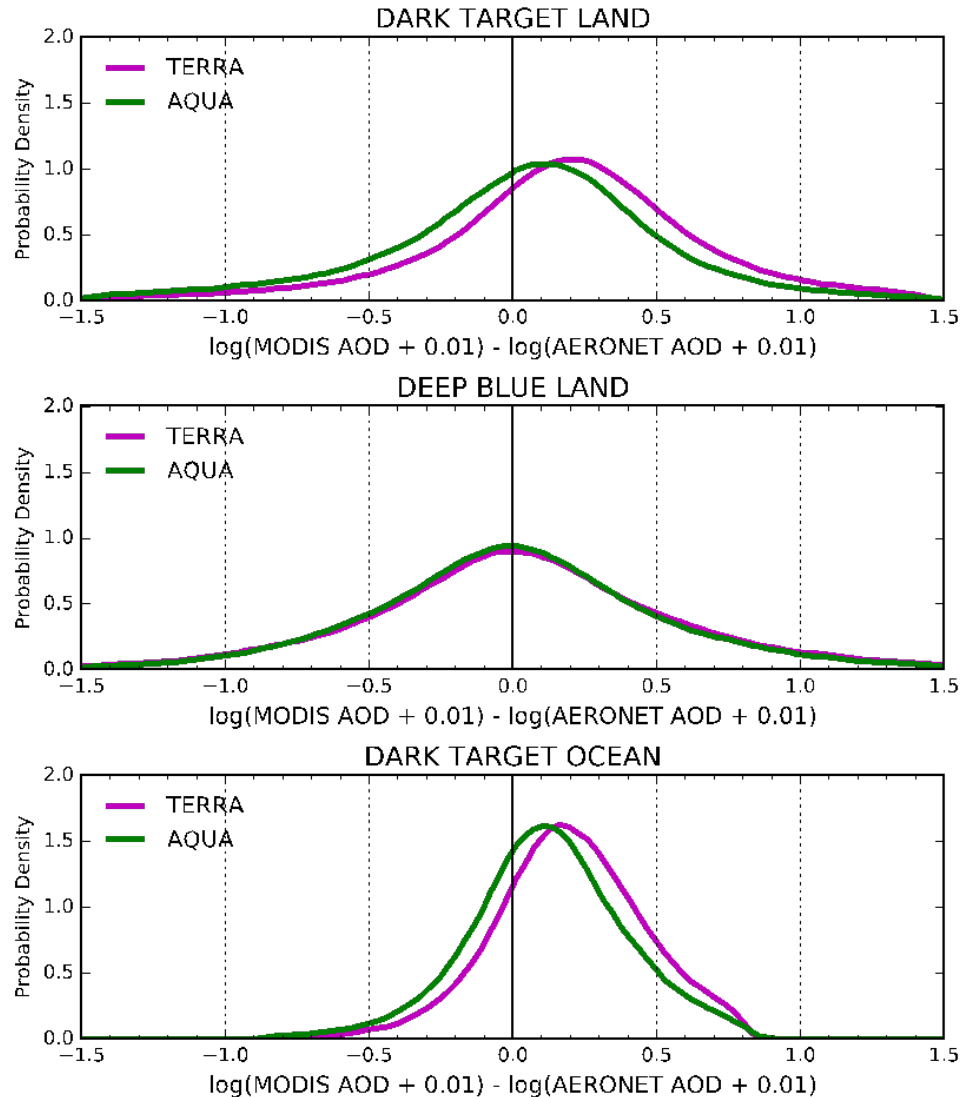
Model is far from perfect, now what?

- Several of these diagnostics are actionable
 - Tuning of emissions can improve speciation
 - $f(\text{RH})$ can in principle be adjusted to reflect measurements; how universal is it?
 - Ditto for prescribed size distributions (up to a point)
 - Assimilation of multi-spectral observations can adjust speciation (up to a point)
 - Assimilation of lidar data can help vertical structure but may not stick when model PBL is too high.
- Others are much tougher
 - There is only so far once can go with bulk aerosol models without explicit microphysics: size and optical properties are not exactly invariant
 - Vertical structure cannot be addressed in isolation of PBL dynamics, injection heights
 - Ditto for removal process (not discussed here) and cloud/precip interactions



GEOS Data Assimilation Update

GEOS Aerosol Observing System

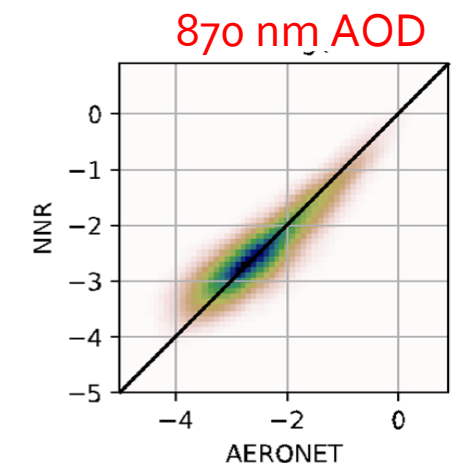
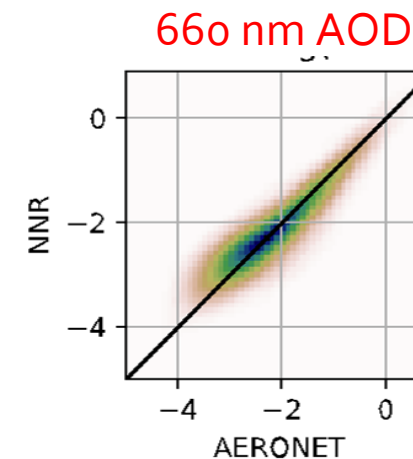
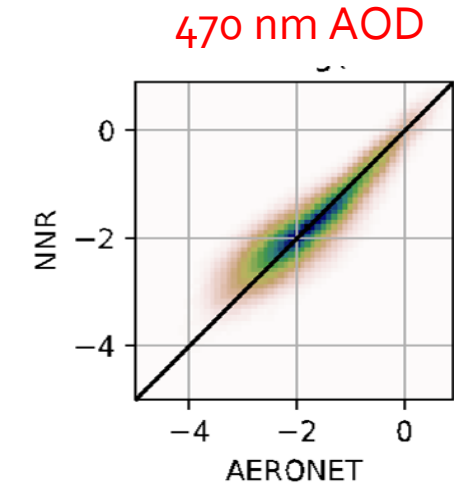
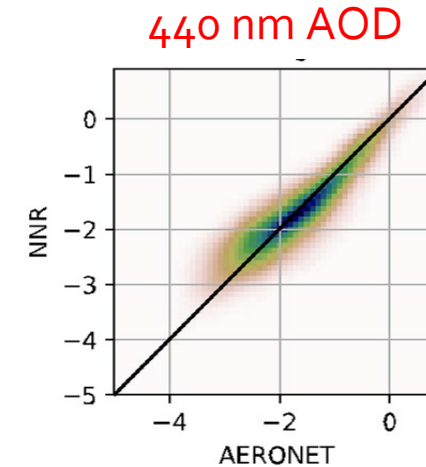


- The aerosol data assimilation problem requires a **homogenized AOD observing system** across different platforms
- Biases between datasets can propagate in the model forecast and lead to **artificial time variability**.

Observing System Homogenization

MODIS

- At GMAO AERONET provides the *calibration reference*
- Originally developed Neural Net retrieval algorithm for bias correction of physical retrievals
- Currently, using multi-channel Neural Net Retrieval (NNR) trained on AERONET
- Multi-channel AOD derived from multi-channel *Level 2 Reflectances*:
 - Generally, can reduce latency for NRT applications
 - No dependency on assumed *aerosol models*
 - Model forecast provides speciation prior



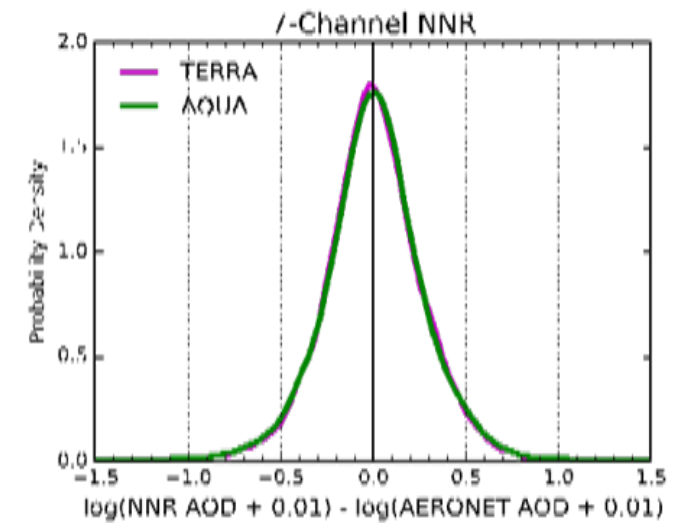
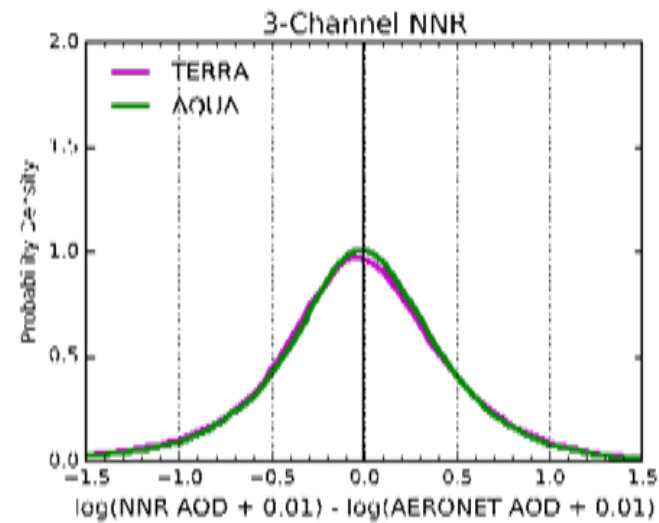
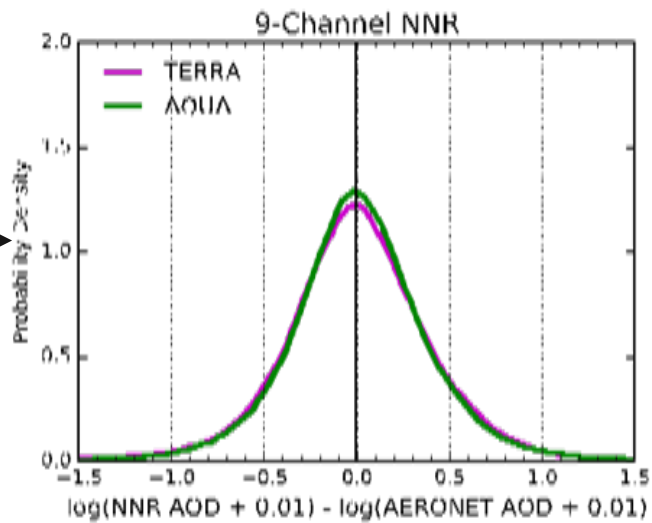
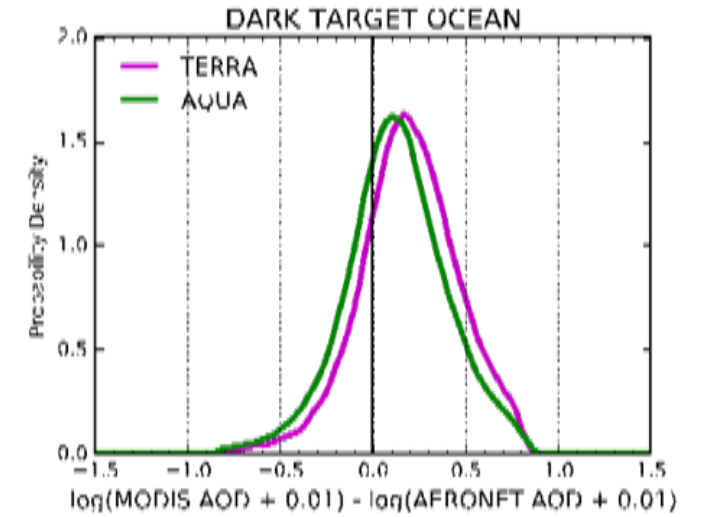
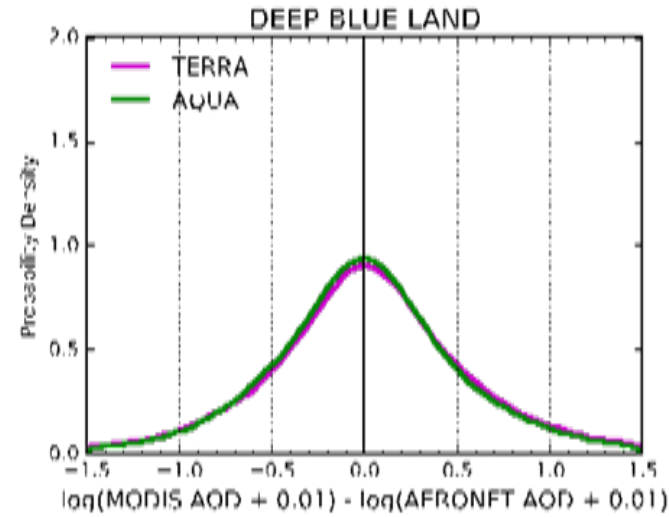
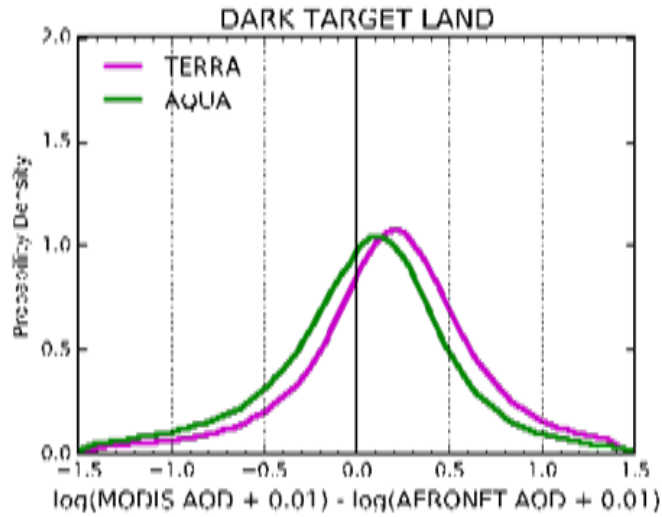


LAND - Dark Surface

LAND - Bright Surface

OCEAN

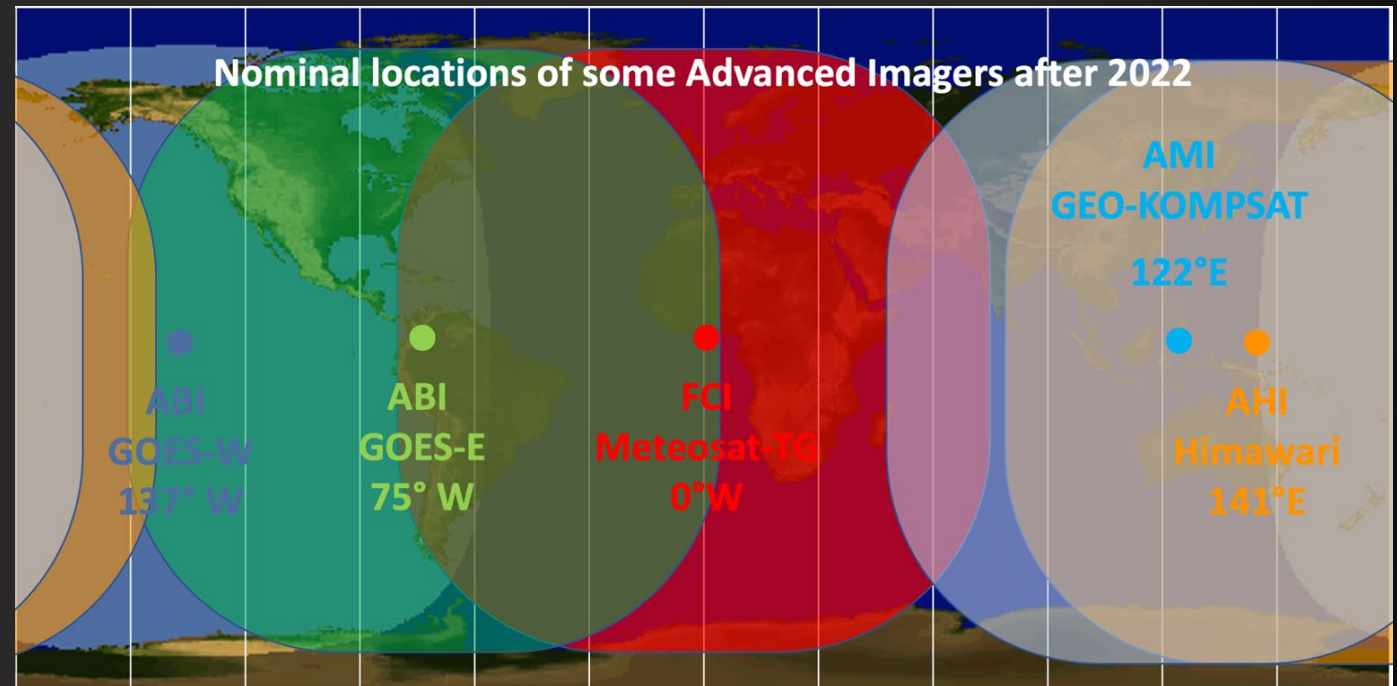
MODIS
Standard
Retrievals



Neural
Network
Retrievals

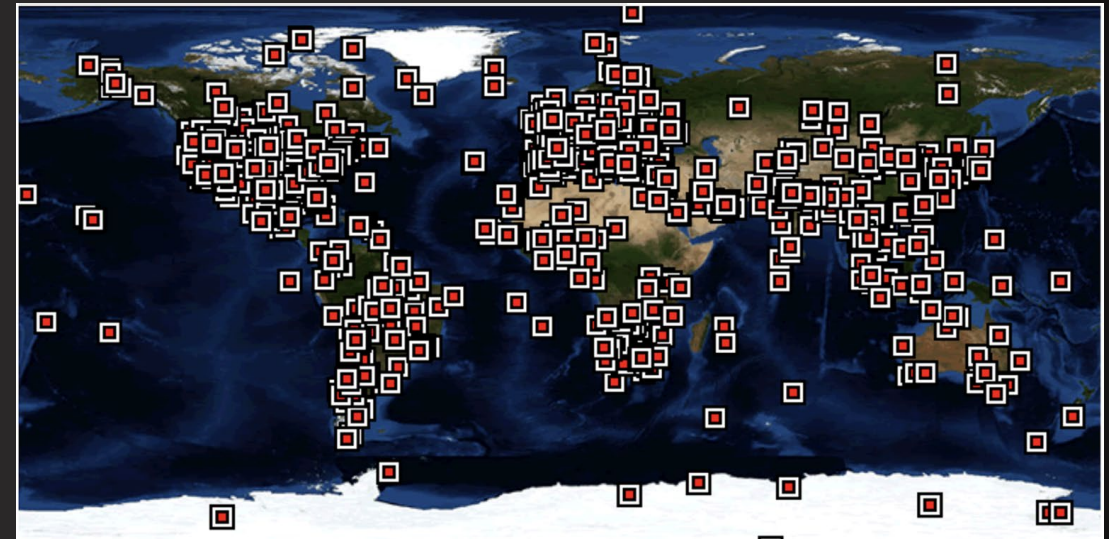
Aerosol Observing System in GEOS

- Current sensors used in GEOS-FP:
 - MODIS
 - AERONET
- Sensors in active development
 - VIIRS
 - Geostationary
 - GOES
 - AHI



Main Limitations of NN AOD Retrievals

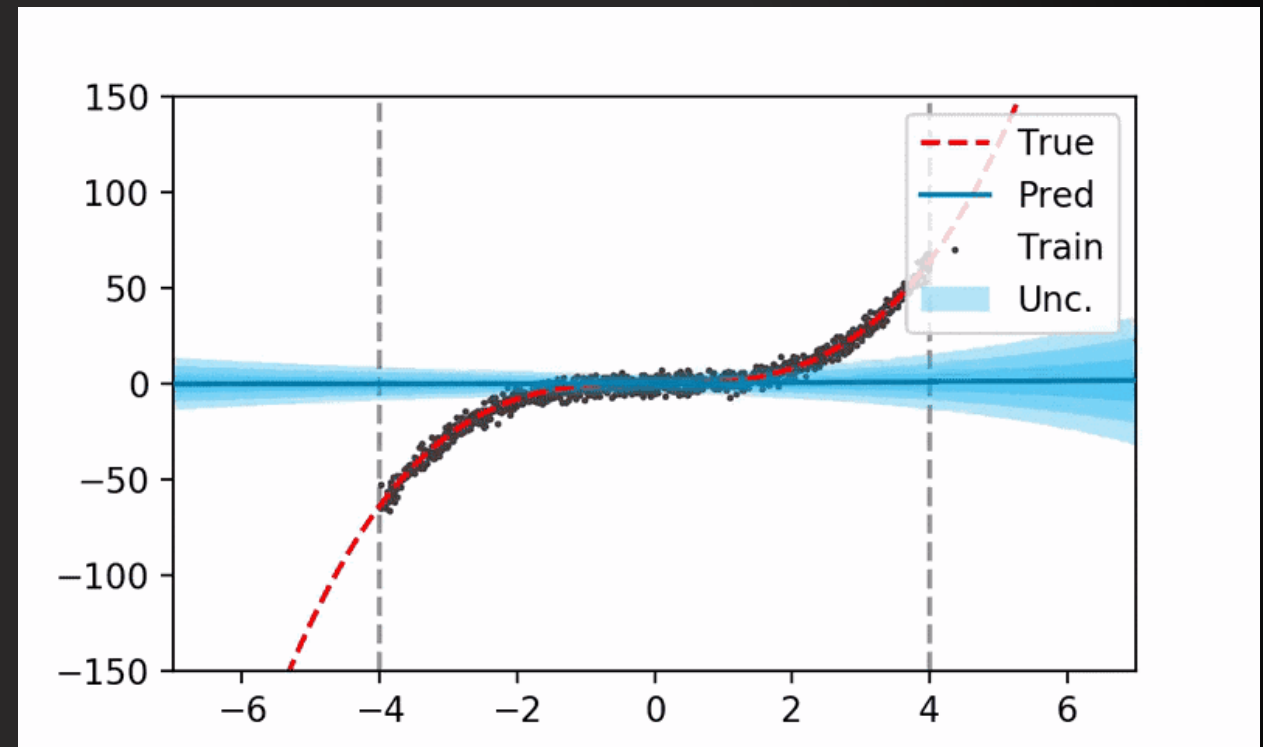
1. Limited by coverage of the training dataset (AERONET)
2. Risk of extrapolation when facing out-of-domain data
3. Lack of *data driven* state dependent error estimates for input into the Data Assimilation system.



In Development: Evidential Deep Learning

All models are wrong, but some — that know when they can be trusted — are useful!
George Box (Adapted)

- Evidential regression simultaneously learns a *continuous target* along with *aleatoric* (data) and *epistemic* (model) uncertainties.
- EDL is able to diagnose *out-of-domain* data (extrapolation)
- EDL provides an essential ingredient for data assimilation: *state dependent observation error estimates*



Amini et al. (2019)

GEOS Aerosol Data Assimilation



- *Current system for Aerosol Analysis: 2D Analysis Splitting*

- **2D-PSAS aerosol analysis with Local Displacement Ensembles**

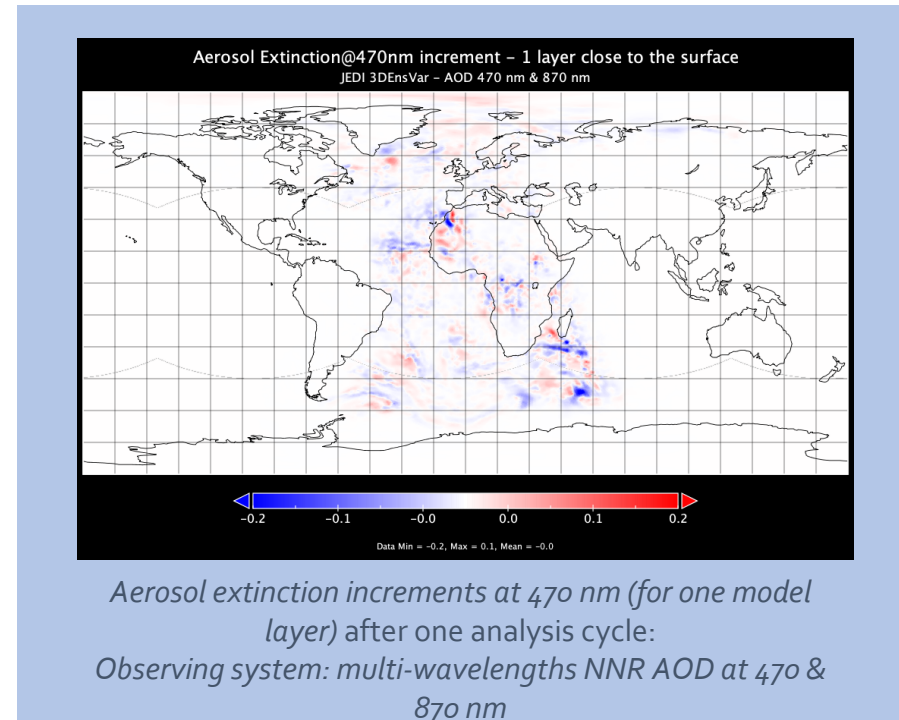
- **control variable:** single-wavelength 2D – AOD (Aerosol optical Depth)
- **observable:** AOD observation at 550nm (NNR)
- single-wavelength AOD measurements primarily constrain the amount of aerosol in a column, with the vertical structure and speciation primarily determined by the specified emissions and the vertical (and horizontal) transport provided by the model.

- *Aerosol Analysis system under development*

- **JCSDA –JEDI hybrid ensemble-variational scheme**

This new scheme brings the flow-dependence in the background error specification inherent in ensemble methods but retains some of the flexibility of variational methods, permitting assimilation of multi-spectral passive and active aerosol measurements.

- **control variable:** vertically resolved aerosol extinction
- **observable:** multi-wavelength AOD (NNR)
- Open doors to future observables: lidar observables, radiances





Summary

- The GEOS model has evolved since 2019 with the addition of scale aware Grell-Freitas deep convection, shallow convection and RRTMG radiation
- The GOCART component has been entirely rewritten for improved efficiency and flexibility and now includes handling of SOA, explicit Brown Carbon Component and updated emissions
- The GEOS aerosol assimilation scheme is evolving toward a JEDI-based hybrid ensemble-variational scheme.
- Additional aerosol observing system under active development includes VIIRS and geostationary reflectance by means of a neural net retrieval.
- Development of the Modal Aerosol Scheme has been dormant since 2019 but it is expected to be revived with increased focus on aerosol-cloud-precipitation processes in support of the AOS mission.



Extra Slides