

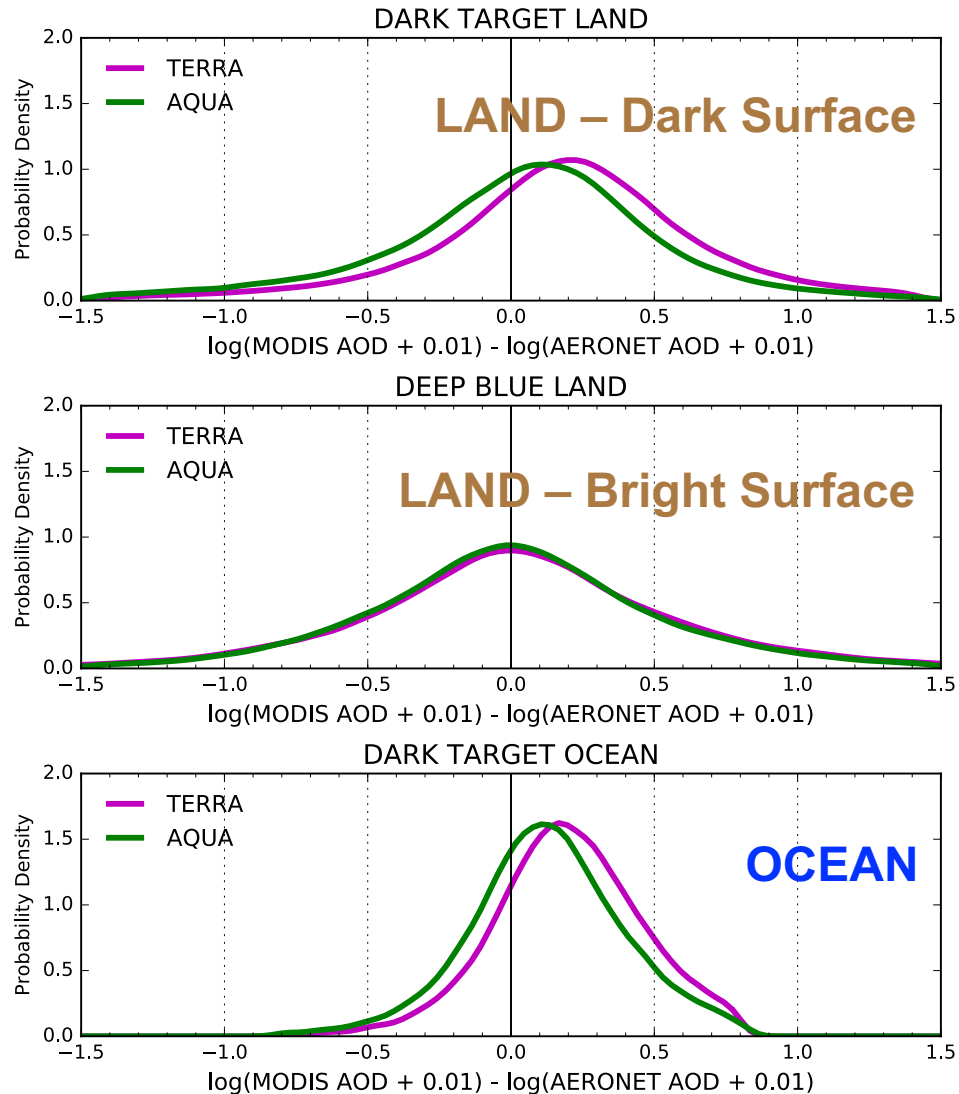
GOES-5 AOD Data Assimilation: Plans for Geostationary Observations

Patricia Castellanos & Arlindo da Silva

CEOS Atmospheric Composition Virtual Constellation AC-VC-14

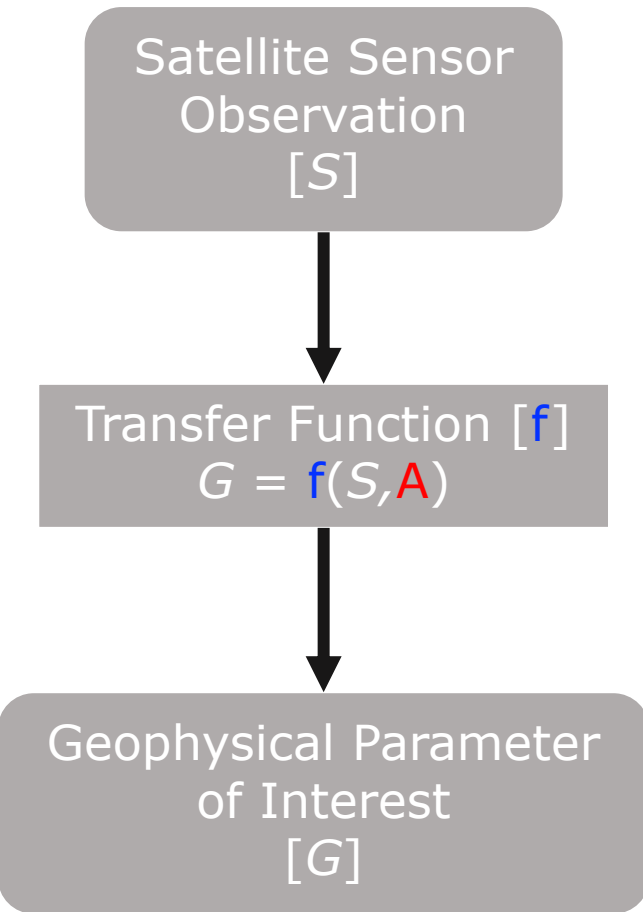
Friday May 4, 2018

Comparison of MODIS Standard AOD Retrievals



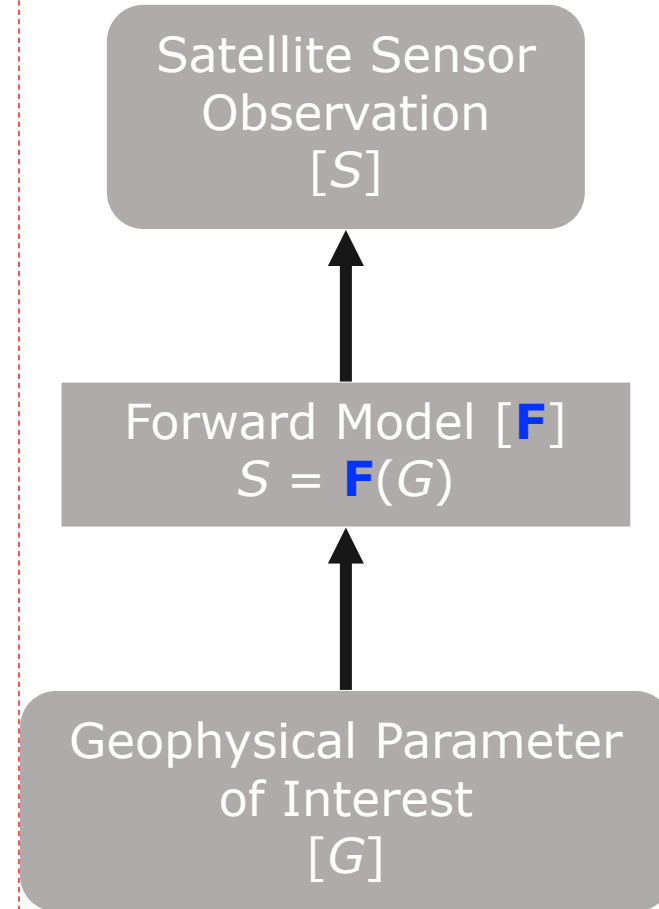
- The aerosol data assimilation problem requires a **homogenized AOD observing** system across different platforms
- Biases between datasets can propagate in the model forecast and lead to **artificial time variability**.

Empirical Retrievals



- f is a continuous function that maps S to G
- Represent f with a mathematical function that contains a set of empirical parameters, A
- A are determined from a training dataset of pairs of G and S observations.
- Training empirically captures physical relationships and tunes away calibration issues.

Physically Based Retrievals



- F is a physical model derived from first principles (e.g. radiative transfer model)
- F is not easily inverted
- The objective of the retrieval algorithm is to search for a G^* that minimizes $\|S - F(G)\|$
- Product quality affected by calibration issues.



L1 Reflectances

Generate L2 Reflectance
 Cloud mask
 Quality control

Collect Relevant Ancillary Data
 Surface reflectance
 Aerosol speciation (forecast)
 Winds, moisture, etc

Machine Learning Algorithm trained with AERONET observations

Do Retrieval

AOD

MODIS Over Land Algorithm
 All procedures applied to individual boxes of 20 x 20 pixels at 500 m resolution (10 km at nadir)

•Ensure angles and reflectance values are valid. If not: **report Fill values and EXIT**
 •Identify and mask (discard) all water, cloudy and snow/ice pixels.
 •Identify "dark target pixels" that have $0.01 \leq \rho_{2.13} \leq 0.25$
 •Discard brightest 50% and darkest 20% of pixels defined with $\rho_{0.66}$
 ... leaving a maximum of 120 pixels

Are there at least 12 (10%) dark target pixels?

Procedure A
 Set QAC=0,1,2 or 3 (based on # of pixels)
 •For all identified 'dark' pixels, Calculate mean $\rho_{0.47}, \rho_{0.66}, \rho_{2.1}, \rho_{1.2}$
 Calculate $NDVI_{SWIR}(\rho_{2.1}, \rho_{1.2})$
 •Assume surface reflectance relationships:
 $\rho_{0.66}^s = f(\rho_{2.12}^s, NDVI_{SWIR}, \Theta); \rho_{0.47}^s = g(\rho_{0.66}^s, \Theta)$
 •Select fine model aerosol type LUT (function of geography and season)
 •Select coarse model aerosol LUT (dust)
 •Correct lookup tables for elevation
 •Interpolate lookup tables on geometry

Do Inversion
 For 13 values of η (-0.1,0.0,0.1,...0.9,1.0,1.1)...
 Find $\tau_{0.55}$ and $\rho_{2.1}^s$ such that $\rho_{MODIS,0.47} - \rho_{TOA,0.47} = 0$,
 where $\rho_{TOA,\lambda} = \eta(\rho_{fine,\lambda}^s) + (1-\eta)(\rho_{coarse,\lambda}^s)$
 Choose η such that $\rho_{MODIS,0.66} - \rho_{TOA,0.66} = \epsilon$ is minimized
Primary products: $\tau_{0.55}, \eta, \rho_{2.1}^s, \epsilon$

•Calculate $\tau_{\lambda}, \rho_{\lambda}^s, \alpha, M_C, \tau_{\lambda}^{fine}$
 •If $\eta = -0.1$ set $\eta = 0.0$; If $\eta = 1.1$ set $\eta = 1.0$
 •If $\tau_{0.55} < 0.2$, then set $\eta = \text{Fill}$
 •If $\epsilon > 0.25$, then set QAC = 0

Procedure B
 Set QAC=0
 Identify and count pixels where $\rho_{2.13} > 0.25$ and $\rho_{2.13} \leq 0.25 G(\mu, \mu_0) < 0.40$
 Are there at least 12 pixels?
 •Assume surface reflectance relationships:
 $\rho_{0.66}^s = f(\rho_{2.12}^s, NDVI_{SWIR}, \Theta); \rho_{0.47}^s = g(\rho_{0.66}^s, \Theta)$
 •Assume Continental aerosol model (only)
 •Correct lookup table for elevation
 •Interpolate lookup table on geometry

Do Single Channel Retrieval
 Find $\tau_{0.55}$ and $\rho_{2.1}^s$ such that $\rho_{MODIS,0.47} - \rho_{TOA,0.47} = 0$,
 where $\rho_{TOA,\lambda} = \rho_{Continental,\lambda}$
Primary products: $\tau_{0.55}, \rho_{2.1}^s$

•Calculate $\tau_{0.47}, M_C$
 •Set $\eta, \tau_{0.66}, \tau_{2.1}, \alpha, \tau_{\lambda}^{fine} = \text{Fill}$

If $\tau_{0.55} \leq 0.0$ then set $\alpha = \text{Fill}, M_C = 0, \tau_{\lambda}^{fine} = 0$
 If $-0.1 < \tau_{0.55} \leq -0.05$, then set $\tau_{\lambda} = -0.05$
 If $\tau_{0.55} \leq -0.10$, then set $\tau_{\lambda}, \alpha, M_C, \tau_{\lambda}^{fine} = \text{Fill}$

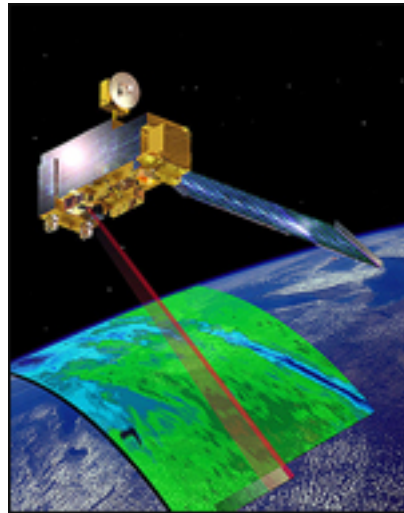
Is $\tau_{0.55} < 0.0$?
 yes: Report: $\tau_{\lambda}, \rho_{\lambda}^s, \alpha, M_C, \tau_{\lambda}^{fine}, QA$, etc EXIT
 no: EXIT

Observations

Satellite Sensor Observation [S]:

MODIS MOD04 /MYD04 Level 2 Reflectance

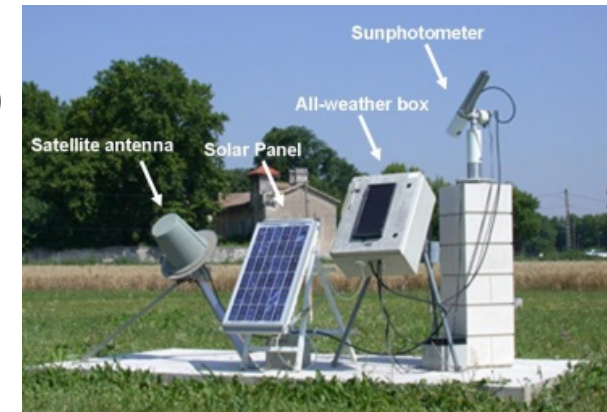
- Cloud masked, quality controlled, 10 km data
- Deep Blue Land
 - 3 channels over bright surfaces
 - 412 nm, 470 nm, and 670 nm
- Dark Target Land
 - 9 channels over dark surfaces
 - 412-2100 nm
- Dark Target Ocean
 - 7 channels over ocean
 - 470-2100 nm



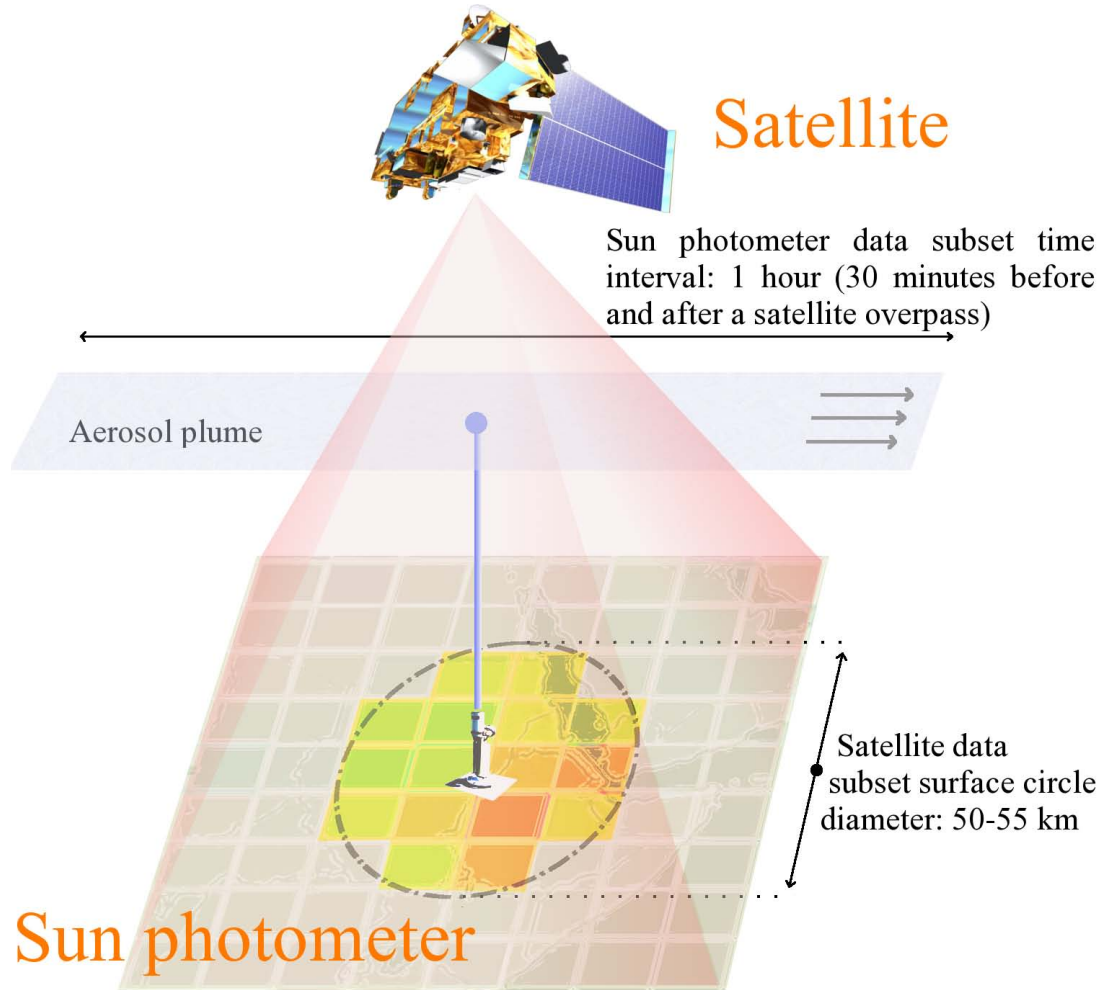
Geophysical Parameter of Interest [G]:

470, 550, 670, 870 nm AOD

- Aerosol Robotic Network (AERONET) observations of AOD
 - Global network of sunphotometers
 - 15 minute sampling
 - Low uncertainty (± 0.01)



MODIS-AERONET Data Pairs



- 15 years of data (2000-2015)
- ~150K Deep Blue data pairs
- ~100K DT-Land data pairs
- ~40K DT-Ocean data pairs

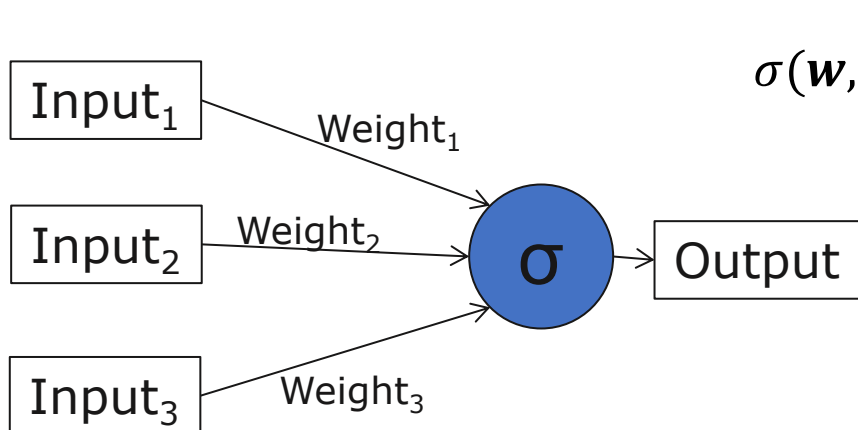
Additional Data Screening

- Outlier removal
- Cloud Fraction < 0.7
- Used MERRA-2 to “balance” the dataset by aerosol type
 - Dust
 - Smoke (Black Carbon + Organic Carbon)
 - Sea Salt
 - Sulfate
- Reduces number of data pairs by half

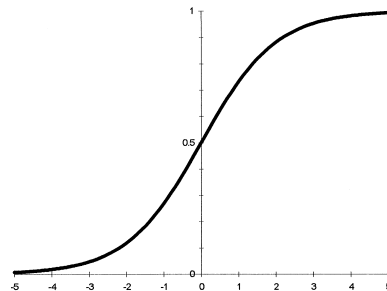
Petrenko, et al. AMT (2012)

Mathematical Function: Neural Network

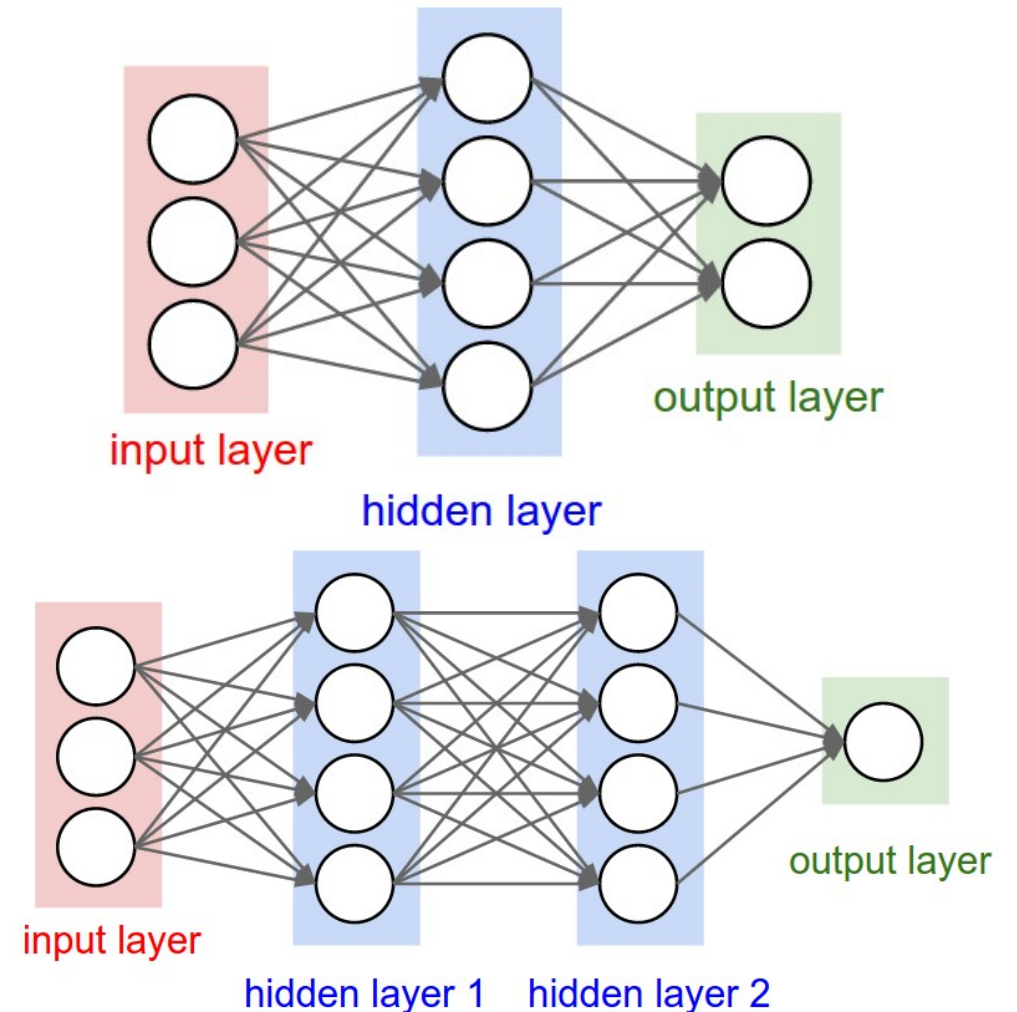
- A set of nodes connected by numerical weights.
- The weights are tuned based on a specific training dataset containing input-output data pairs.
- The superposition of many nonlinear transfer functions (nodes) allow NN's to approximate extremely nonlinear functions



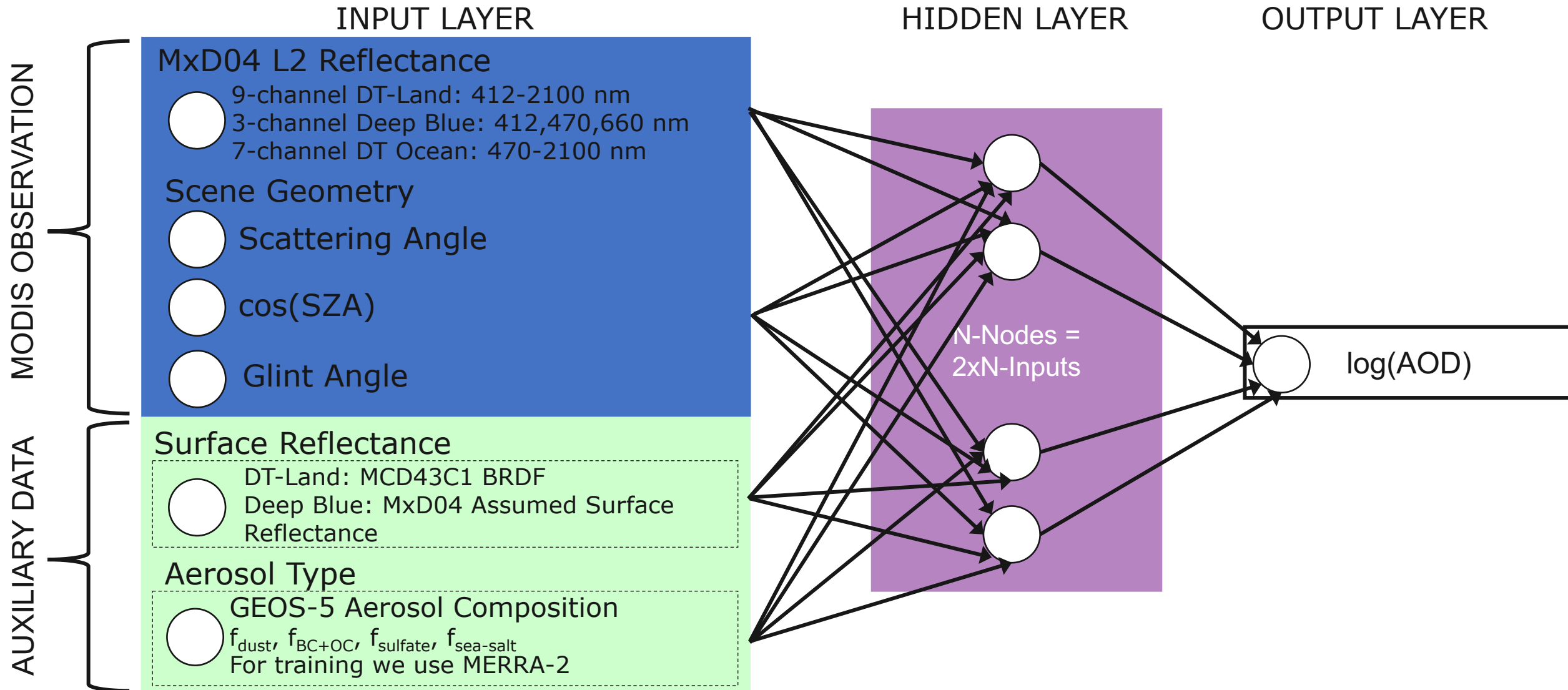
$$\sigma(\mathbf{w}, \mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w} \cdot \mathbf{x} - c)}$$



Feed-forward Neural Network



GEOS-5 NNR for AOD



NNR Training, Testing, Validation

□ Train & Test

- Iteratively train and test adjusting input variables, architecture, etc. to optimize neural network
- Cross Validation
 - K-folding: create K subsets of data, using K-1 for training, and 1 for testing. Iterate K times.

□ Validate

- Use a separate dataset, not used to train/test
- Observations after 2015

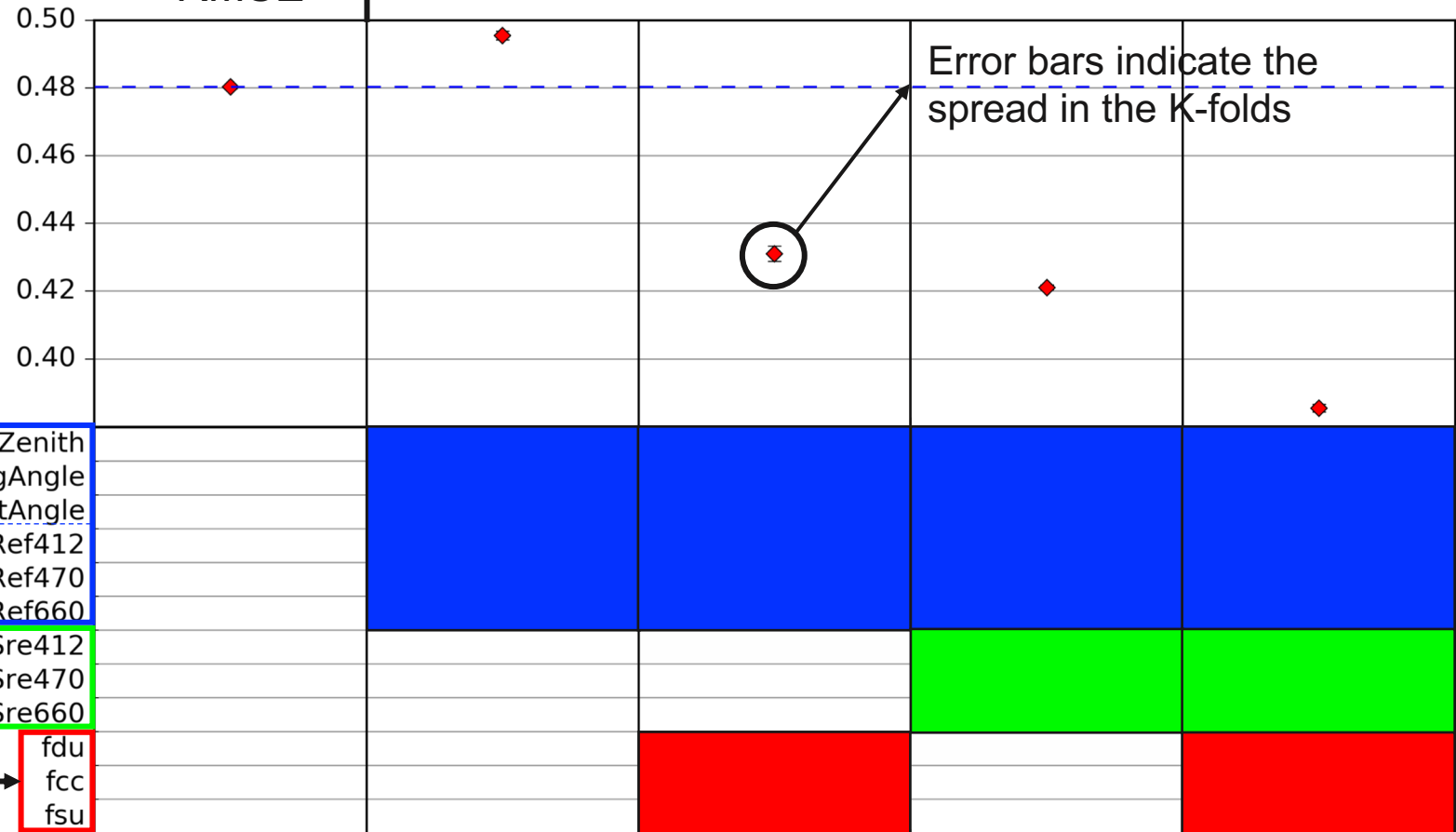


NNR Training & Testing

LAND - Bright Surface Retrieval

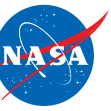
MYD04
RMSE

AQUA DEEP BLUE NNR RMSE



MODIS
AUXILIARY
OBSERVATION
DATA

NNR Testing

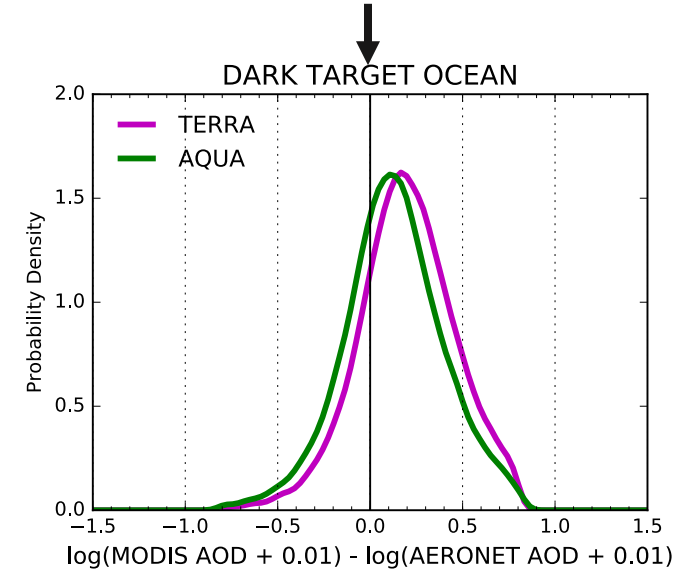
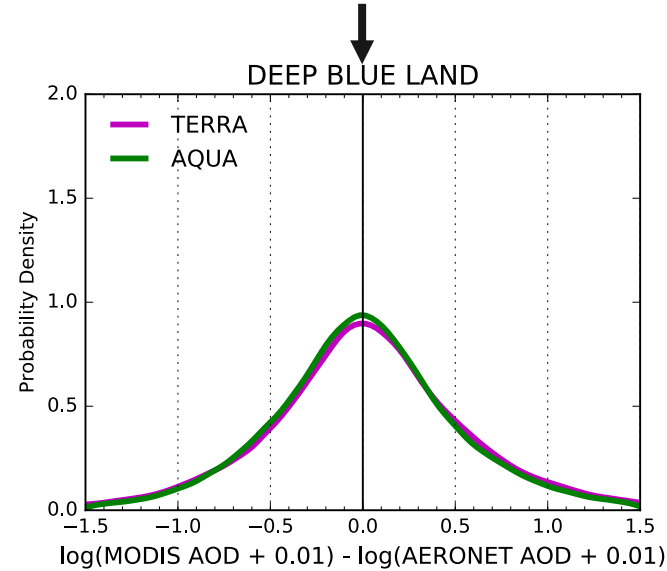
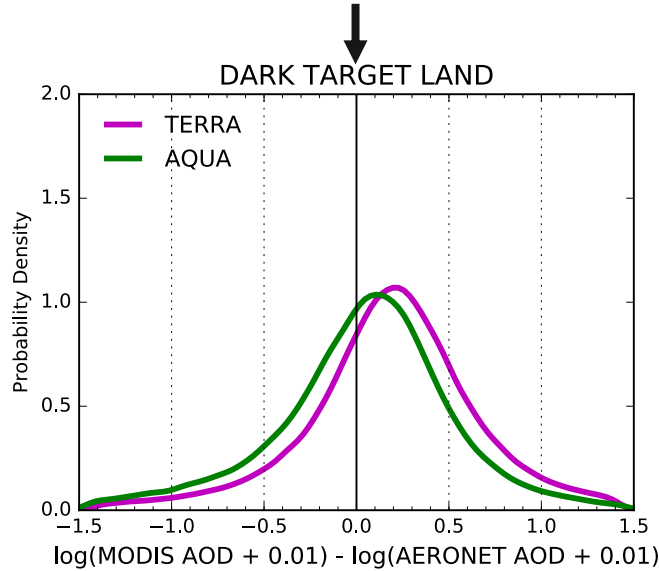


LAND - Dark Surface

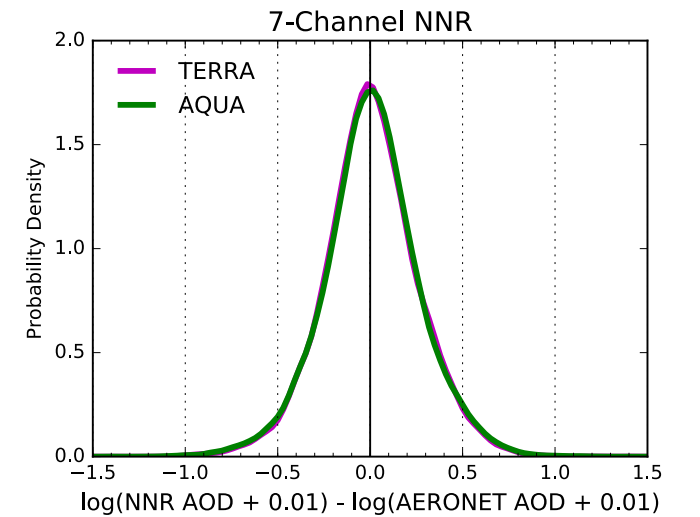
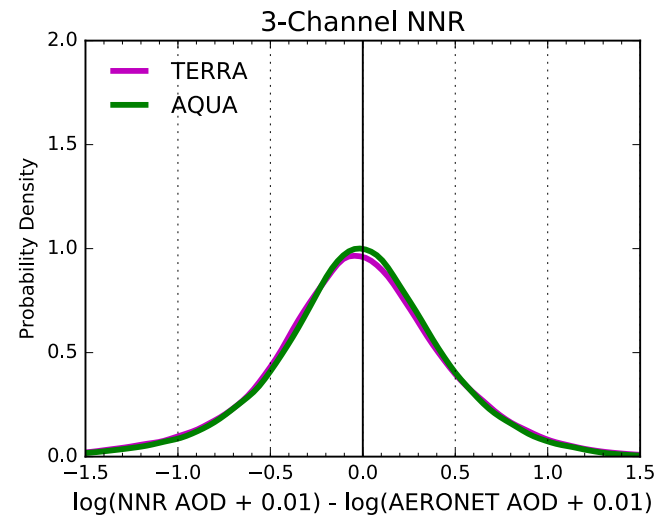
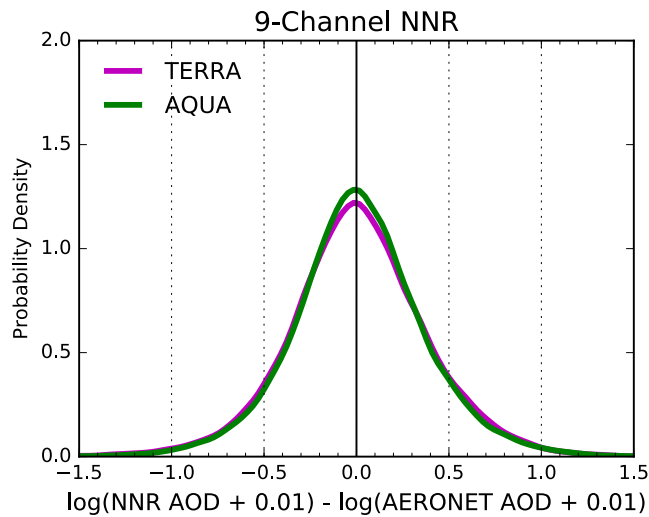
LAND - Bright Surface

OCEAN

MODIS
Standard
Retrievals

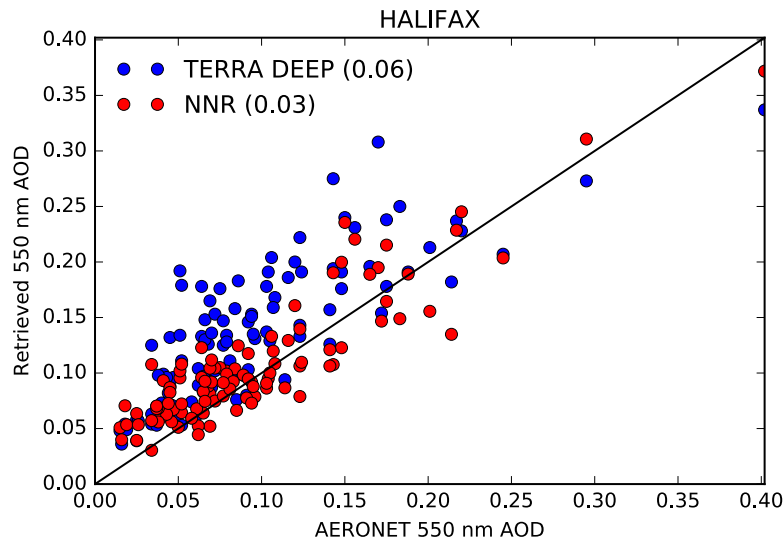


Neural
Network
Retrievals

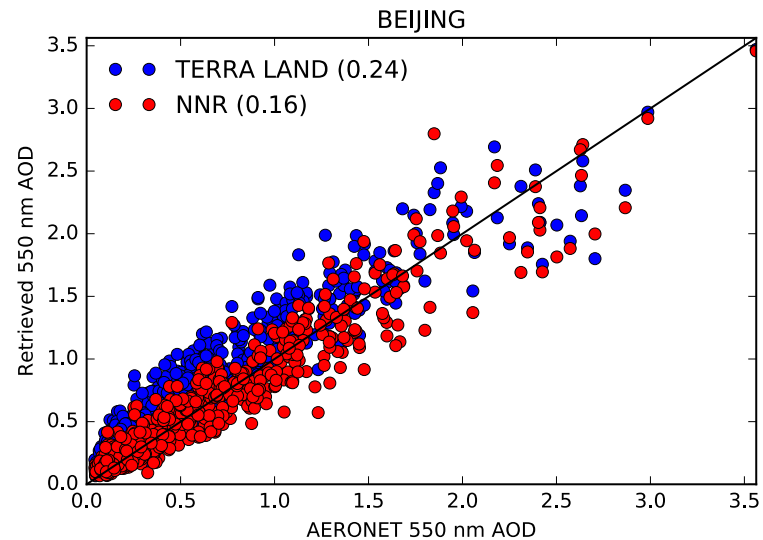


NNR Testing at Some Individual Sites

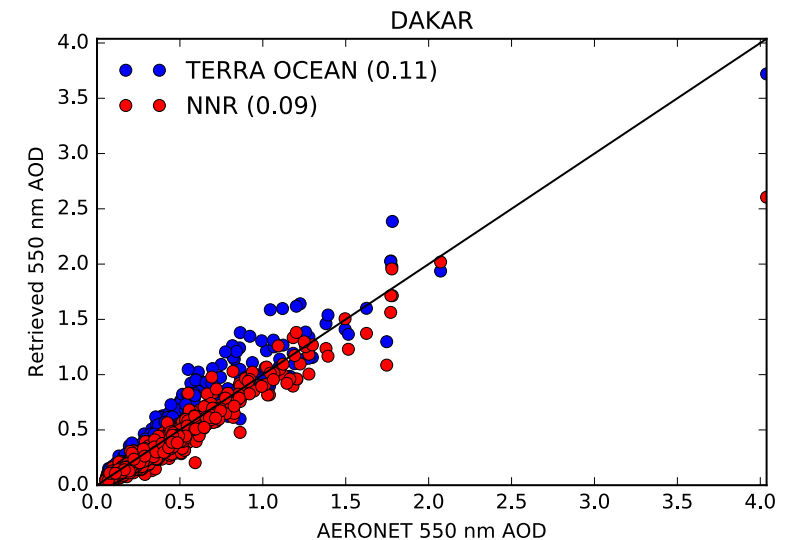
LAND - Bright Surface



LAND - Dark Surface



OCEAN



NNR Validation (Observations after 2015)

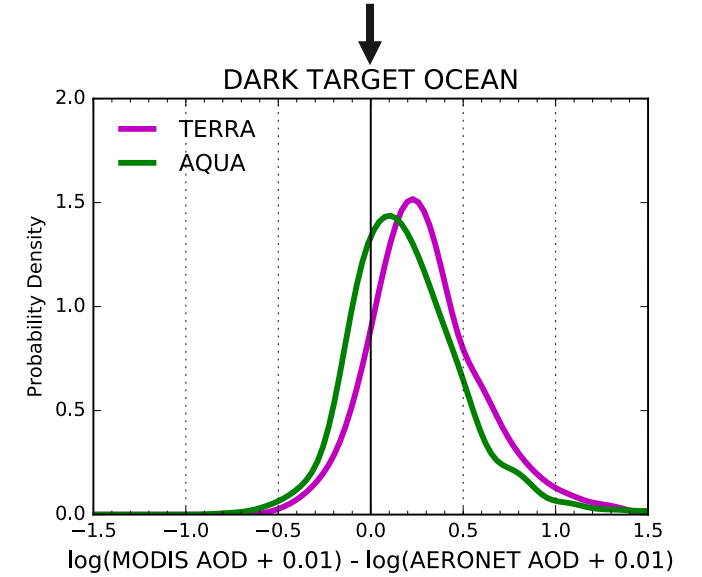
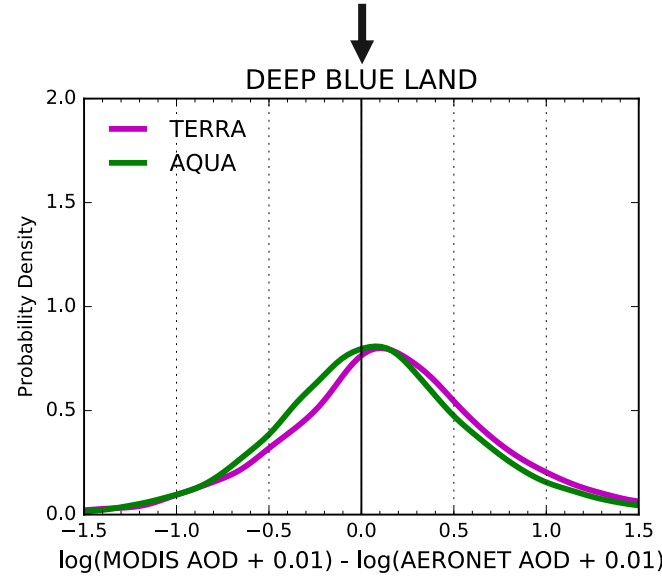
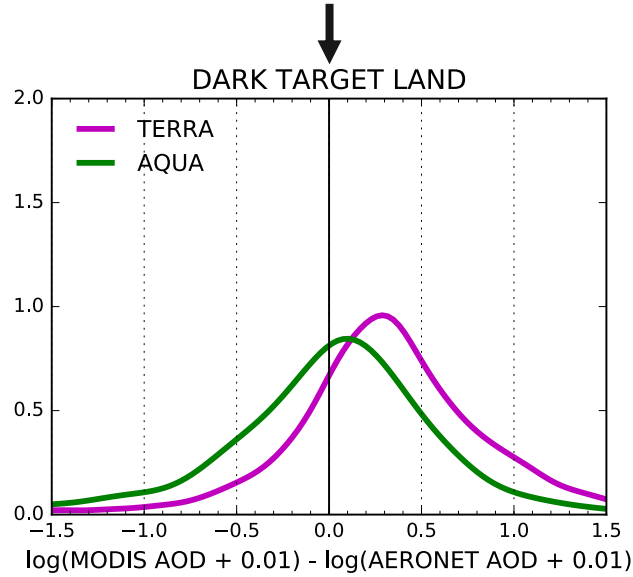


LAND - Dark Surface

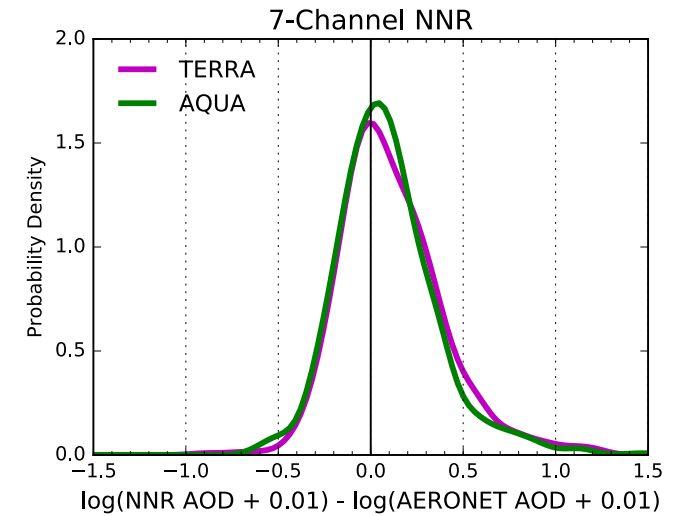
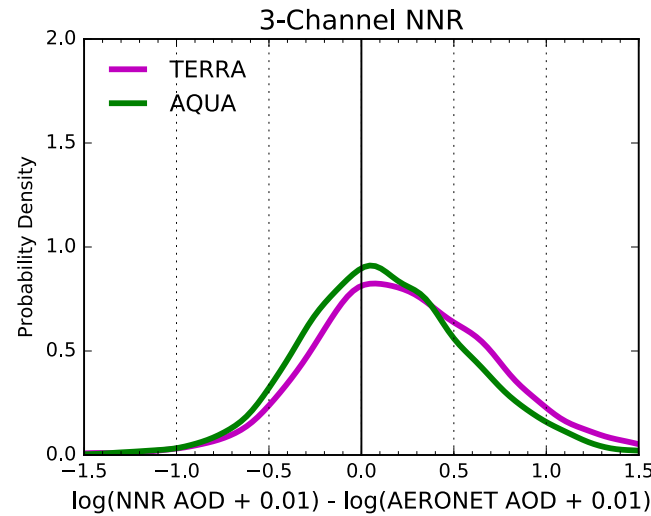
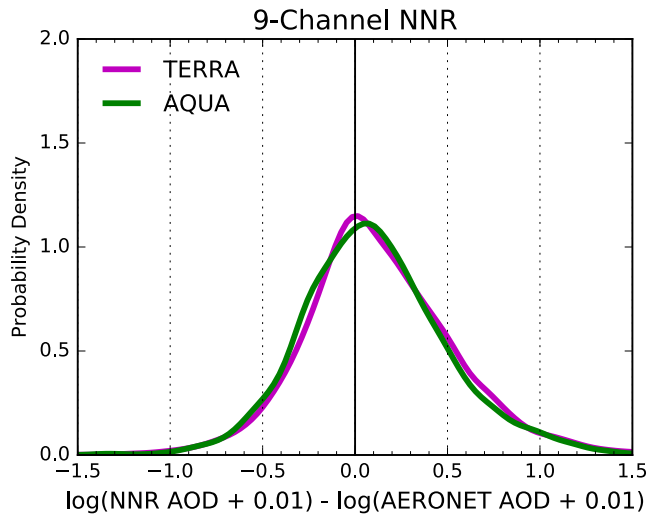
LAND - Bright Surface

OCEAN

MODIS
Standard
Retrievals



Neural
Network
Retrievals

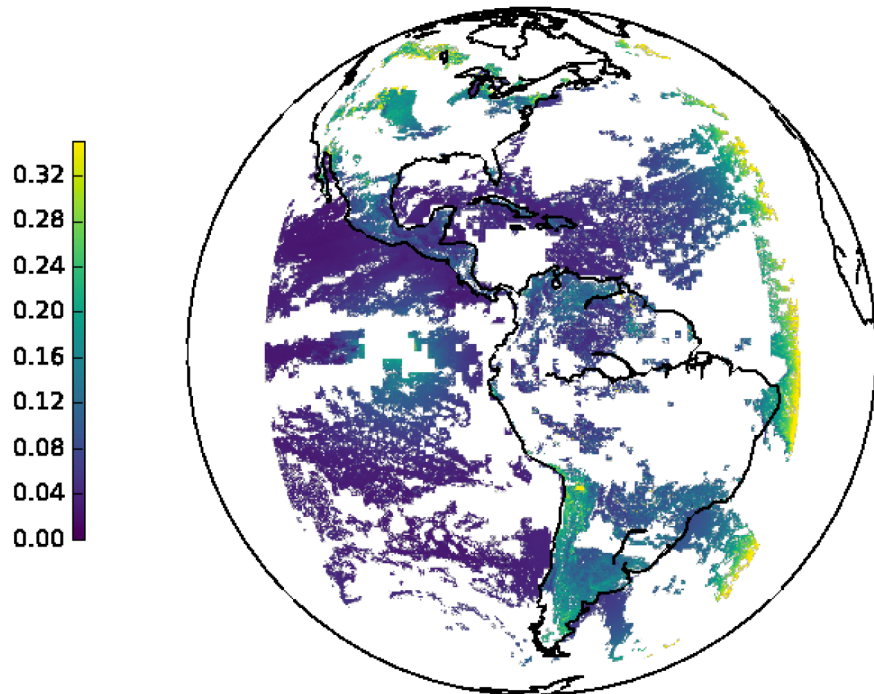


From LEO to GEO: Calibration Transfer

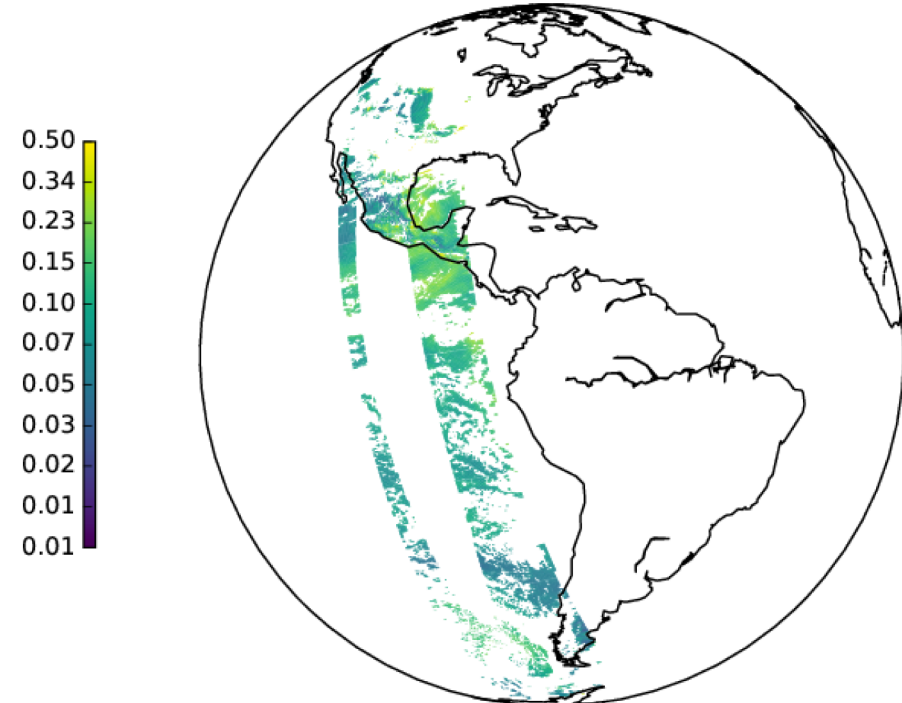
- NRT SatCORPS cloud cleared GOES-16 and AHI-8 TOA reflectances
 - Provided by NASA Langley SatCORPS Group (R. Palikonda, W. Smith)
 - 1 full disk scan per hour
- Use MODIS-NNR AOD as targets for training GEO Reflectance observations

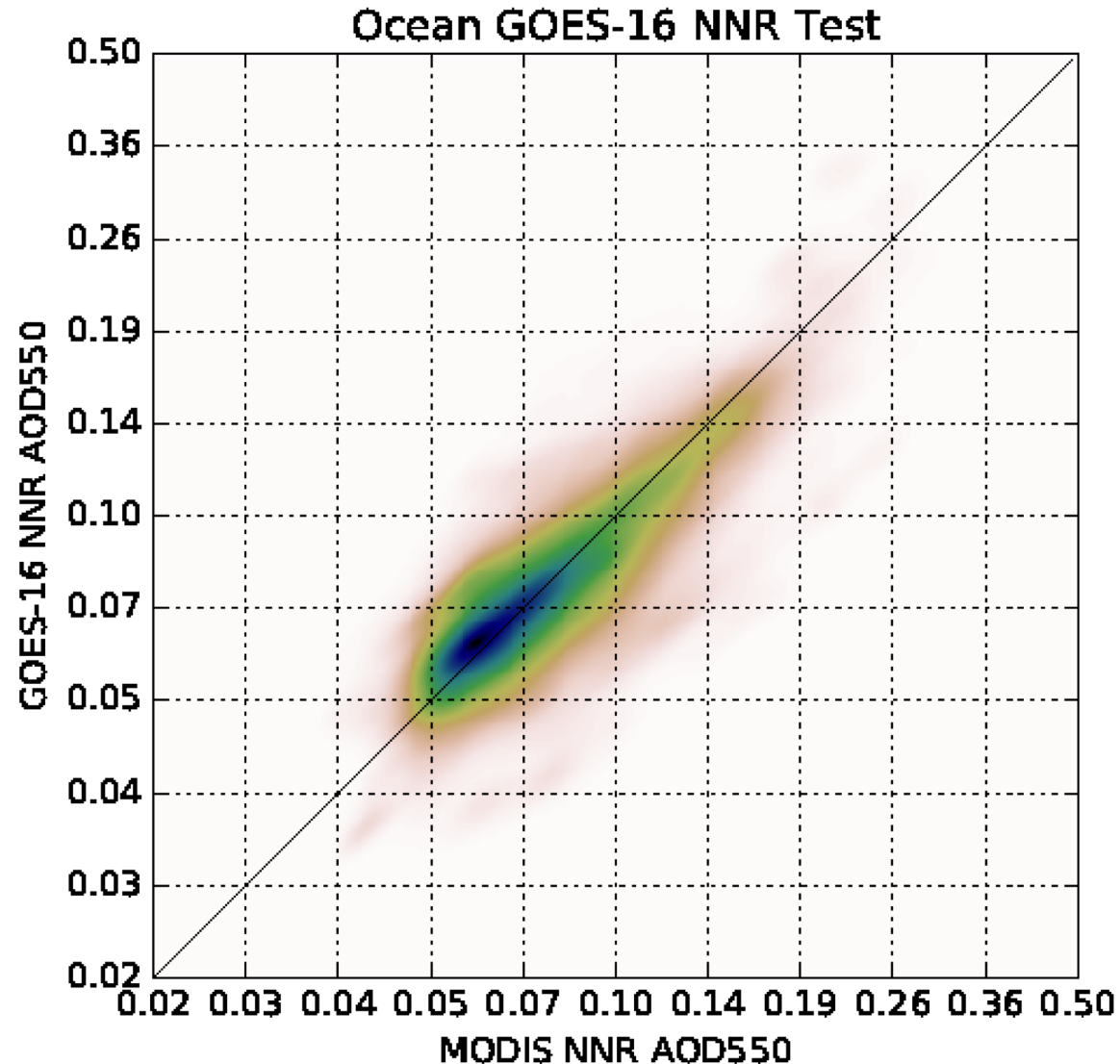
INPUTS  **TARGETS**

GOES-16 TOA 640 Reflectance 2018-03-11 20Z



MODIS Aqua NNR AOD 2018-03-11 20Z

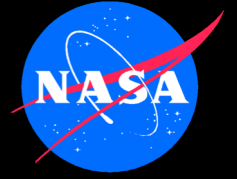




Preliminary Test with Ocean Data

- Trained NNR with 2-months of MODIS/GOES-16 collocated observations
- ~100K data points
- Currently only 640, 860, and 1600 nm channels provided
- No water vapor correction

Current Aerosol Analysis: Splitting



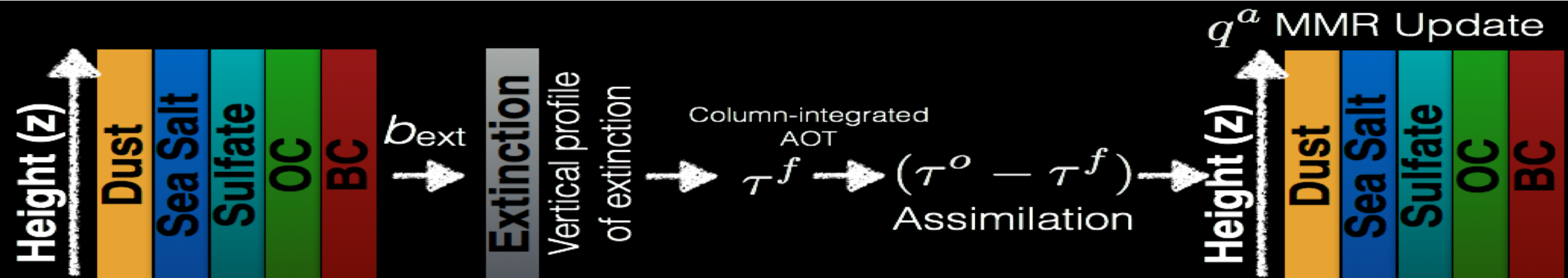
2D AOD ANALYSIS

- Observable 550 nm AOD is 2D
 - MODIS Aqua/Terra: Ocean, Land, Deep Blue channels
 - Constrains column averaged optics
 - Cannot constrain speciation or vertical distribution
- Analysis in observation space:

$$\begin{aligned}\tau^a &\equiv Hq^a = H(q^b + \delta q^a) \\ &= \tau^b + \delta\tau^a\end{aligned}$$

GOING TO 3D CONCENTRATIONS

- Based on error covariances:
$$\delta q^a = BH^T (HBH^T)^{-1} \delta\tau^a$$
- Using ensemble perturbations,
$$\delta q^a = XY^T (YY^T)^{-1} \delta\tau^a$$
- NRT GEOS-5 uses Local Displacement Ensembles (LDE), in 1D
- Developing EnKF for Aerosols

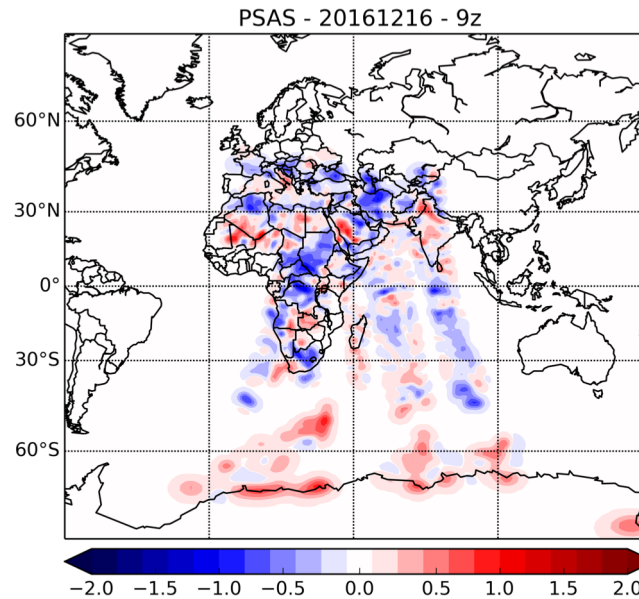


In Development: Aerosol EnKF

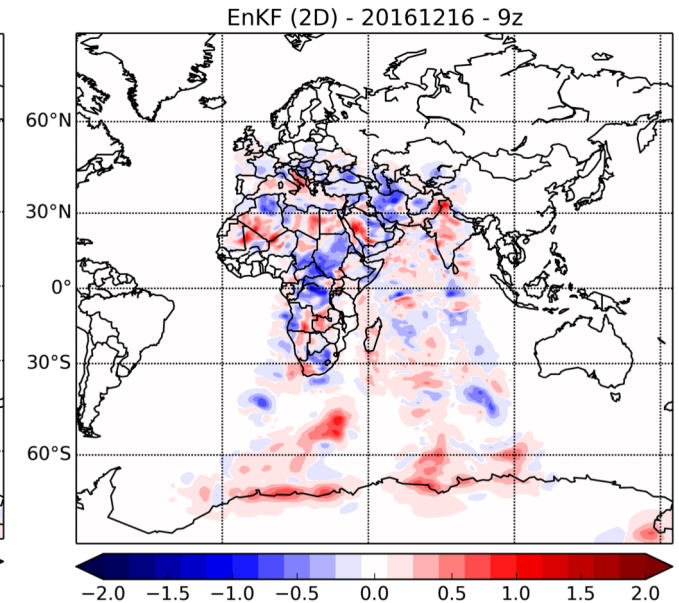


- ❑ As part of GMAO's hybrid system, aerosol ensemble members are produced as a matter of routine
- ❑ The same Whitaker-Hamill EnKF used the hybrid Meteorological assimilation has been adapted for aerosols
- ❑ Target observation systems
 - Multi-spectral AOD: 470, 550 and 870 nm
 - Lidar attenuated backscatter
 - Sensors: MODIS, VIIRS, **GEO**, CATS/CALIOP, TropOMI

PSAS AOD inc (current method)



EnKF AOD inc Ensmean



Summary & Outlook

- The NNR provides a way to homogenize the AOD observing system for data assimilation
- A NNR for GOES-16 and AHI-8 will be developed using the MODIS-NNR AOD data as targets
 - Demonstrates the need for continuity in the observing system
- Innovate the training methodology
 - Multi-channel AOD training allows for physical constraints on cost function
 - Use p.d.f. type of targets – spread in the solution indicates the uncertainty in the NNR AOD.

