GEOS Aerosol Update

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Outline

- Recent developments in GEOS aerosol modeling
  - GOCART-2G
  - MAM
- GEOS Aerosol Data Assimilation & Observing System
- Biomass Burning Emissions
  - QFED with VIIRS
  - FILDA, McBEF
- Summary and Outlook

Recent Developments in GEOS Aerosol Modeling

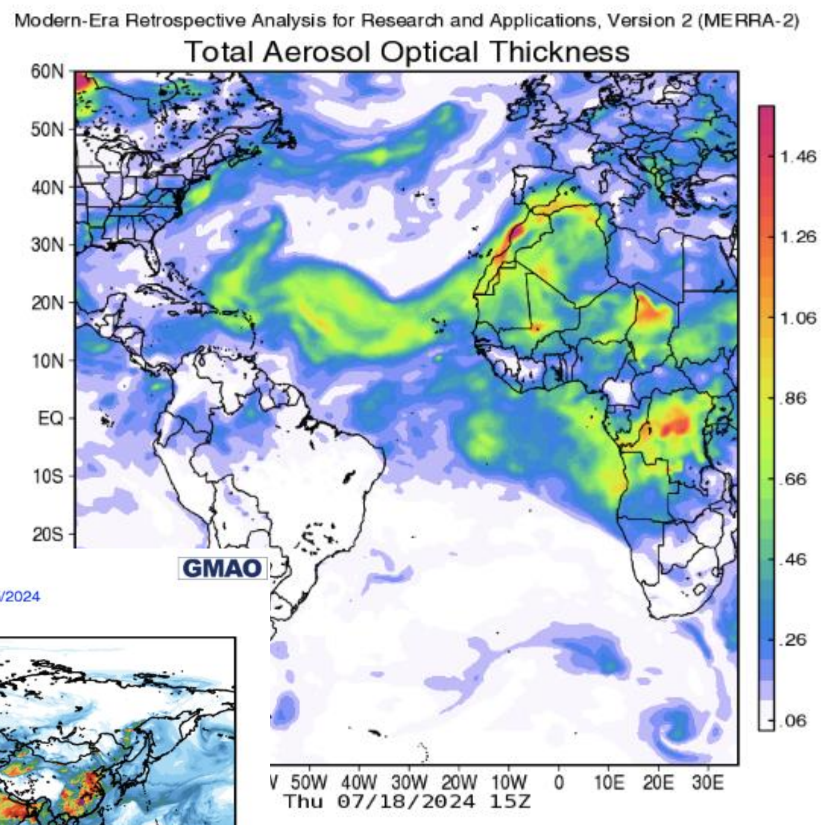
Bulk and modal schemes

GEOS Main Systems

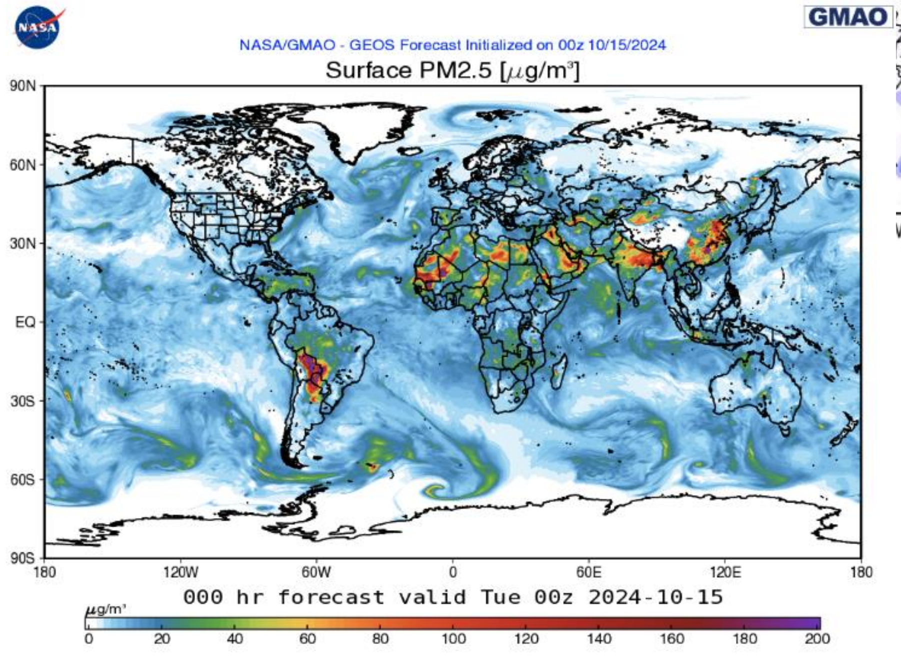
- Aerosols are an integral part of the GEOS forecasting system
- Aerosols runs interactively at the model highest resolution

GEOS products	Purpose	Nominal Res	Aerosol DA
GEOS-FP	Weather/aerosols analyses and forecasts	12 km	√
GEOS-S2S	Coupled system for S2S predictions	50 km	(√)
GEOS-CF	Composition Forecast Full reactive gas chemistry	25 km	(√)
Reanalysis			
MERRA-2	Gelaro et la, 2016, Randles et al., 2017	50 km	√
GEOS-IT	N.R.T analysis system for Instrument Teams	50 km	√
MERRA-21C	Current reanalysis on production	25 km	√

Total AOD at 550nm from MERRA-2



Surface PM2.5 form GEOS-FP



https://fluid.nccs.nasa.gov/weather/

- The prognostic model underlying the data assimilation system is based on the **GEOS earth system model radiatively coupled to GOCART aerosol Module** (recently refactored as GOCART2G (*Collow et al., 2023, GMD*) *(https://github.com/GEOS-ESM/GOCART)*

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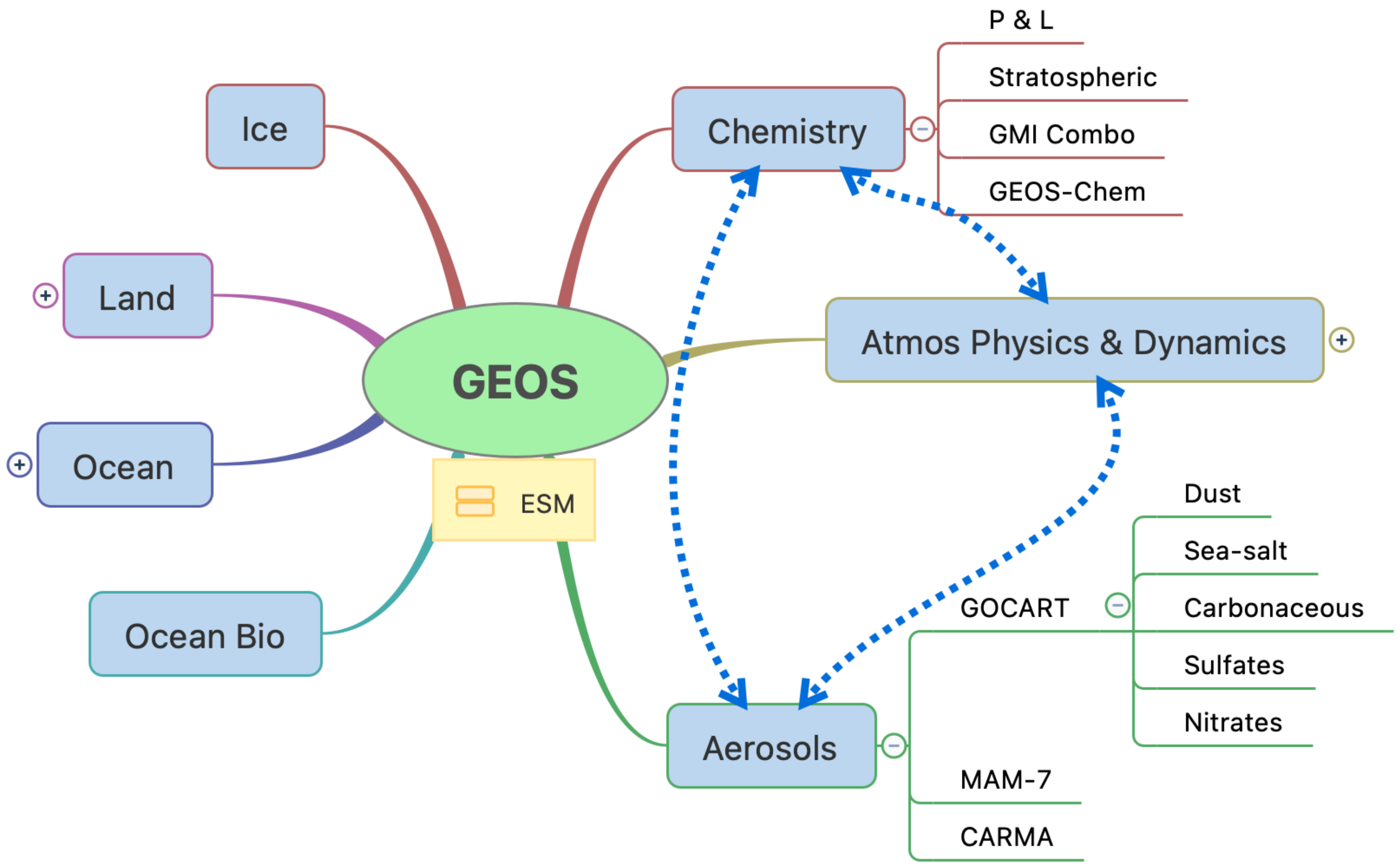
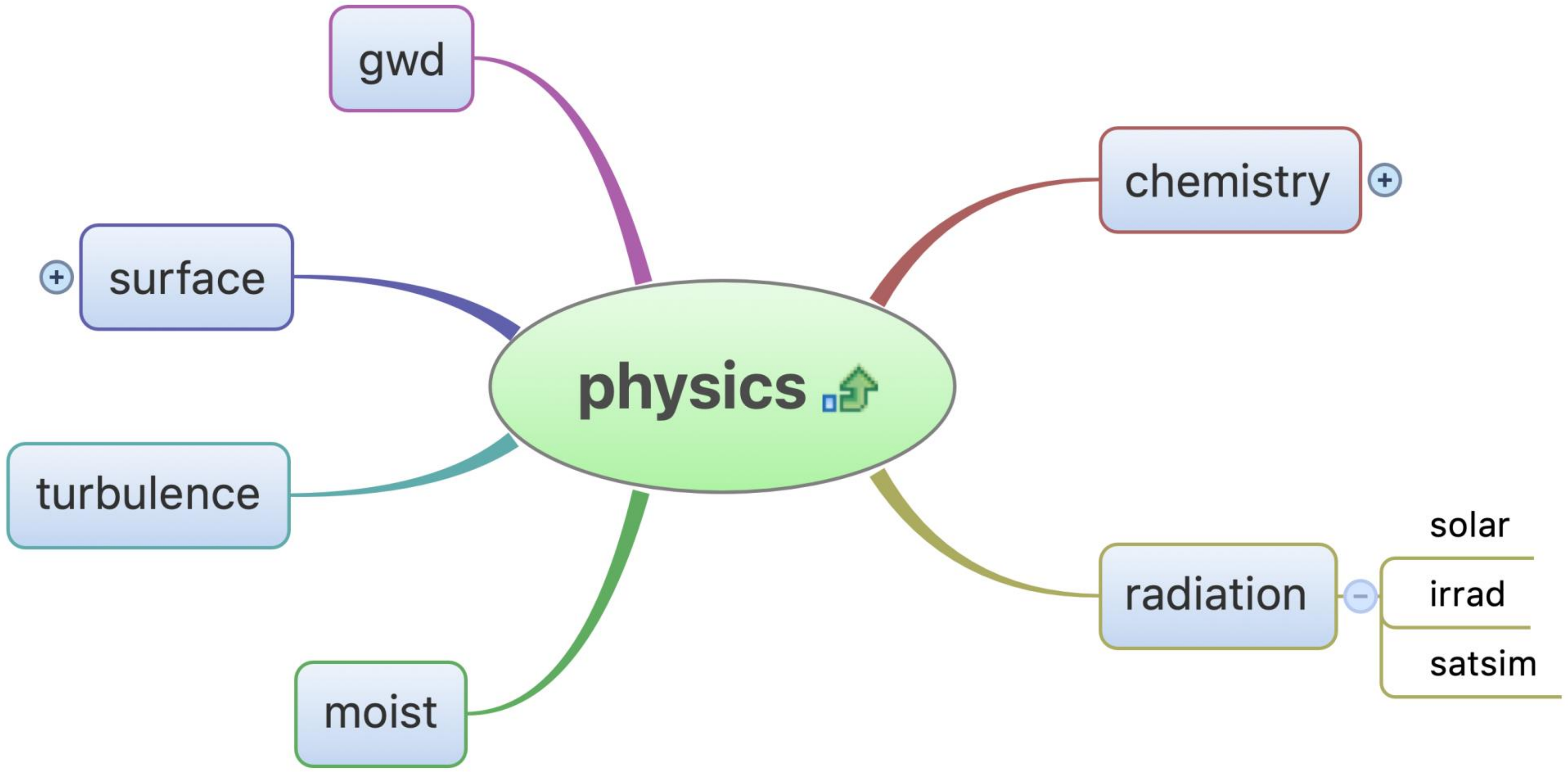
GEOS Earth System Model



- The GEOS-ESM contains all major components of the Earth system
- GEOS is global, running at multiple resolutions
- **Software Architecture**
  - All components coupled with the Earth System Modeling Framework (ESMF), down to physics parameterizations
  - GEOS uses the MAPL usability later for facilitating hierarchical coupling of components
- **Applications of GEOS**
  - NASA reanalyzes
  - Forecasting: NWP, S2S, aerosols, chemistry
  - GEOS analyzes and forecasts provide ancillary information to **NASA instrument teams**
  - GEOS atmospheric composition forecasts play important role in flight planning for **NASA suborbital campaigns**
  - Observation System Simulation Experiments (OSSEs) for support the development of NASA space missions

GEOS Earth System Model



Every entry in this diagram is an ESMF Component

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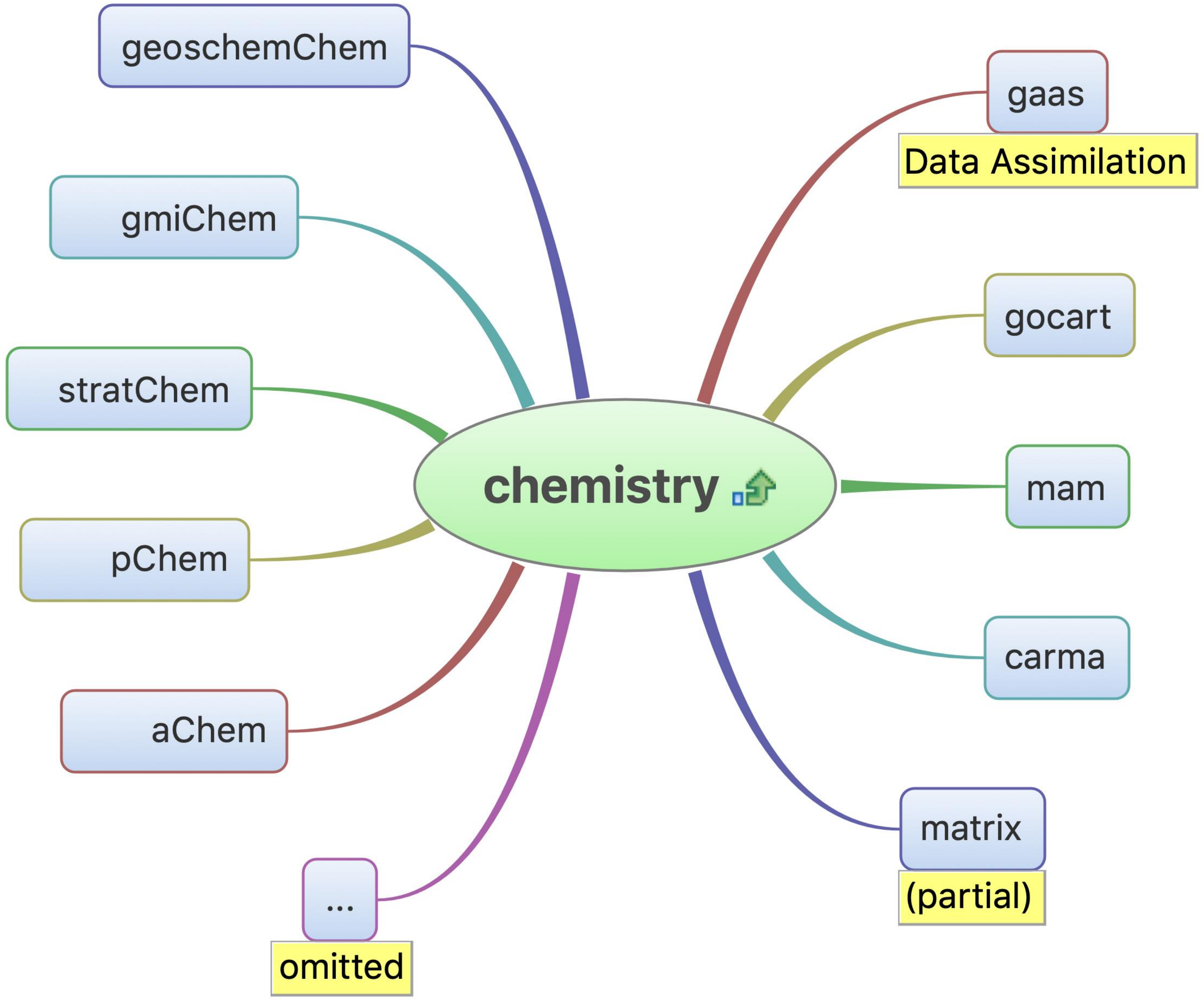

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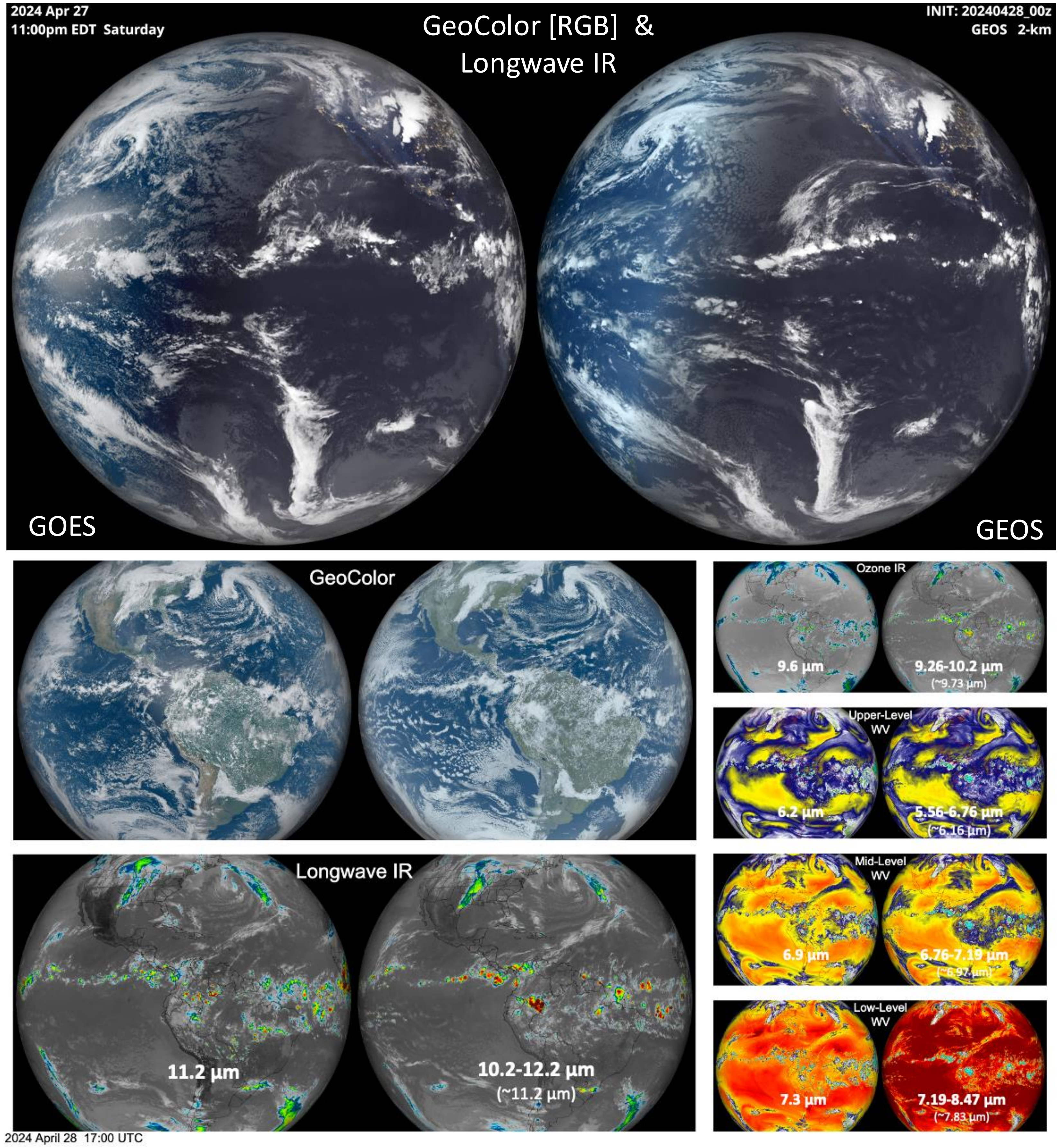
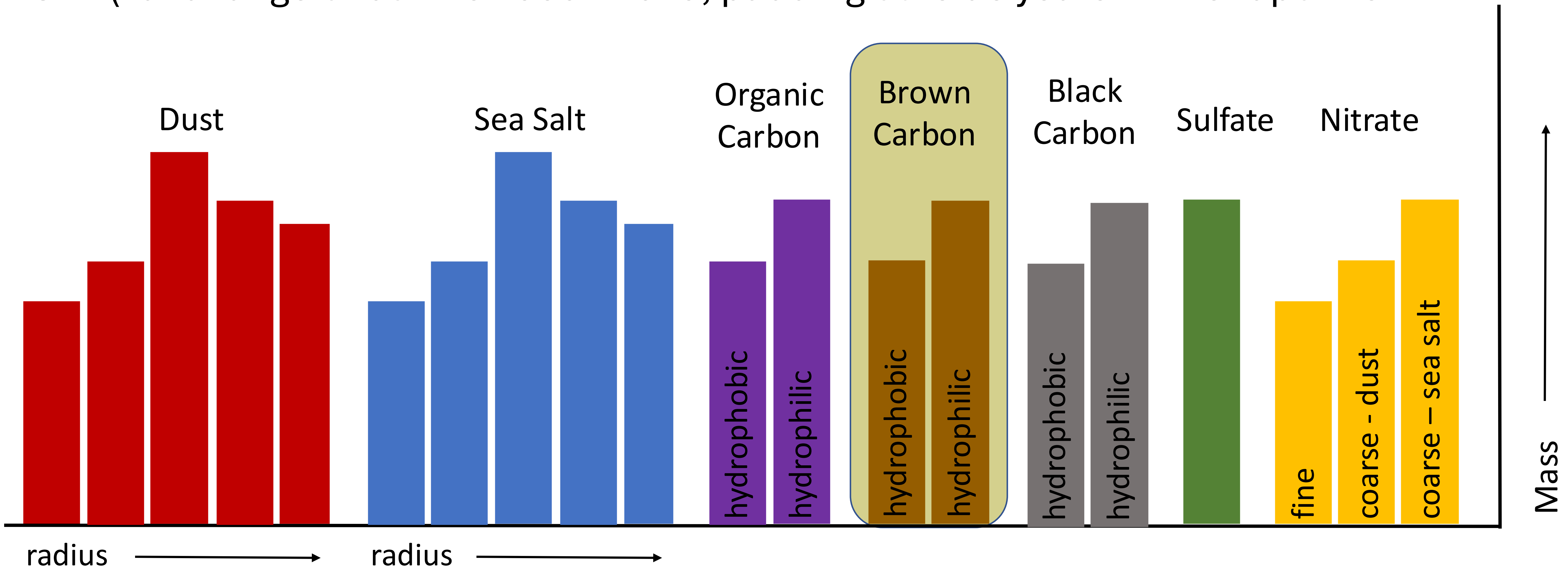
Latest GEOS Modeling Updates

- ✓ Non-Hydrostatic 181L + GWD tuning
  - ✓ NCAR new GWD [background and mountain ridge orographic schemes]
  - ✓ BKG: Richter et al, 2010: https://doi.org/10.1175/2009JAS3112.1
  - ✓ ORO: Scinocca and McFarlane, 2000: https://doi.org/10.1002/qj.49712656802
- ✓ FV3/TRB/GWD/MST/UW [reduce vertical resolution sensitivity]
- ✓ Improved FV3 vertical remapping [stability and performance]
- ✓ RRTMG new orbital settings & diagnostics [RRTMGP Evaluation]
- ✓ GOCART-2G [Improved efficiency and reduced code complexity]
- ✓ GEOS-Chem [accelerated chemistry]
- ✓ GFv2 [Grell-Freitas Deep convective updates and tunings]
- ✓ GFDL-Microphysics [6-phase, single moment]
- ✓ MGB2-Microphysics [6-phase, two moment]
- ✓ New land surface boundary conditions [SMAP and MODIS based]
- ✓ Flexible physics time-stepping
  - ✓ Improved performance at coarse resolution
  - ✓ Improved stability at fine resolution
  - ✓ Better dynamics/physics coupling
- ✓ Coupled MOM6+CICE6 verification with stock Atmosphere
- ✓ WaveWatch III Integration
- ○ SHOC-EDMF Unified Boundary Layer integration near completion



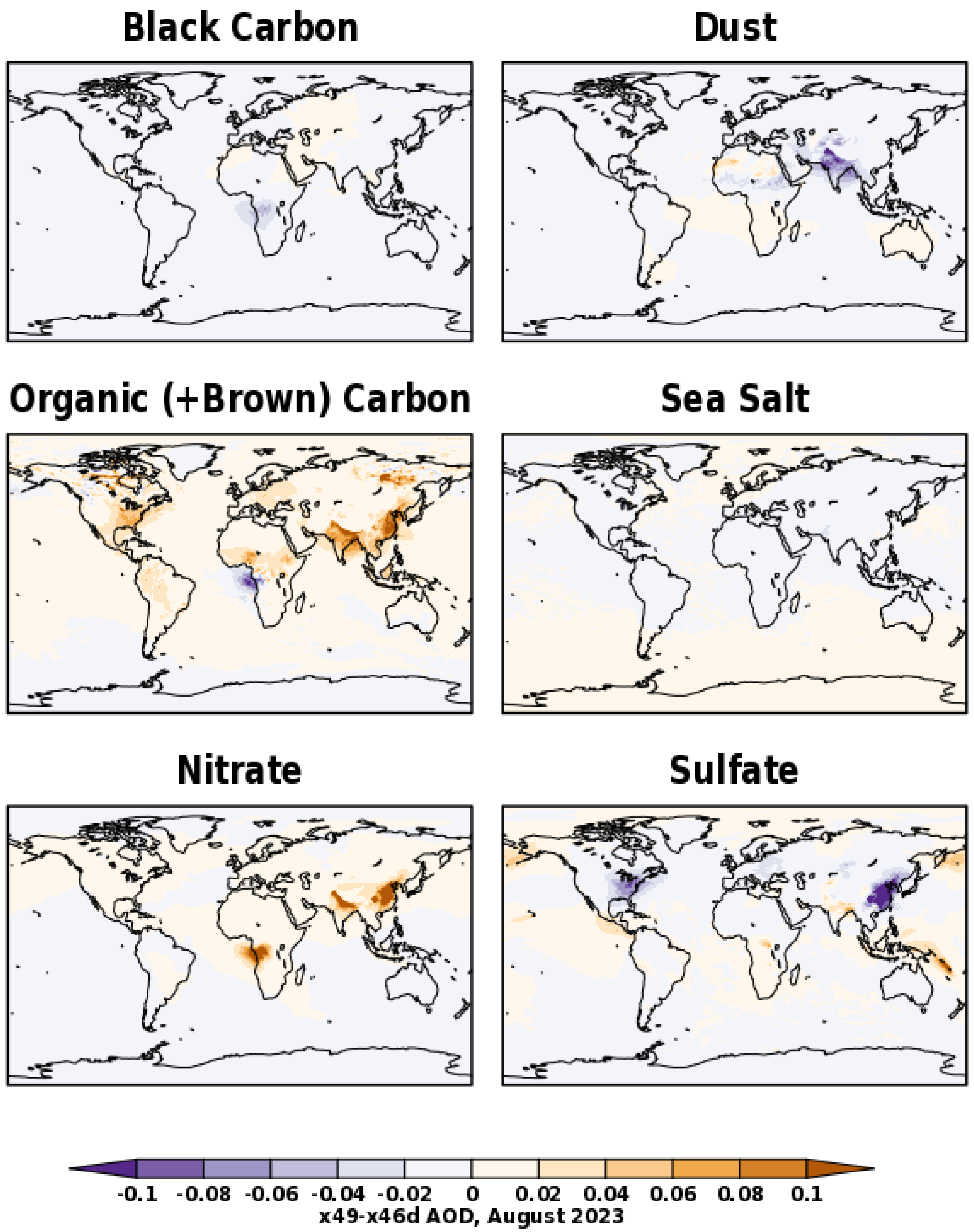
Science Changes Bundled with GOCART-2G

- 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



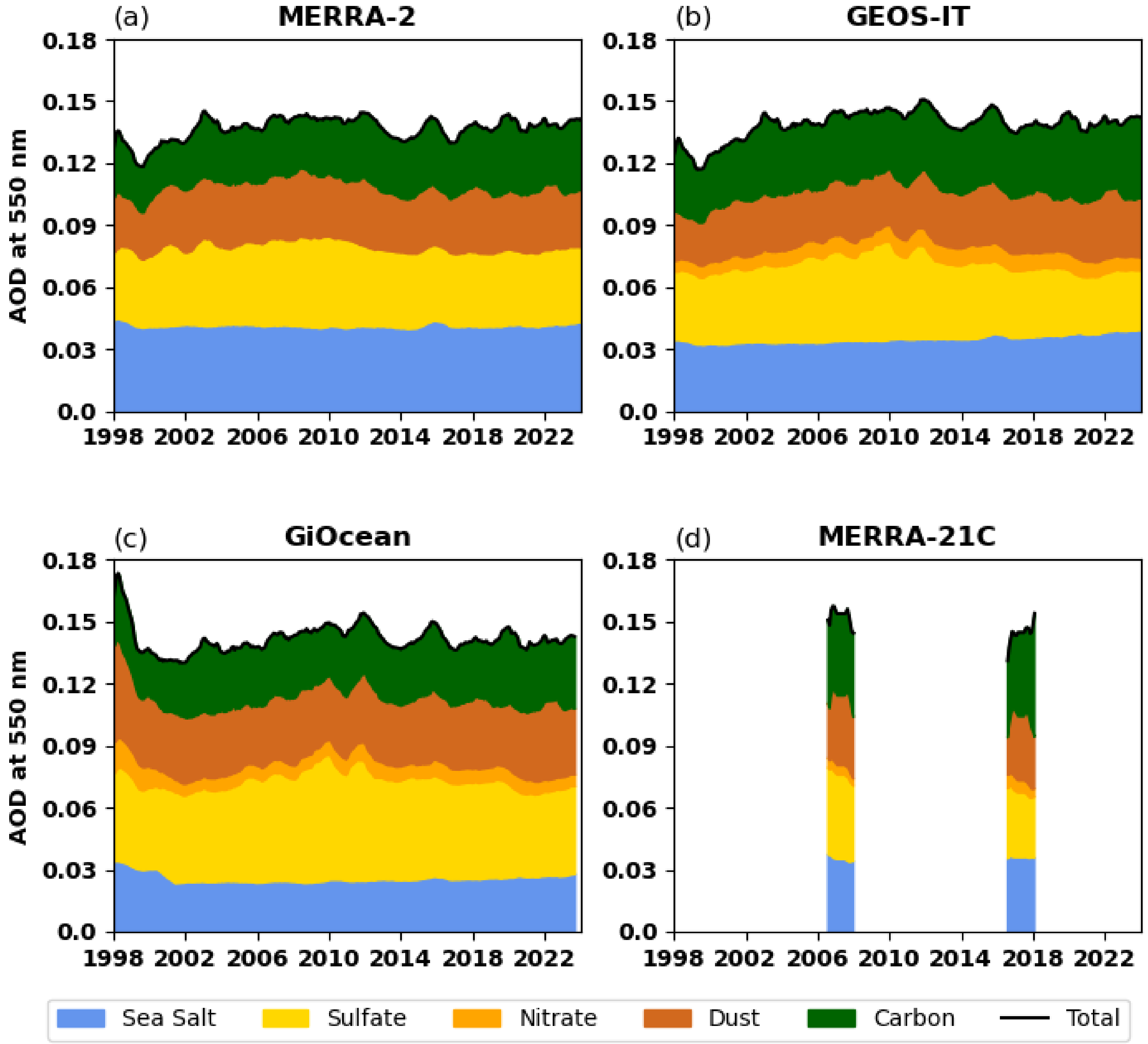
Progress Towards Promoting GOCART-2G to Production

GOCART2G – Legacy GOCART AOD



- GOCART-2G has undergone protocol testing for incorporation in the next version of GEOS-FP, including experiments with a full cycling data assimilation system and the generation of forecasts
- A general increase in carbon occurs in response to the inclusion of brown carbon and secondary organic aerosol
- Other changes, predominantly for nitrate and sulfate, are due to an update in the dataset used for anthropogenic emissions
- It is anticipated that GOCART-2G will be included in the next update for GEOS FP, along with other significant model updates

Aerosols in GEOS Reanalyses

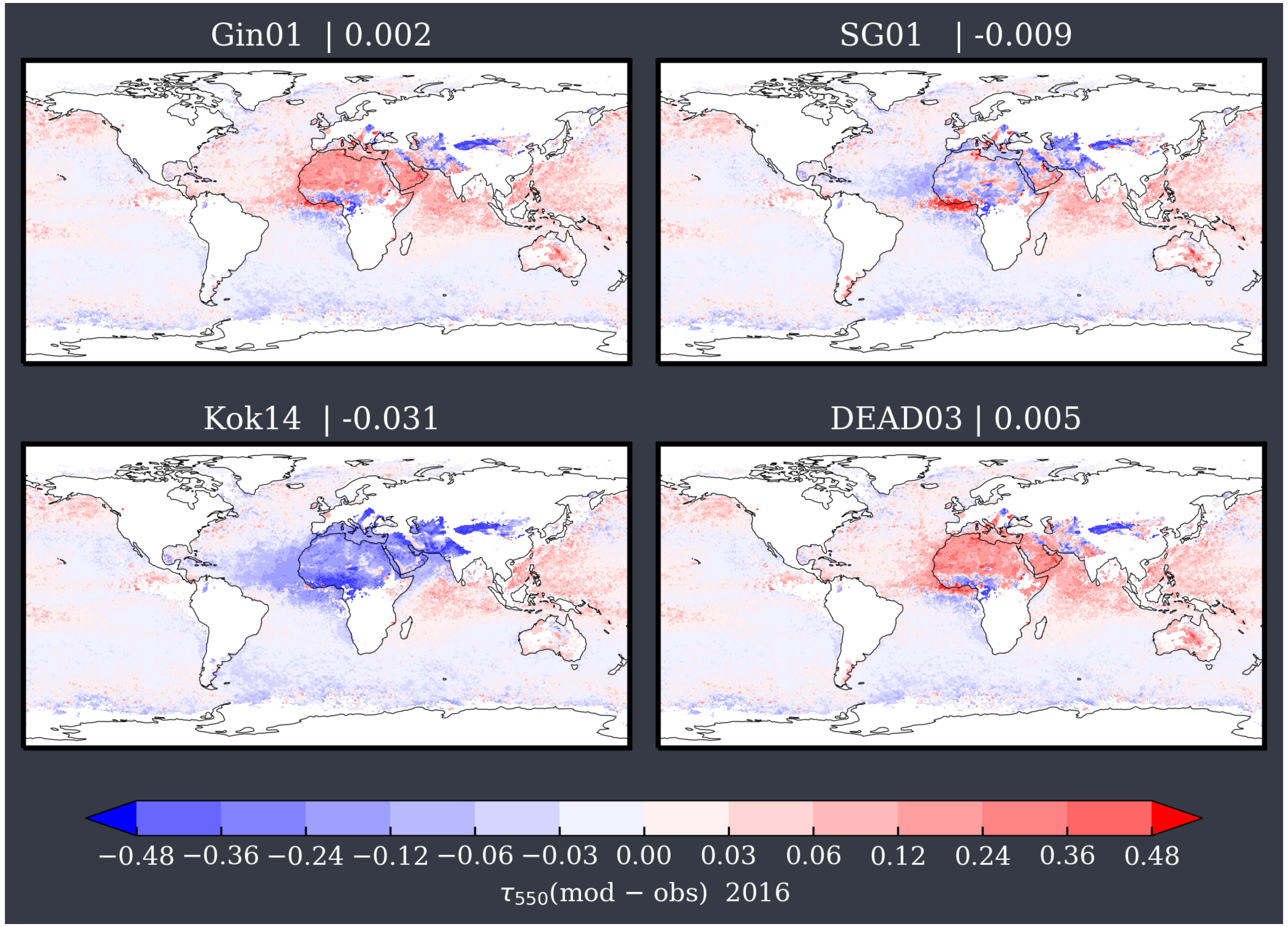


- Each GEOS reanalysis has a unique configuration for representing aerosols
- The Modern Era Retrospective analysis for Research and Applications in the 21st century (**MERRA-21C**) will be the first GEOS operational product to use GOCART-2G
- MERRA-21C will be completed in three streams, covering the period of 1998 through present and is currently in the spin-up phase
- MERRA-21C will also assimilate AOD retrievals not available for MERRA-2 including those produced using MODIS Deep Blue radiances
- Behind the scenes, an emphasis was placed on improving usability of the data through updating metadata, documentation, and adding highly requested output variables such as $PM_{2.5}$

Revisiting the Dust Emission Schemes

- GOCART-2G standard configuration carries 5 size bins of dust
- Several emission schemes are currently implemented
  - Ginoux and its variants
  - Kok 2014
  - DEAD
  - Fengsha (NOAA contribution)
- Recent tweaks
  - Mask for vegetation, snow/ice, and frozen-soil
  - Global tuning constant and dry threshold
  - Model-predicted, rather than fixed, air density

τ_{550} Simulated – NNR Observed



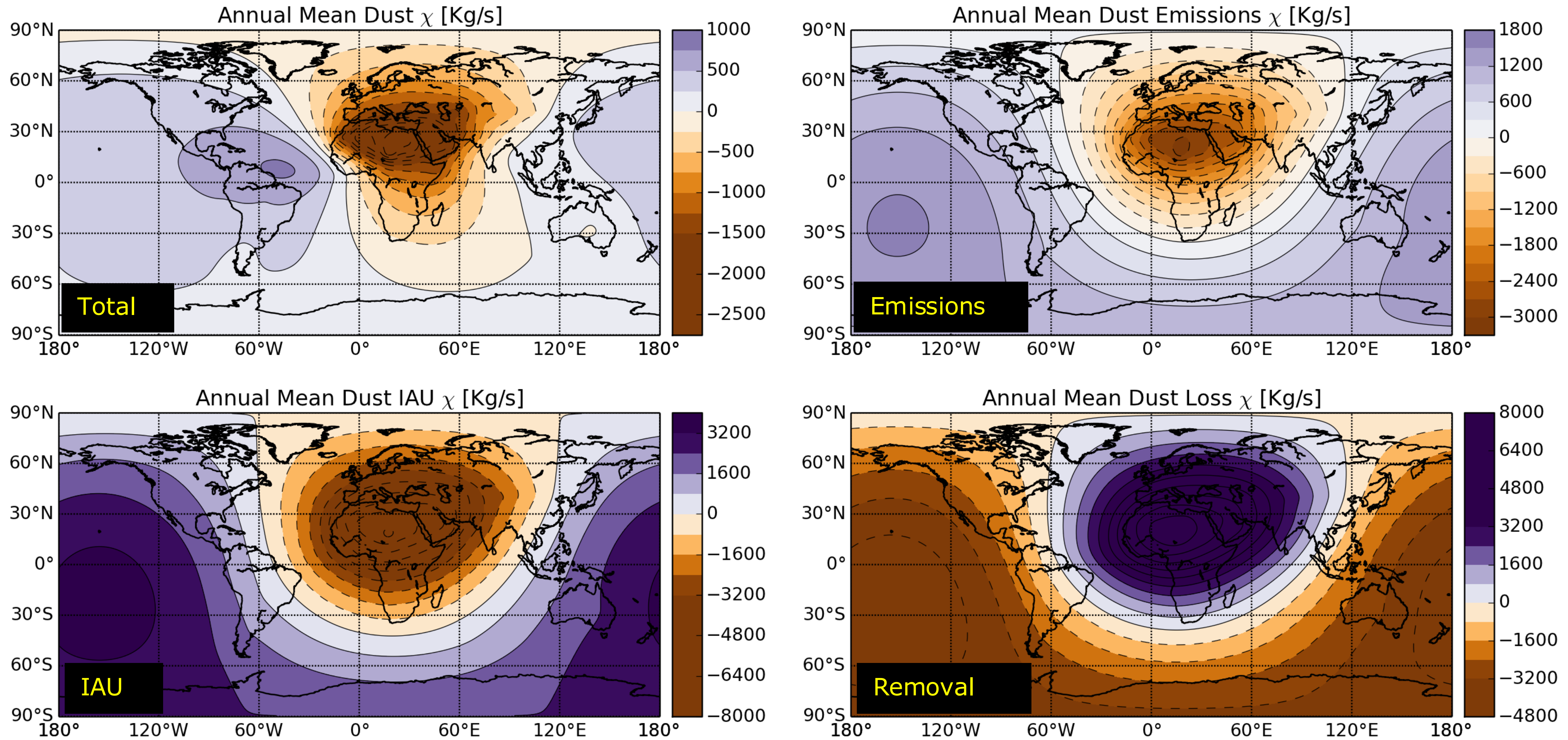
SG01: 'Simplified' Ginoux scheme, Gin01, with dry threshold speed set to 4 m/s

Revisiting the Dust Emission Schemes

- Before any fine-tuning dust AOD simulation from the various schemes show ...
  - Seasonal and regional dependence
  - Underprediction over Taklimakan desert
- Currently undergoing development of systematic tuning mechanism based on the continuity equation

$$\nabla \cdot \overline{\langle \mathbf{u} q \rangle} = \overline{E} + \overline{P} - \overline{L} + \overline{\frac{\langle \Delta q^a \rangle}{\tau}}$$

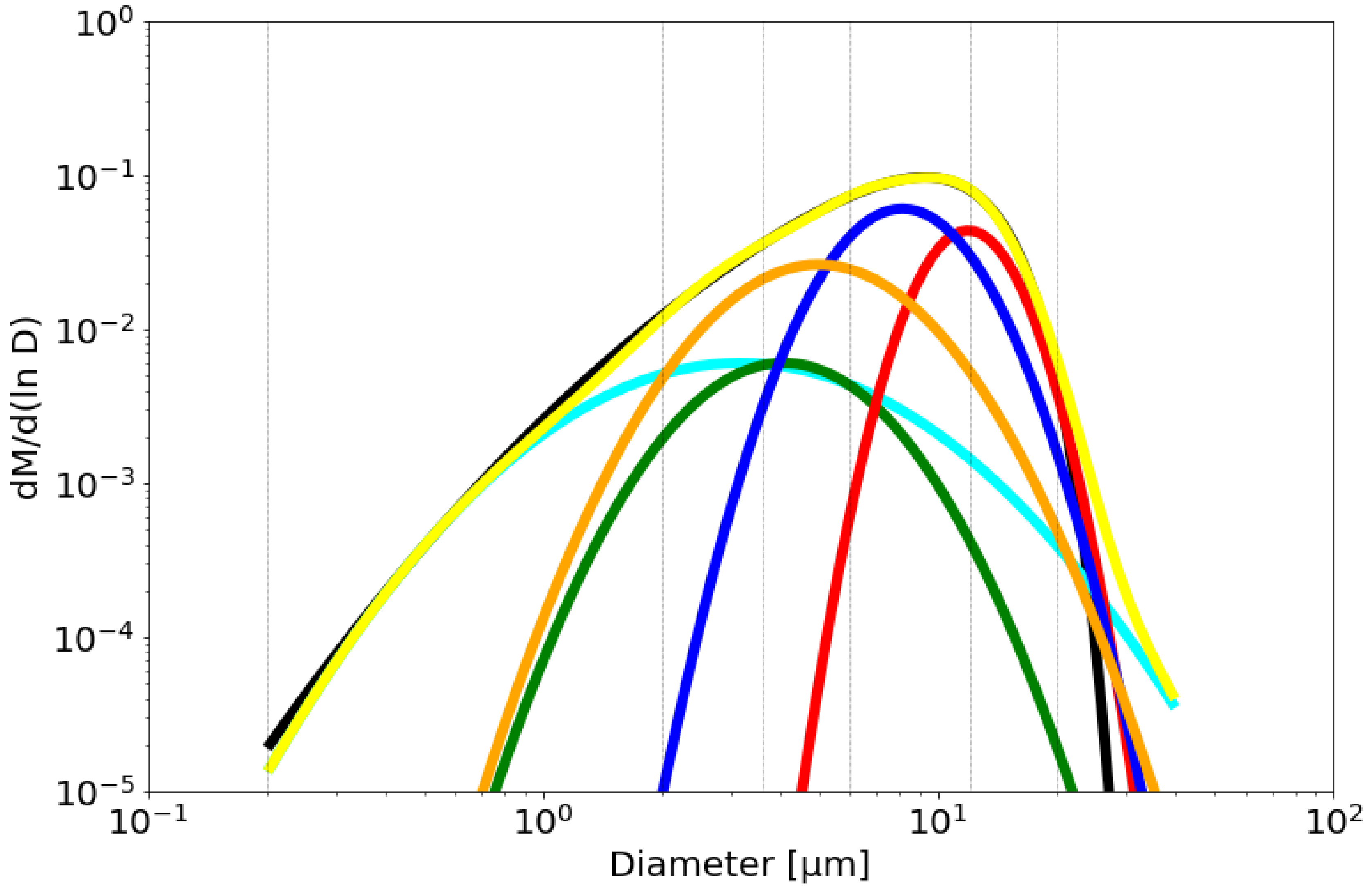
- Tuning of removal processes, away from sources must precede tuning of emissions.



$$\chi = \nabla^{-2}\left[(\overline{E} + \overline{P} - \overline{L} + \overline{\frac{\langle \Delta q^a \rangle}{\tau}}\right]$$

Mass Flux Potential

Modal Approach to Dust Particle Size Distribution



Kok, J. F.: A scaling theory for the size distribution of emitted dust aerosols suggests climate models underestimate the size of the global dust cycle, Proc National Acad Sci, 108, 1016–1021, https://doi.org/10.1073/pnas.1014798108, 2011.

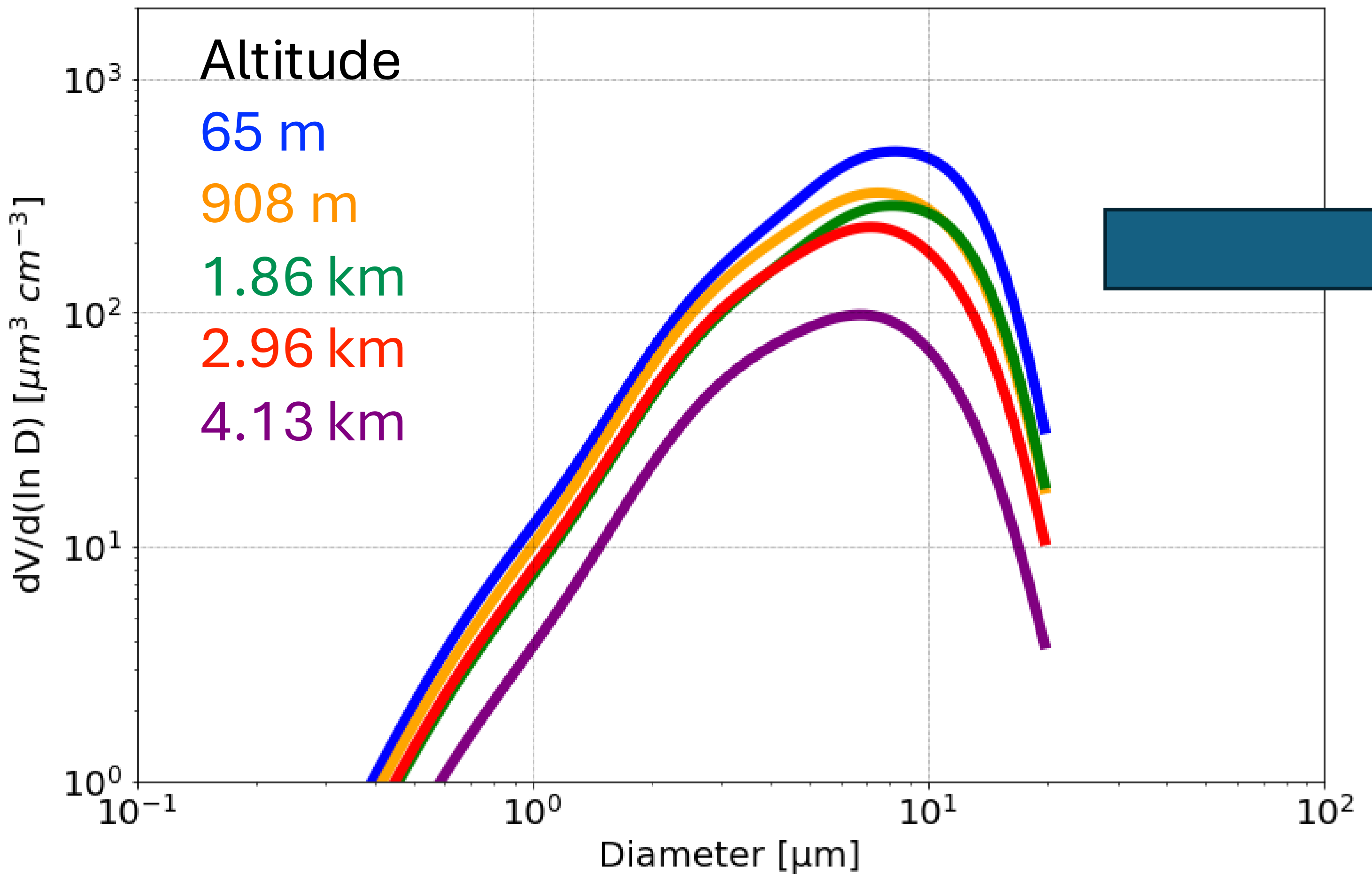
- Assume a continuous function at emissions (Kok 2011, **black line**)
- Fit a series of lognormal modes to describe this distribution
- This allows a smoother representation of the particle size distribution and optical properties versus the piecewise bin approach used currently

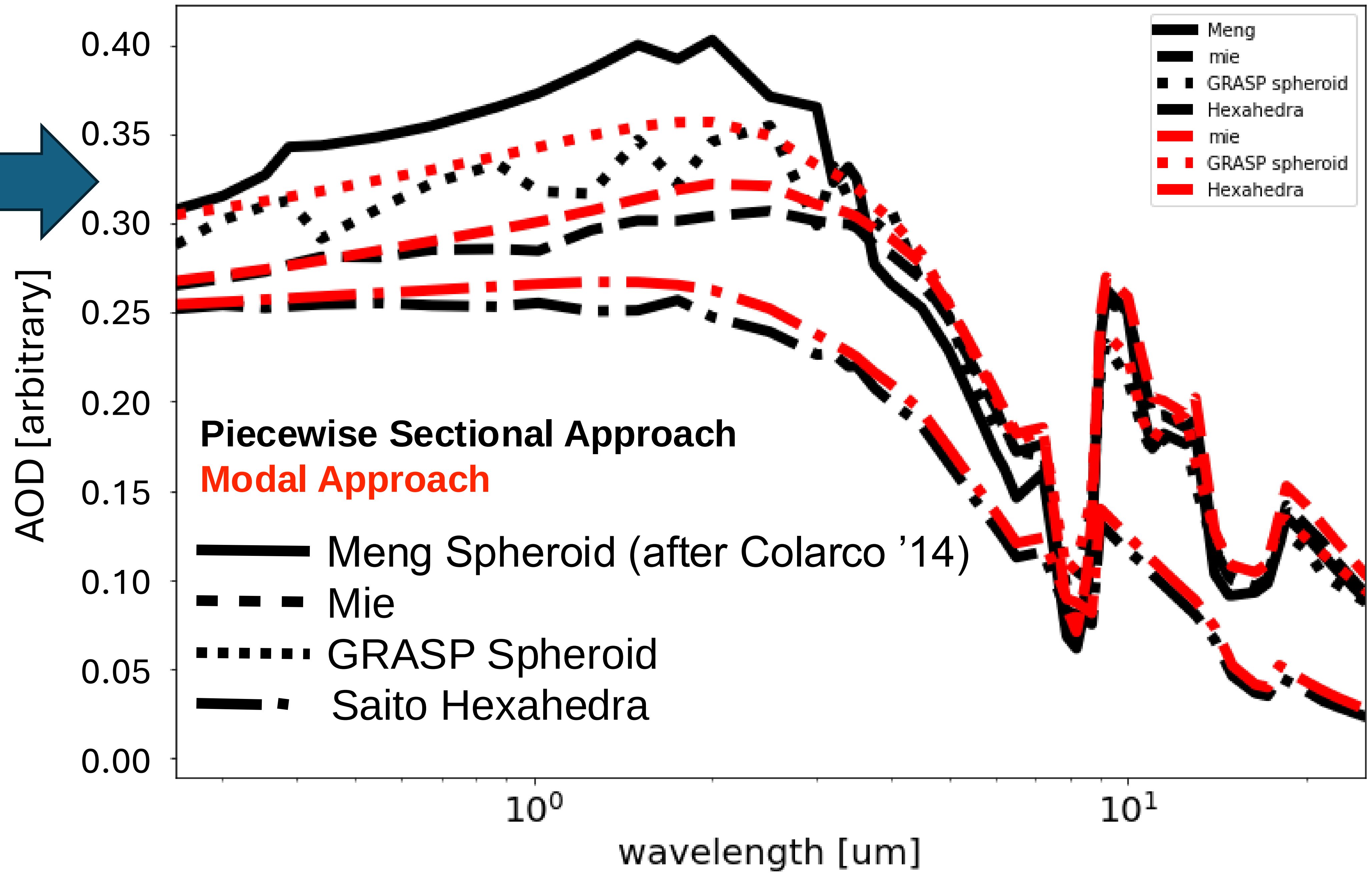
Slide credit: Pete Colarco

Modal Approach to Dust Particle Size Distribution

Simulated dust PSD

September 22, 2022 @ 3km, near Cape Verde



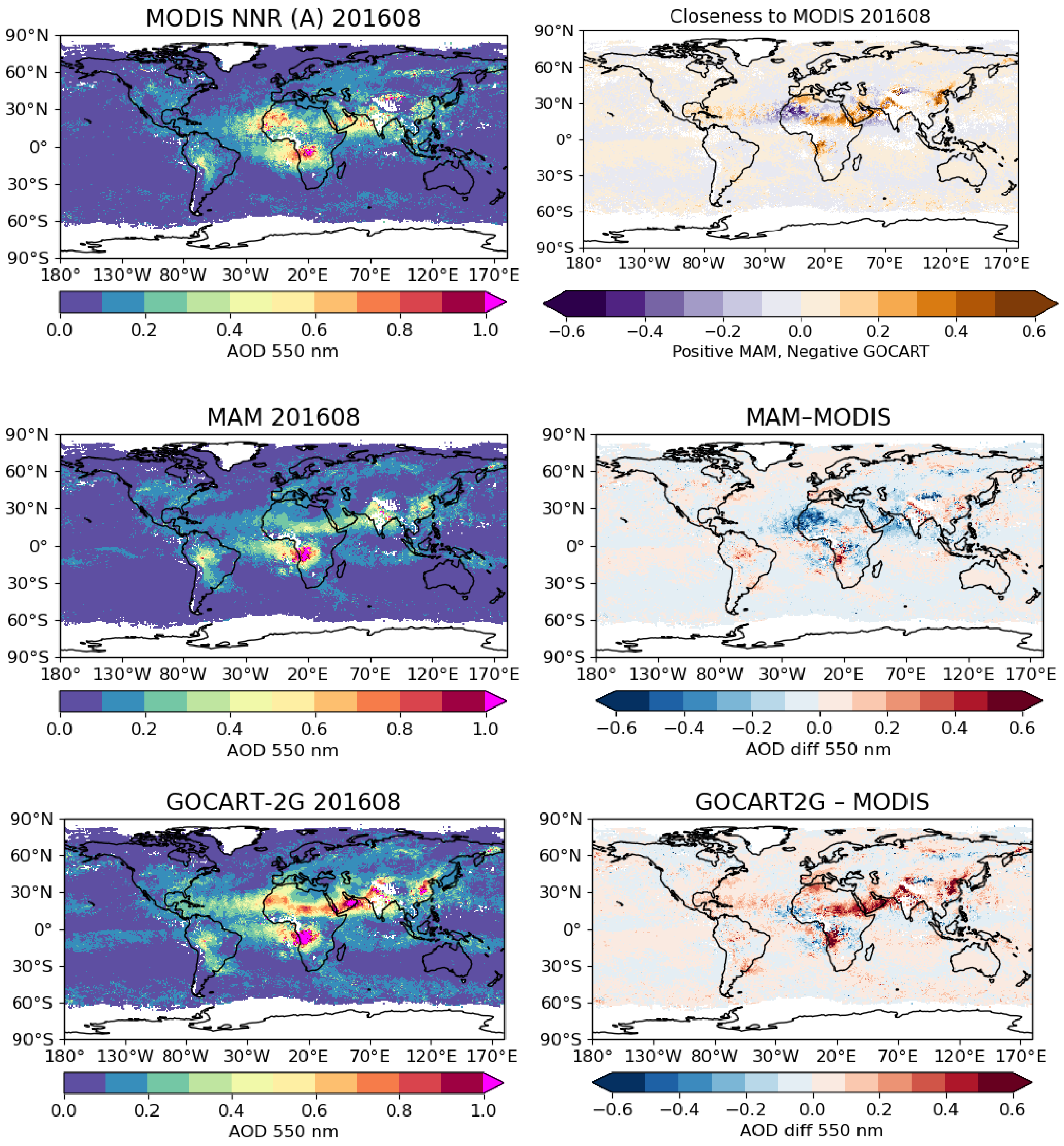


Modal approach to distributing dust into our five size bins results in a **smoother representation of integrated dust optical properties**

Slide credit: Pete Colarco

Modal Aerosol Module (MAM) within GEOS

- Efforts are underway to revive the MAM scheme within GEOS and to bring it up to speed with the current GEOS model version
- **GEOS (v11.6.0) replay to MERRA-2** experiments were set-up at c180 resolution such that GOCART-2G and MAM aerosol schemes are run in parallel with similar aerosol and gas emissions.
- POM:OC ratio was changed from 1.4 to 1.8 to align with the assumptions within GOCART-2G
- The run period was chosen as **July-September 2016** to allow evaluations using ATom1 and ORACLES-I observations in addition to satellite retrievals.
- Comparisons to **MODIS (Aqua) NNR retrievals** for **August 2016** are depicted here, with **MAM AOD being closer to observations for most of the globe**, especially over dust source, east Asian pollution and southern African biomass burning regions.

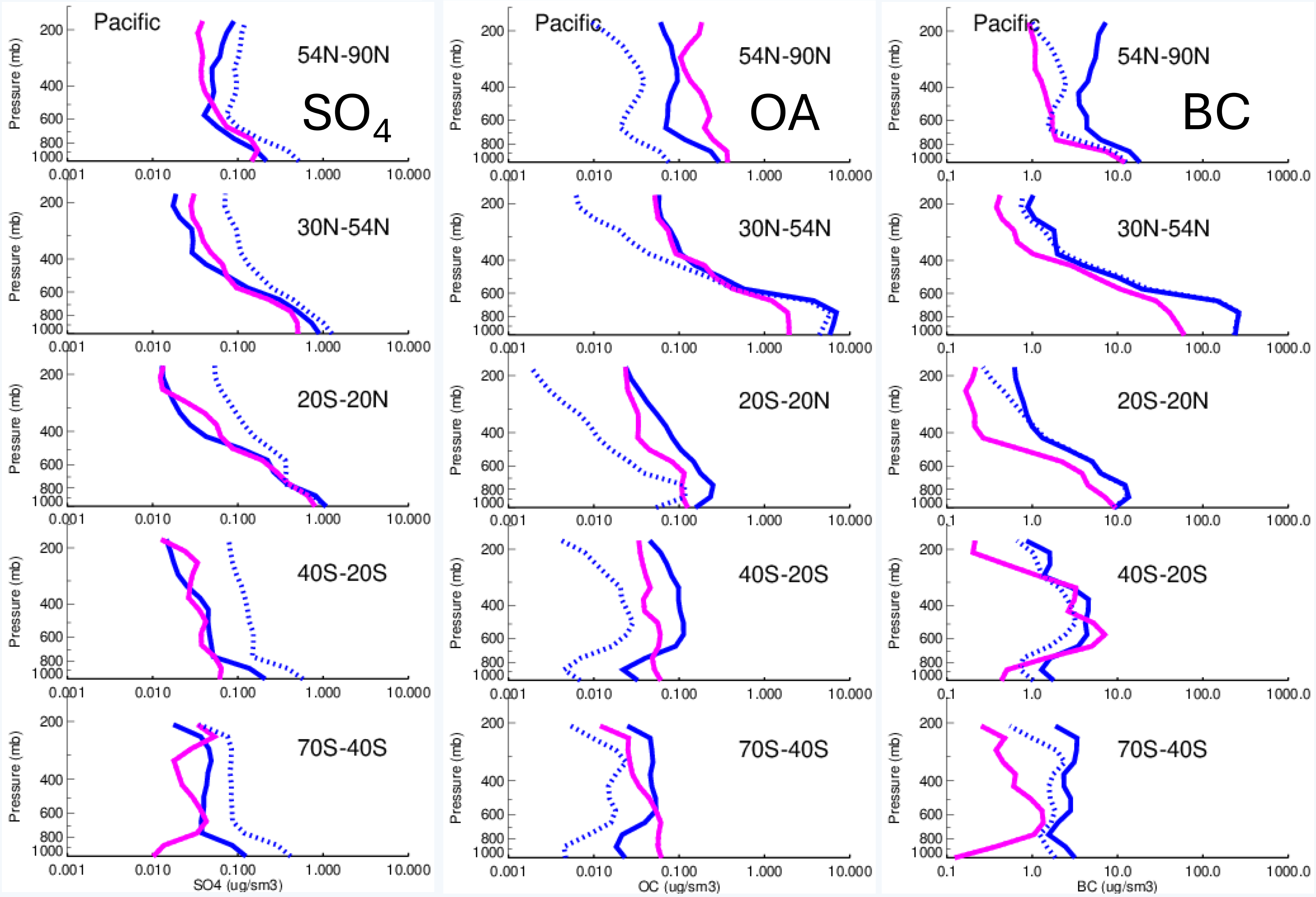


Slide credit: Sampa Das and Huisheng Bian

MAM: Comparisons to ATom1

GOCART2G
MAM
ATom1 PALMS

MASS (μg/sm3)

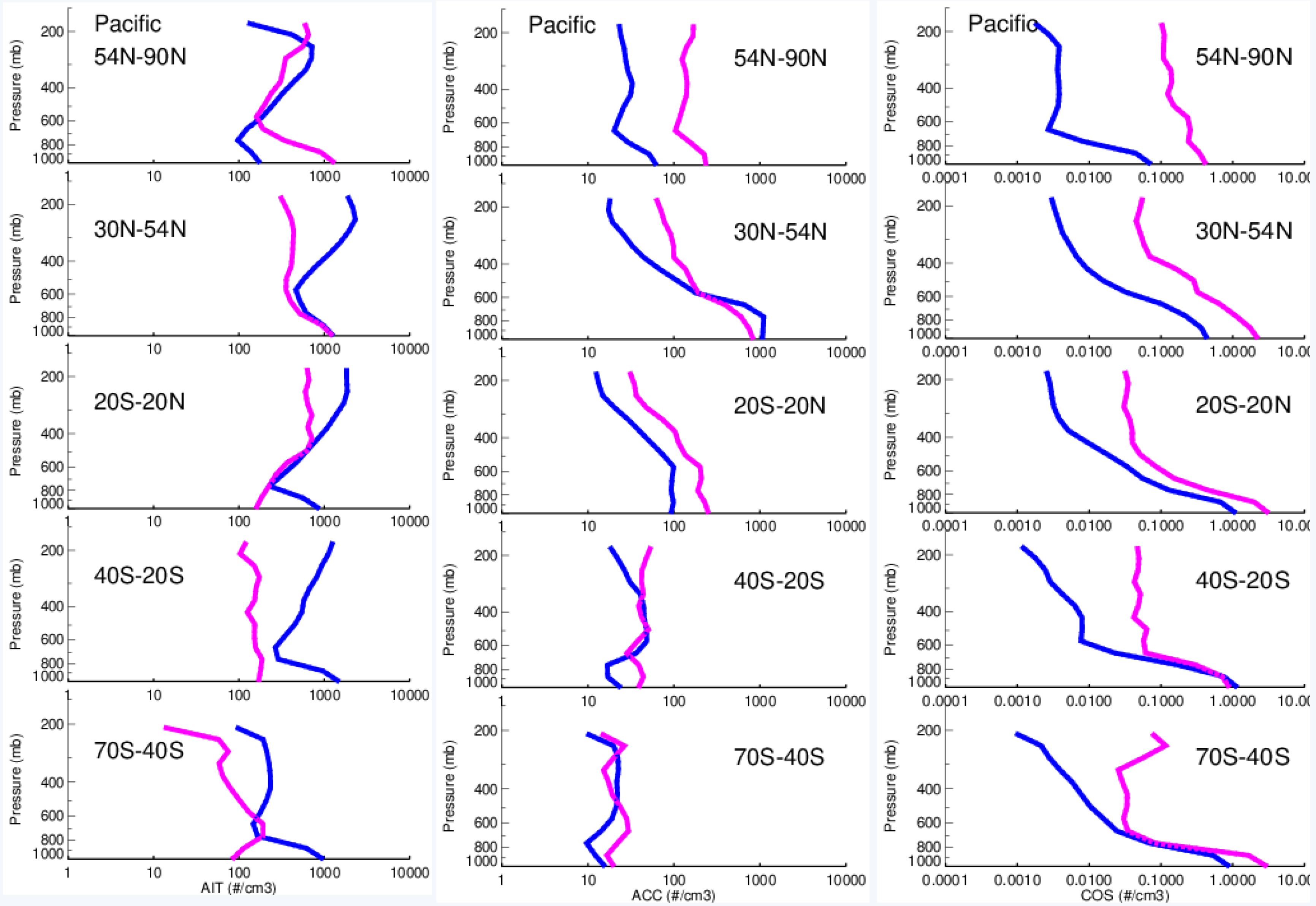


- ❑ MAM SO4 is consistently higher, OA is consistently lower, while BC is closer compared to GOCART-2G simulations and PALMS observations.
- ❑ Higher MAM SO4 is possibly due to higher DMS component.

MAM
ATom1 AMP

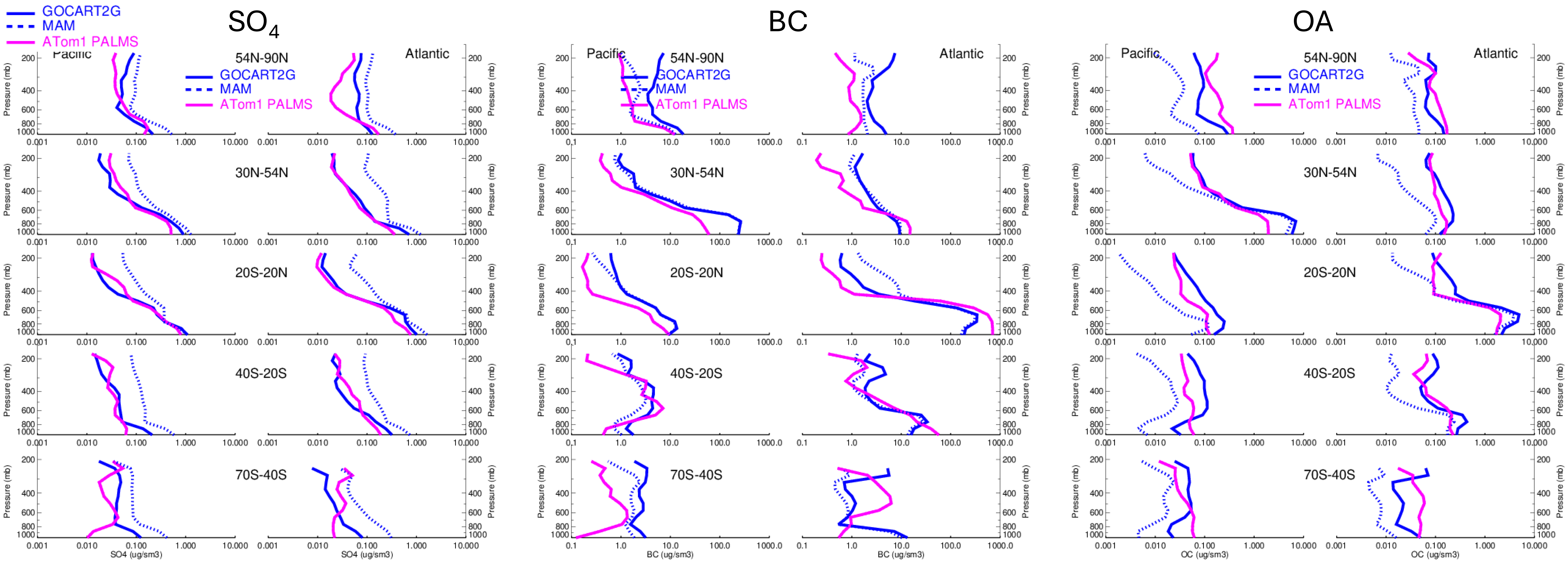
NUMBER (#/cm3)

AIT (0.012–0.06 μm) ACC (0.06-0.5 μm) COS (0.5-4.8 μm)



- ❑ Compared to AMP observations, MAM aerosol number concentrations are consistently higher in the Aitken mode (AIT), consistently lower in the coarse mode (COS), and closer in the accumulated mode (ACC).

MAM: Comparisons to ATom1



- Sulfate is consistently higher in MAM compared to both GOCART-2G and PALMS observations possibly due to higher DMS component.
- MAM OA (organic aerosol) on the other hand are consistently lower than observations barring over Atlantic (20N-20S)
- MAM BC profiles are in closer agreement with GOCART-2G and observations, compared to other aerosol species.

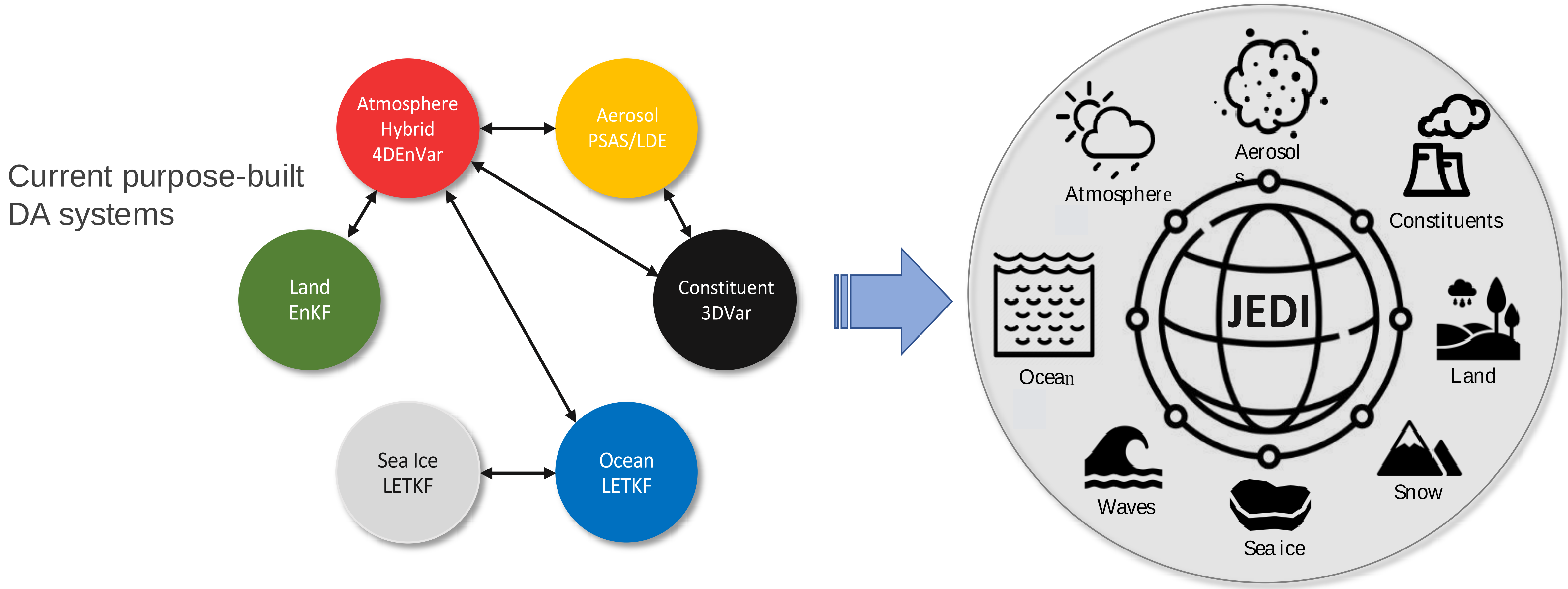
Slide credit: Sampa Das and Huisheng Bian

Aerosol Data Assimilation & Observing System Homogenization

JEDI based Data Assimilation and NNR Multispectral AOD Retrievals

The context for JEDI at GMAO

GMAO is developing a unified coupled data assimilation system based on the GEOS model and JEDI, for weather analysis and prediction, reanalysis, composition forecasting, and S2S prediction.



- Eliminate GMAO's dependence on legacy, purpose-built assimilation systems
- Use coupled models to exploit the full range NASA's diverse set of Earth-system observations
- Capitalize on JEDI's multi-agency adoption to accelerate R2O transition of NASA's observations

GEOS JEDI Aerosol DA Status

Observation operator for multi-wavelength AOD developed and merged into JEDI/UFO

- ✓ Developed using multi-wavelength extinction profiles (2 or 3) as the control variable
- ✓ Updated with log option (AOD closer to log-normal distribution)
- ✓ Updated with an option to select which observation wavelengths to simulate

IODA Python App

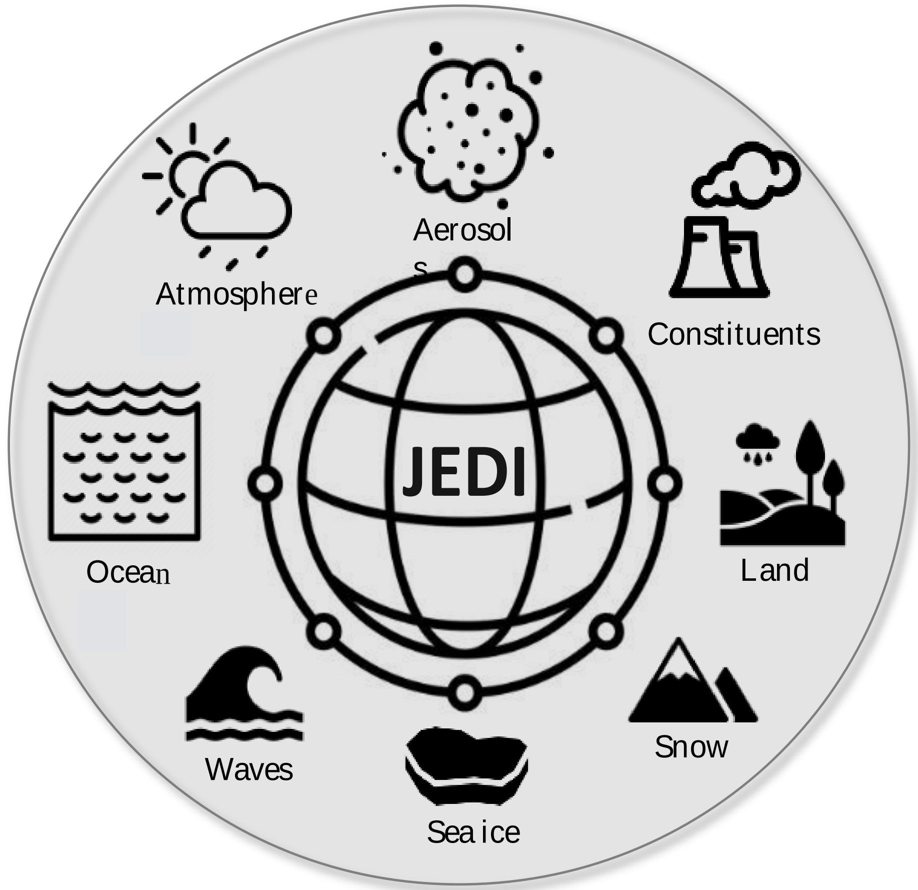
- ✓ Conversion of current native aerosol observation to JEDI/IODA format
- o Integration into current NNR codes to include model information for quality control; ongoing

Quality control of aerosol observations

- Current quality control for aerosols in GEOS-FP is not available in the JEDI framework
- o Background and buddy-check codes are being written in Python performed outside JEDI; ongoing

Cycling the model with the JEDI-based DA system

- Model extinction profile control variable
  - ✓ Multiple-λ extinction profiles available in refactored and more flexible GOCART-2G aerosol module; completed
- Updating current GAAS modules inside GEOS model
  - o Transform of extinction increments into mass mixing ratio required by the model; requires development



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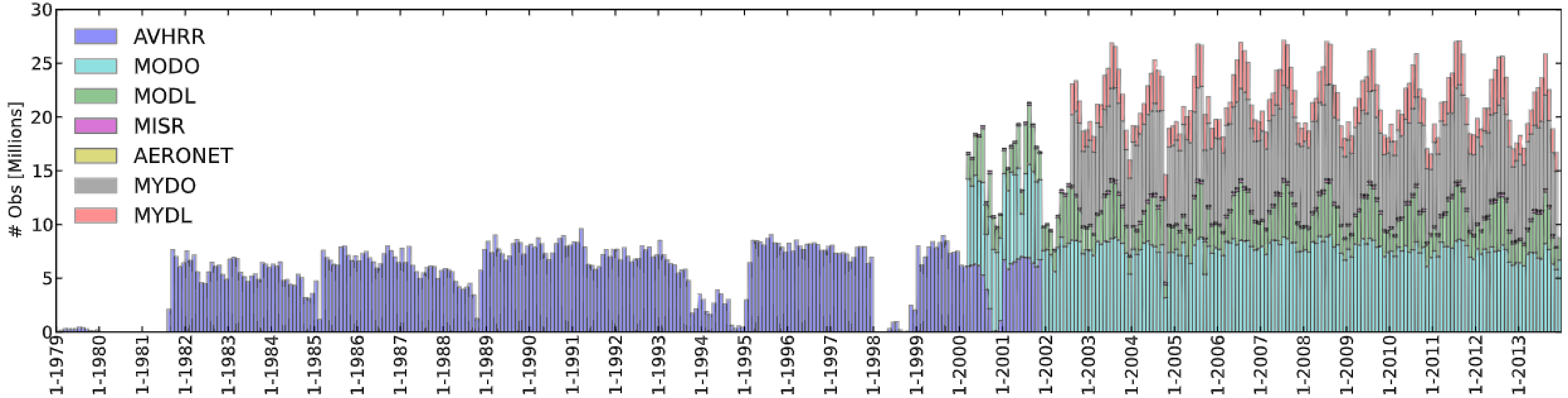
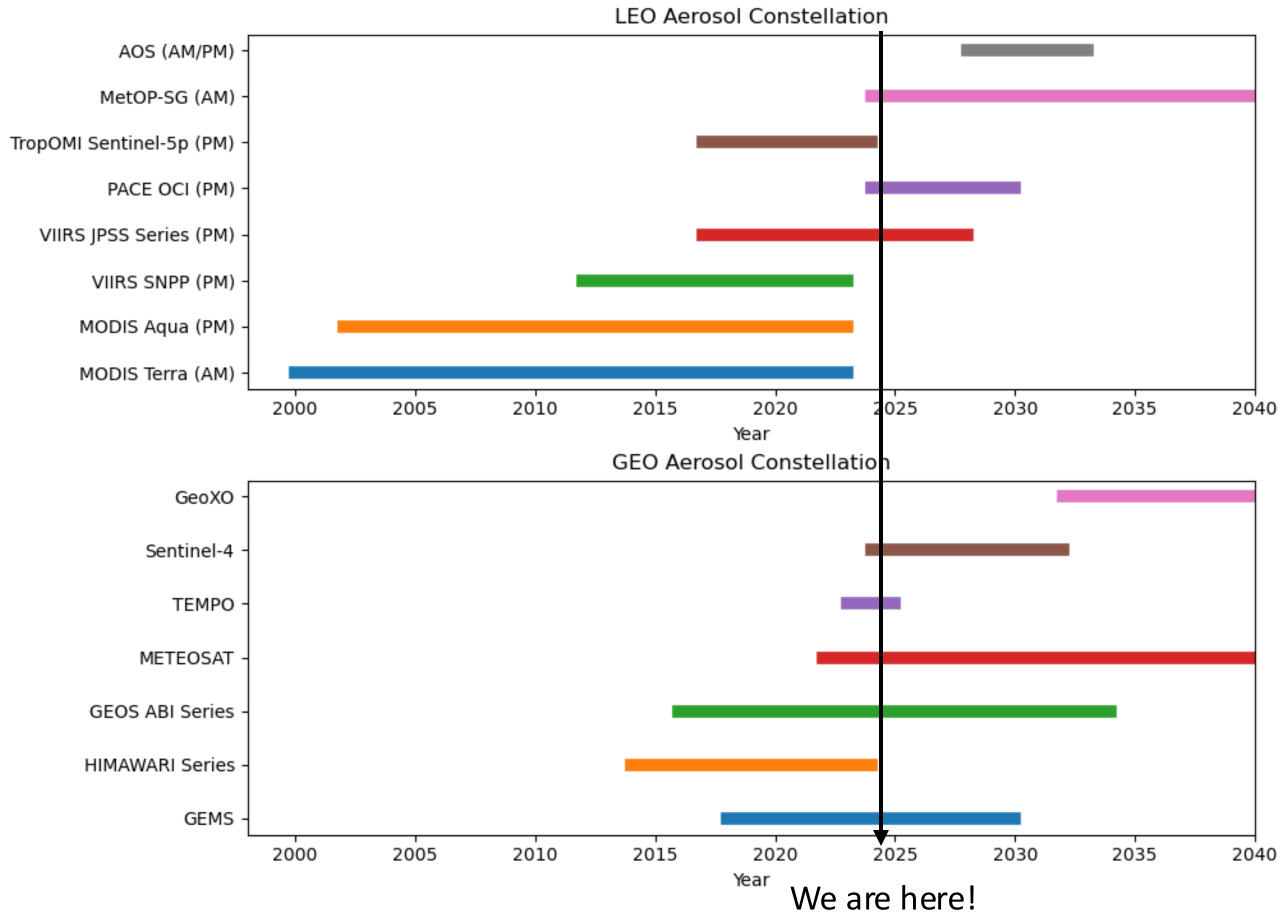
GEOS Aerosol Observing System



- MODIS Terra & Aqua observations of 550 nm AOD have been, by far, the main sources of aerosol observations for the GEOS aerosol DA system

- Actively working to include VIIRS NNR dataset in the GEOS system

- Will follow with the GEO dataset



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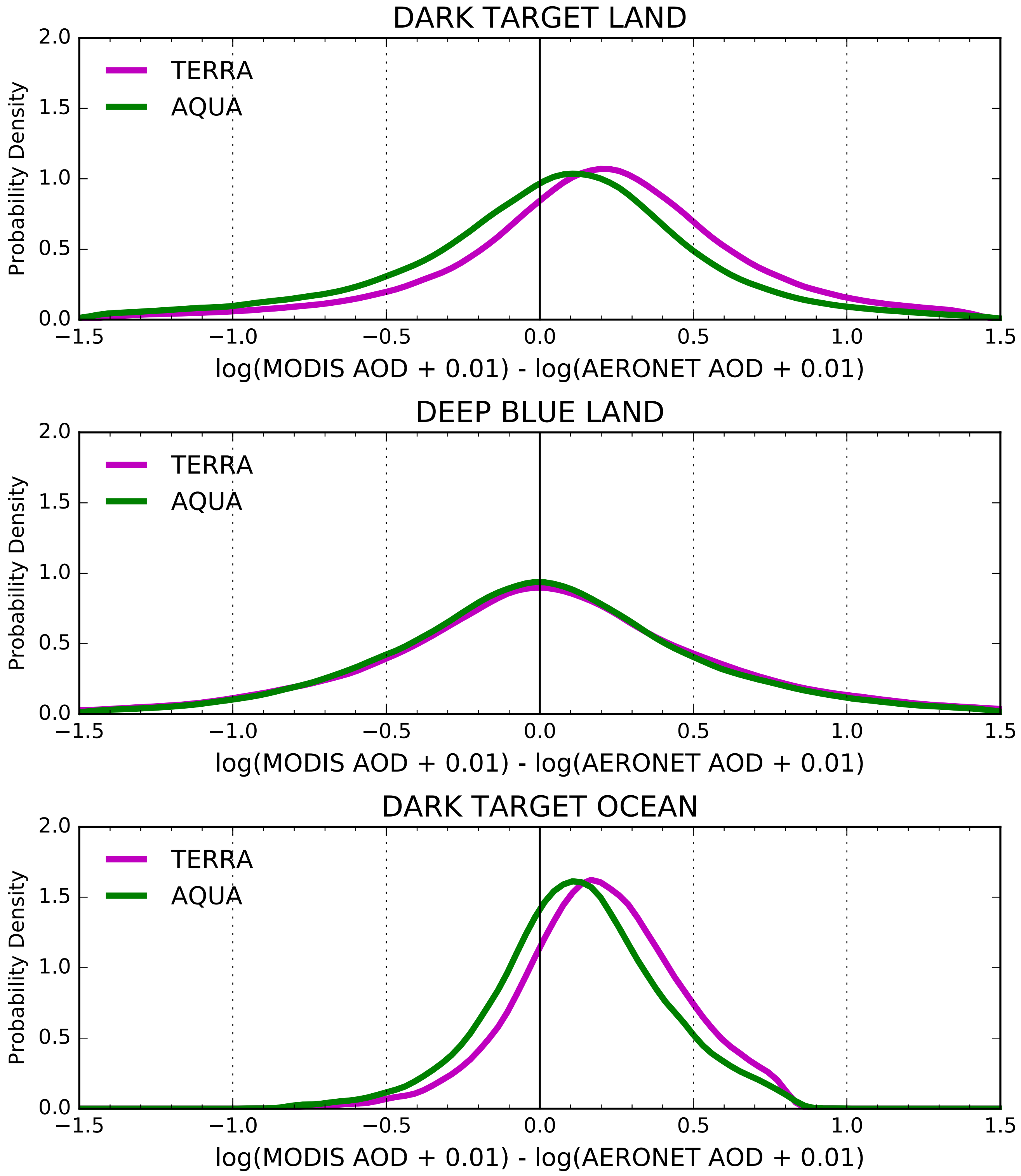
Homogenization of Aerosol Observing System

- The aerosol DA problem requires a homogenized AOD observing system across many different platforms

- Biases between datasets can propagate in the model forecast and lead to artificial variability

- Approach: ML algorithm based on Level 2 reflectances



NNR Algorithm Updates

NNR for MODIS

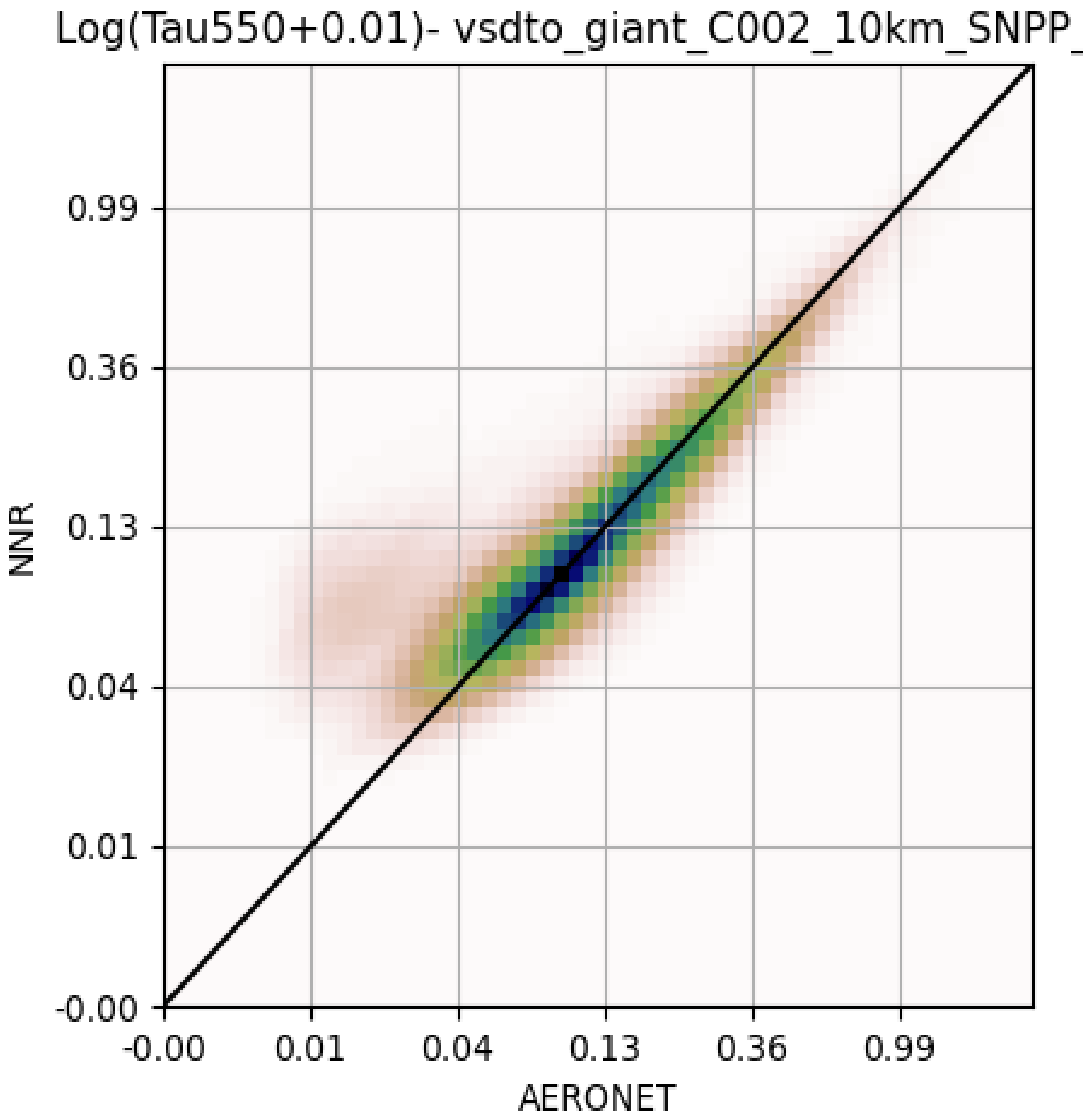
- **Fixes**
  - Target AOD balancing (spc_aod_balance), improves systematic overestimation at low values, underestimation at high values
- **Changes**
  - Input/Target standard scaling
  - Extends training data through 2023-12-31
    - Refactors code to more easily update training
  - Use 412 nm channel over ocean (previously left out, a bit better performance for dust)

NNR for VIIRS

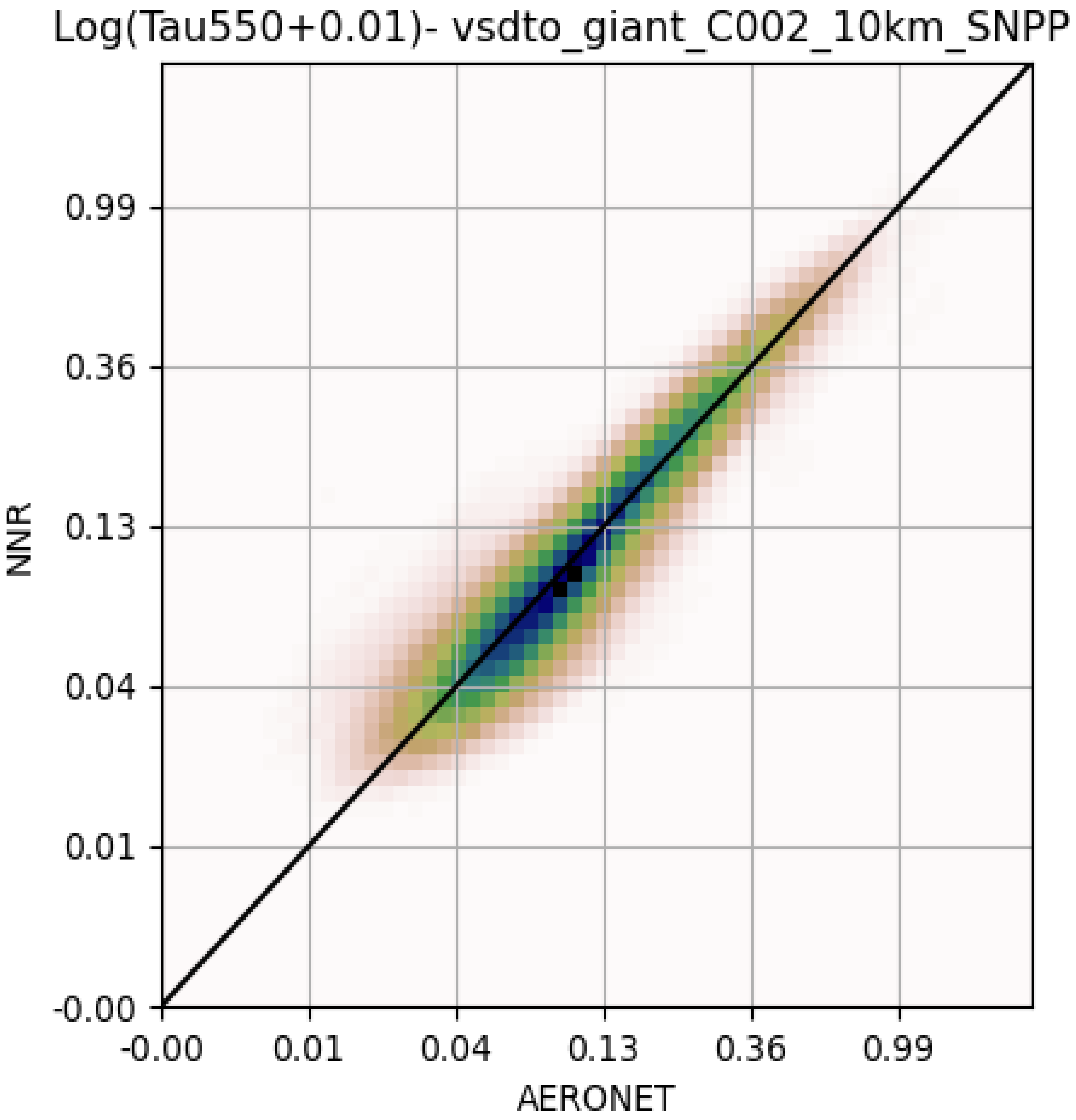
- **Fixes**
  - Target AOD balancing (spc_aod_balance), improves systematic overestimation at low values, underestimation at high values
- **Changes**
  - Input/Target standard scaling
  - Much stricter cloud filtering. MODIS uses CF<0.7, had to reduce down to CF<0.1
    - MODIS and VIIRS CF definition is fundamentally different
  - Exclude 1640 nm channel over ocean – it was noisy
  - Over land had to add original Tau550 as a predictor

NNR for VIIRS: AOD 550nm (Ocean)

NNR v001



NNR v011



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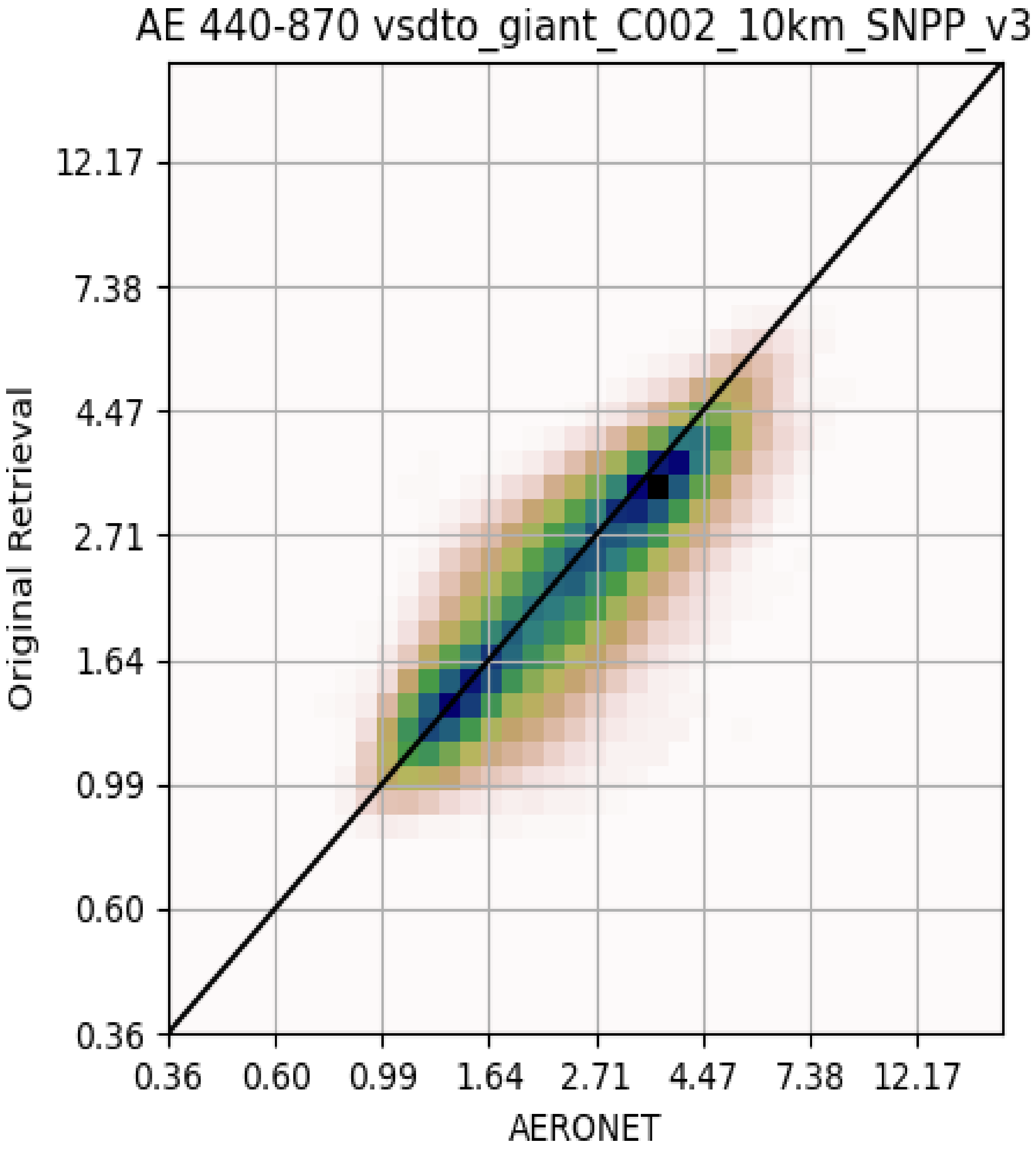
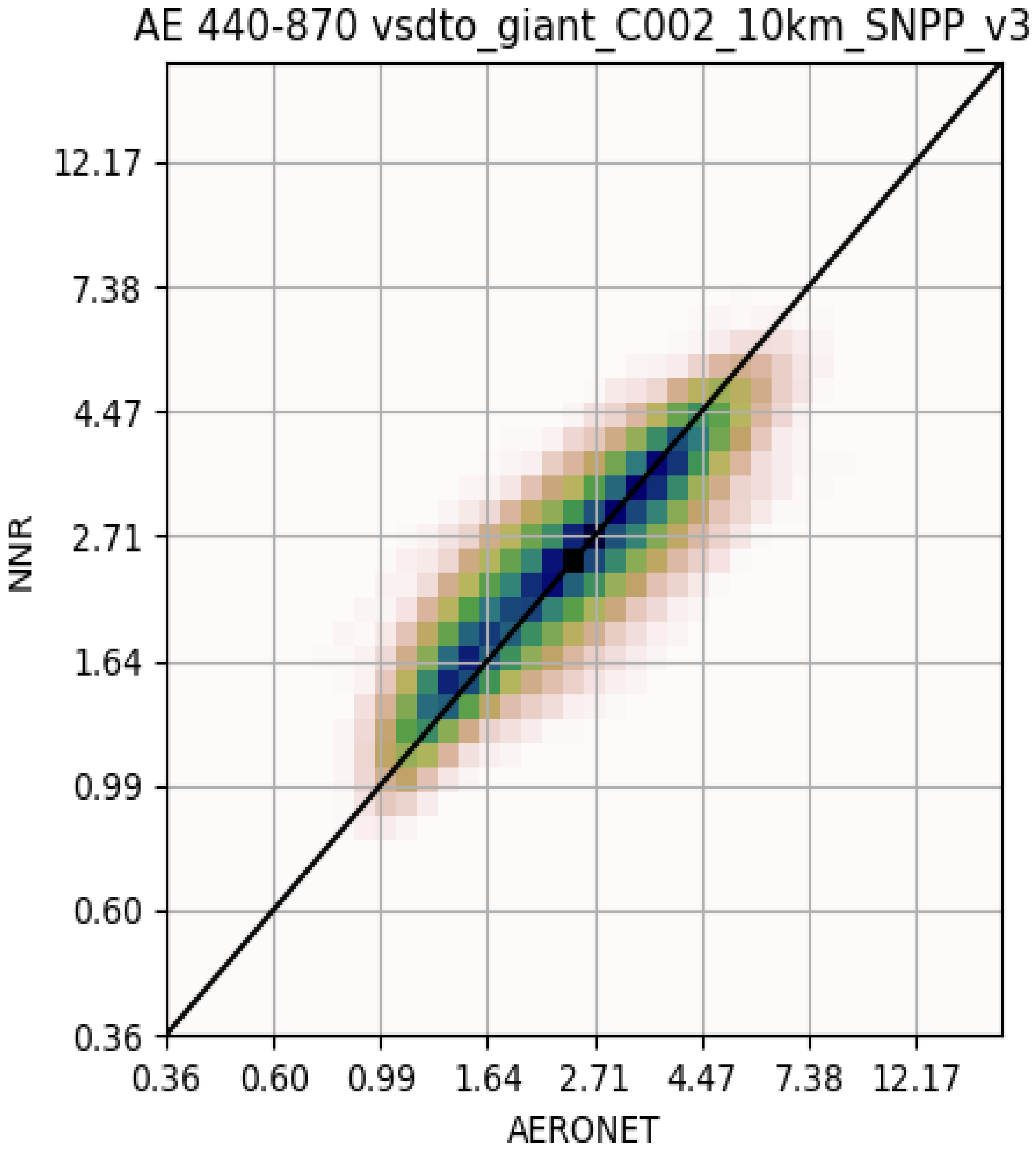
Slide Credit: P. Castellanos

NNR for VIIRS: Angström 440-870n(Ocean)

NNR v001



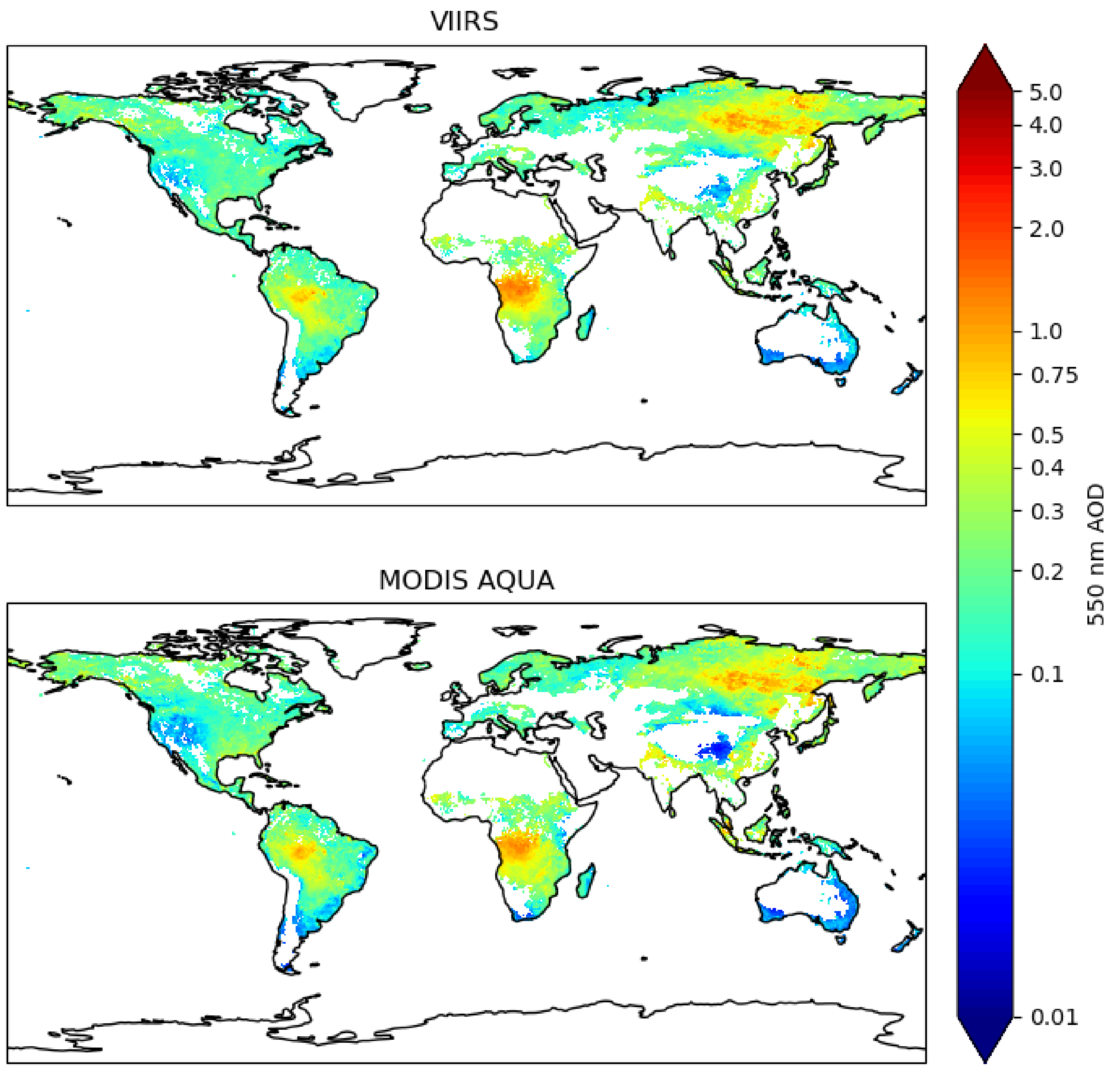
NNR v011



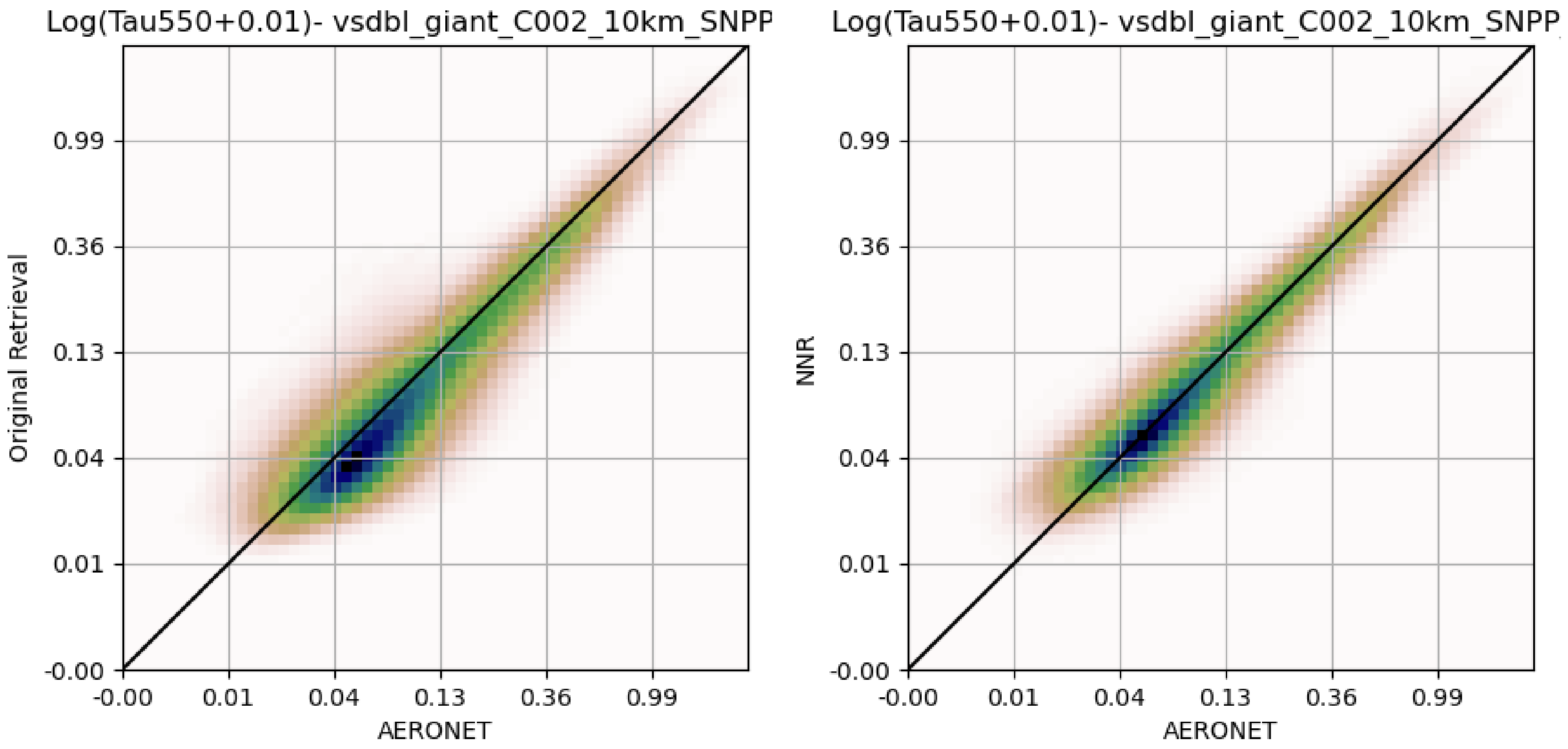
Slide Credit: P. Castellanos

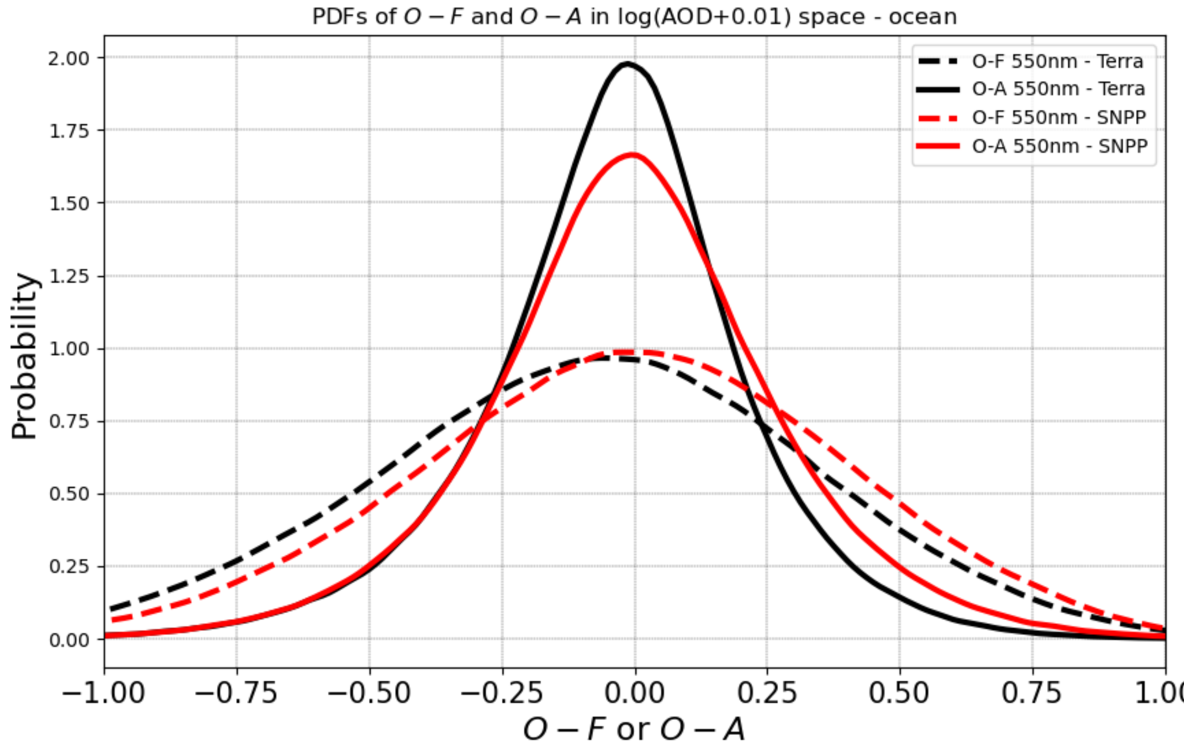
MODIS-VIIRS Consistency

NNR implementation on VIIRS dataset



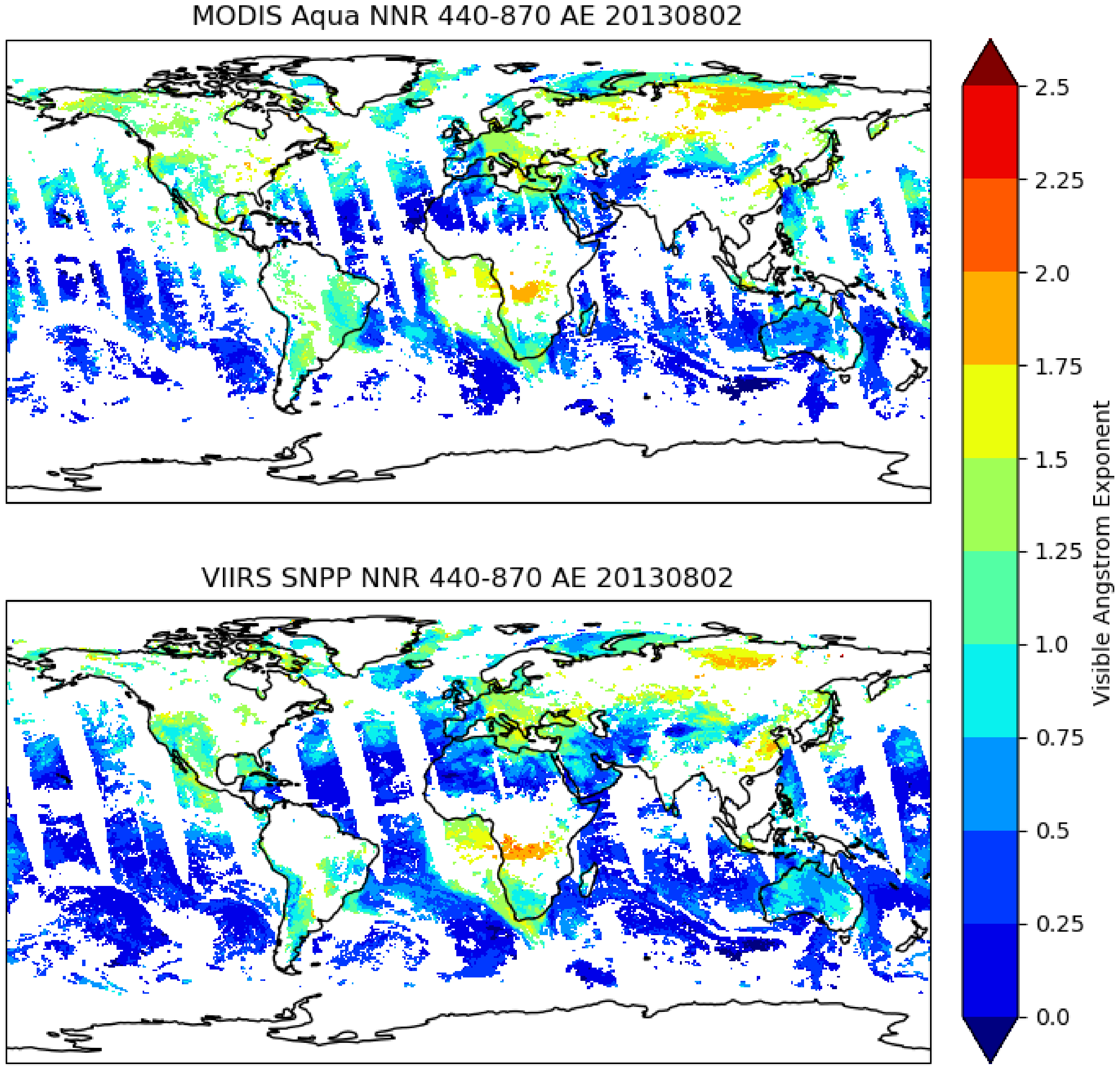
August 2019





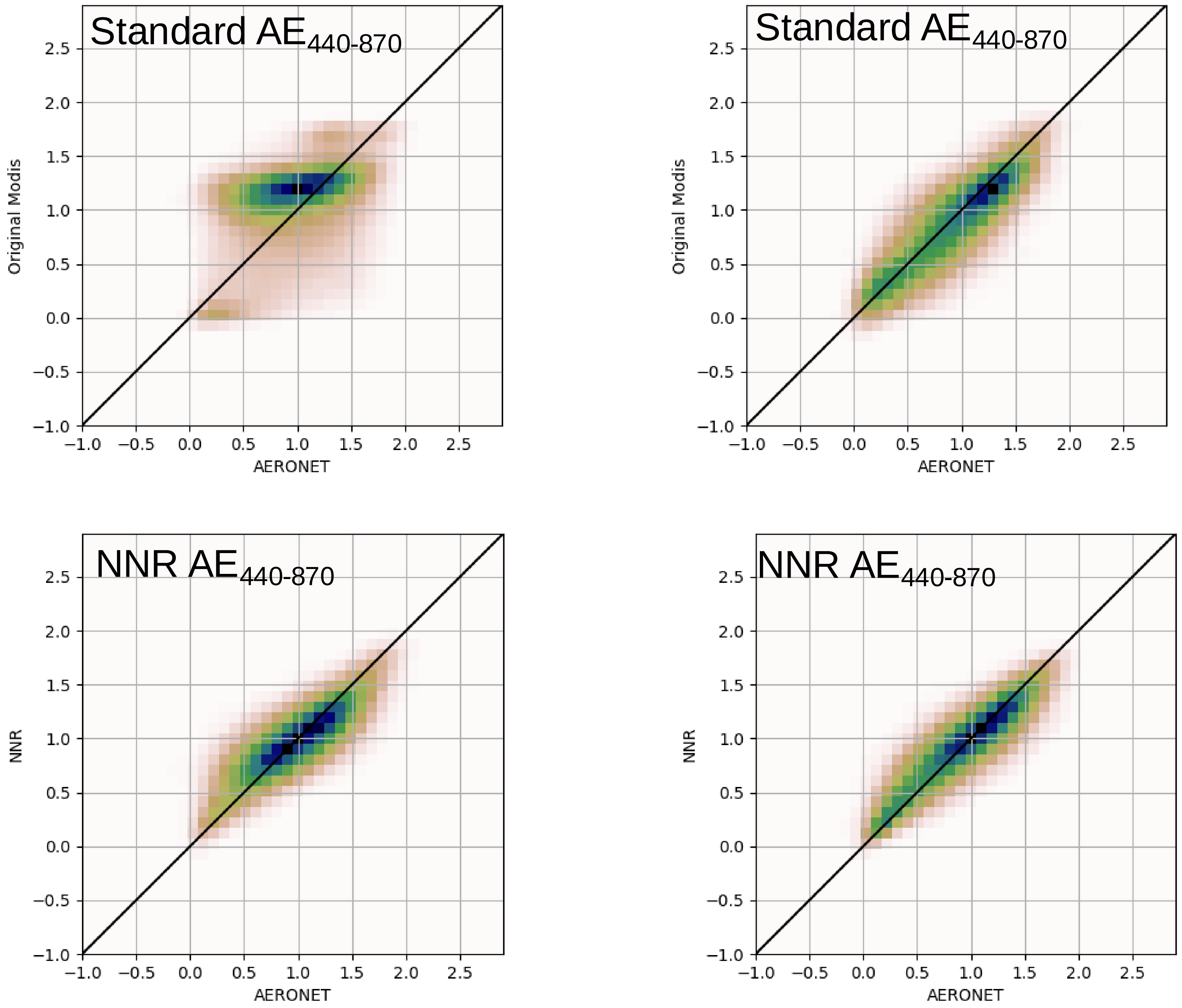
Slide Credit: V. Buchard, P. Castellanos

NNR Algorithm now Includes Visible Angstrom Exponent



Land Surface

Ocean



VIIRS

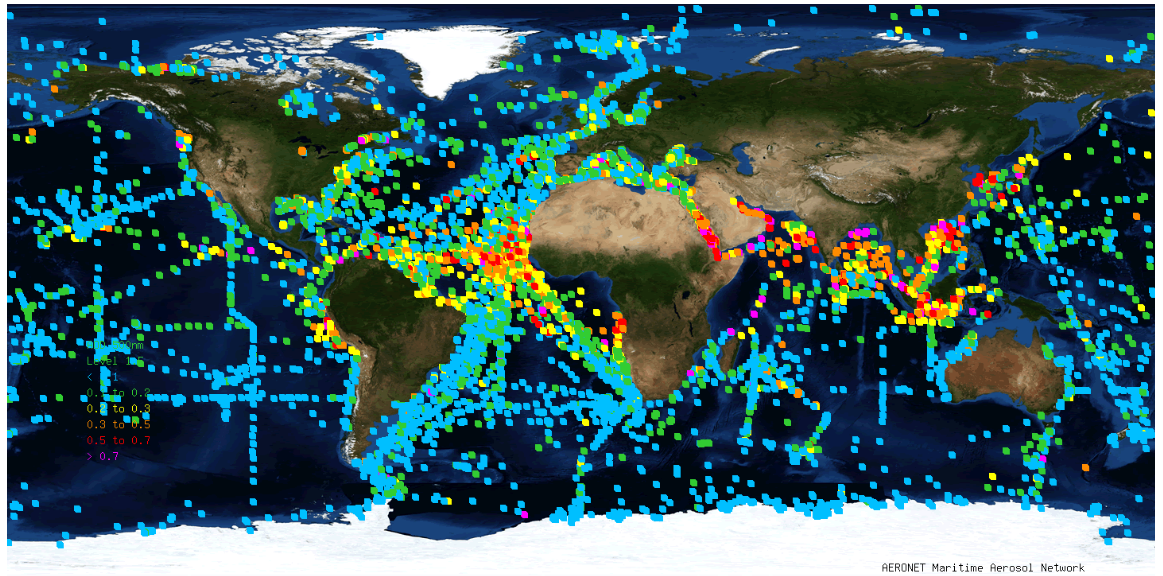
VIIRS

Slide Credit: P. Castellanos

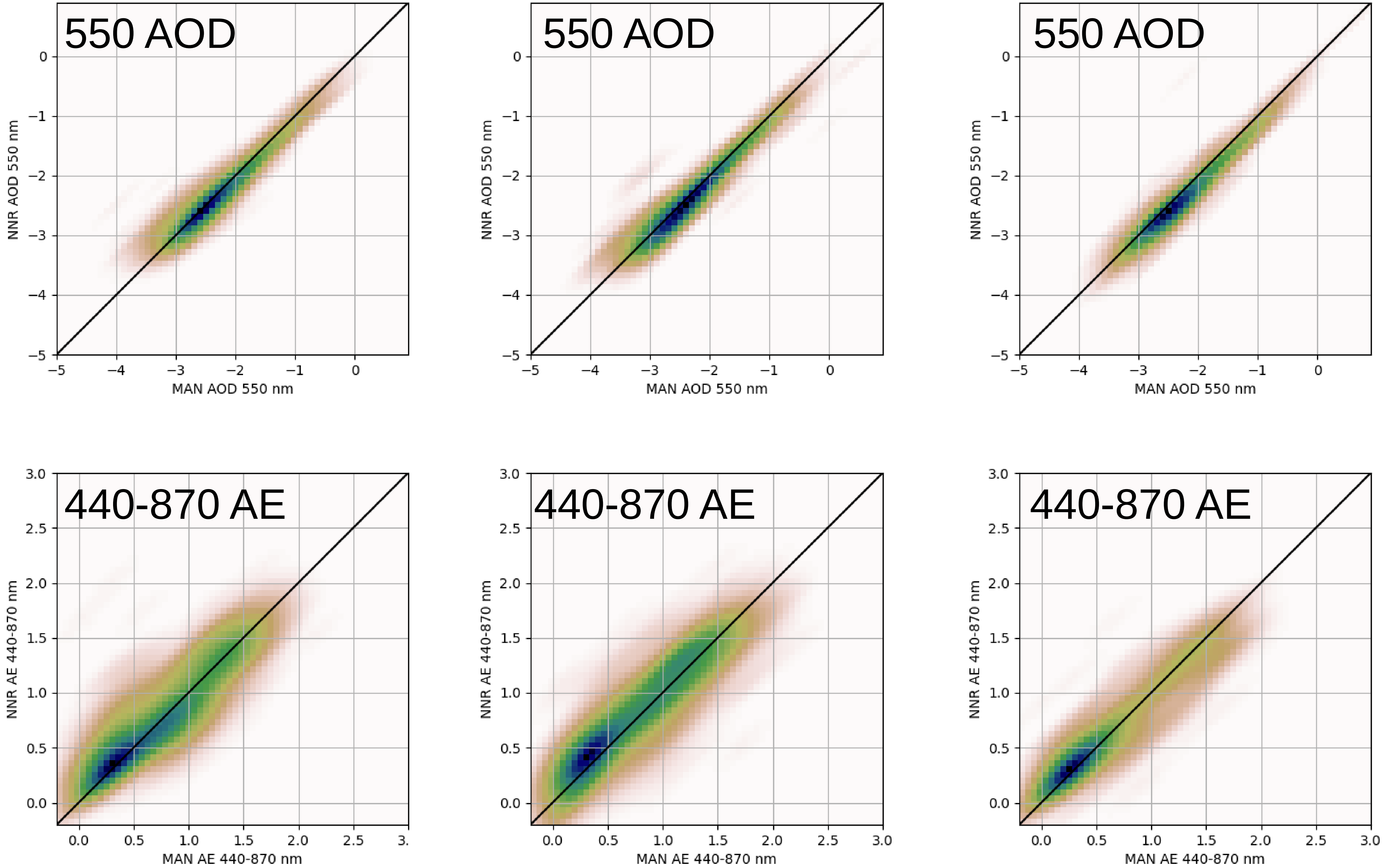
Comparison to Maritime Aerosol Network

Handheld sun photometers are deployed during research cruises

MAN Cruise Tracks



MODIS TERRA | MODIS AQUA | VIIRS SNPP



Slide Credit: P. Castellanos

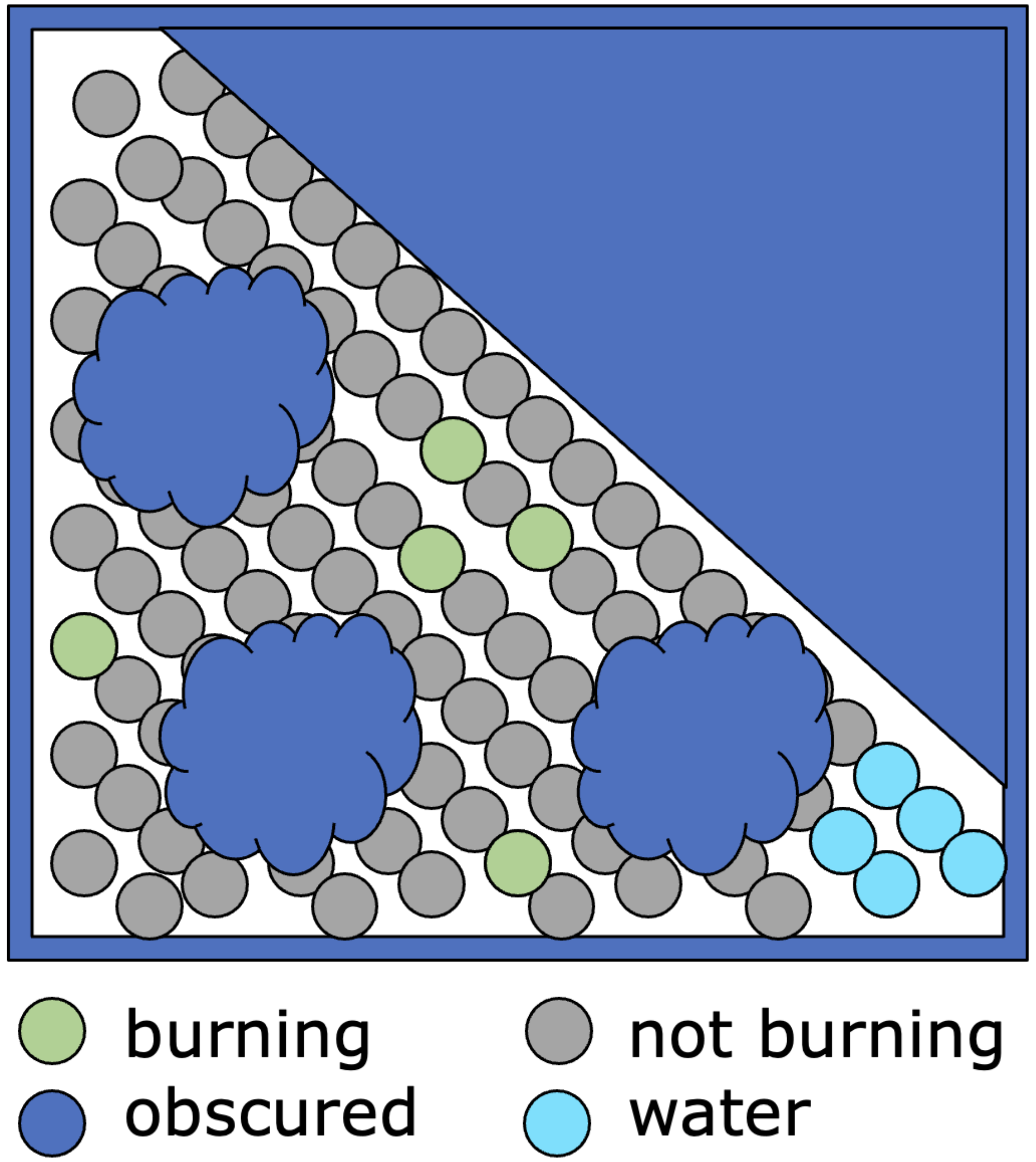
Biomass Burning Emissions

Components, parameterizations and computational implementations

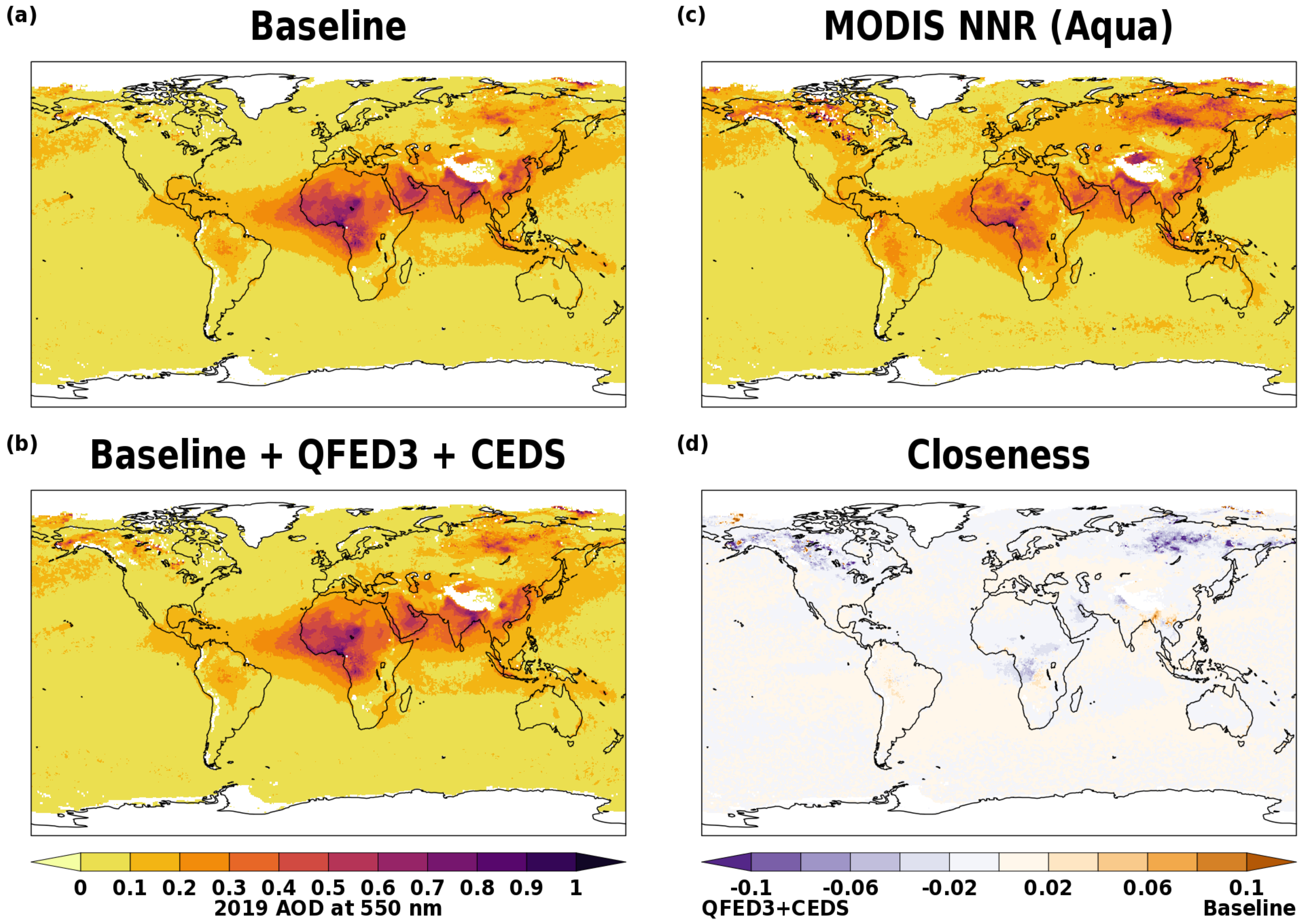
QFED: Quick Fire Emissions Dataset

- Emission estimates based on simple sequential DA algorithm which addresses obscured pixels
- Estimates daily fire emissions based on FRP data
  - Tradiitonally: MODIS
  - Just in: VIIRS
  - In development: GEO
- Two-step calibration
  - Trace gas emissions are calibrated against GFED
  - Aerosol emissions are calibrated against MODIS AOD resulting in ~3x enhancement vs GFED
- Emissions are persisted during GMAO forecasts (climatology used for S2S), with prescribed diurnal cycle.

Model grid-box



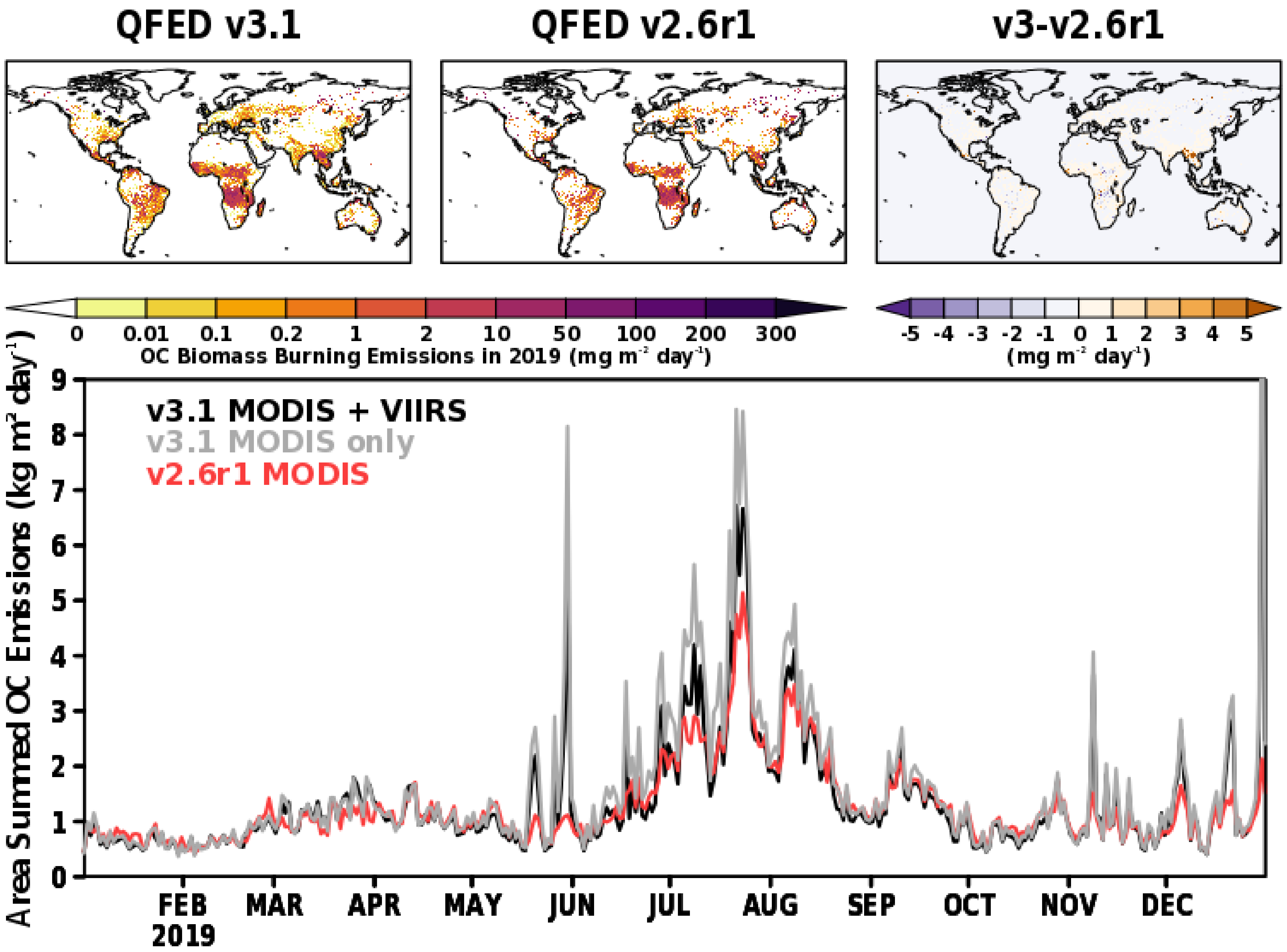
QFED 3.1 Adds VIIRS



- One year simulations with constrained meteorology were completed for 2019 with a “baseline”, updated biomass burning emissions, and updated anthropogenic emissions
- Data assimilation for AOD was turned off
- A comparison to MODIS NNR demonstrates an improvement in total AOD, primarily in response to using QFED 3.1over the northern hemisphere boreal forests and central Africa
- In the closeness plot, purple indicates the updated emissions result in a AOD that is closer to MODIS NNR observations

In QFED 3.1 VIIRS derived emissions Have been calibrated for consistency with MODIS.

QFED 3.1 Adds VIIRS



- QFED provides biomass burning emissions for all (quasi)operational GEOS systems
- Major features of version 3.1 include a code refactoring and the inclusion of Fire Radiative Power (FRP) from VIIRS on SNPP and NOAA-20
- VIIRS detects more and smaller fires compared to MODIS (indicated by larger regions of yellow on the spatial map)

Going Forward:
Addressing Issues with VIIRS Fire Detections

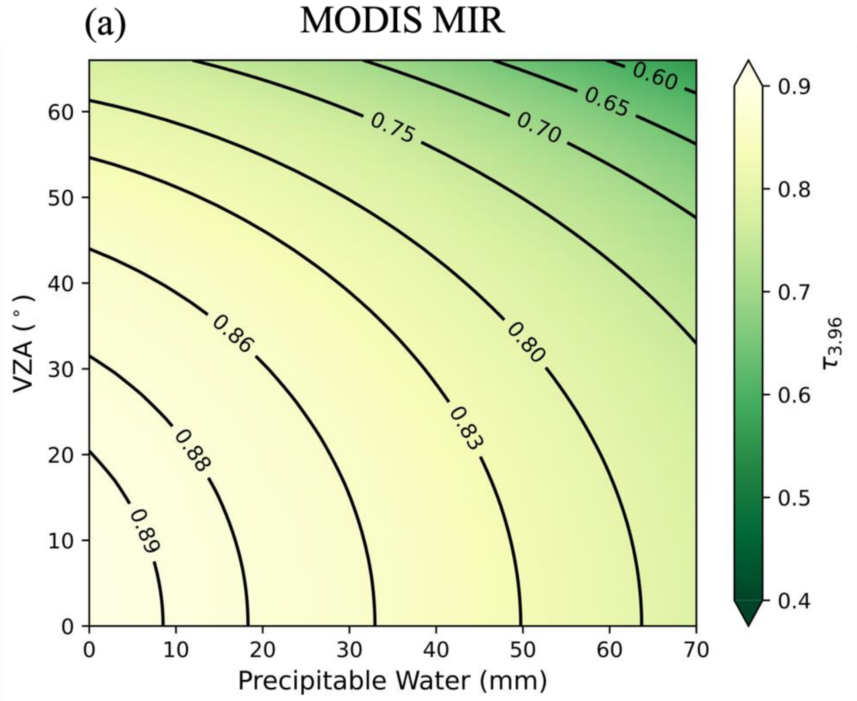
Housekeeping Issues

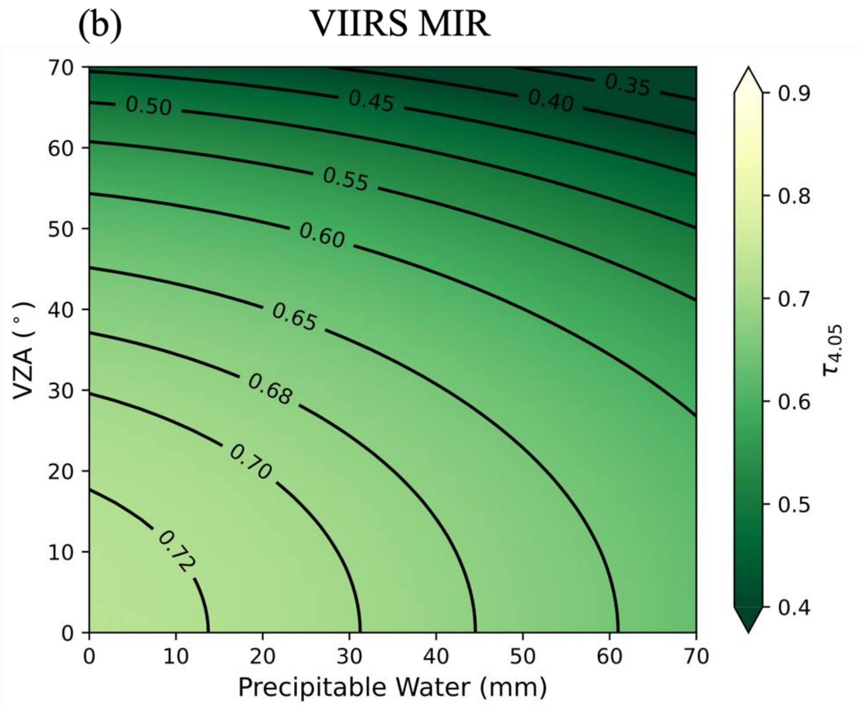
- Need for Atmospheric Correction
- Those pesky bowties…
- Addressed in FILDA-2 during night, being extended to daytime.

Algorithmic Issues

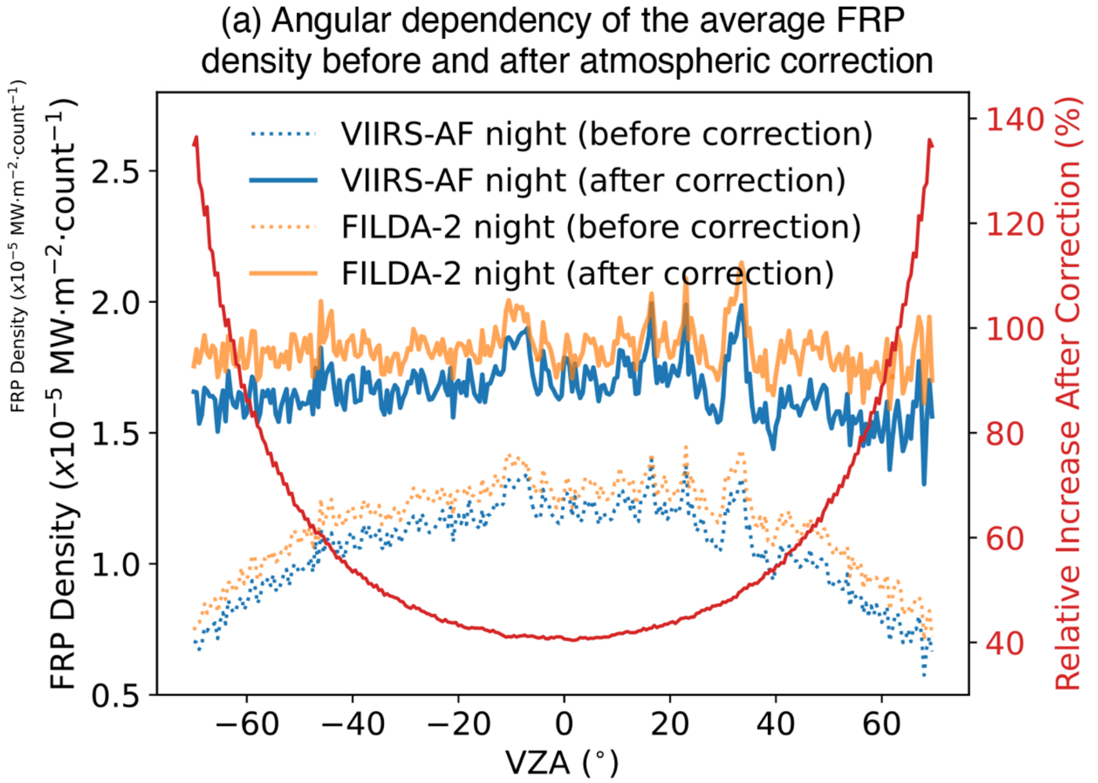
- Retrieving FRP
  - Importance of multi-spectral data
- Retrieving MCE
- Parameterizing emission factors/coefficients in terms of MCE

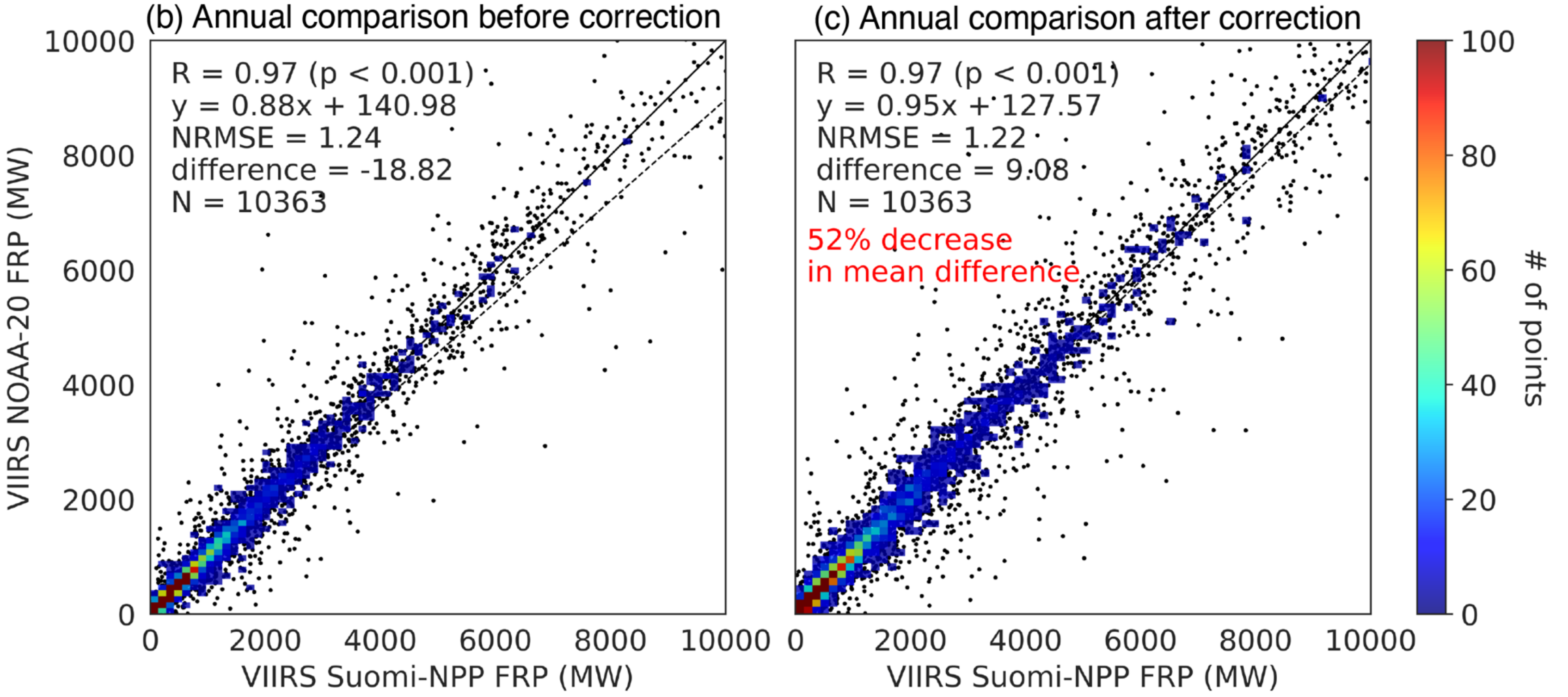
Importance of Atmospheric Correction

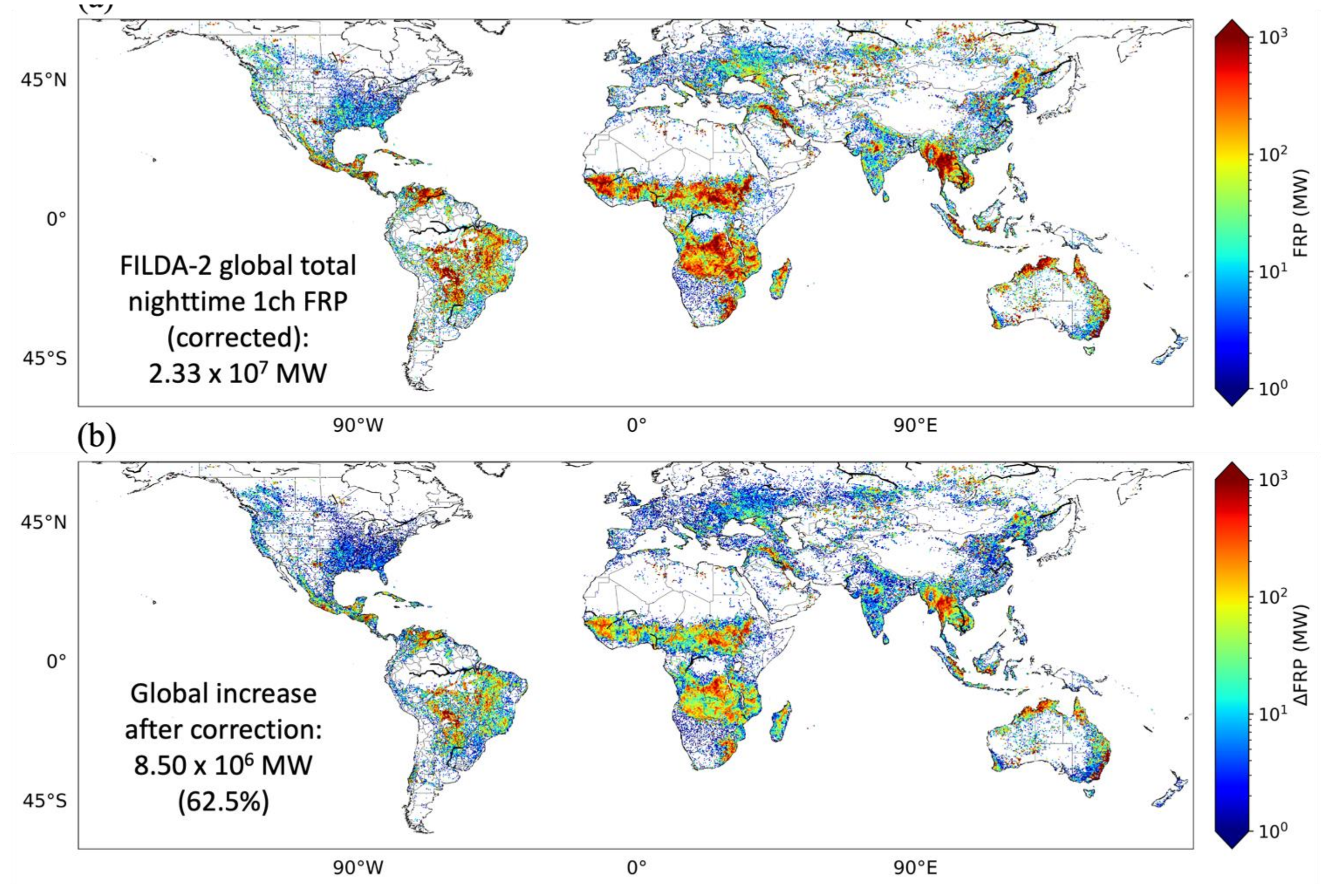




Water vapor absorbs significant amount radiance at ~4 µm





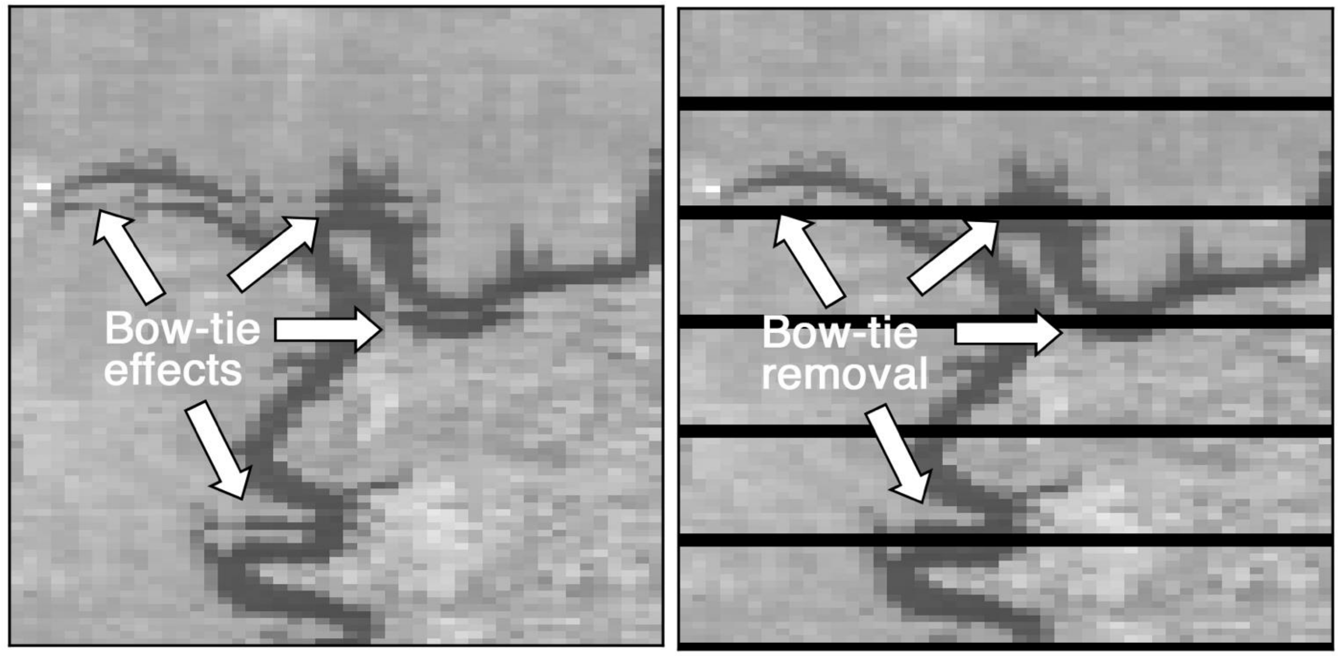


Proper atmospheric correction greatly improves the consistency between VIIRS on SNPP and NOAA-20 platforms.

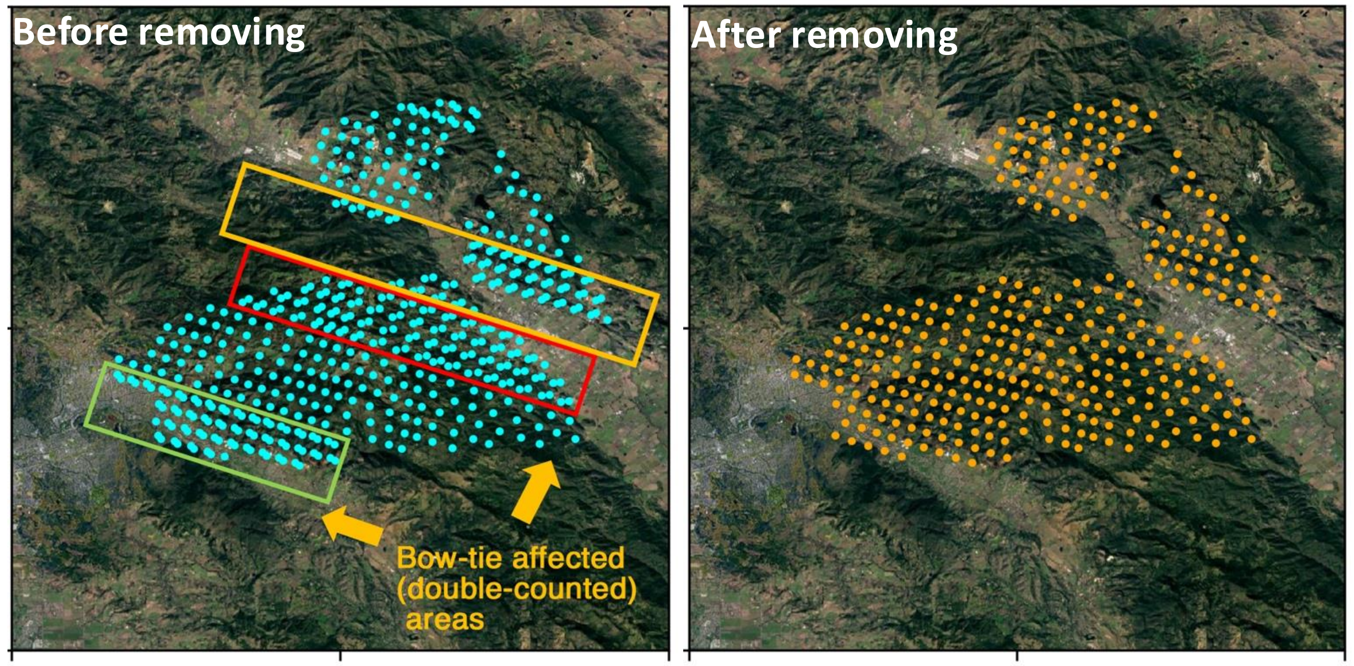
Slide Credit: Meng Zhou, Weizhi Deng, Jun Wang

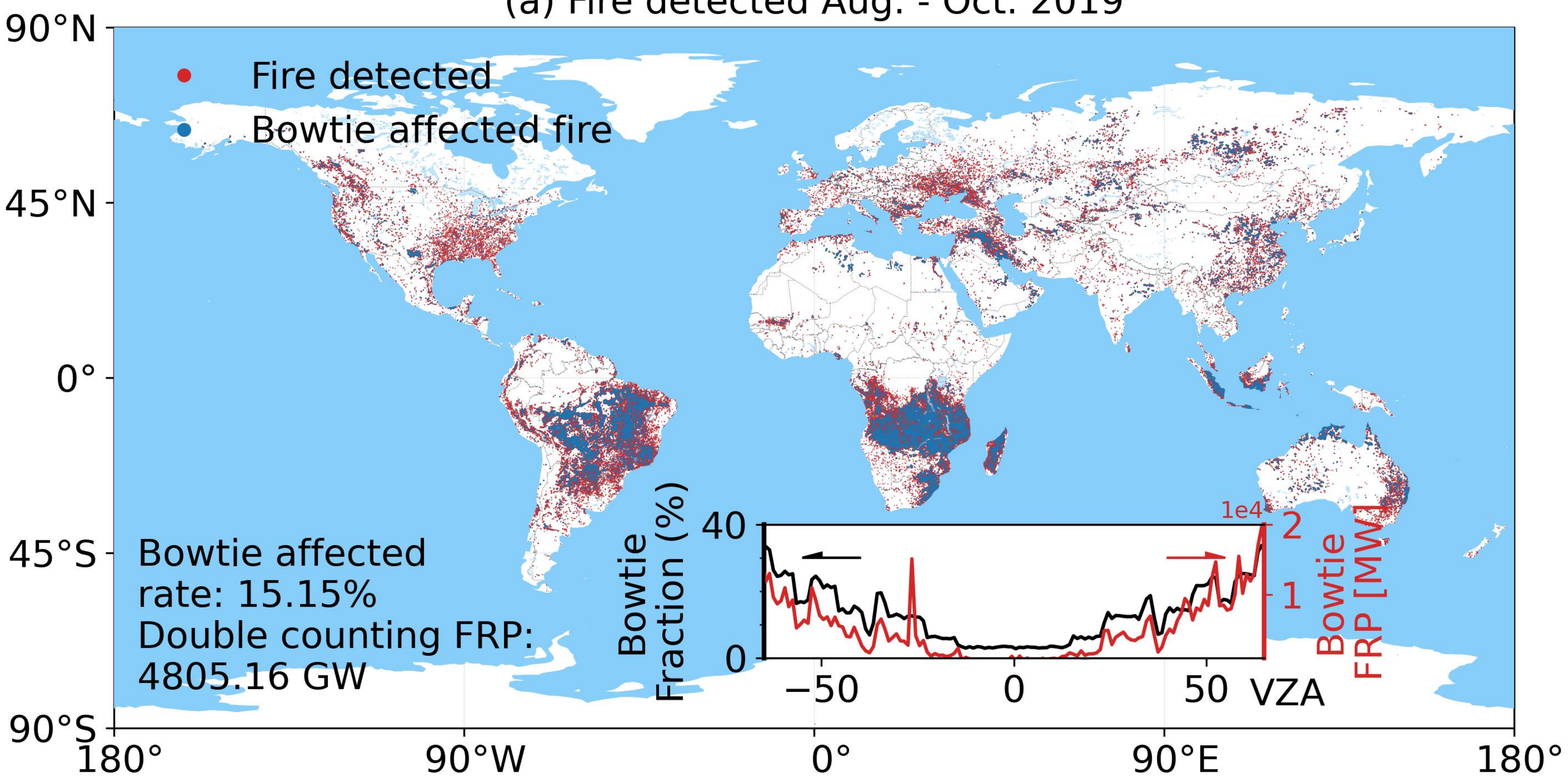
Bowtie Correction

Bowtie effects on polar orbit imaging



Bowtie effects on polar orbit fire detection





Zhou et al. 2023: Enhancement of Nighttime Fire Detection and Combustion Efficiency Characterization using Suomi-NPP and NOAA20 VIIRS Instruments, TGRS 2023

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Slide Credit: Meng Zhou

McBEF: MCMC Biphasic, Multispectral Estimation of Fire Properties

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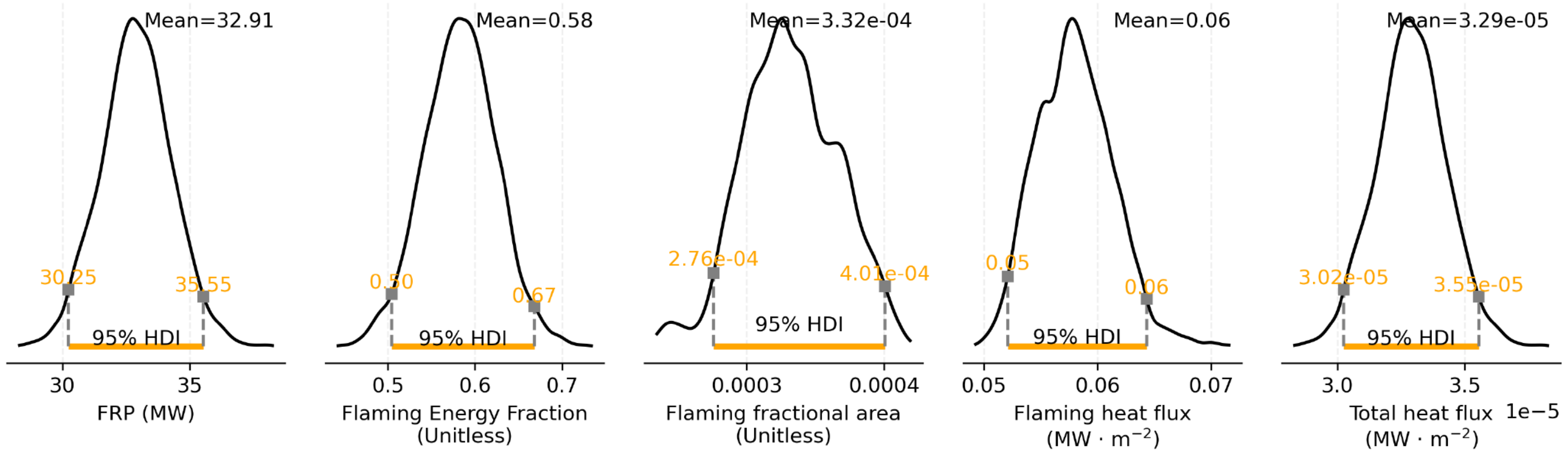
NASA

- Generalization of (uniphasic) Dozier bi-spectral algorithm by explicitly considering considering flaming and smoldering phases of a single fire:

$$L_\lambda = p_F * B_\lambda(T_F) + p_S * B_\lambda(T_S) + (1 - p_F - p_S) * B_\lambda(T_B)$$

- The 4 parameters (T_F, T_S, p_F, p_S) are estimated by means of an Markov-chain Monte-Carlo (MCMC) algorithm using multiple wavelengths.
- This algorithm allows for the FRP to be decomposed in terms of flaming and smoldering components, and calculation of flaming heat fluxes needed for Plume Rise calculations



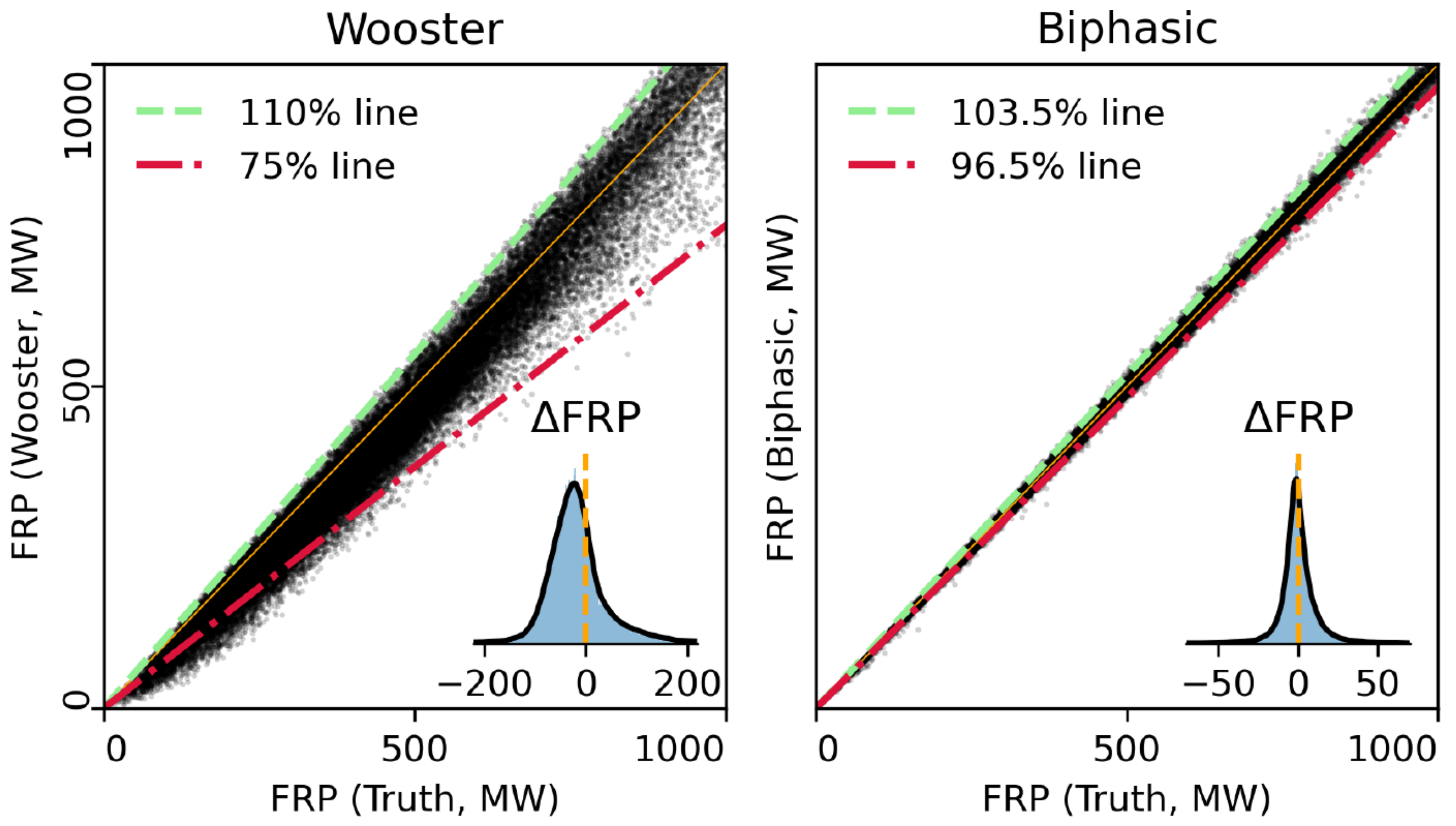
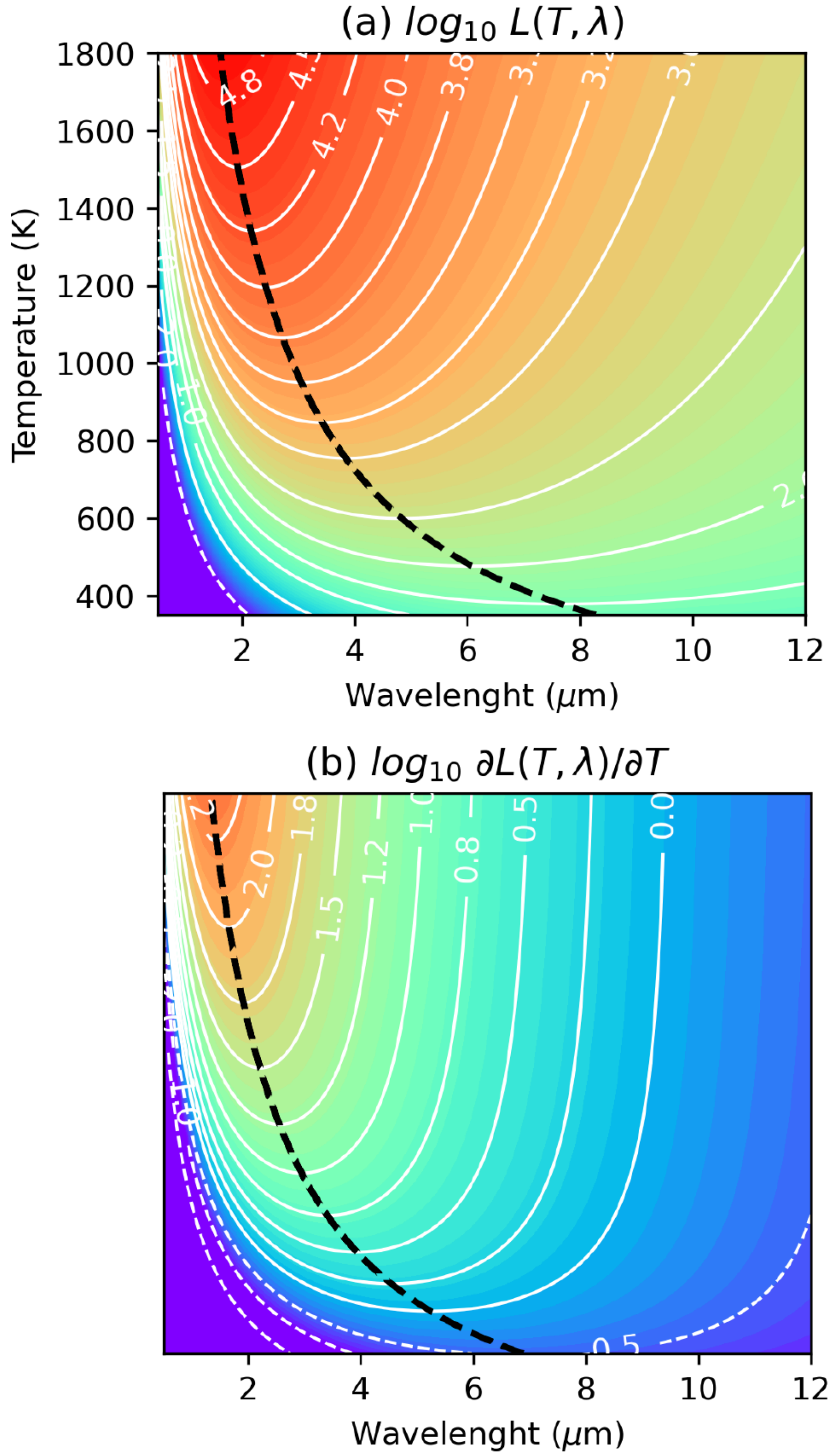


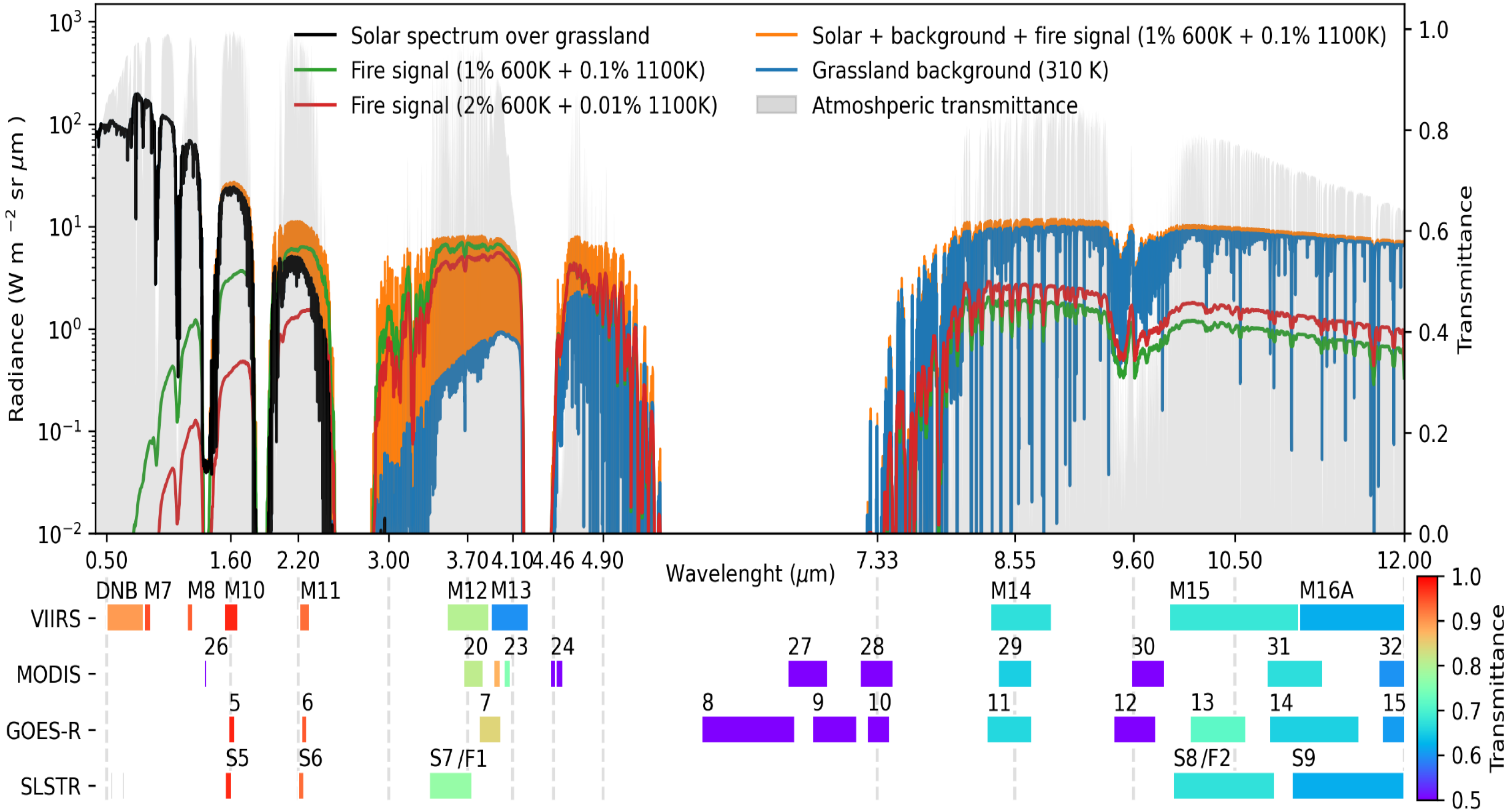
Figure 2: Comparison of the FRP estimates from Wooster and MC-MC biphasic method.

The flaming energy fraction can be used to parameterize ***Modified Combustion Efficiency*** (MCE) and ultimately modulate emission factors/coefficients (see Jun Wang's presentation)

Wavelengths for Biphasic Algorithm



Channel Sensitivity



Slide Credit: Meng Zhou

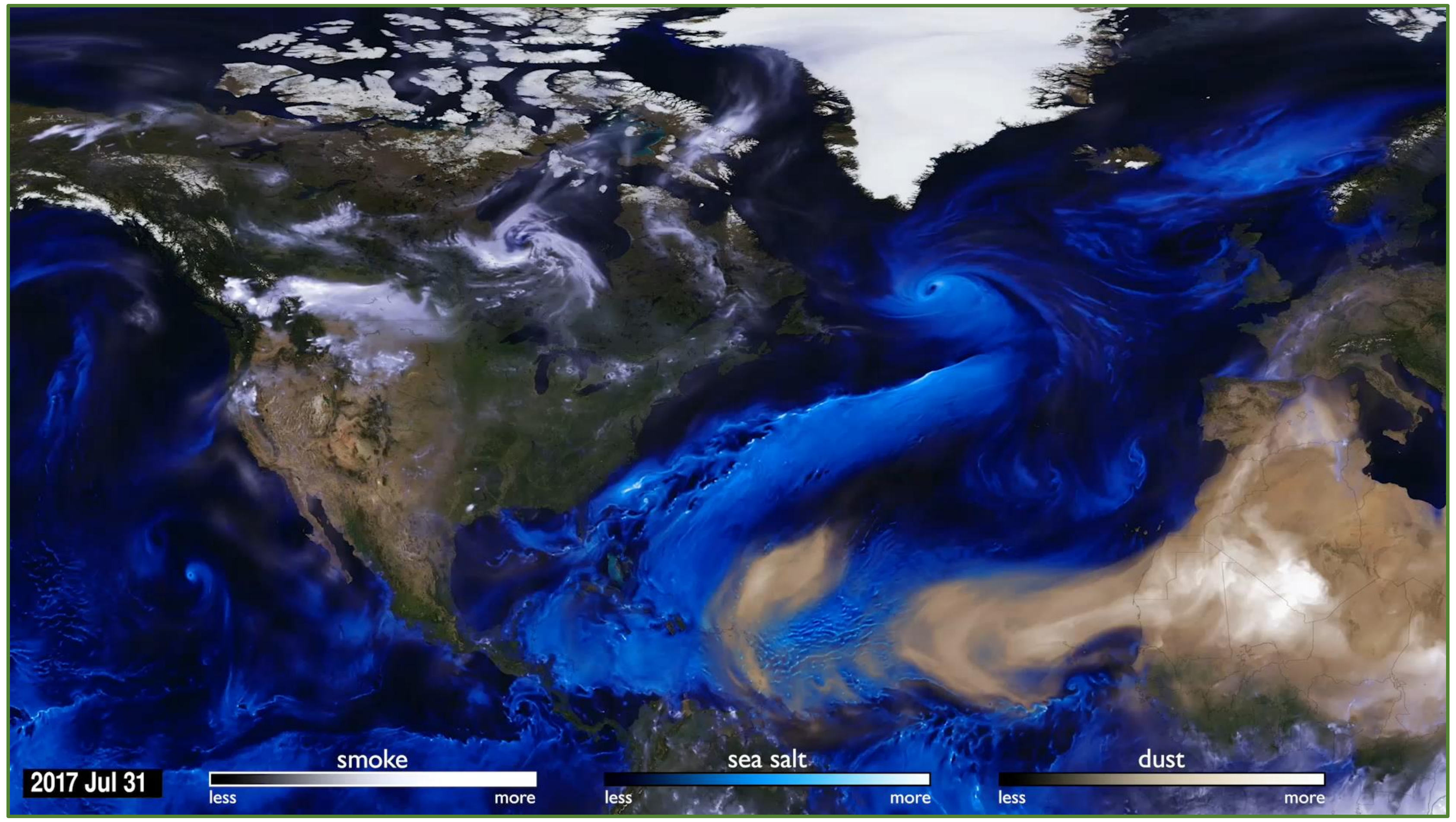
Short to Mid-term Outlook

Aerosol Modeling

- Concerted effort for tunning aerosol emissions:
  - Concurrent tuning of removal processes
  - ML , ensemble of adjoint based inverse calculations
- Improve representation of dust size distributions
- Continue of Modal Aerosol Module (MAM) and coupling to 2M cloud scheme

Data Assimilation and Observing System

- Complete JEDI-based aerosol DA scheme
- Extend NNR to geostationary sensors
- Extend NNR to hyperspectral sensors
  - Alternative to "Aerosol Layer Height" retrievals
  - Single scattering properties such as SSA
- Adjustment of aerosol single scattering properties as a sequential bias estimation problem
- Dust mineralogy



Biomass Burning Emissions

- Extend QFED with additional Functional Biome Types (FBTs), including treating of gas flares
- Extend FILDA/McBEF to daytime
- Implement McBEF estimates of FRP and MCE in QFED
- Implement Freitas Plume Rise based on McBEF estimates of flaming heat fluxes.

QFED Evolution

- Adopting University of Iowa Fire Light Detection Algorithm (FILDA) for VIIRS
  - Muti-spectral BTs, including DNB
  - Improved atmospheric correction
  - Estimation of Modified Combustion Efficiency
- Developing a bayesian, biphasic algorithm for FRP estimation
  - Based on multi-spectral IR data
  - Smoldering/flaming phase resolving estimation of FRP, sizes and heat fluxes
  - Will provide more targeted inputs for the Freitas Plume Rise Model
- Designing AI/ML for the fire evolution model used in the QFED sequential estimation (proper handling of obscured pixels)
- Integration of VIIRS and GEO fire detection using proper observations operators developed by means of AI/ML models

Table 1: configurations of the non-homogeneous fire model

Phase	Temperature	Total fractional area	Number of seeds
Flaming	$T_f \sim N(1100, 300)$	$ln\ p_f \sim N(-4, 1)$	$N_f \sim U(0, 5)$
Smoldering	$T_s \sim N(600, 200)$	$ln\ p_s \sim N(-3, 1)$	$N_s \sim U(1, 5)$
Cooling	$T_c \sim N(350, 50)$	$ln\ p_c \sim N(-3, 1)$	$N_c \sim U(1, 5)$
Background	$T_b \sim N(300, 10)$	$1 - p_f - p_s - p_c$	1

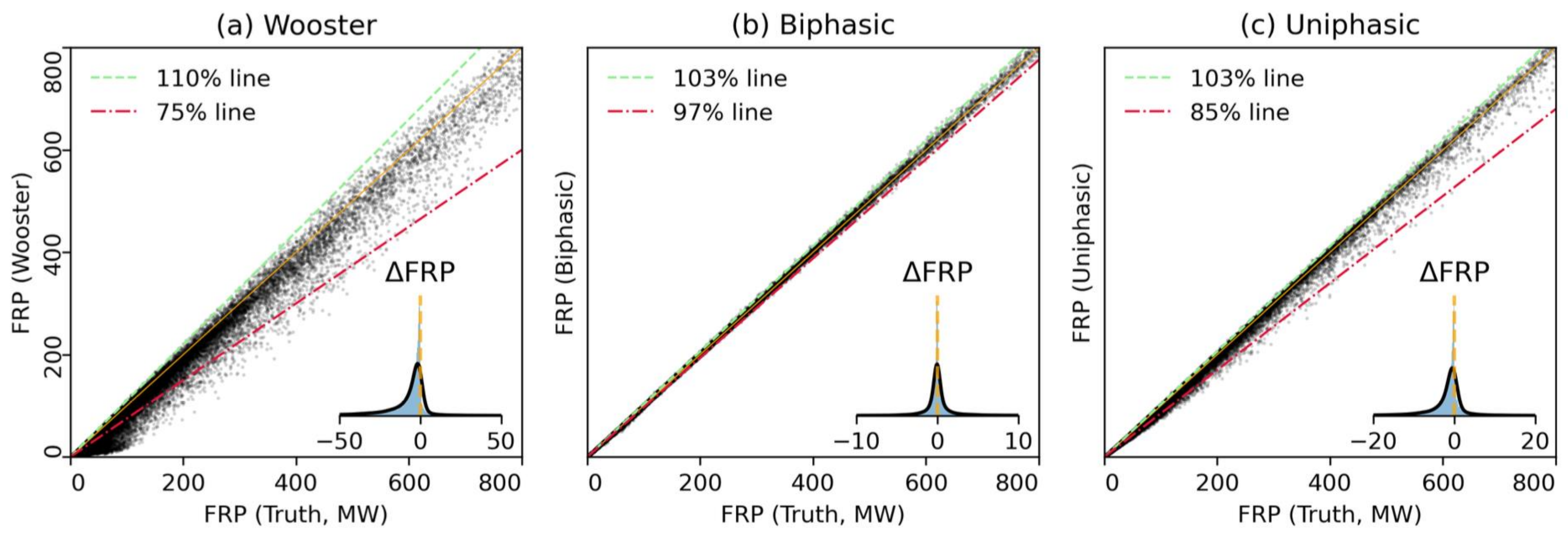


Figure 5: Comparison of FRP estimations for different methods against ground truth. (a) Wooster; (b) Biphasic; (b) Uniphasic. The embedded graphs are the error distributions.