Aerosol Modeling and Data Assimilation at GMAO: An Update

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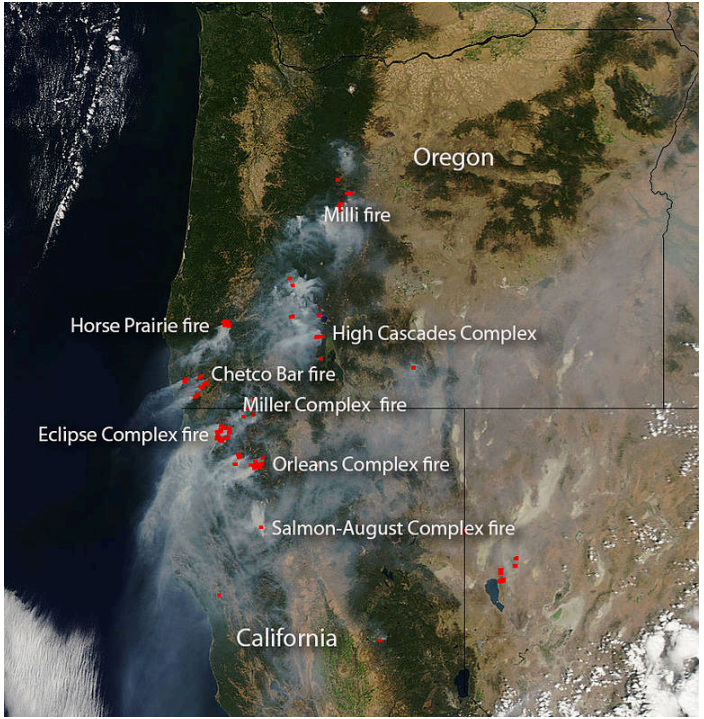
With contributions from: Cynthia Randles, Virginie Buchard, Anton Darmenov, Peter Colarco, Bill Putman, Ravi Govindaraju, Hongbin Yu, Sasha Smirnov and many others

CERES Science Team Meeting

Greenbelt, September 26-28, 2017

Outline

- **Overview: Aerosol Activities at GMAO**
- **Aerosols in the GEOS Earth System Model**
  - Bulk and modal aerosol schemes: GOCART & MAM
  - QFED: GMAO's NRT biomass burning emission
- **Aerosol Data Assimilation**
  - Homogenizing the aerosol observing system
  - AOD assimilation with Local Displacement Ensembles
  - Going forward: Aerosol Ensemble Kalman Filter
- **Applications:**
  - Aerosol in MERRA-2
  - Aerosol impact on meteorological analysis
- **Concluding Remarks**

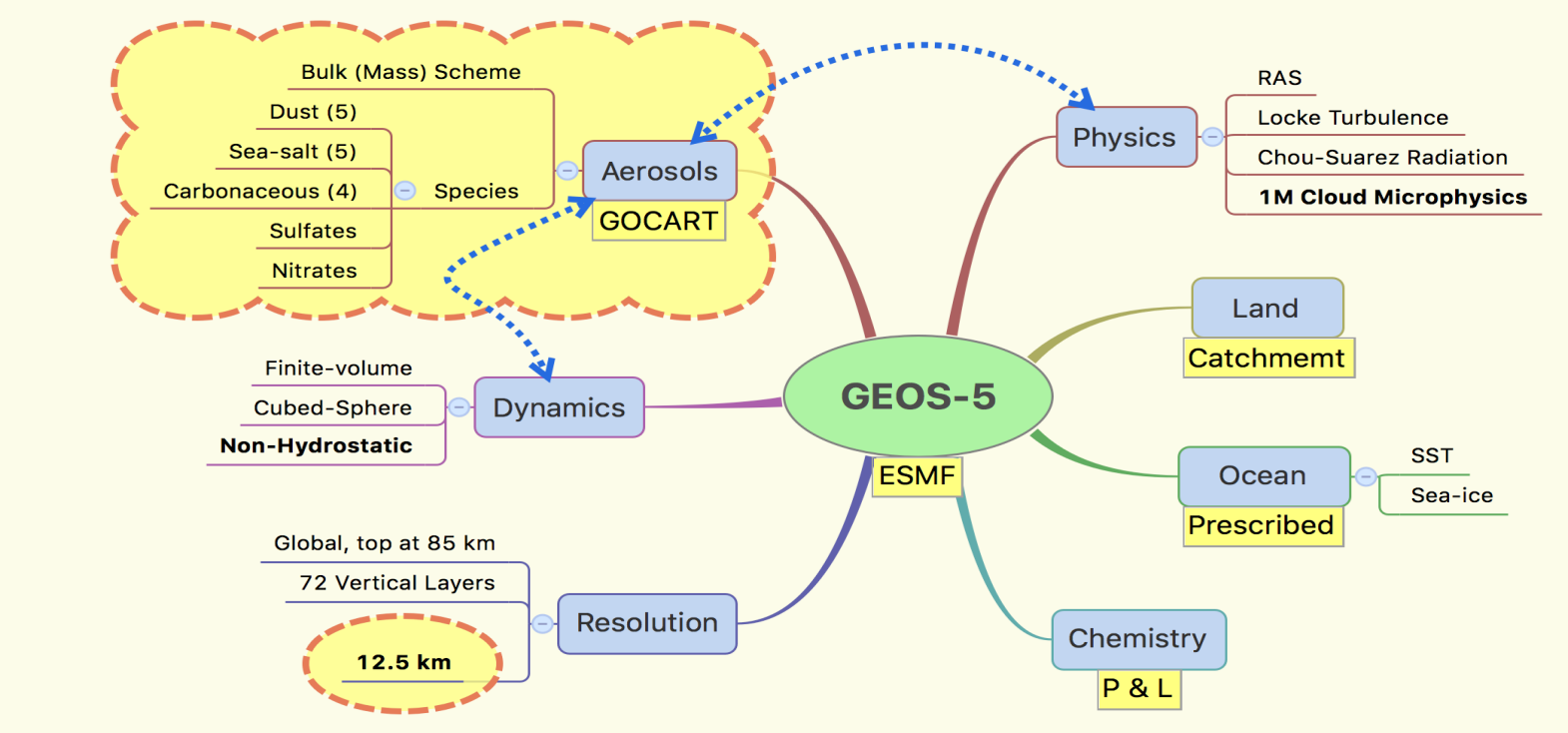


MODIS Aqua true-color image on August 31, 2017

Aerosol Activities at GMAO

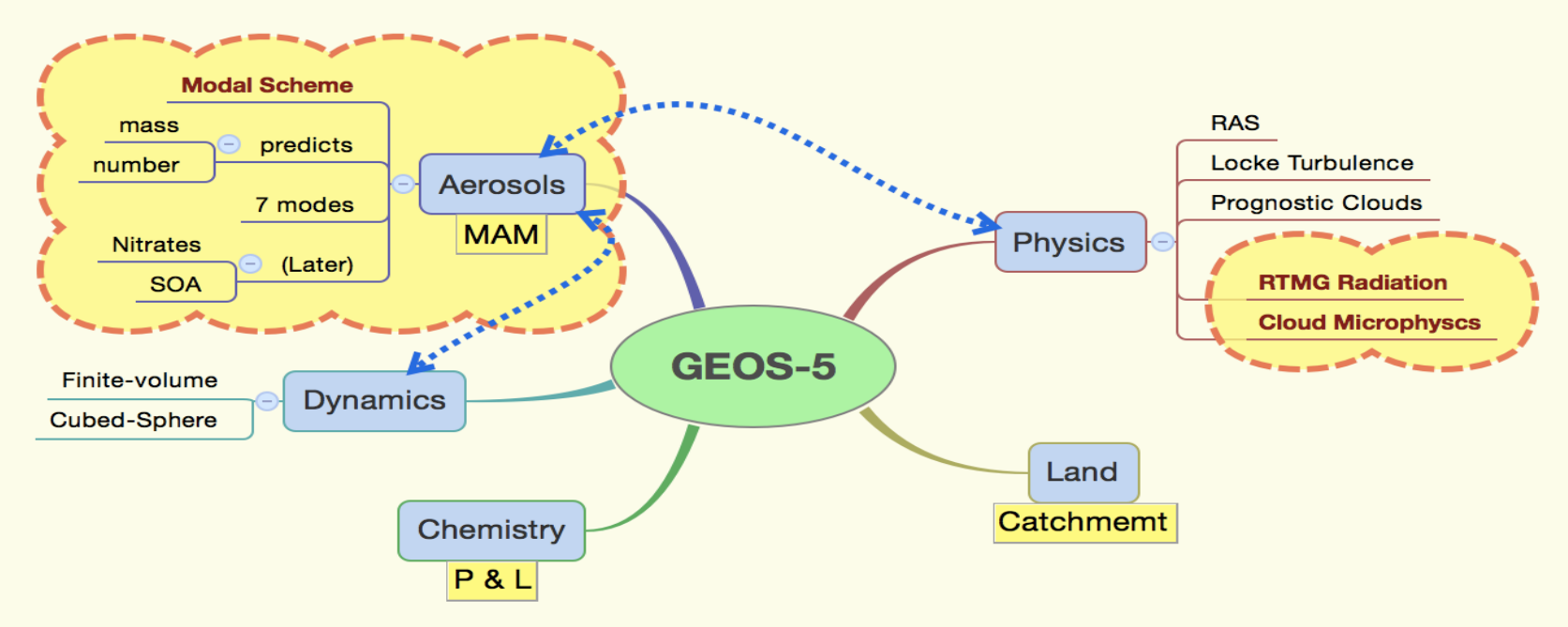
- **Developing a hierarchy of *global* models capable of skillfully representing**
  - the global aerosol distribution as depicted by available in-situ and remotely-sensed measurements
  - the microphysical processes needed for parameterizing cloud/precipitation-aerosol feedbacks
  - Aerosol interaction with earth-system components
- **Developing a comprehensive aerosol data assimilation capability for constraining and calibrating aerosol transport models, including the estimation of emissions needed for driving such models**
- **Developing an aerosol forecasting capability in support of NASA field campaigns.**
- **Developing an aerosol reanalysis capability as a component of a larger IESA**
- **Developing an aerosol observing system simulation capability for aiding planning of future NASA observing missions.**

GEOS-5 Model Configuration for current Forward Processing System



Global, 12.5 km, 72 Levels, top at 0.01 hPa

Current GEOS-5 Development: Aerosol & Clouds Microphysics



Global, **12.5 km**, **72** Levels, top at 0.01 hPa

Biomass Burning

QFED: Quick Fire Emission Dataset

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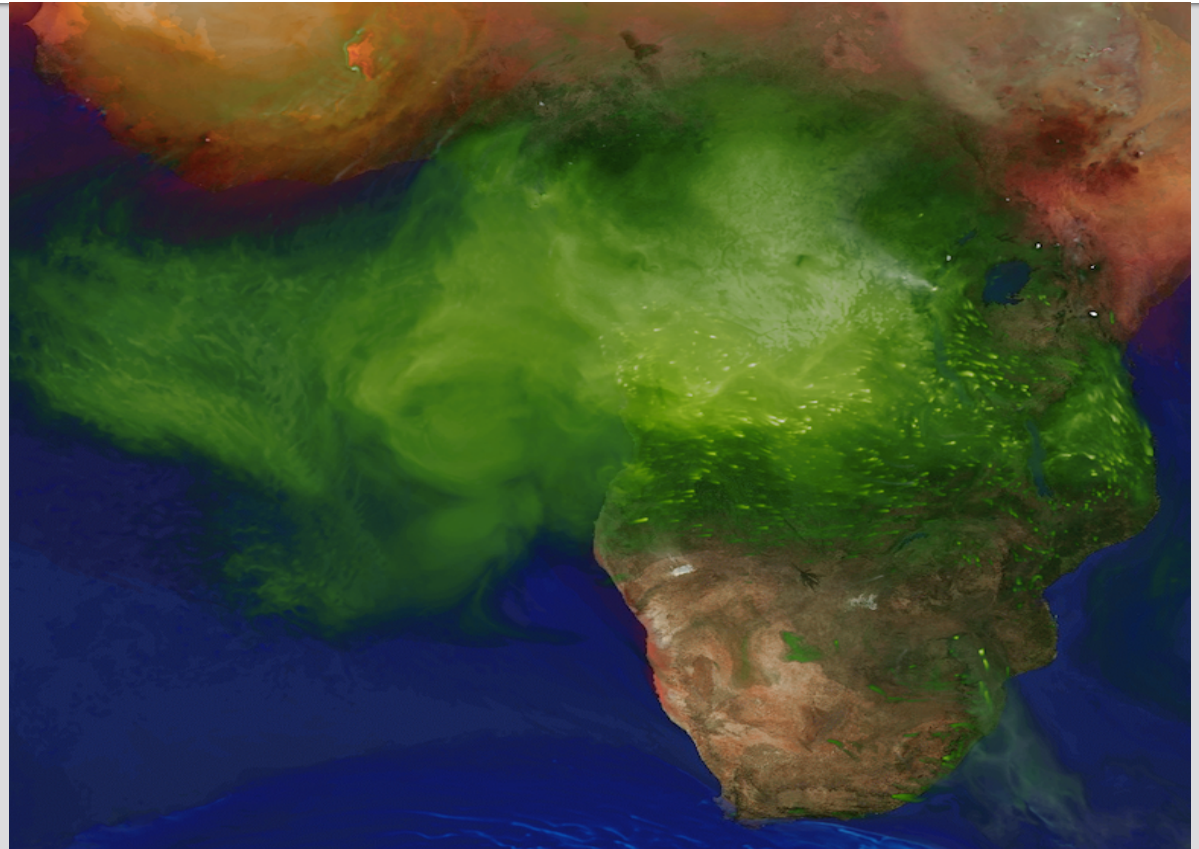
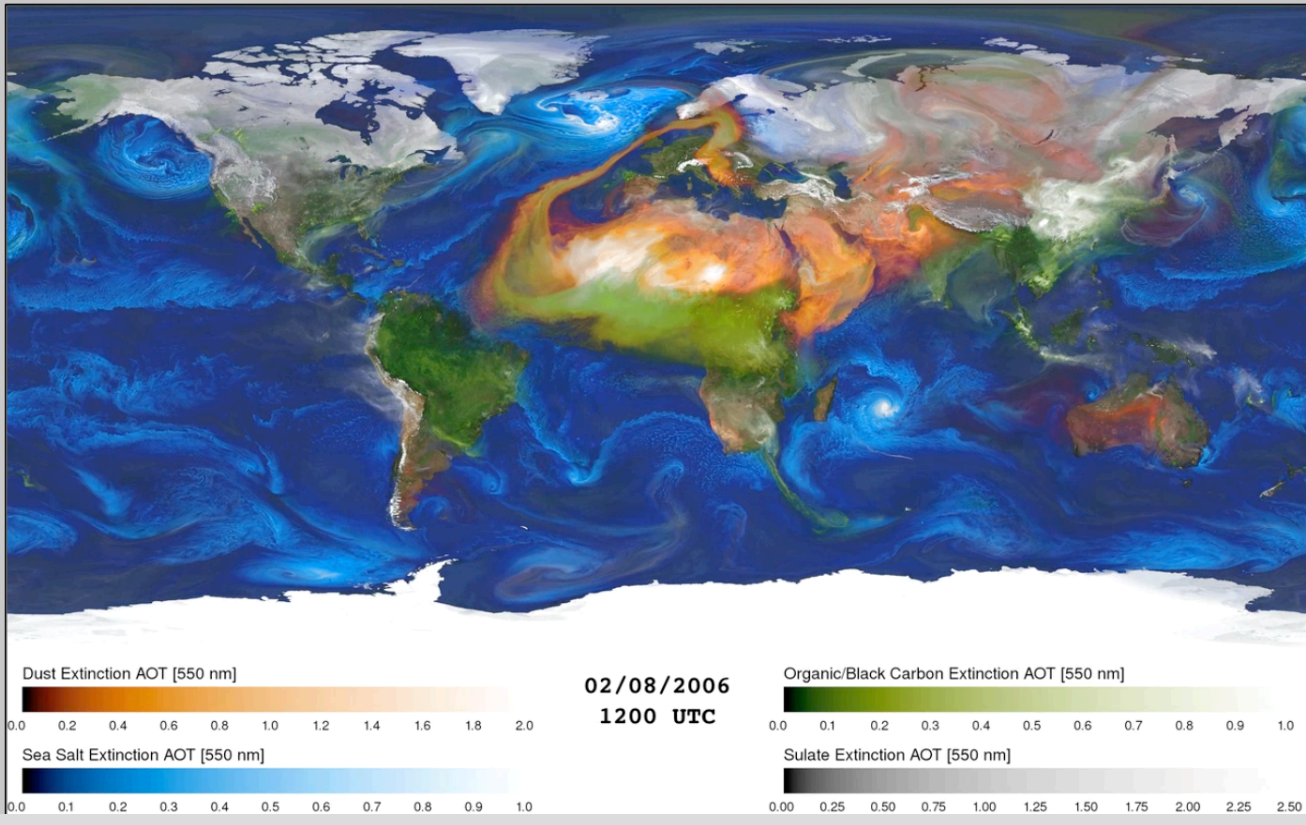
- Top-down algorithm based on MODIS Fire Radiative Power (AQUA/TERRA)
- FRP Emission factors tuned by means of inverse calculation based on MODIS AOD data.
- Daily mean emissions, NRT
- Prescribed diurnal cycle
- In GEOS-5 BB emissions are deposited in the PBL.



Global Aerosols

7 km GEOS-5 Nature Run Global Mesoscale Simulation

Aerosols play an important role in both weather and climate. They are transported around the globe far from their source regions, interacting with weather systems, scattering and absorbing solar and terrestrial radiation, and modifying cloud micro- and macro-physical properties. They are recognized as one of the most important forcing agents in the climate system.



Sulfur Dioxide
Sulfate Aerosols

7 km GEOS-5 Nature Run
Global Mesoscale Simulation

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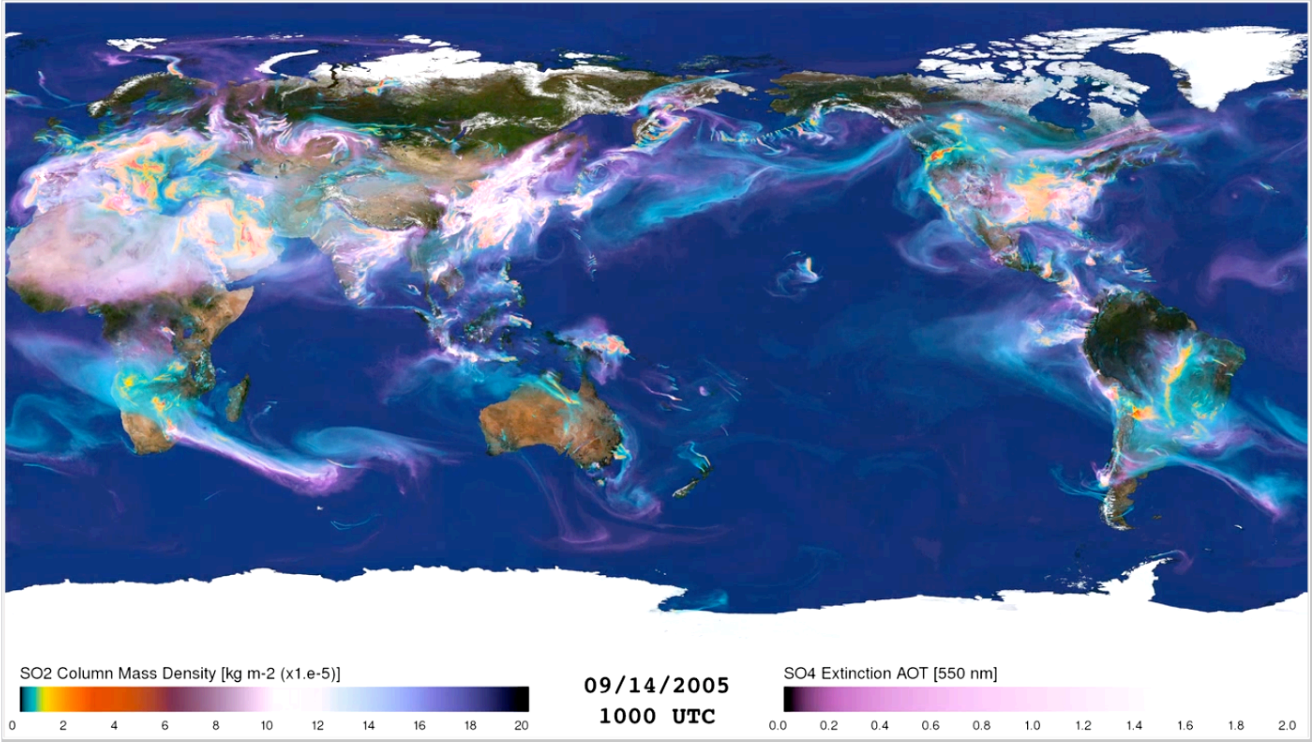
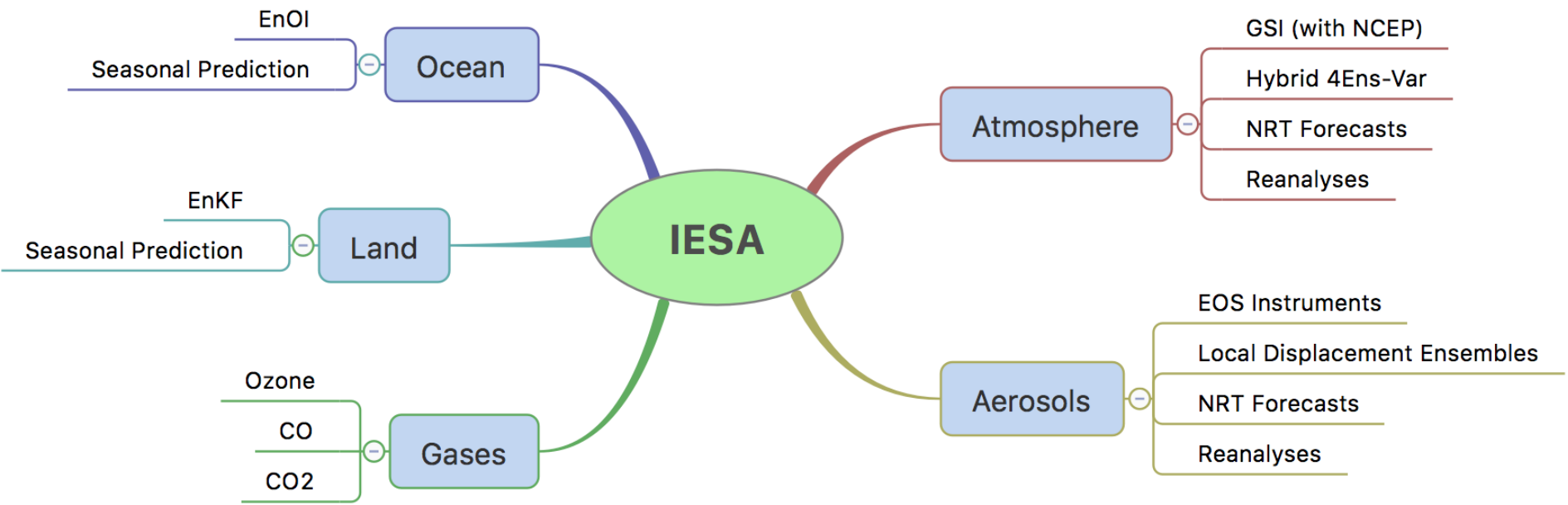
Sulfur dioxide (SO_2), produced during the burning of fossil fuels and from volcanic eruptions, is a short lived gas which can act as pollutant near the surface with detrimental health and acidifying effects. With a mean life time of just a couple of days in the troposphere, emitted SO_2 is quickly converted to sulfate aerosol (SO_4) through oxidation by OH or by reaction with H_2O_2 within clouds. The resulting SO_4 exerts a direct radiative effect on the atmosphere and it can also have an indirect radiative effect by inducing changes in cloud and precipitation microphysics.



Why Aerosol Data Assimilation?

- **Models are useful but difficulty in specifying emissions, microphysical processes and transport lead to large uncertainties**
- **While there are a large number of aerosol sensors, there are still large blind spots:**
  - Measurements are usually vertically integrated
  - Diurnal cycle is not represented by polar orbiters
- **Data assimilation can act as an integrator of model/obs information and as a conveyor of past observations**

Integrated Earth System Analysis (IESA) Data Assimilation for the Earth System



Aerosol Data Assimilation

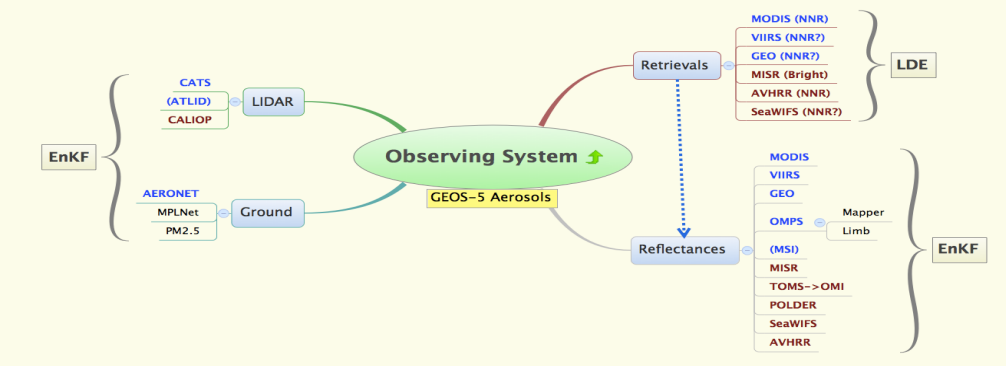
- **State representation**
  - Multiple 3D concentrations
    - Mass
    - Number (modal schemes)
    - Bin sizes (sectional schemes)
  - Number of tracers: tens to hundreds
- **Emissions:**
    - Dynamic: dust, marine, biogenic aerosols
    - Remotely sensed: biomass burning
    - Inventories: anthropogenic
- **Observation operators**
  - Intrinsic aerosol optical properties needed for 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:

$$\tau = \beta \bullet M$$

  - Given diversity of aerosol representation in models, *DA software should not hardwire optical properties.*

Aerosol Observing System

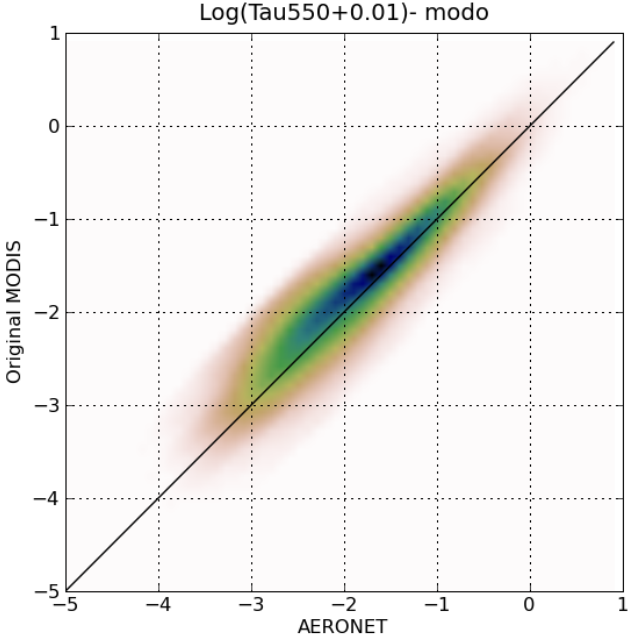
- **Aerosol Optical Depth (AOD) is the most commonly available observable**
  - Vertically integrated mass weighted by extinction coefficient, summed over multiple species: *low observability*
  - Available multi-spectral AOD measurements are not really measured
- **Radiance assimilation:**
  - Vector scattering calculations needed for UV-VIS measurements are not cheap
  - Surface BRDF characterization is a challenge
- **Surface PM 2.5**
  - Single level
  - Often plagued by representativeness



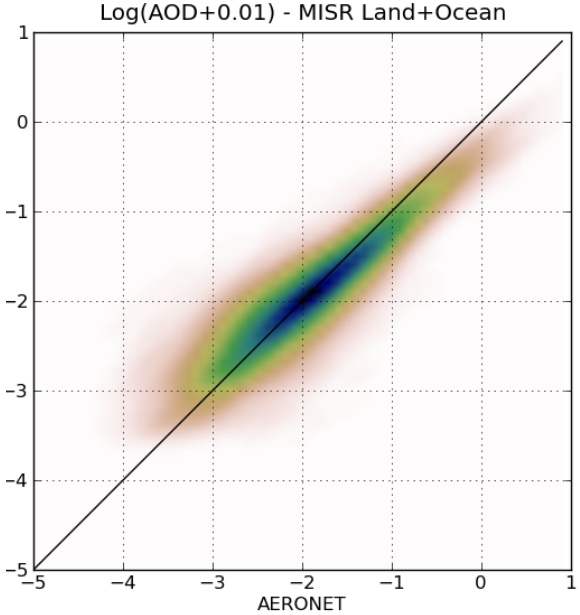
- **Lidar measurements provide vertical info**
  - Spatially coverage is poor (pencil thin)
  - Attenuated backscatter again requires optical assumptions which are not directly measured
    - New HSRL concept is promising

AERONET-MODIS/MISR Joint PDF

C5 MODIS-Terra (Ocean)



MISR (Ocean+Land)



Observation bias correction is necessary.

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NRL Empirical AOD Corrections

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 111, D22207, doi:10.1029/2005JD006898, 2006

Click Here for Full Article

MODIS aerosol product analysis for data assimilation: Assessment of over-ocean level 2 aerosol optical thickness retrievals

Jianglong Zhang[1,2] and Jeffrey S. Reid[1]

Received 16 November 2005; revised 1 March 2006; accepted 10 July 2006; published 18 November 2006.

[1] Currently, the Moderate-resolution Imaging Spectroradiometers (MODIS) level II aerosol product (MOD04/MYD04) is the best aerosol optical depth product suitable for near-real-time aerosol data assimilation. However, a careful analysis of biases and error variances in MOD04/MYD04 aerosol optical depth product is necessary before implementing the MODIS aerosol product in aerosol forecasting applications. Using 1 year's worth of Sun photometer and MOD04/MYD04 aerosol optical depth (τ) data over global oceans, we studied the major biases in MODIS aerosol over-ocean product due to wind speed, cloud contamination, and aerosol microphysical properties. For τ less than 0.6, we found similar uncertainties in the mean MOD04/MYD04 τ as suggested by the MODIS aerosol group, while biases are nonlinear for τ larger than 0.6. We showed that

An over-land aerosol optical depth data set for data assimilation by filtering, correction, and aggregation of MODIS Collection 5 optical depth retrievals

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Neural Net for MODIS C5 AOD Empirical Retrievals

- **Ocean Predictors**
  - Multi-channel
    - TOA Reflectances
    - ~~Retrieved AOD~~
  - Angles
    - Glint
    - Solar
    - Sensor
  - Cloud fraction (<70%)
  - Wind speed
- **Target: AERONET**
  - Log(AOD+0.01)

- **Land Predictors**
  - Multi-channel
    - TOA Reflectances
    - ~~Retrieved AOD~~
  - Angles
    - Solar
    - Sensor
  - Cloud fraction (<70%)
  - Surface Albedo or BRDF Kernels
- **Target: AERONET**
  - Log(AOD+0.01)

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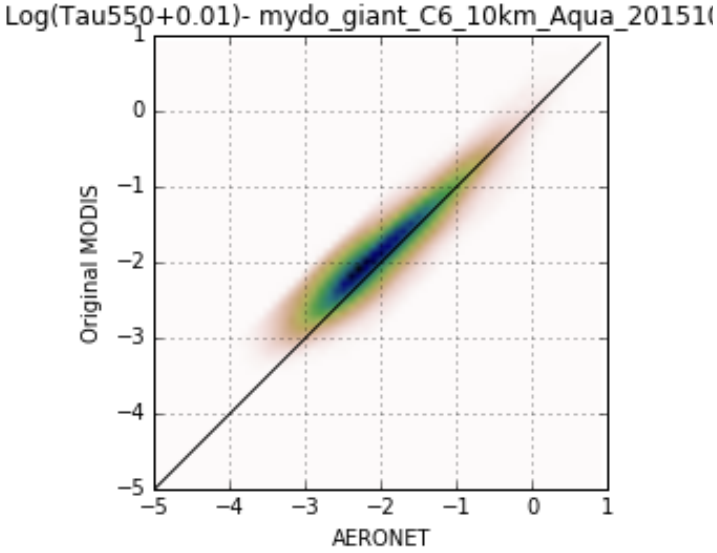
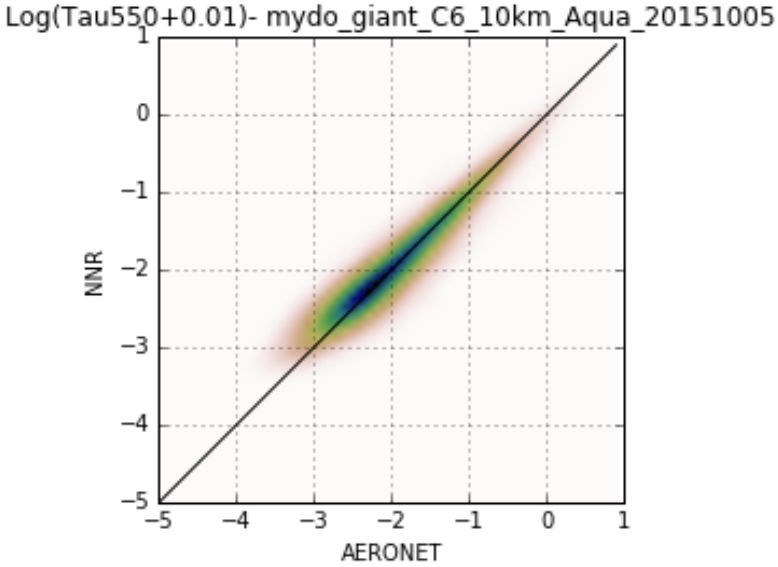
Observational Bias

ORIGINAL MODIS C6 AOD

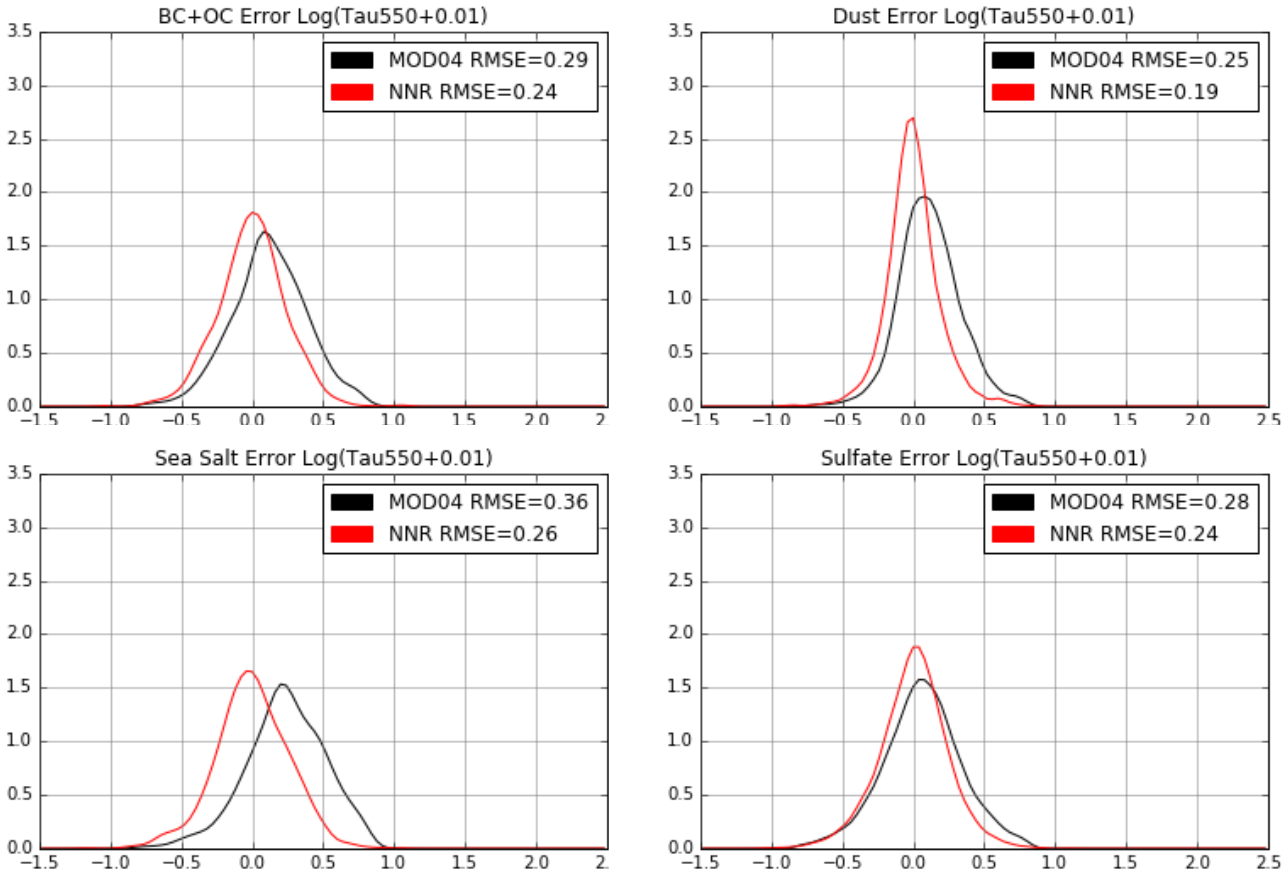


BIAS CORRECTED AOD



MODIS Neural Net AOD Retrievals trained on AERONET

MODIS Collection 6: Aqua



Analysis Splitting

3D Aerosol Concentration Analysis

$$x^a = x^f + P^f H^T \left(HP^f H^T + R\right)^{-1} \left(y^o - Hx^f\right) \equiv x^f + \delta x^a$$

where y is AOD, and x is aerosol concentration.

2D AOD Analysis

Since the AOD observable is 2D is common to solve the AOD analysis equation:

$$y^a \equiv Hx^a = y^f + HP^f H^T \left(HP^f H^T + R\right)^{-1} \left(y^o - Hx^f\right) \equiv y^f + \delta y^a$$

Projecting AOD into Concentration Increments

The 3D concetration increments is related to the 2D AOD increments by:

$$\delta x^a = P^f H^T \left(HP^f H^T\right)^{-1} \delta y^a$$

For efficiency, this last equation can be solved in 1D (vertical).

Analysis Splitting with Ensembles

If the background error covariance P^f is parameterized in terms of ensemble perturbations, say

$$\begin{aligned} X &= \begin{pmatrix} x_1 & x_2 & \cdots & x_E \end{pmatrix} \\ Y &= HX \\ &= \begin{pmatrix} Hx_1 & Hx_2 & \cdots & Hx_E \end{pmatrix} \\ &= \begin{pmatrix} y_1 & y_2 & \cdots & y_E \end{pmatrix} \end{aligned}$$

so that

$$P^f \sim XX^T$$

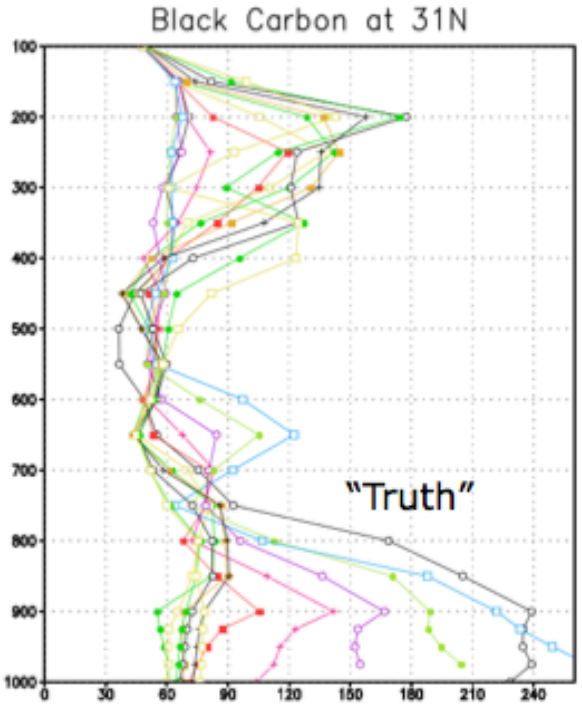
it follows that

$$\delta x^a = XY^T \left(YY^T\right)^{-1} \delta y^a$$

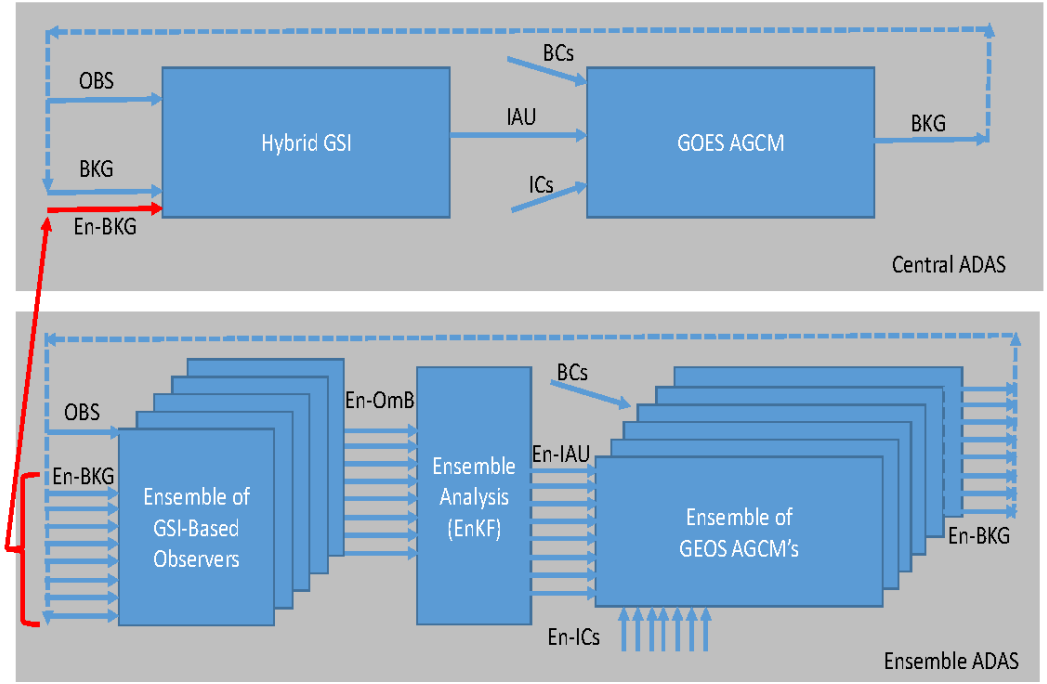
This is the well known (unbiased) linear regression equation.

Local Displacement Ensembles (LDE)

- Construct perturbation ensembles by means of isotropic displacements around gridbox
- Weigh each ensemble member by its fit to 2D AOD analysis
- For efficiency, perform the AOD-to-mixing ratio calculation in 1D



GEOS-5 Hybrid Data Assimilation

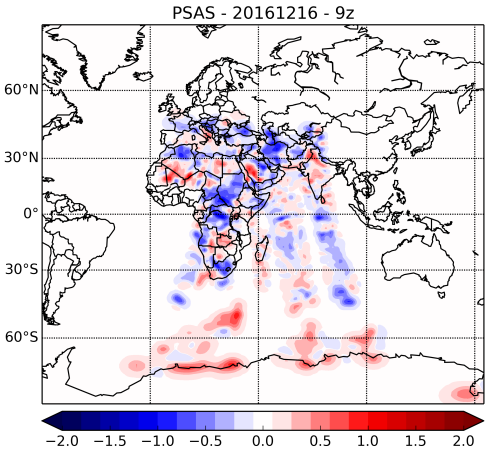


Remark: Ensemble analyses are not re-centered around central (top) DAS analysis.

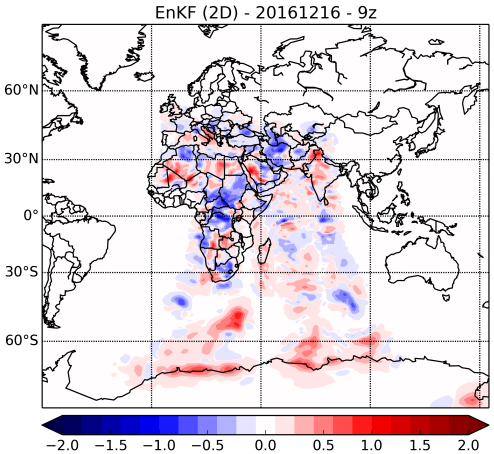
In Development: Aerosol EnKF

- **As part of GMAO's hybrid system, aerosol ensemble members are produced as a matter of routine**
- **The same Whitaker-Hamill EnKF used for 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



GMAO Data Products

Product	Brief Description	Links
GEOS FP	Analyses and forecasts produced in real time, using the most recent validated GEOS system	GEOS NRT Product Table GEOS Wx Maps
GEOS FP-IT	Analyses produced for Instrument Teams, using a stable version of GEOS	Available by subscription only: please contact Rob Lucchesi (rob.lucchesi@nasa.gov) GEOS NRT Product Table
Seasonal Forecasts	Ocean analyses and nine-month atmosphere-ocean forecasts	Seasonal-Decadal Analysis & Prediction Products
MERRA-2	A reanalysis of the period 1979 to the present, including aerosols	MERRA-2 data archive at the GES-DISC GMAO Reanalysis Products
7km-G5NR	A "Nature Run" using a high-resolution version of GEOS, spanning two years and including aerosols and carbon gases	7km-G5NR data archive at the NCCS Data Portal
SMAP L4	Soil moisture and carbon fluxes produced as part of the SMAP mission	GMAO SMAP Level 4 Products page SMAP data at the NSIDC

https://gmao.gsfc.nasa.gov/products/

Applications

AEROSOLS IN MERRA-2

The MERRA-2 Aerosol Reanalysis, 1980 Onward. Part I: System Description and Data Assimilation Evaluation

6823–6850

SC

C. A. Randles, A. M. da Silva, V. Buchard, P. R. Colarco, A. Darmenov, R. Govindaraju, A. Smirnov, B. Holben, R. Ferrare, J. Hair, Y. Shinozuka, and C. J. Flynn

Journal of Climate

September 2017, Vol. 30, No. 17

Published online on 27 Jul 2017.

Abstract | Full Text | PDF | Supplemental Material

The MERRA-2 Aerosol Reanalysis, 1980 Onward. Part II: Evaluation and Case Studies

6851–6872

SC

V. Buchard, C. A. Randles, A. M. da Silva, A. Darmenov, P. R. Colarco, R. Govindaraju, R. Ferrare, J. Hair, A. J. Beyersdorf, L. D. Ziemba, and H. Yu

Journal of Climate

September 2017, Vol. 30, No. 17

Published online on 27 Jul 2017.

Abstract | Full Text | PDF | Supplemental Material

http://journals.ametsoc.org/topic/merra-2

Why we make a reanalysis?

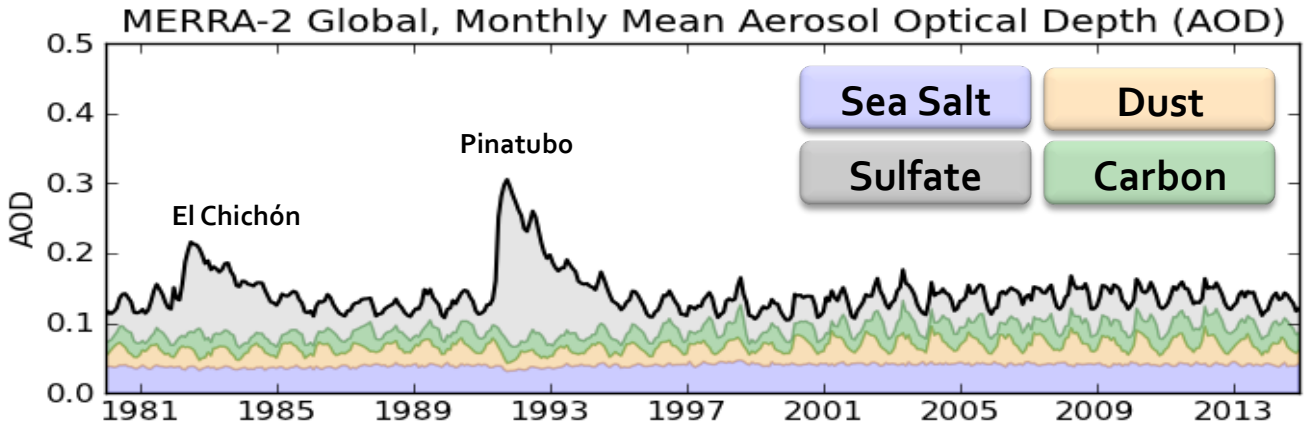
A consistent reprocessing of Earth system observations using a modern, unchanging data assimilation system

- Relies on models to interpret, relate and combine many different observations from multiple sources
- Produces multi-decadal gridded data sets that estimate a large variety of Earth system variables, including ones that are not directly observed
- Has become fundamental to research and education in the Earth Sciences

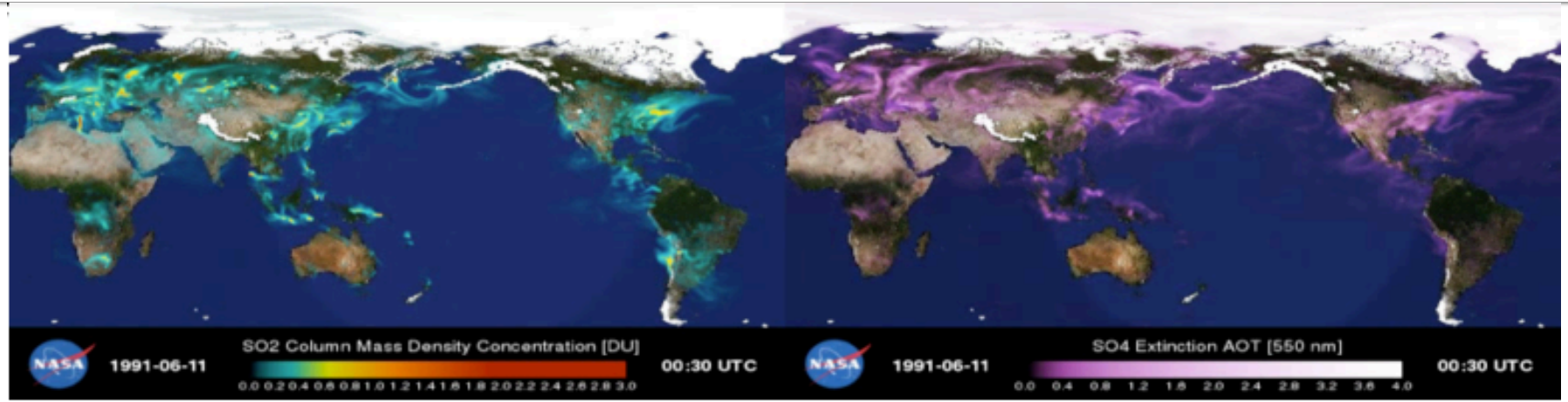
A successful reanalysis ***requires*** a good forecast model combined with bias-corrected/quality controlled observations

MERRA-2 Global Mean AOD Analysis: 1980 - Onward

- Unique amongst its peers, the MERRA-2 reanalysis now includes an aerosol reanalysis for the modern satellite era (1980 – onward).
- Aerosols are ***coupled*** to the meteorological reanalysis (both radiatively and through emissions/loss processes).



MERRA-2: Pinatubo Eruption



- First aerosol assimilation to include major historic volcanic events like El Chichón (1982) and Pinatubo (June, 1991).
- Movie shows the co-evolution of gaseous SO_2 emissions from Pinatubo (left) and formation of the the sulfate aerosol plume (right) as SO_2 is converted into particles.
- SO_2 (g) is from emissions inventories and unconstrained by assimilation. Sulfate aerosol AOD (right), however, is impacted by the assimilation of total aerosol AOD.

MERRA-2 Emissions

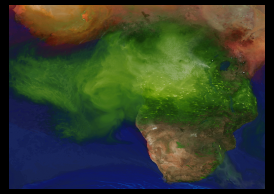


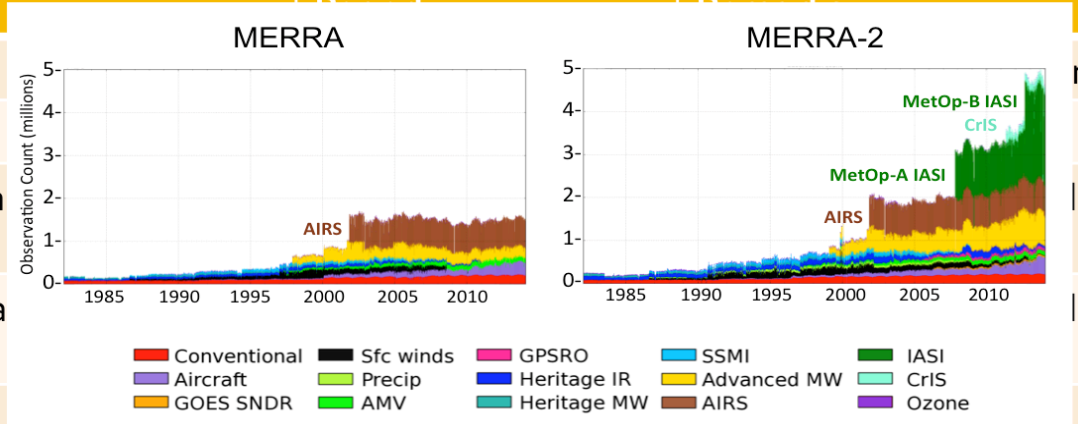
Table 1: Aerosol emissions databases (native temporal and spatial resolutions).

Aerosol Type	Source	Temporal Resolution	Spatial Resolution[a,b]
Dust[c]	Wind-driven emissions w/? source	Annual-mean climatology	0.3125° × 0.25°
Sea Salt	Wind-driven emissions	Model	Model
Volcanic (SO_2)	AeroCom Phase II (HCA0 v2)	Daily	Point-sources
Biogenic terpene	GEIA	Monthly-mean climatology	2° × 2.5°
DMS	Lana *et al.* 2011	Monthly-mean climatology	1° × 1°
Biomass Burning (SO_2, OC and BC)[d]	HFED	Monthly-varying	0.5
Biomass Burning (SO_2, OC and BC)[e]	QFED-2.4r6	Daily	0.3125° × 0.25°
Anthropogenic SO_2 and SO_4	EDGARv4.2 (Energy + Non-Energy)	Annually-varying	1° × 1°
Anthropogenic OC and BC	AeroCom Phase II (HCA0 v1)	Annually-varying	1° × 1°
Ship (SO_2, SO_4, OC, BC)	EDGARv4.1 and ?	Annually-varying	1° × 1°
Aircraft (SO_2)	AeroCom Phase II (HCA0 v1)	Monthly-varying	1° × 1.25° × 72-levels

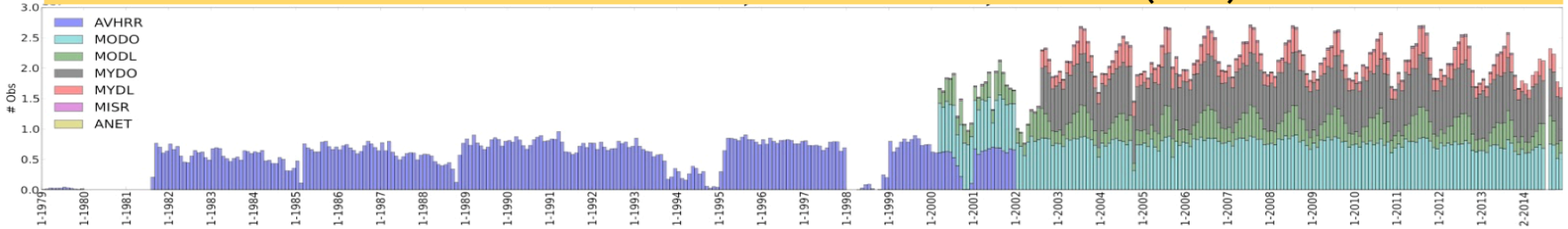
[a] Model = MERRA-2 time-step of 30 minutes with spatial resolution of 0.5° latitude × 0.625° longitude.
[b] latitude × longitude
[c] Resolution is for source map (Ginoux *et al.* 2001); wind-driven emissions at model time-step.
[d] Streams 1-3; Y1979-Y2010
[e] Stream 4; Y2010-onward

Aerosol Observing System

Sensor		
AVHRR*		n Only
AERONET		
MODIS Terra		l & ocean
MODIS Aqua		l & ocean
MISR	2000 – 2014	Bright surfaces (albedo > 0.15)

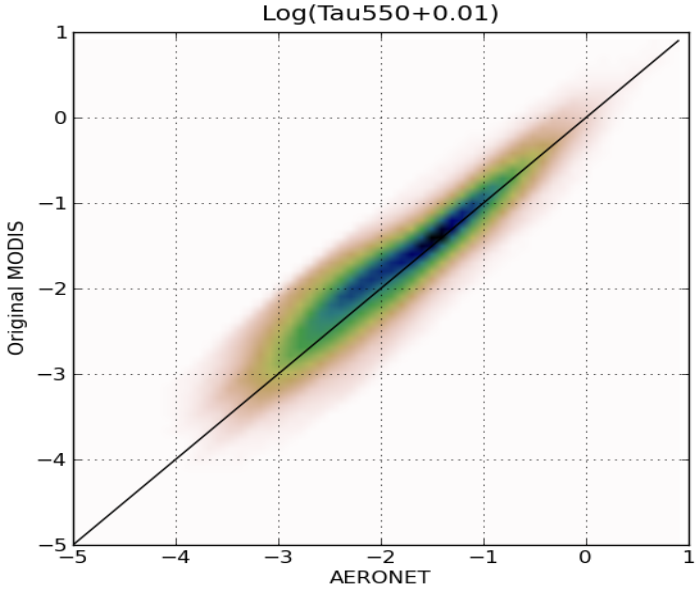


TOTAL GLOBAL MONTHLY NUMBER OF AOD OBSERVATIONS (× 10^7) BY SENSOR

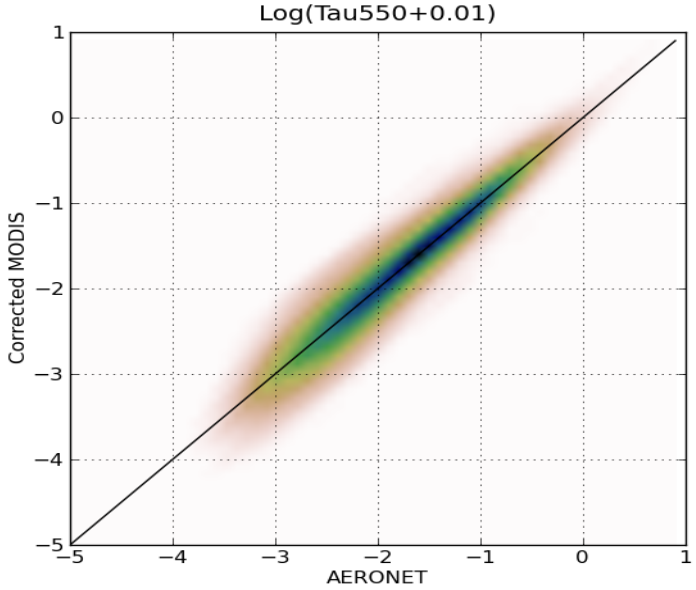


Observational Bias

ORIGINAL MODIS AOD



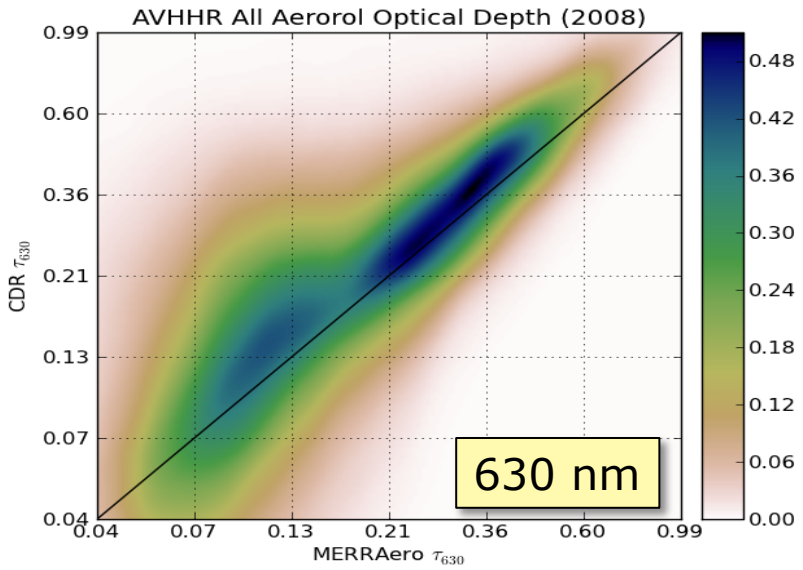
BIAS CORRECTED AOD



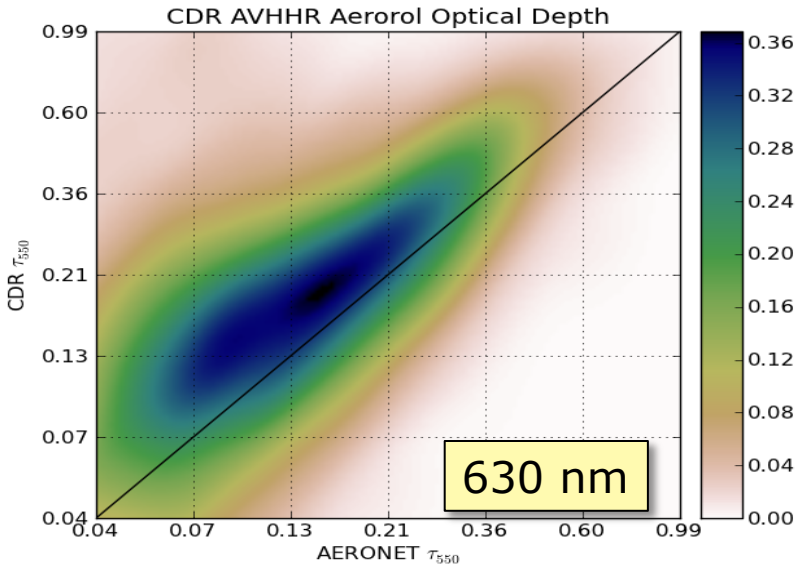
MODIS Neural Net AOD Retrievals trained on AERONET

AVHRR NOAA CDR AOD

MERRAero, AERONET Comparison

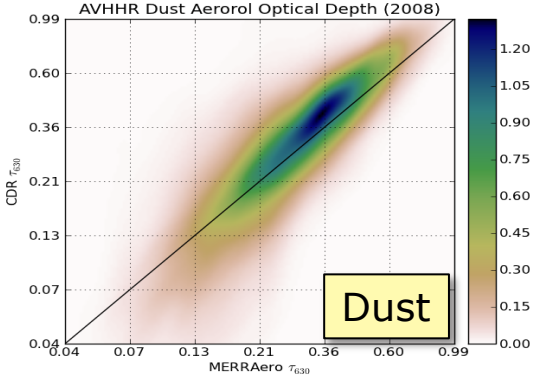


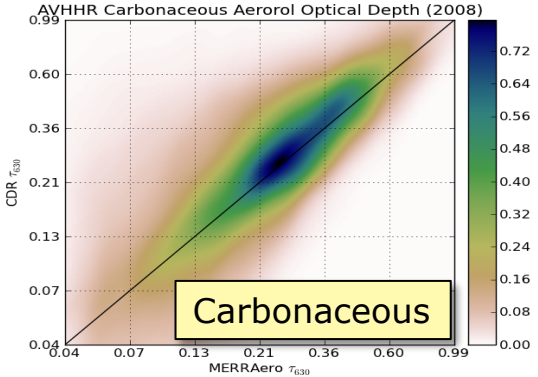
MERRAero

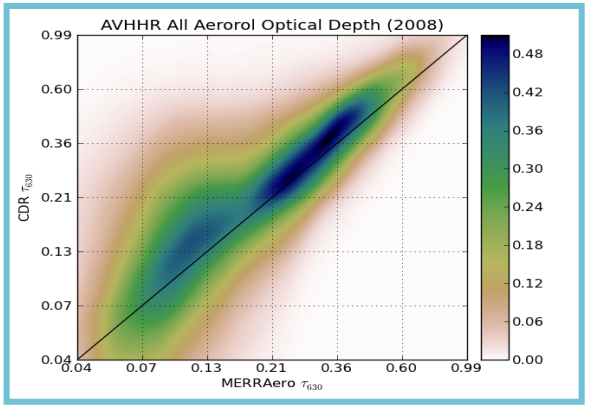


AERONET

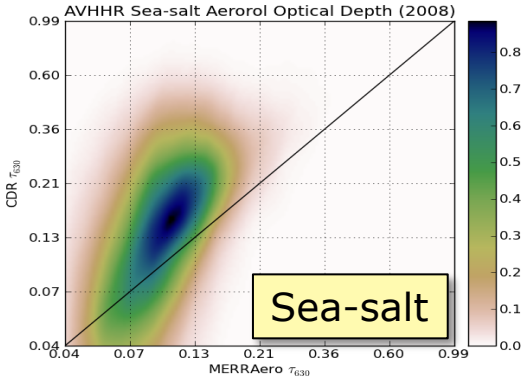
CDR: 2008

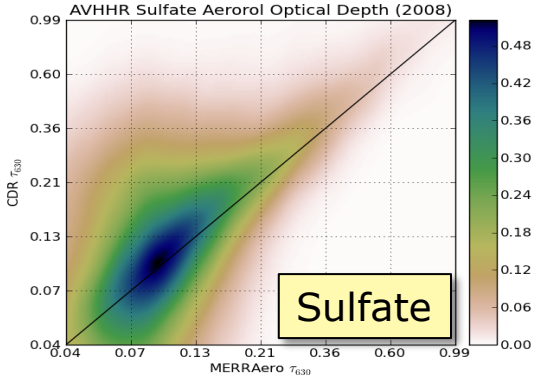






Multiple Species





PATMOS-x

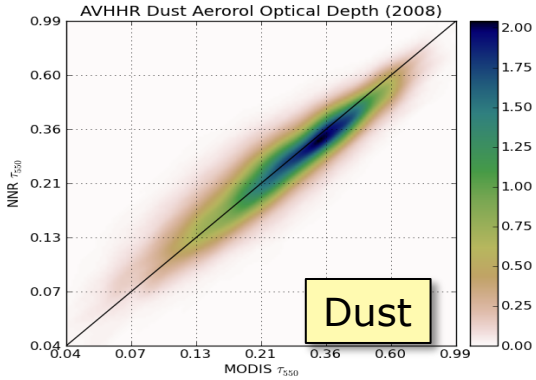
AVHRR Pathfinder Atmospheres - Extended

PATMOS-X DATASET

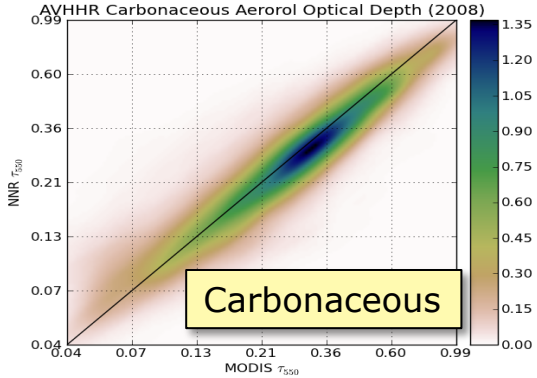
- Version 5 Level 2B
- 0.1 degree sampling (not average)
- Period: 1978-2009
- Inter satellite calibration (MODIS reference)
- Bayesian probabilistic cloud detection (CALIPSO reference)
  - **cpd <0.5%**

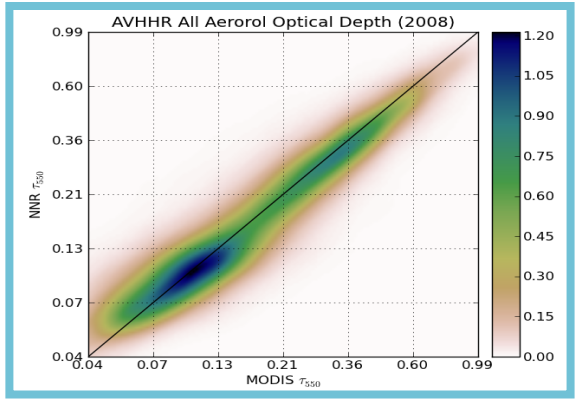
NEURAL NET RETRIEVAL

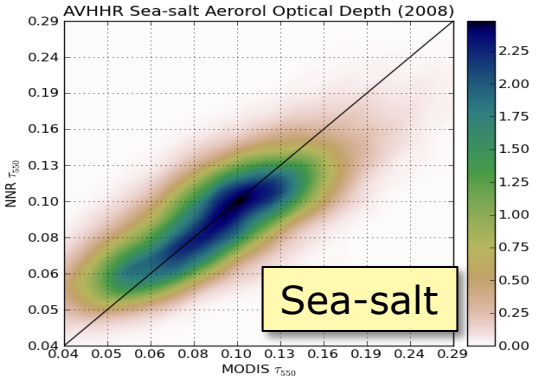
- Ocean Predictors
  - TOA Reflectances
  - 630 and 860 nm
  - TPW
  - Ocean albedo (wind)
  - Solar and sensor angles
  - GEOS-5 fractional AOD speciation
- Target:
  - AOD at 550 nm
  - Balanced MODIS NNR



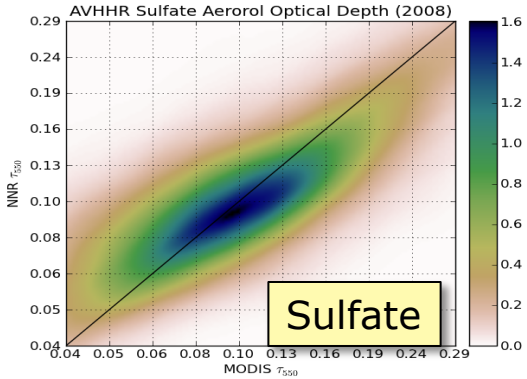
2008







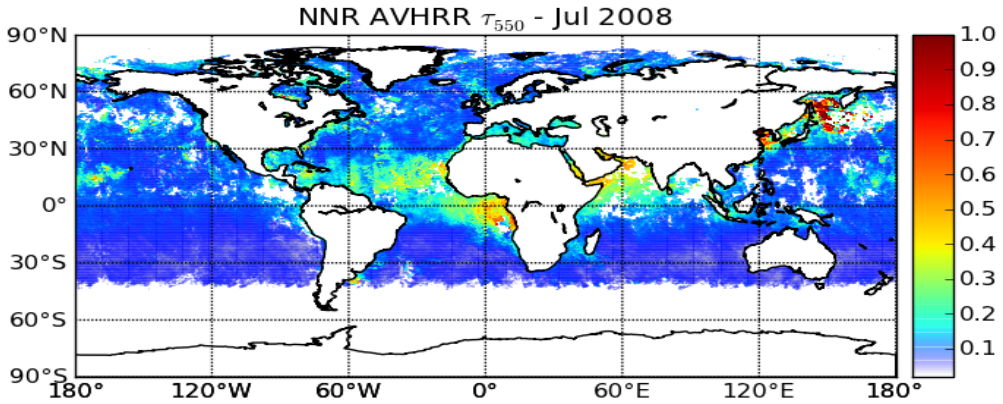
Multiple Species

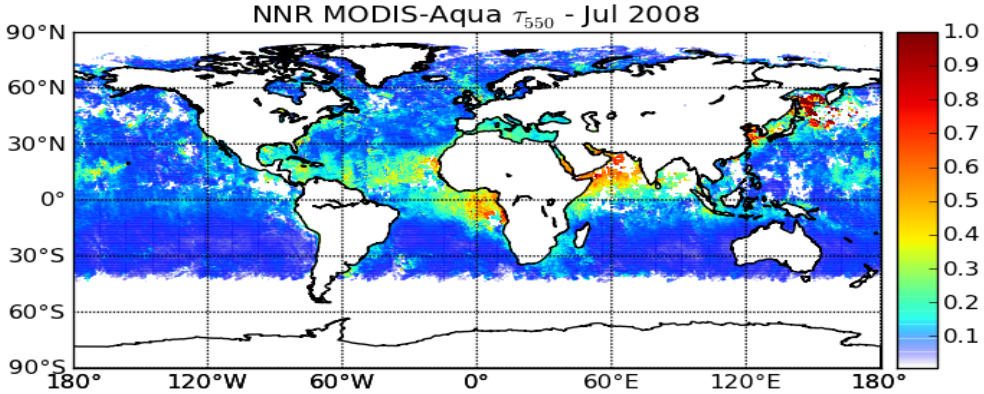


Observing System Homogenization

In order to minimize spurious jumps due relative instrument biases MERRA-2 uses AERONET as reference in a series of Neural Net Retrievals (NNR) based on reflectances from:

- MODIS Collection 5
- PATMOS/X AVHRR





Aerosol Analysis: Splitting

2D AOD ANALYSIS

- Observable 550 nm AOD is 2D
  - Constrains column averaged optics
  - Cannot constrain speciation or vertical distribution
- Analysis in observation space:

$$\tau^a \equiv Hq^a = H\left(q^b + \delta q^a\right)$$
$$= \tau^b + \delta\tau^a$$

GOING TO 3D CONCENTRATIONS

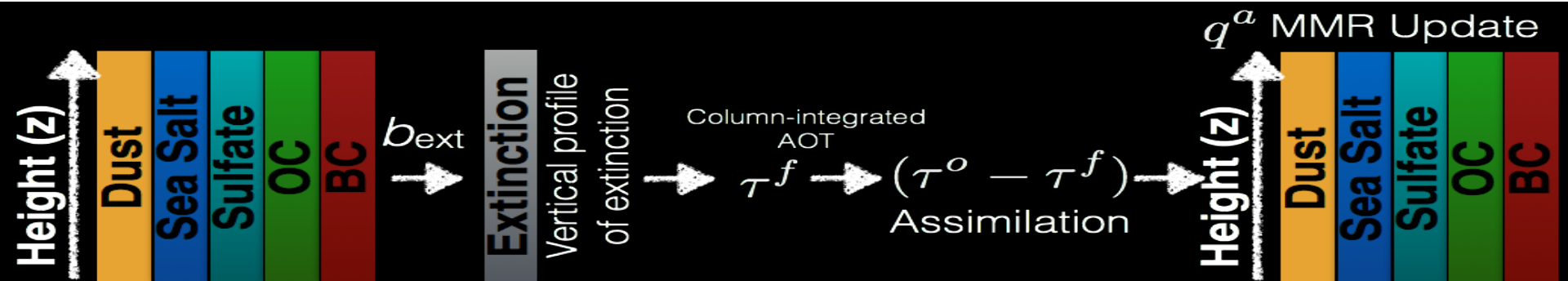
- Based on error covariances:

$$\delta q^a = BH^T\left(HBH^T\right)^{-1}\delta\tau^a$$

- Using ensemble perturbations,

$$\delta q^a = XY^T\left(YY^T\right)^{-1}\delta\tau^a$$

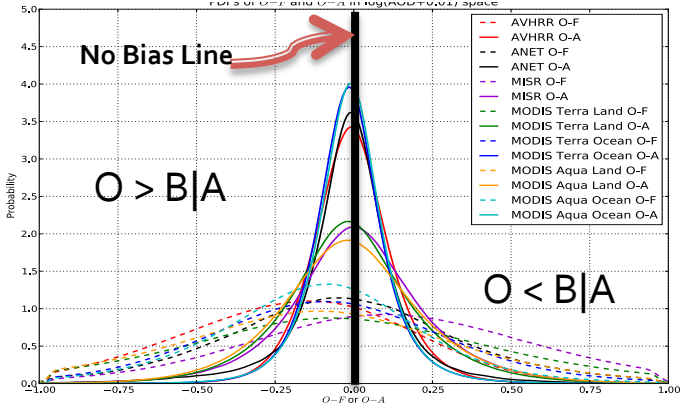
- NRT GEOS-5 uses Local Displacement Ensembles (LDE), in 1D



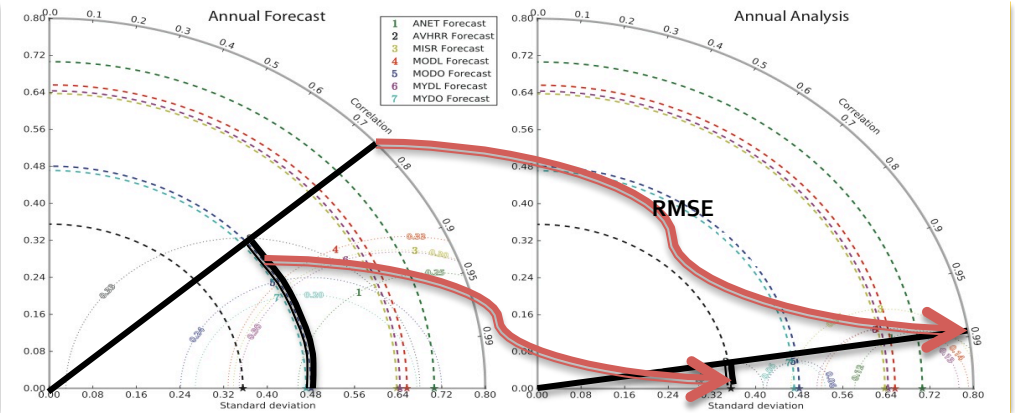
Innovation Statistics

- O-F and O-A computed at Level 2 observation locations
- Analysis relatively unbiased, spread indicative of error of representativeness
- Background generally has low AOD bias, and spread reflects extreme events that are tamed by analysis

PDFs of *O – B* (dashed) and *O – A* (solid)

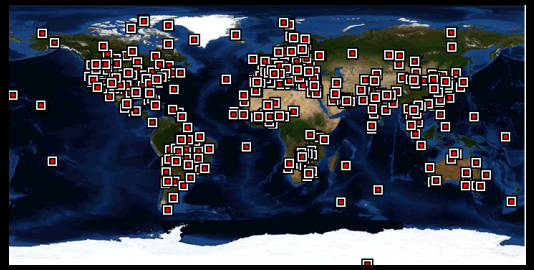


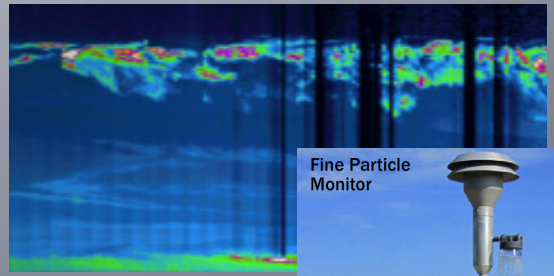
Taylor Diagrams for Forecast (left) and Analysis (right)



MERRA-2 Aerosols Evaluation Highlights

Using Independent Observations

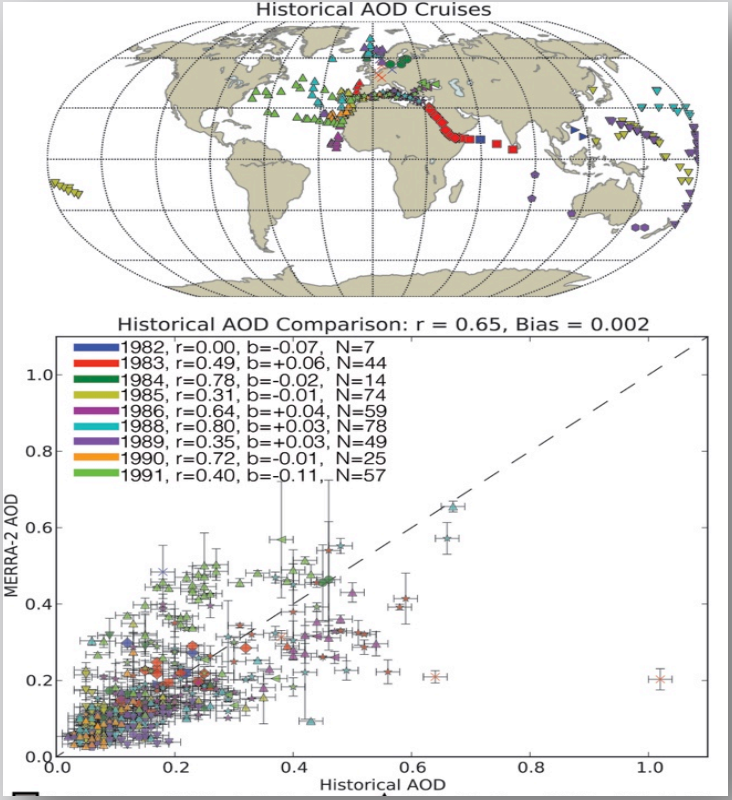




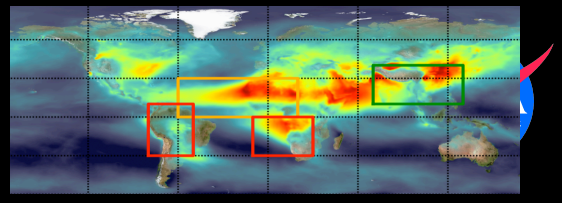
Historical Cruises

Independent AOD data is scant before the EOS Period.

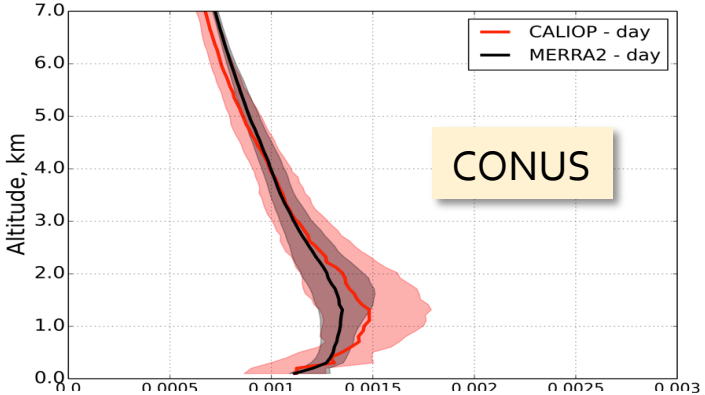
These historical ship cruises provides an unique opportunity to evaluate the assimilation of AVHRR data for the pre-EOS era.

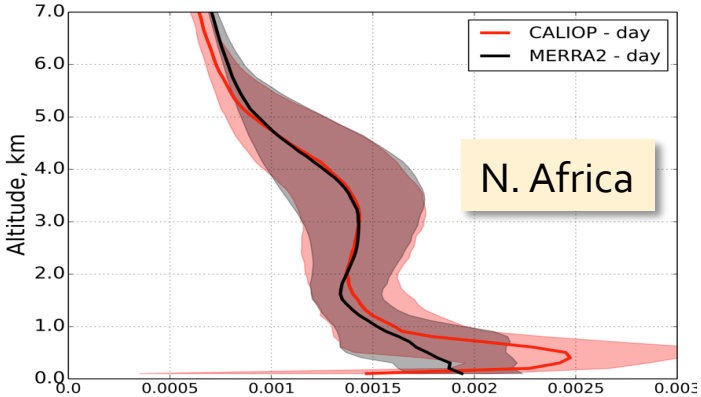


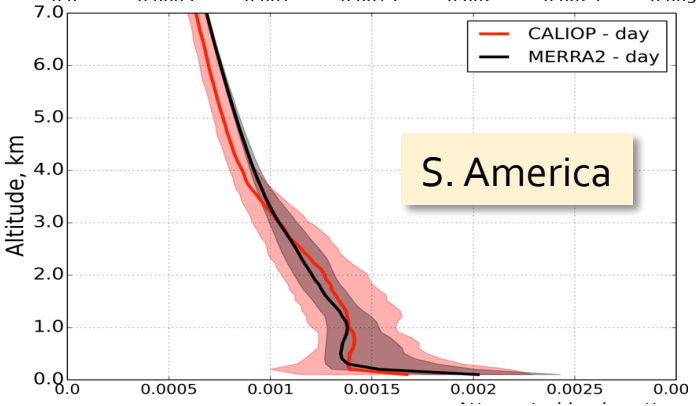
Vertical Structure: Comparison to CALIOP

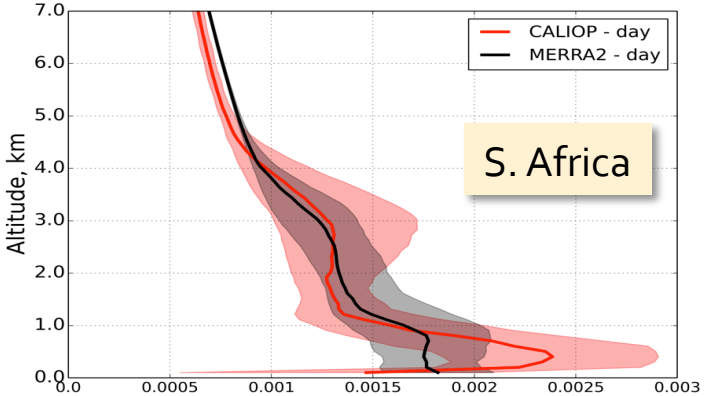


Attenuated Backscatter $km^{-1} sr^{-1}$

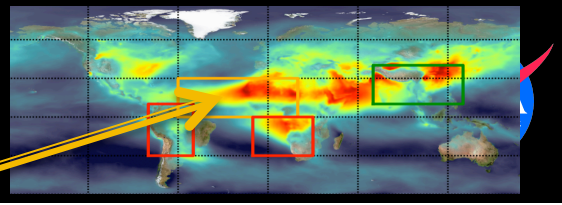


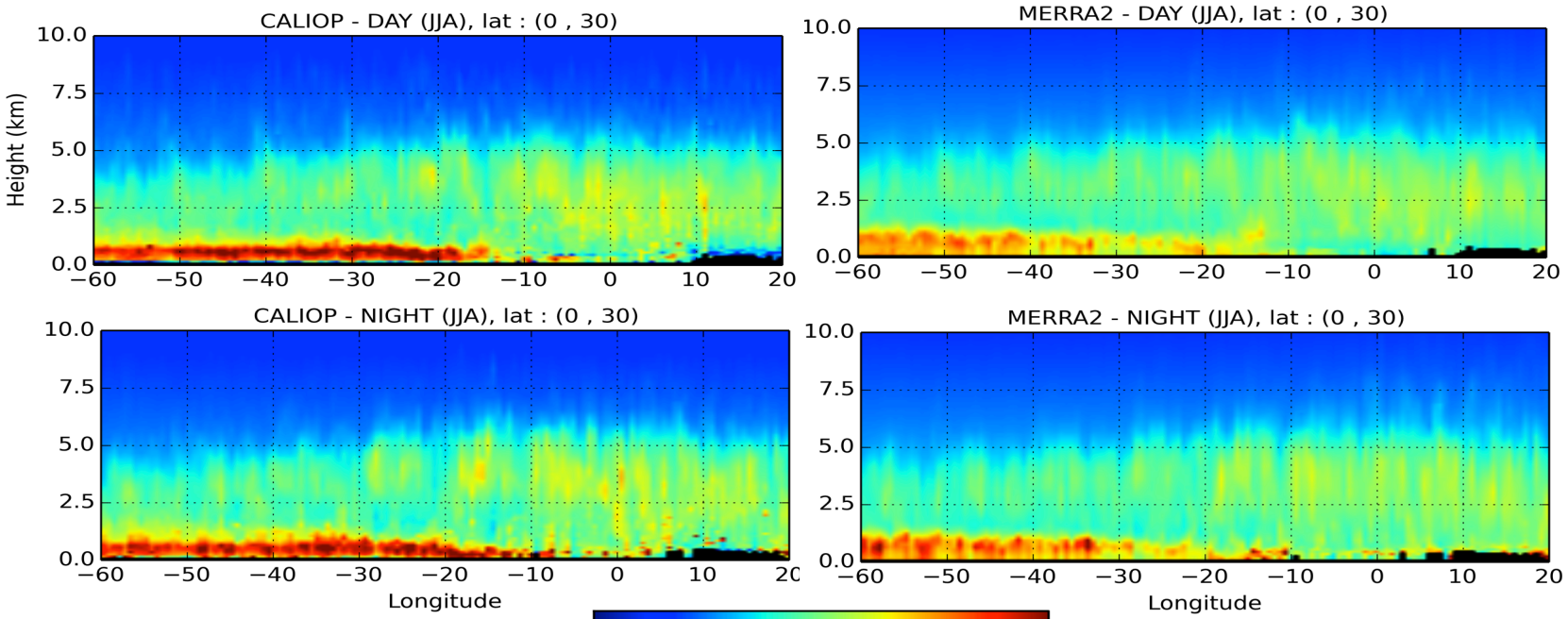






Vertical Structure: Comparison to CALIOP





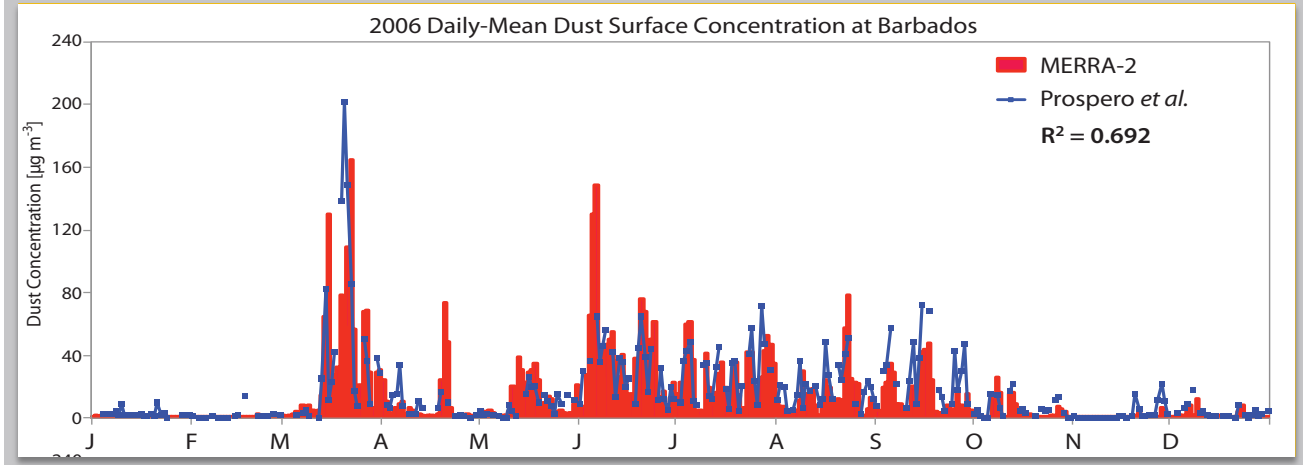
Attenuated Backscatter

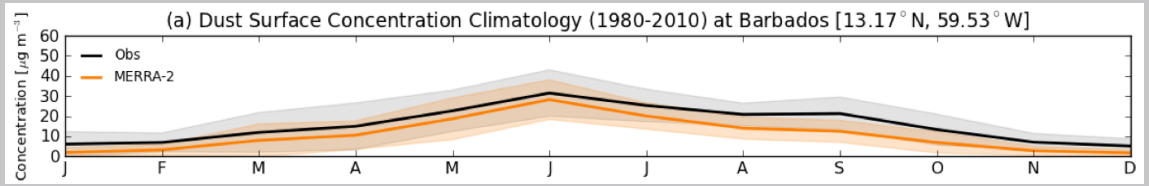
JJA

MERRA-2
Evaluation Highlights

Dust Transport: Barbados

- High correlation with in-situ dust concentration measurements in Barbados
- Dust concentration seasonal cycle well captured in Barbados

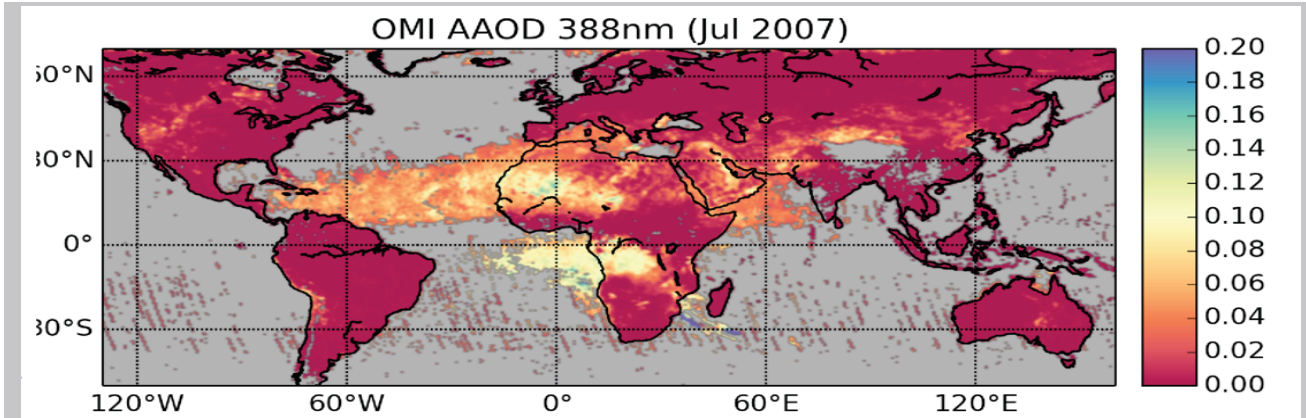


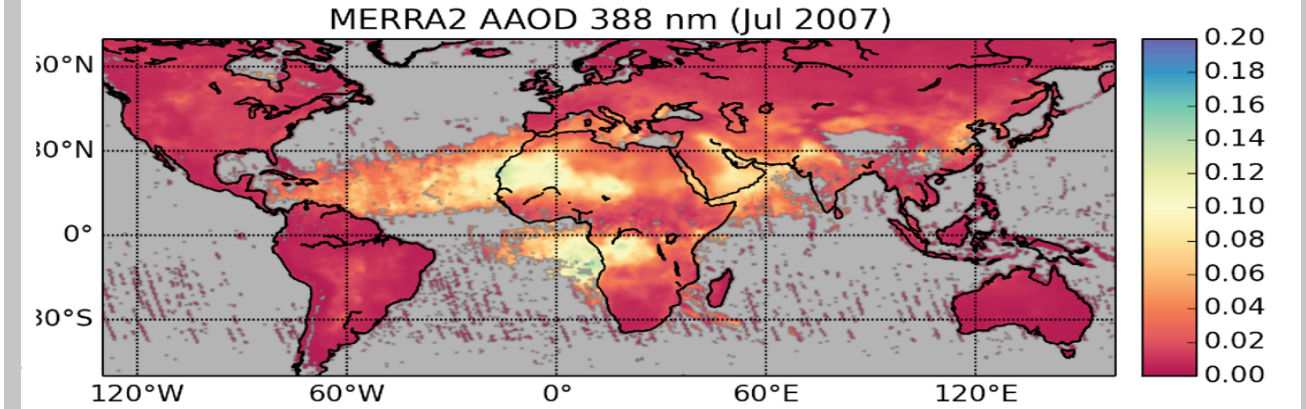


MERRA-2
Evaluation Highlights

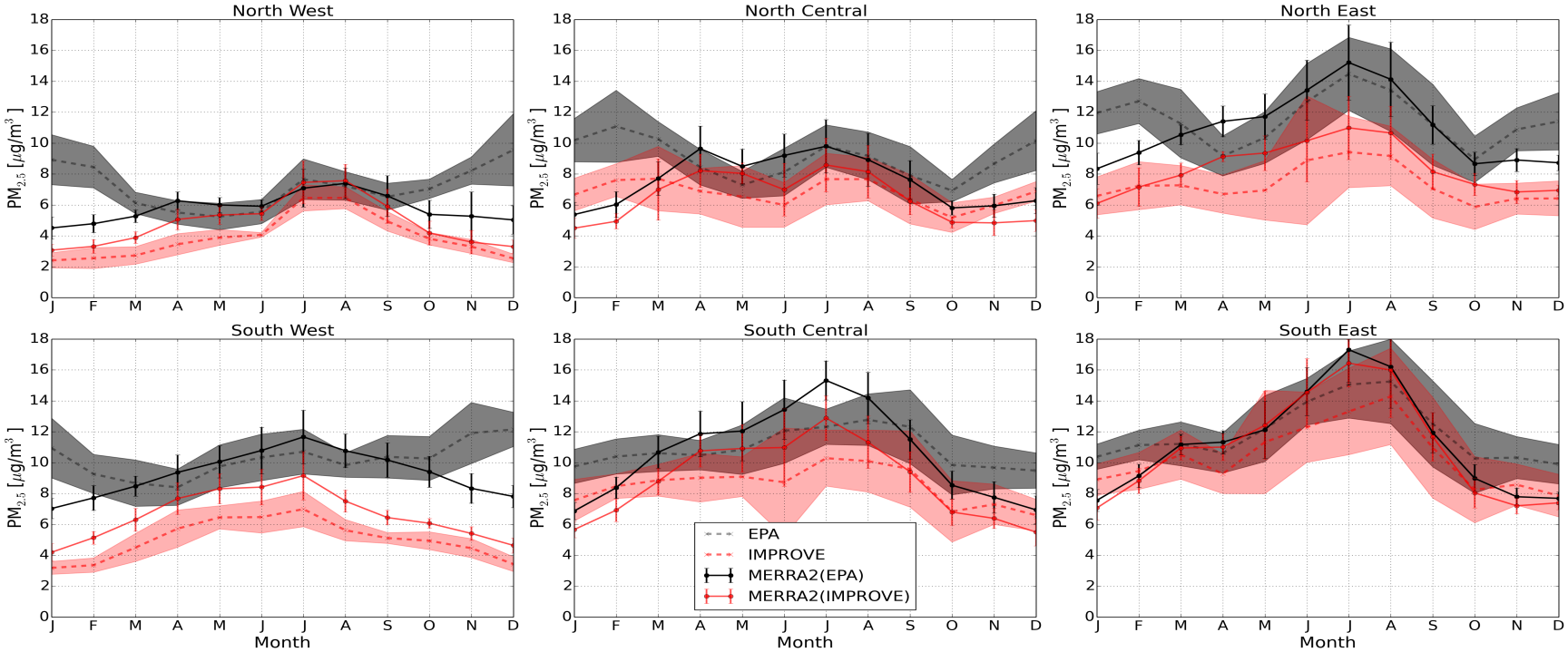
Aerosol Absorption

- Comparison of MERRA-2 Absorption Optical Depth (AAOD) with OMI retrievals
- Good agreement for African dust and smoke
- North American biomass burning underestimated according to OMI





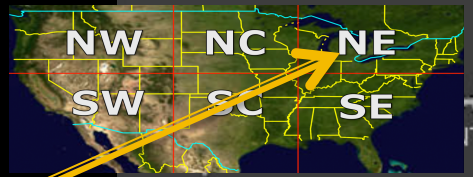
$PM_{2.5}$ (Total) Regional Climatology



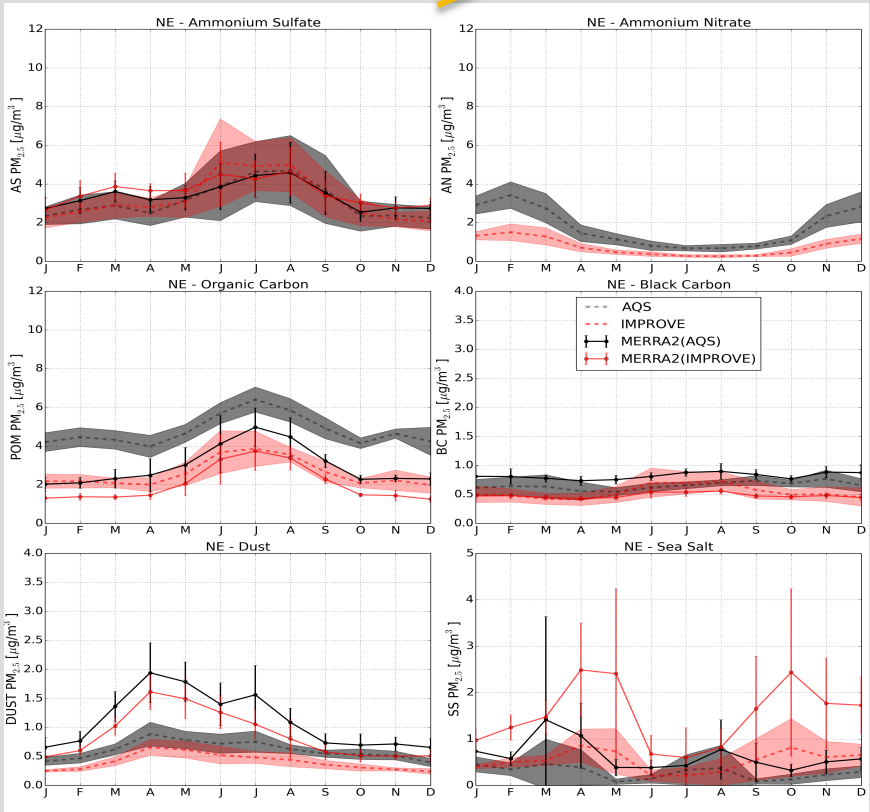
Comparison with in-situ measurements after *Buddy Check*

MERRA-2
Evaluation Highlights

PM2.5 by Species At Northeast



- Relatively good agreement for **Sulfates**
- MERRA-2 lacks **Nitrates** altogether
- Underestimation of **Carbonaceous** near urban areas
- Too much **dust**
- Too much **sea-salt** at coastal stations



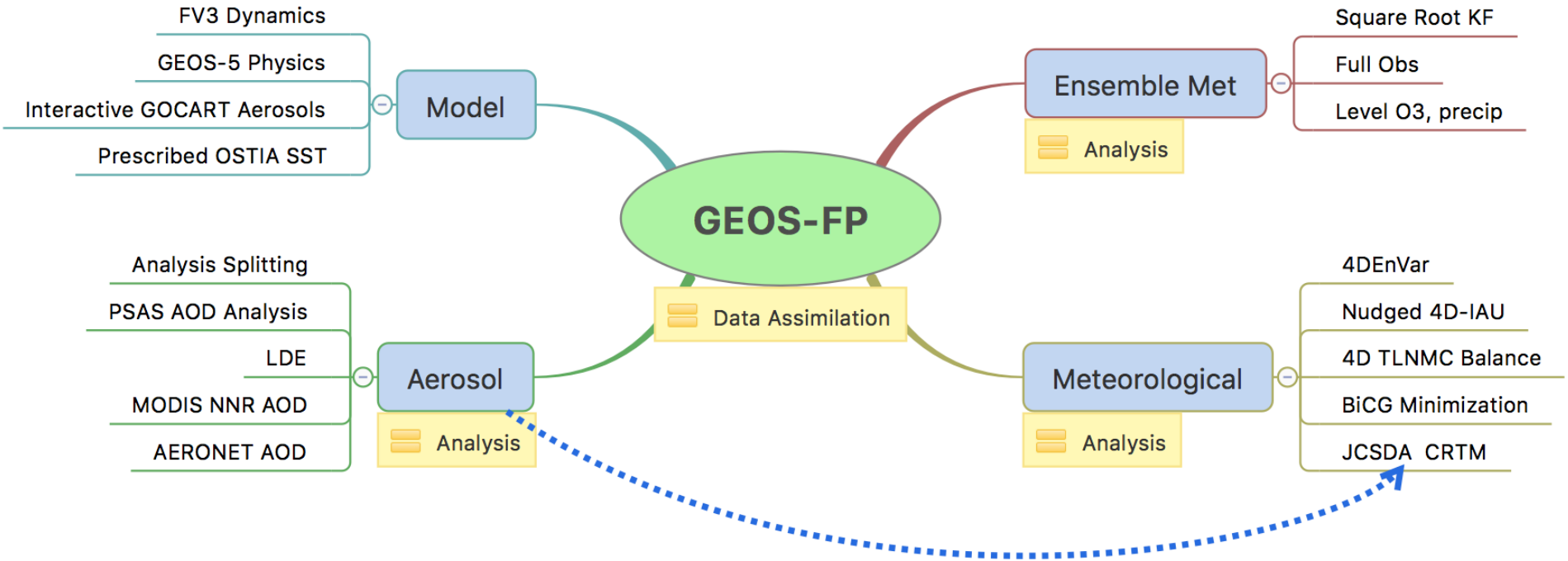
MERRA-2 Summary

- MERRA-2 provides the first integrated aerosol-meteorology reanalysis for the satellite era
  - Aerosols impact the meteorological "first guess"
- Compared to MERRAero, MERRA-2 adds AVHRR, MISR and AERONET data to MODIS
- Caveats:
  - Monthly mean biomass burning emissions inadvertently used during 2000-2010
  - Due to forward processing constraints, MISR/AERONET have been dropped around mid/late 2014.
- MERRA-2dd: 12.5 km downscaling under evaluation

Aerosol Impact on the GEOS-5 Meteorological Analysis

With contributions from: Jong Kim, Santha Akella, Ricardo Todling

GEOS-FP: Meteorological & Aerosol DA



Aerosols in GSI

- CRTM allows for the inclusion of (GOCART) aerosols
- The GEOS-5 GOCART aerosol species have been introduced as *state variables* in GSI
  - No aerosol increments for now
  - Aerosol effects included in the observation operators for AIRS, HIRS, IASI, CRIS, SEVIRI, AVHRR
- Optical properties hardwired inside CRTM
  - Inconsistent with GEOS-5 VIS channels but
  - OK for IR channels

Aerosol Contamination of GSI Radiances

CONTROL EXPERIMENT

- Aerosols fully interactive in GEOS-5 model
  - Standard, decoupled AOD assimilation
- Standard GSI global analysis
- Period
  - August 2016
- Resolution:
  - C360 (~25 km)

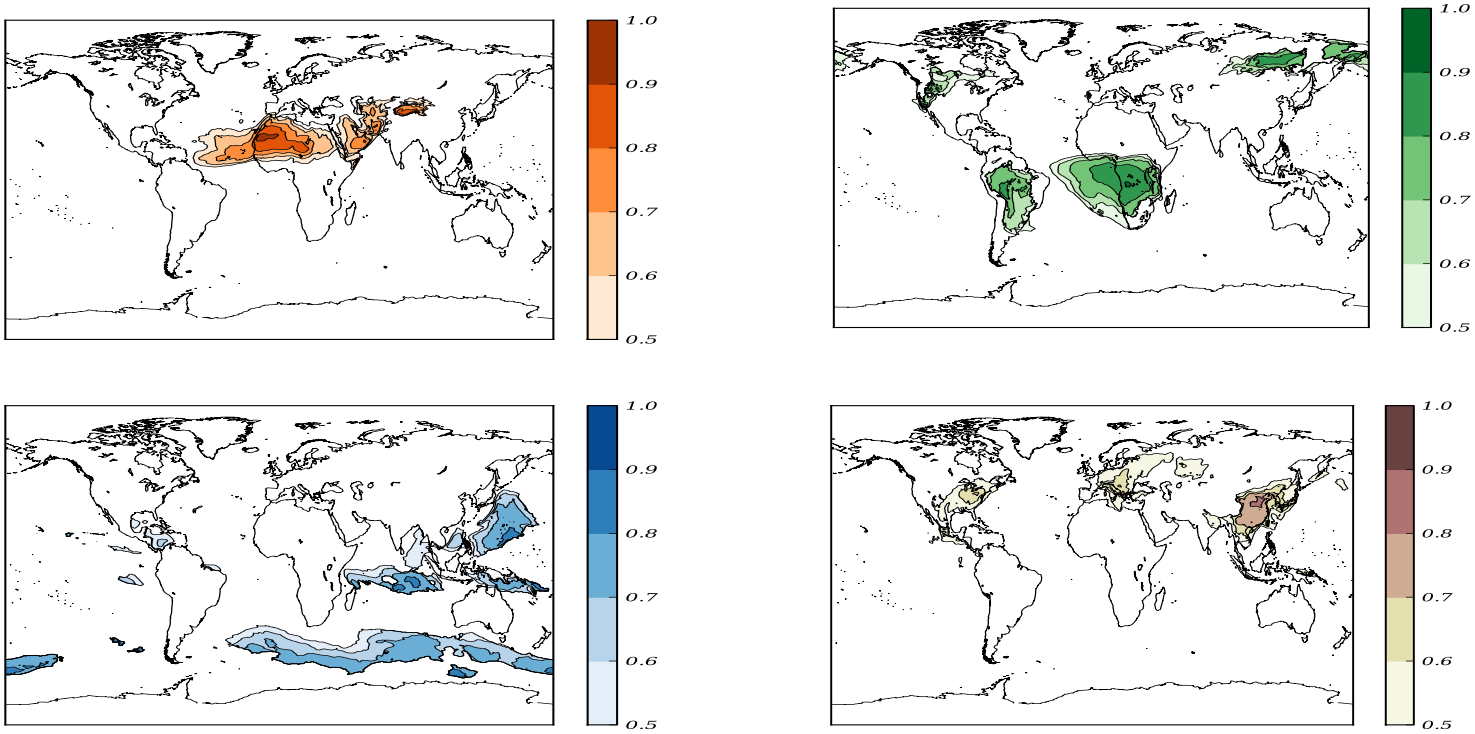
AEROSOL IMPACT EXPERIMENT

- Aerosols fully interactive in GEOS-5 model
  - Standard AOD assimilation
- GSI observation operators:
  - 15 GOCART species
  - Concentration
  - Effective radius
  - Optical parameters internally determined by CRTM

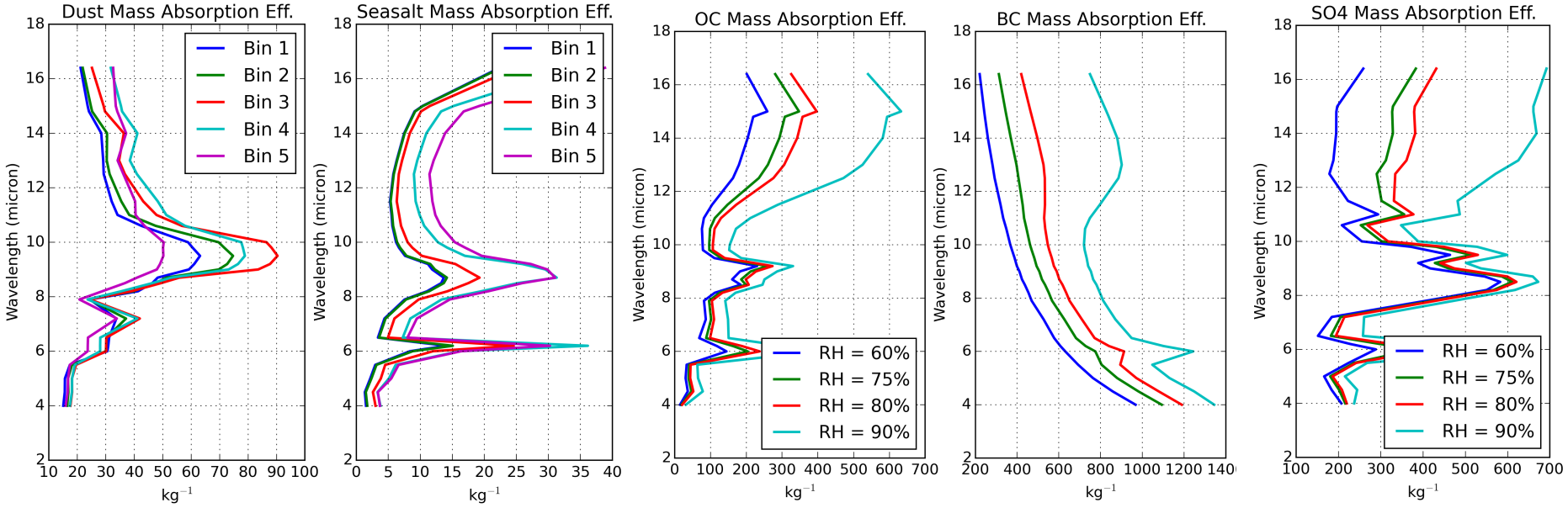
Non-cycling Experiment

IMPACT OF AEROSOLS ON SIMULATED BRIGHTNESS TEMPERATURE

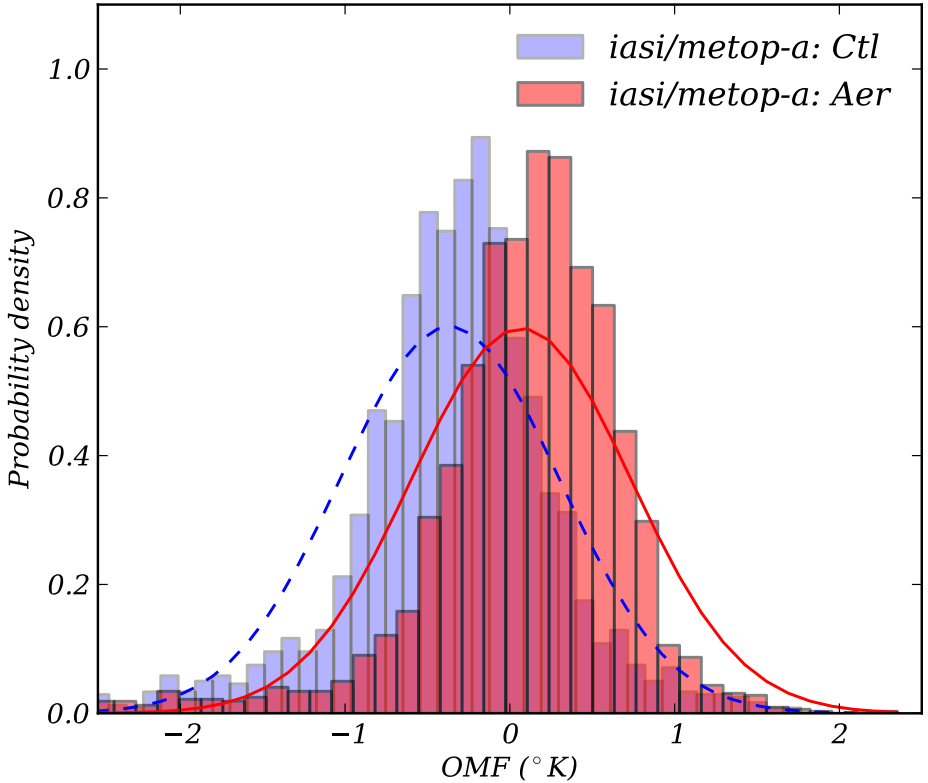
Aerosol AOD Speciation: Aug 2016



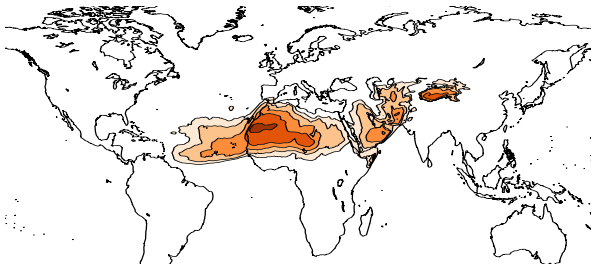
OPAC Aerosol Optical Properties

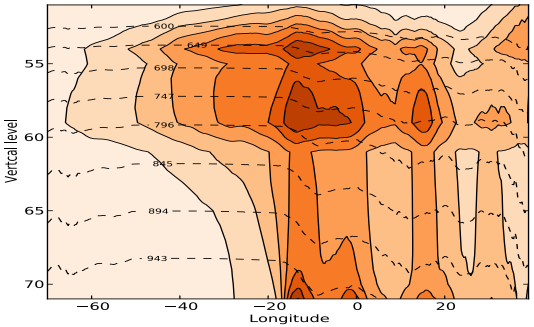


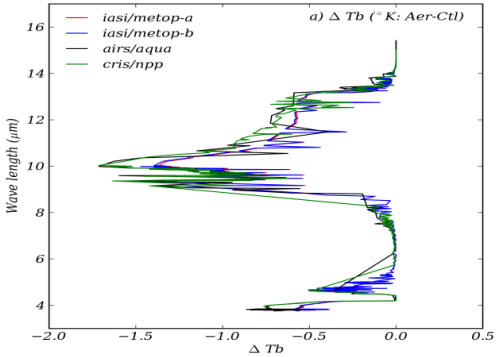
IASI Innovations

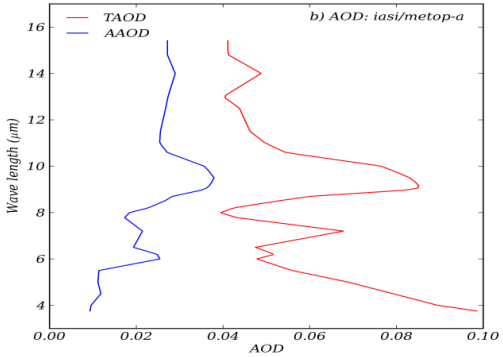


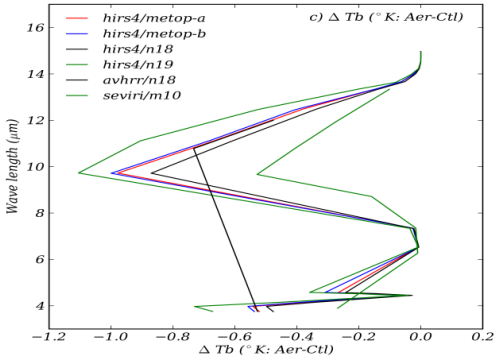
Dusty Pixels: T_b(aer) – T_b(ctl)

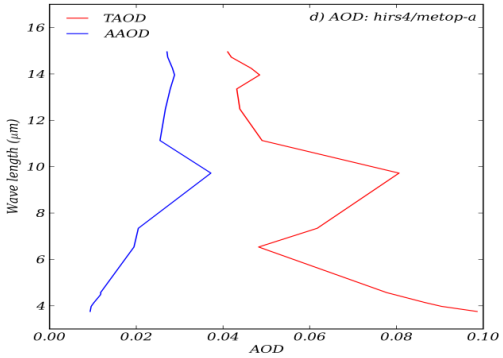




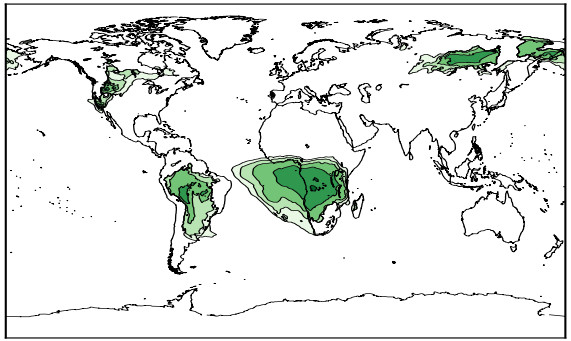


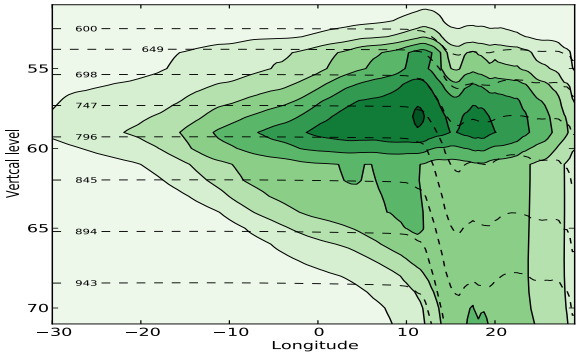


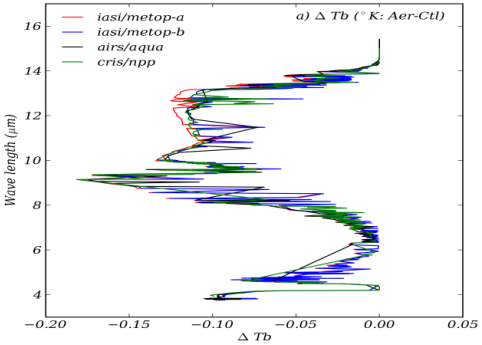


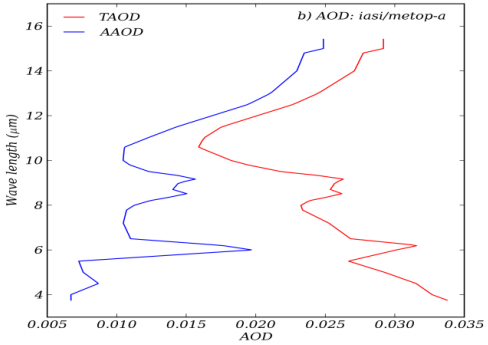


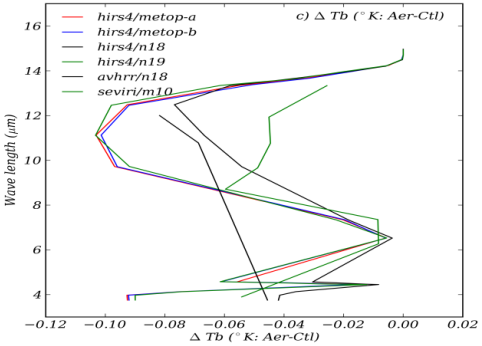
Smoky Pixels: T_b(aer) – T_b(ctl)

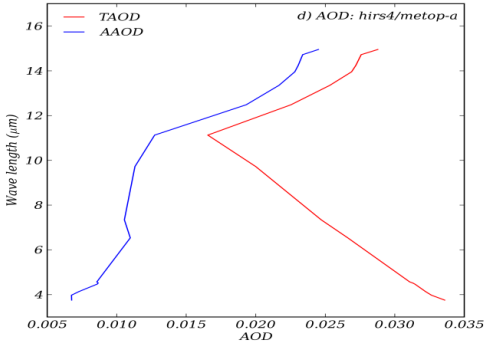




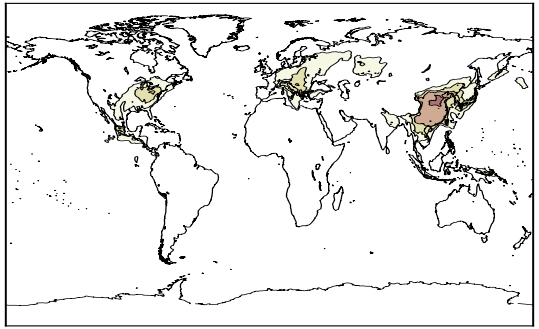


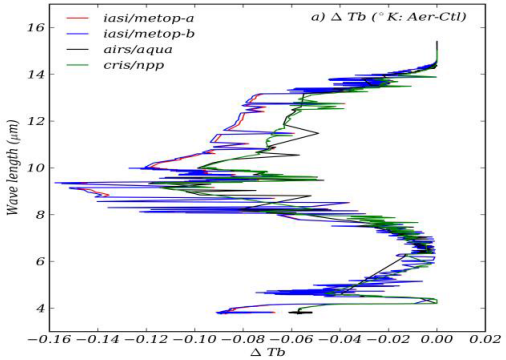


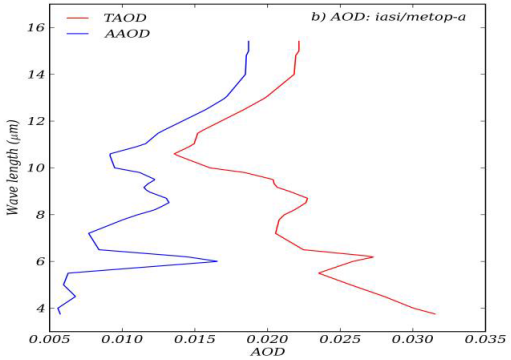


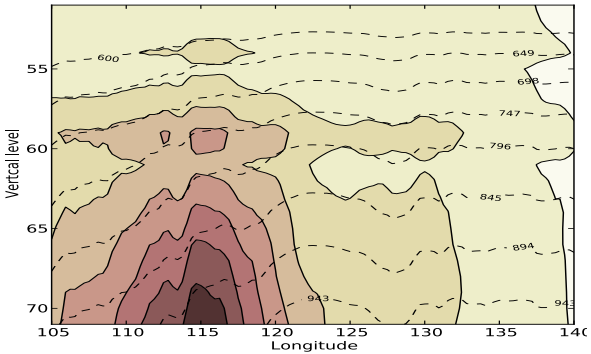


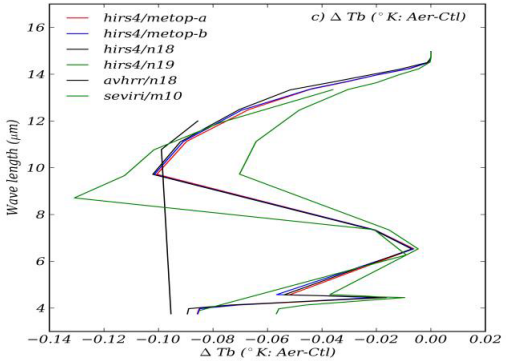
Sulfate Pixels: T_b(aer) – T_b(ctl)

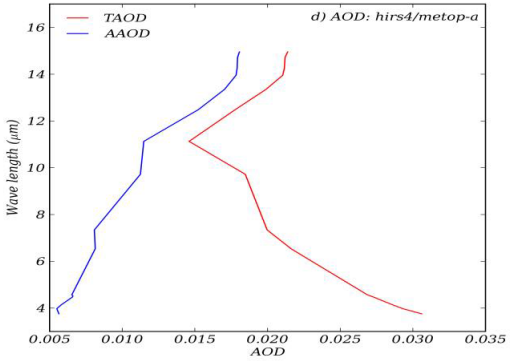




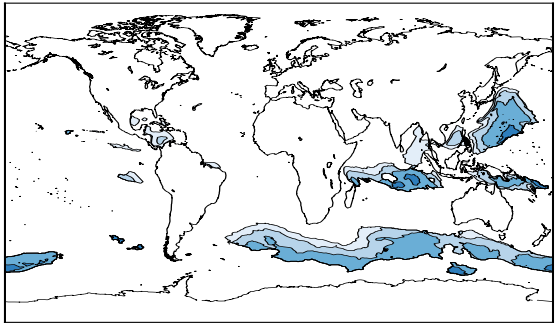


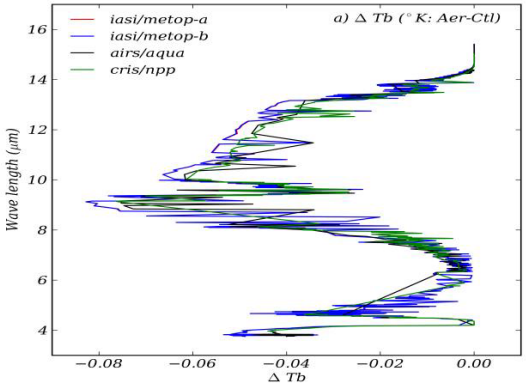


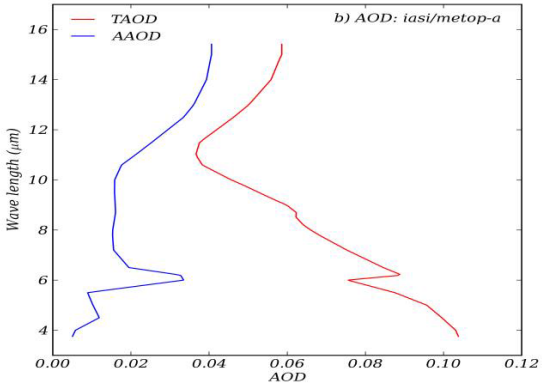


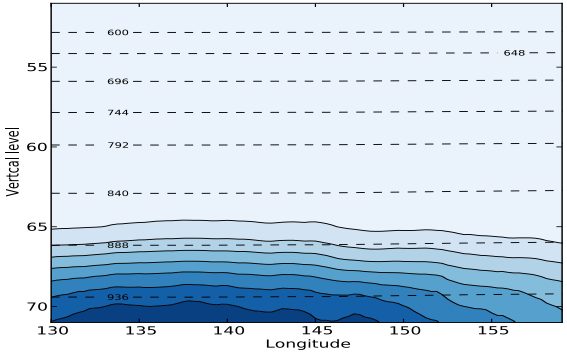


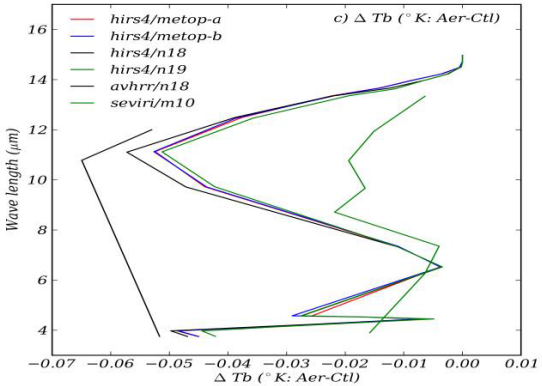
Salty Pixels: T_b(aer) – T_b(ctl)

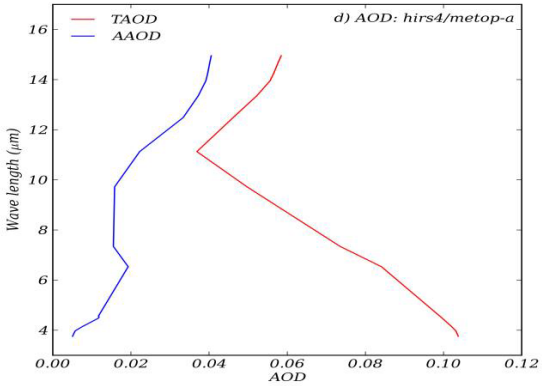






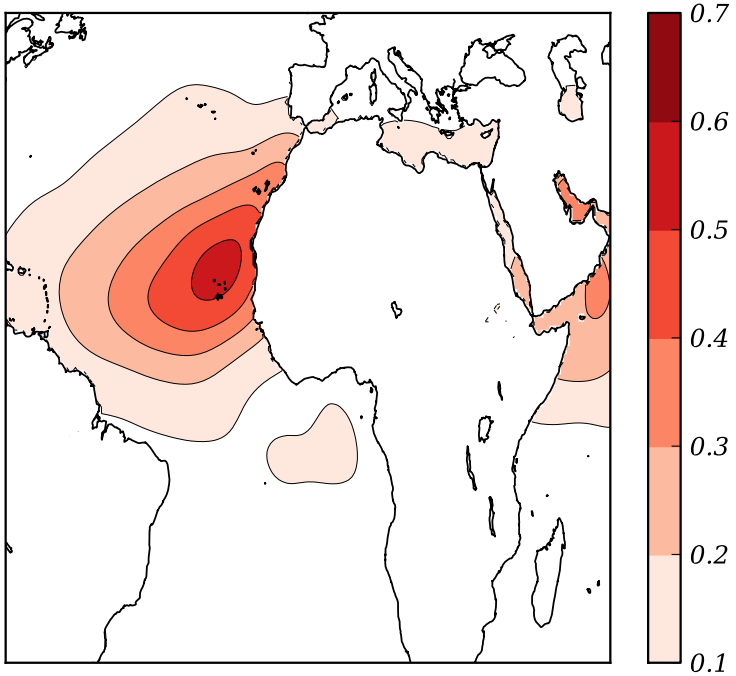






Impact on Temperature Analysis

SST



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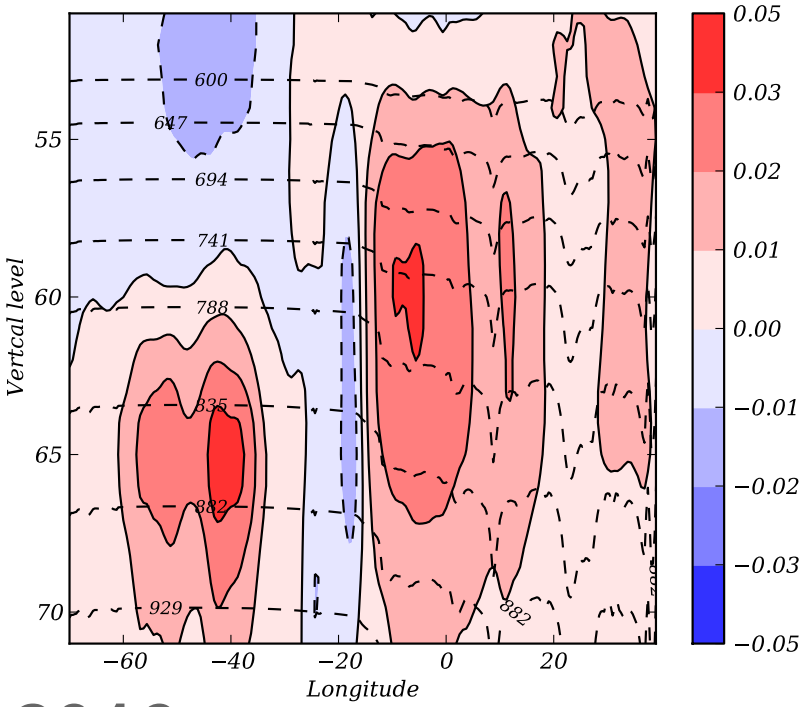


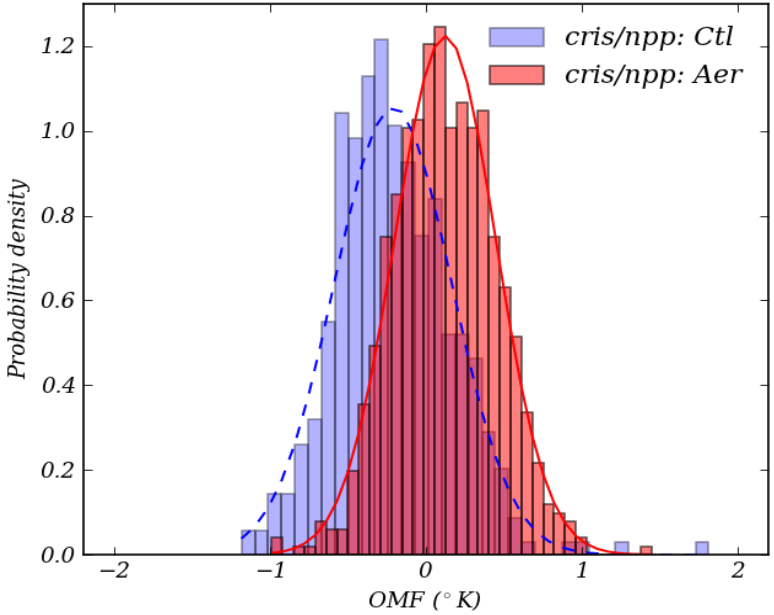
Aug 2016

Cycling Experiment: July 2015 & August 2016

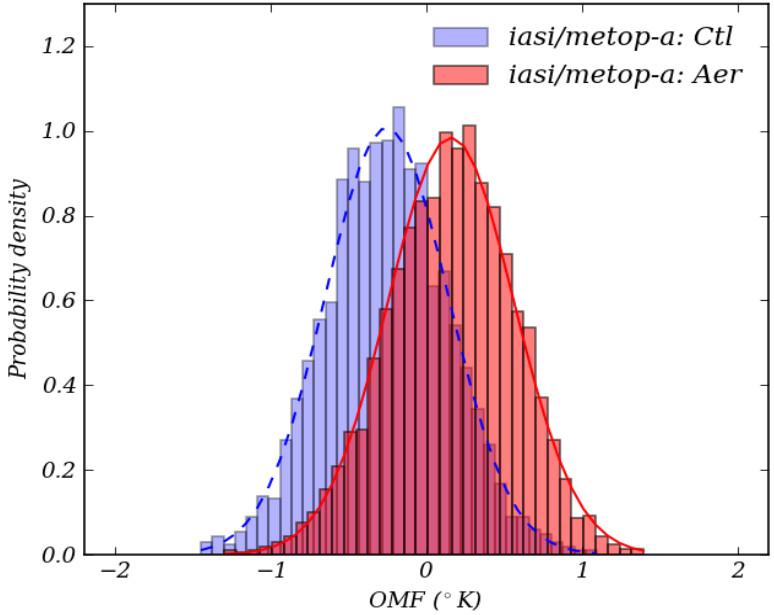
IMPACT OF AEROSOLS ON METEOROLOGICAL ASSIMILATION

Impact on Innovations (After QC & VBC)

CRIS (10.5μm)

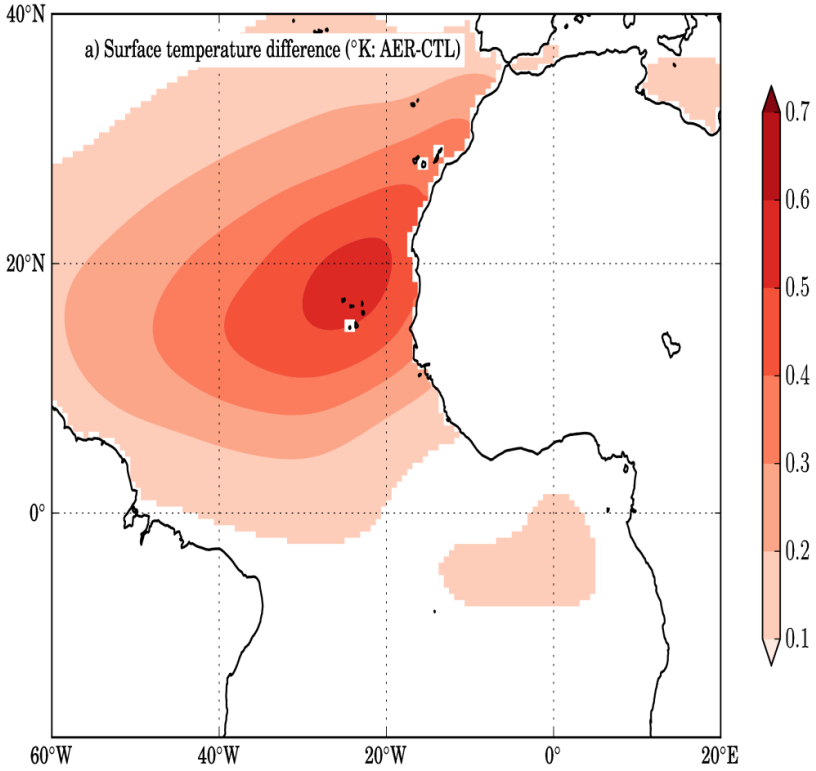


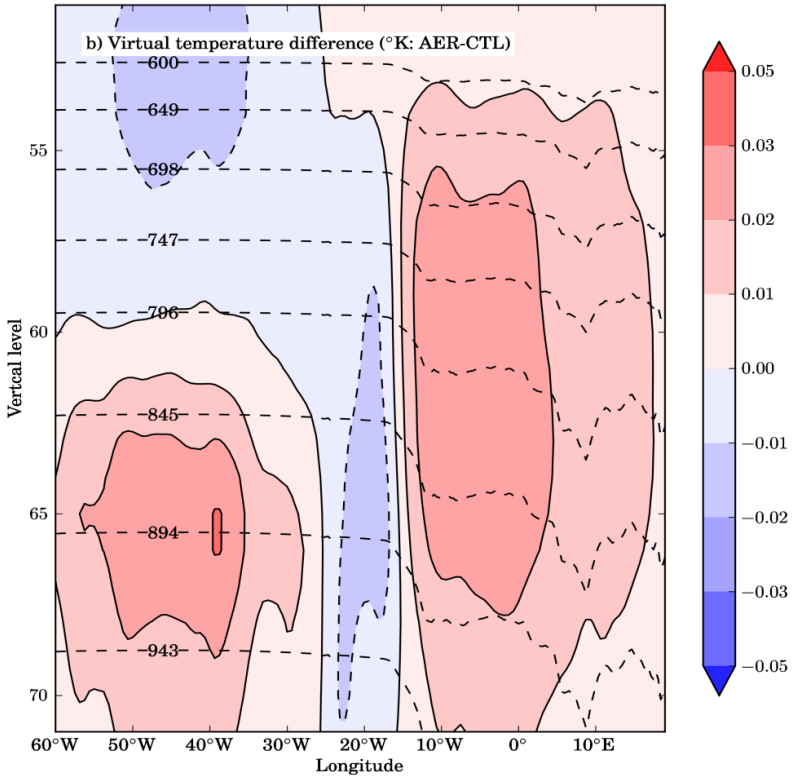
IASI (10.4μm)



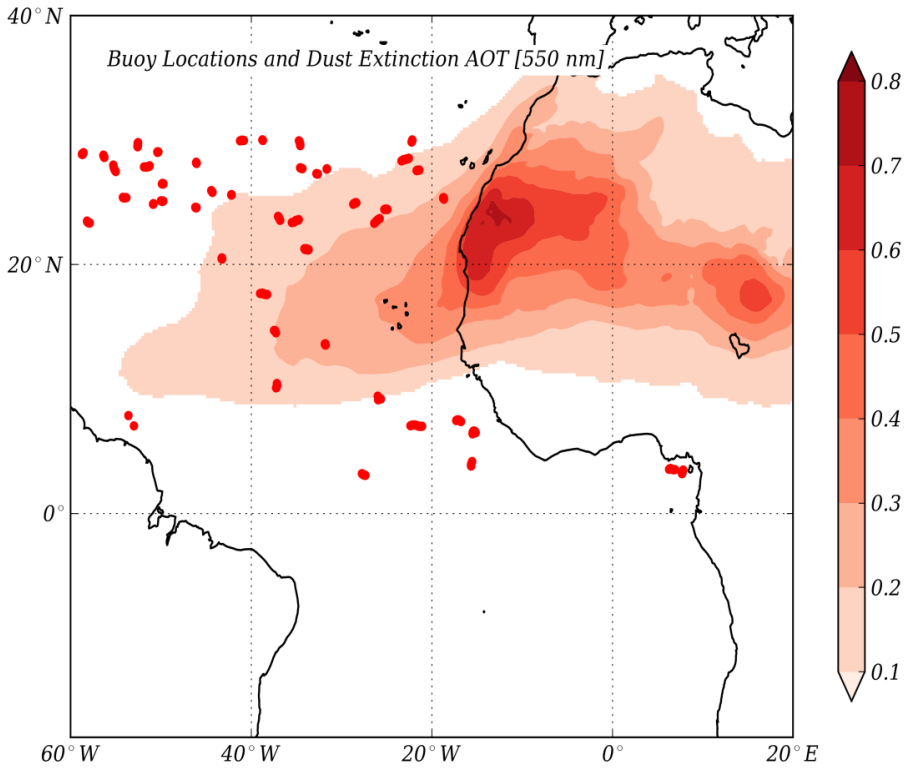
Aug 2016

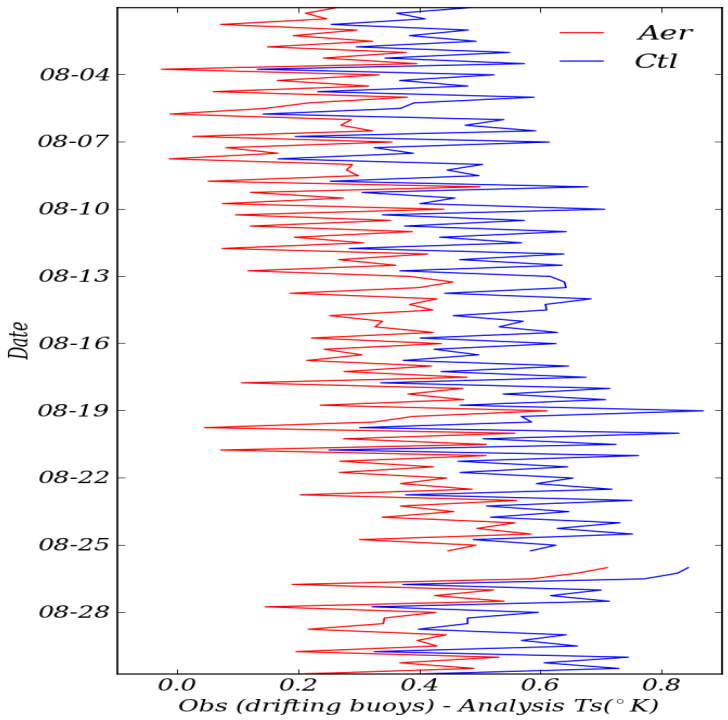
ΔSST Analysis (Aer-Ctl): Aug 2016



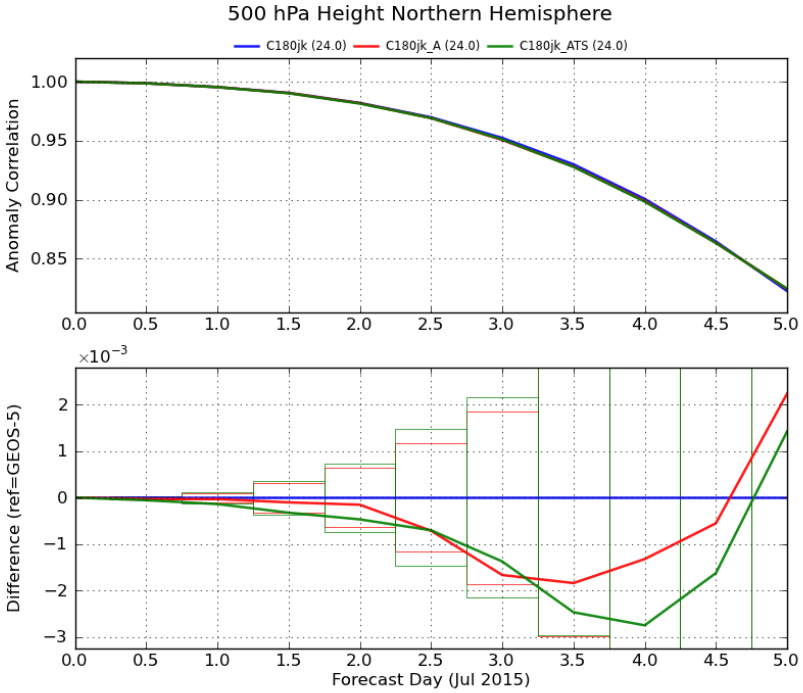


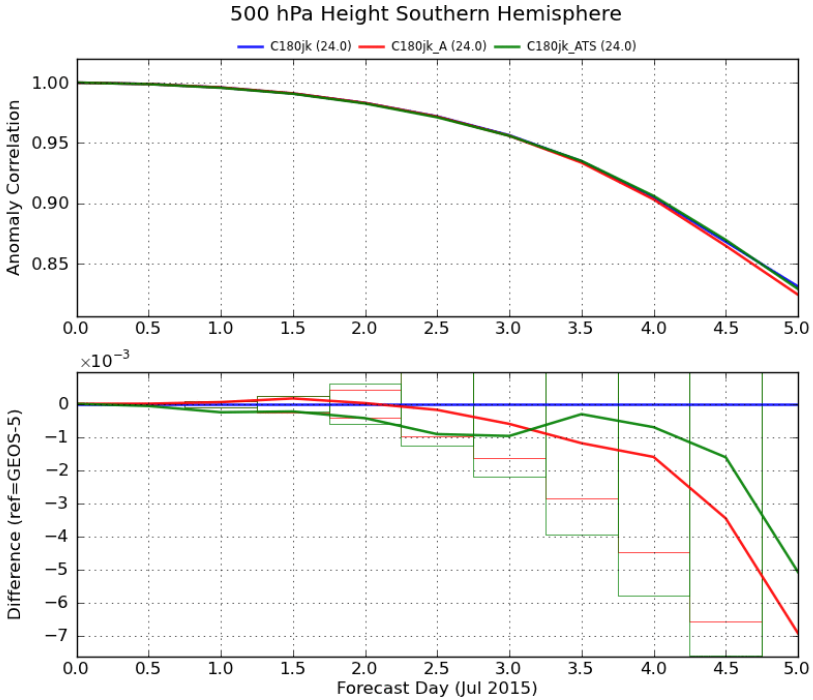
SST: Comparison to Buoys: Aug 2016



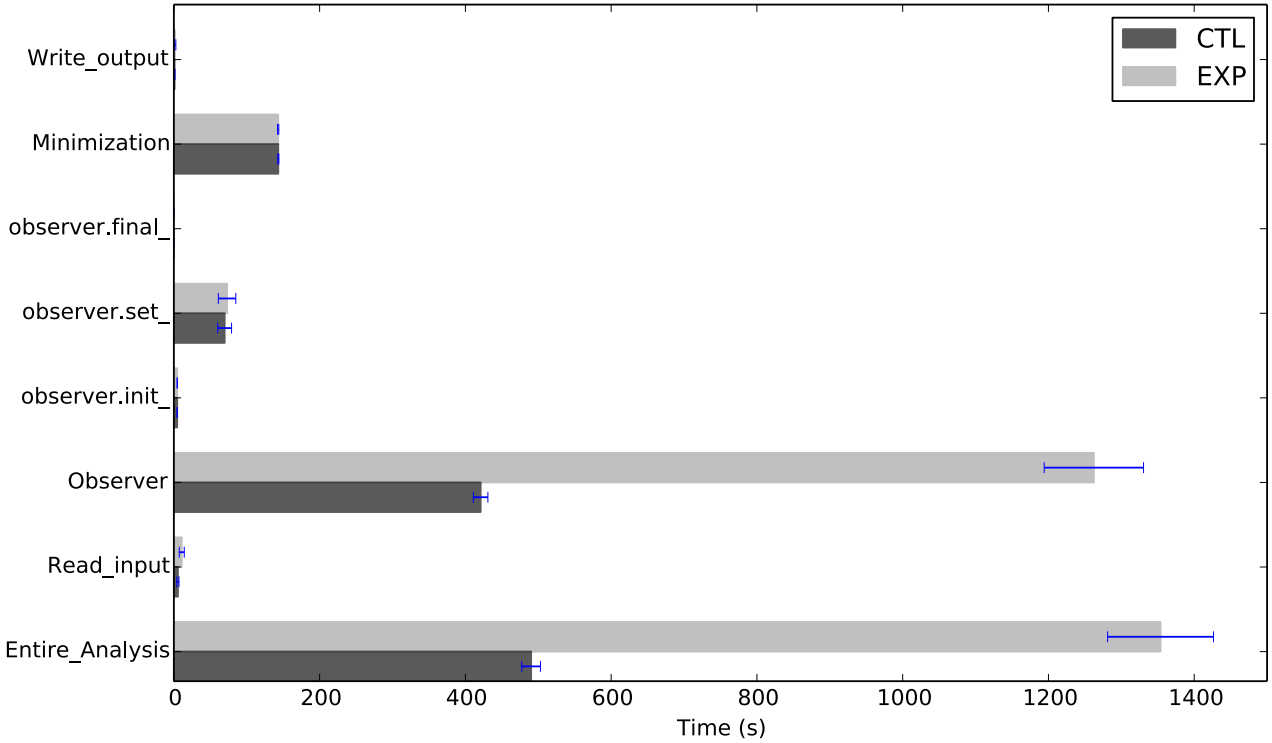


500 hPA Anomaly Correlation





Computational Cost



Aerosol Impact on Met Analysis: Summary

- **The impact of the GEOS-5 assimilated aerosols on meteorological assimilation has been examined**
  - One way interaction: 3D aerosol concentrations impact on the CRTM calculation of IR BTs
- **Larger effect over predominantly dusty pixels**
- **Cooling effect of aerosols on T_b calculation leads to warming in SST analysis**
  - Nearly 1K effect on SST analysis over the Saharan dust plume
- **Impact on 5-day forecast skill is negligible**
- **Slightly more data were accepted in the cycled experiments: HIRS, AIRS, IASI, CRIS**
- **SST verification against drifting buoy indicates that the aerosol experiments had slightly improved surface temperature in the tropical Atlantic**
- **Neural Net based approximations being investigated as a device to reduce cost**
  - Possibly a better parameterization for the variational bias correction

Concluding Remarks

- **Aerosols are an integral part of the GEOS-5 N.R.T. and re-analysis systems**
  - Aerosols are run at the same resolution as the main meteorological model
- **MERRA-2 provides the first integrated aerosol-meteorology reanalysis for the satellite era**
- **Current GEOS-5 developments incorporate cloud and aerosol microphysics**
  - Aerosol-cloud interactions, better representation of aerosol mixing state
  - There is great need for in-situ and remotely sensed data to evaluate/validate new parameterizations
- **QFED biomass burning emissions to include diurnal cycle from GEO satellites**
- **Aerosol analysis migrating to an EnKF based system**
  - New observables: multi-spectral AOD, attenuated backscatter
  - New active/passive sensors: VIIRS, GEO, CATS/CALIOP, TropOMI

EXTRA SLIDES

GEOS-5 Reanalysis Activities

Name	Nominal Resolution	Period	Aerosol Data	Availability
MERRA-1	50 km	1979-present	NONE	now
MERRAero	50 km	2002-2016	MODIS C5	now
FP for Inst. Teams	50 km	2000-	MODIS C5	now
NCA	25 km	2010-11	MODIS C5, MISR	now
MERRA-2	50 km	1980-ongoing	AVHRR, MODIS C5, MISR, AERONET	now
MERRA-2 Dynamical Downscaling	12.5 km	2000-2014	AVHRR, MODIS C5, MISR, AERONET	(Not yet released)

MERRA-2 Advances

Builds on the successes of MERRA by updating the GEOS-5 model, analysis code, and observing system:

- Include modern satellite observation types not available to MERRA
- Reduce spurious trends and jumps related to changes in the observing system
- Reduce biases and imbalances in the water cycle

Steps towards a full Earth System Reanalysis

- Improved representation of cryospheric processes
- Improved representation of the stratosphere, including ozone

For the first time, a coupled aerosol-meteorological reanalysis for the entire satellite era (1980 – onward)