Aerosol modeling, observations, and data assimilation

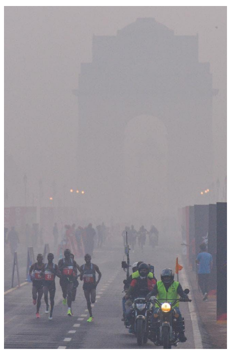
Mariusz Pagowski
Cooperative Institute for Research in Environmental Sciences, University of Colorado
and
NOAA/Global Systems Laboratory
Boulder, CO

Sources: NASA, NOAA, JCSDA, IPCC, WHO, news

Aerosol Intro

Importance

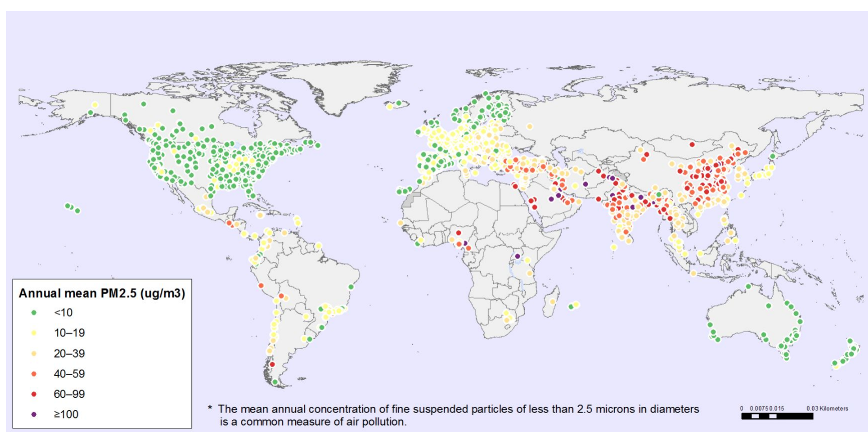
- Pivotal contributor to atmospheric pollution (smog)
  - Particulate matter with diameter smaller than 2.5 um (PM2.5) is the single most critical factor affecting human mortality due to air pollution (U.S. EPA)



Marathon runners

New Delhi (CNN called “the most polluted city on Earth”)

Denver

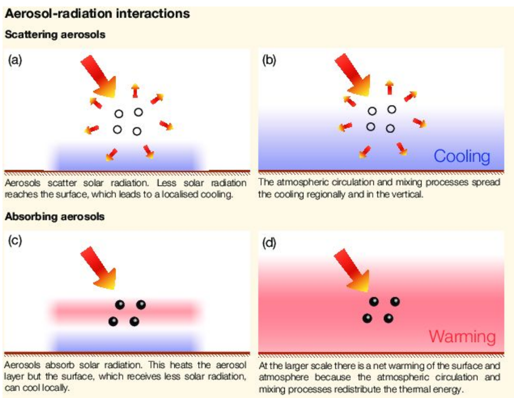


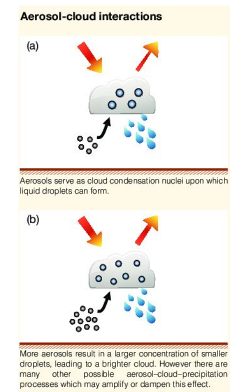
World Health Organization

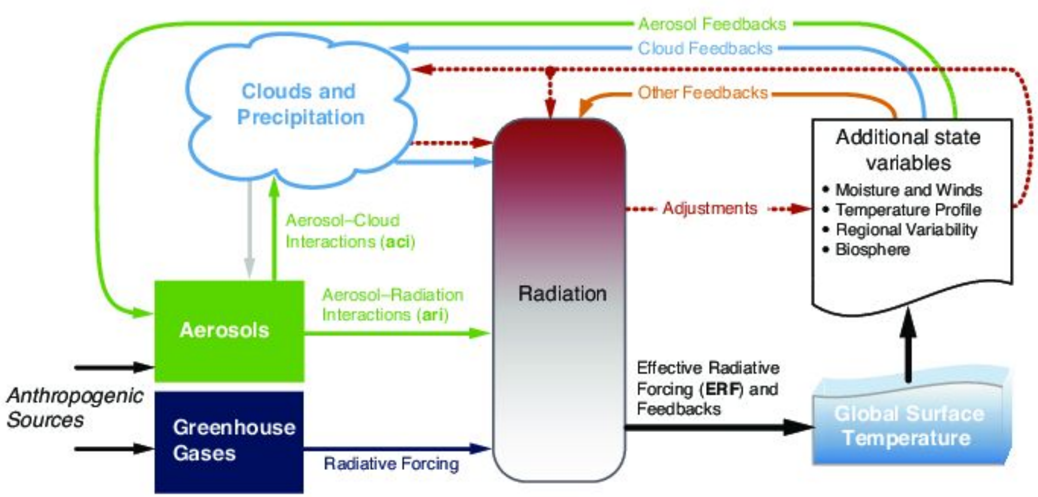
Aerosol Intro

Importance

- Pivotal contributor to atmospheric pollution (smog)
- Impacts weather and climate
  - Aerosol-radiation interactions (ari)
  - Aerosol-cloud interactions (aci)





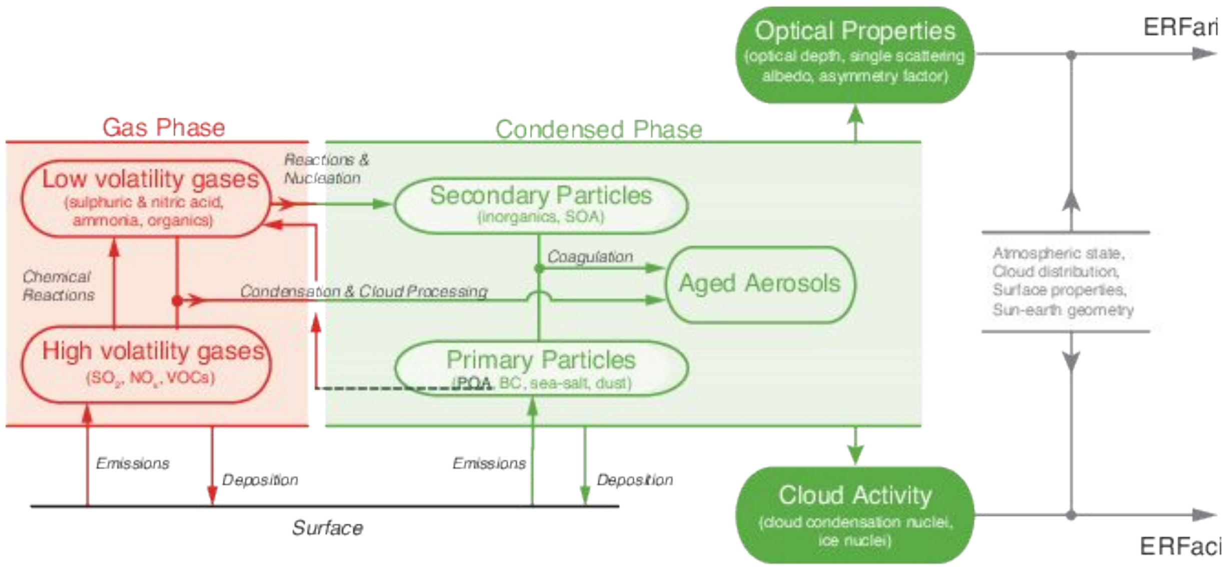


Fifth Assessment IPCC (2014):

“Clouds and aerosols continue to contribute the largest uncertainty to estimates and interpretations of the Earth’s changing energy budget.”

Global Mean
Effective Radiative Forcing (ari+aci)
-0.9 (-1.9:+0.1) Wm^{-2}

Aerosol Intro



Effective Radiative Forcing due to aerosol-radiation interactions

Effective Radiative Forcing due to aerosol-cloud interactions

Emission sources (fluxes similar to heat/moisture but usually with larger uncertainties)

- Natural (e.g. mineral dust or sea salt, ~biomass burning)
- Anthropogenic (e.g. industry/agriculture/other human activities)

Because of importance of sources as much initial as boundary value problem

Aerosol modeling options

- Complex chemistry involving gaseous with more than a hundred of species (usually regional scale)
- Marginal chemistry so that mostly driven by physical processes (usually global scale)

Aerosol Intro
A simple aerosol model

Physics
- Emission fluxes
  - meteorology dependent e.g. mineral dust (wind, geomorphology) or sea salt (wind, ocean state)
  - anthropogenic (emission inventories)
  - biomass burning (satellite observations)
  - episodic volcanic ash
- Boundary layer mixing
- Ground uptake (dry deposition)
- Gravitational settling
- Thermal uplift in forest fires (plume-rise)
- Rain washout (wet deposition, grid-resolved and convective)
- Convective mixing (updraft/downdraft)
- Microphysics (hygroscopic growth of hydrophilic aerosols, CCNs in interactive meteorology-chemistry model)
- Radiative processes (in interactive meteorology-chemistry model).

Chemistry (minimal)
- Conversion of gas SO_2, to sulfate aerosol using climatological background
- Aging of carbonaceous aerosols (hydrophobic -> hydrophilic).

GOCART (Chin et al., 2000, Ginoux et al., 2001)
- Aerosol species: BC (hydrophobic/philic), OC (hydrophobic/philic), sulfate (hphl), dust (hphb), sea salt (hphl)
  - size bins for dust (five) and sea-salt (four), other species in one microscopic bin (total 14 tracers)
- Three gas species: SO_2, DMS, MSA plus climatological backgrounds of H_2O_2, OH, NO_3(total 3 tracers)
- Most serious deficiencies: missing Secondary Organic Aerosols and nitrogen based compounds (nitrates)
- NOAA's GEFS-Aerosols model.

Modeling <-> Observations

Aerosol Optical Depth (AOD) - the most common type of aerosol observation globally

An integral measure of extinction of radiation by aerosols throughout an atmospheric column

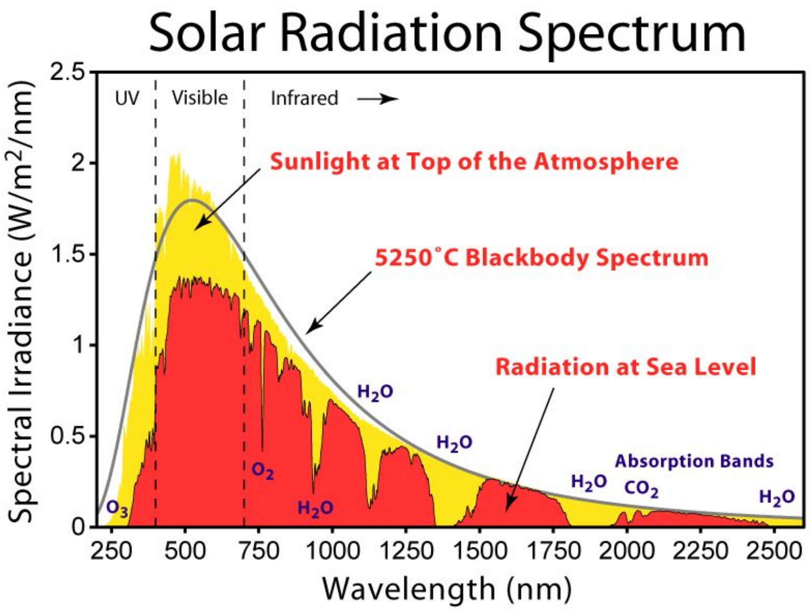
$$\tau(\lambda) = \sum_{i=1}^{n} \sum_{k=1}^{ktop} E_{ext}\left(\lambda, n_{r_i}, r_{eff_i}\right) \times c_{ik} \times \rho_{d_k} \times d_k,$$

E_{ext} - the extinction coefficient (wavelength λ, refractive index n_r, and effective radius r_{eff}),
c - aerosol mixing ratio, d - layer depth, i and k - aerosol species and model layers respectively

Extinction coefficients calculated using a radiative transfer model; dependent on aerosol species, their size distribution including hygroscopic growth, particle shapes, mixture types. Operational RTMs have aerosol capabilities for GOCART or similar.

Observations

Aerosol Optical Depth (AOD)



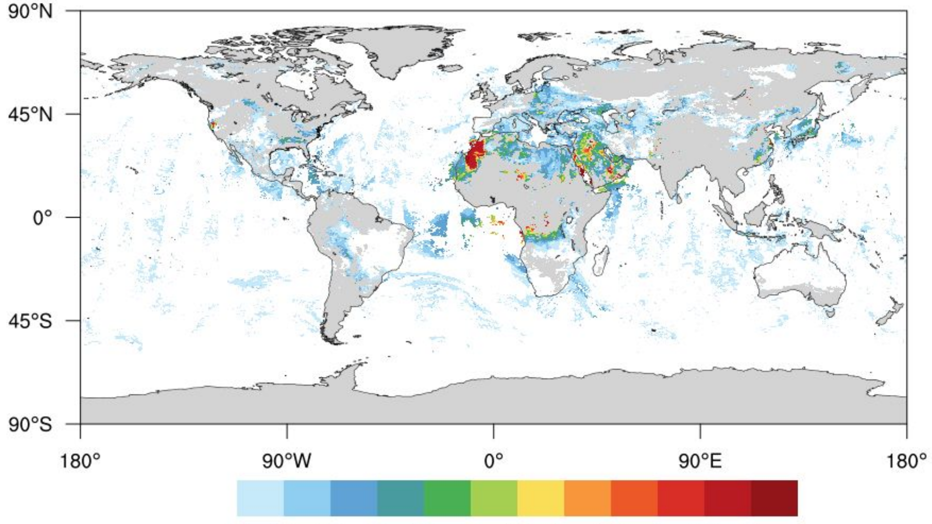
(*from Wikipedia*)

- Aerosols interact with radiation in ~300 – 2100 nm range
- Absorption and scattering depend on particle size and surface properties
  - Assimilation of multispectral AODs can help infer speciation and size distribution of aerosols
- Requires strict quality control, especially for cloud screening.
- Even though aerosol concentrations usually highest in the boundary layer total value of AOD largely determined by aerosols in mid- and upper tropospheric layers.
  - Caution needed when correlating high surface concentrations with AOD.

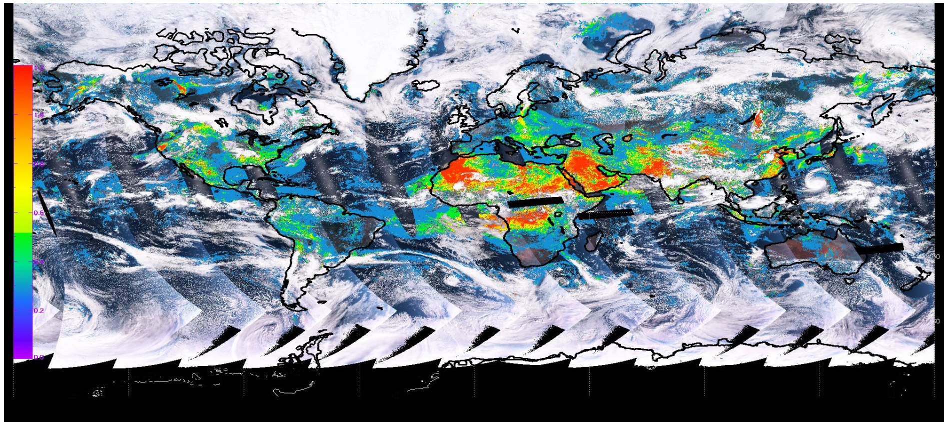
Observations – space based

ɪtical Depth

20150805



MODIS Aqua and Terra NNR at 550 nm



VIIRS L2 at 550 nm

NASA

MODIS

AOD@ 550 nm retrievals at 10 km resolution

NOAA/NESDIS

VIIRS

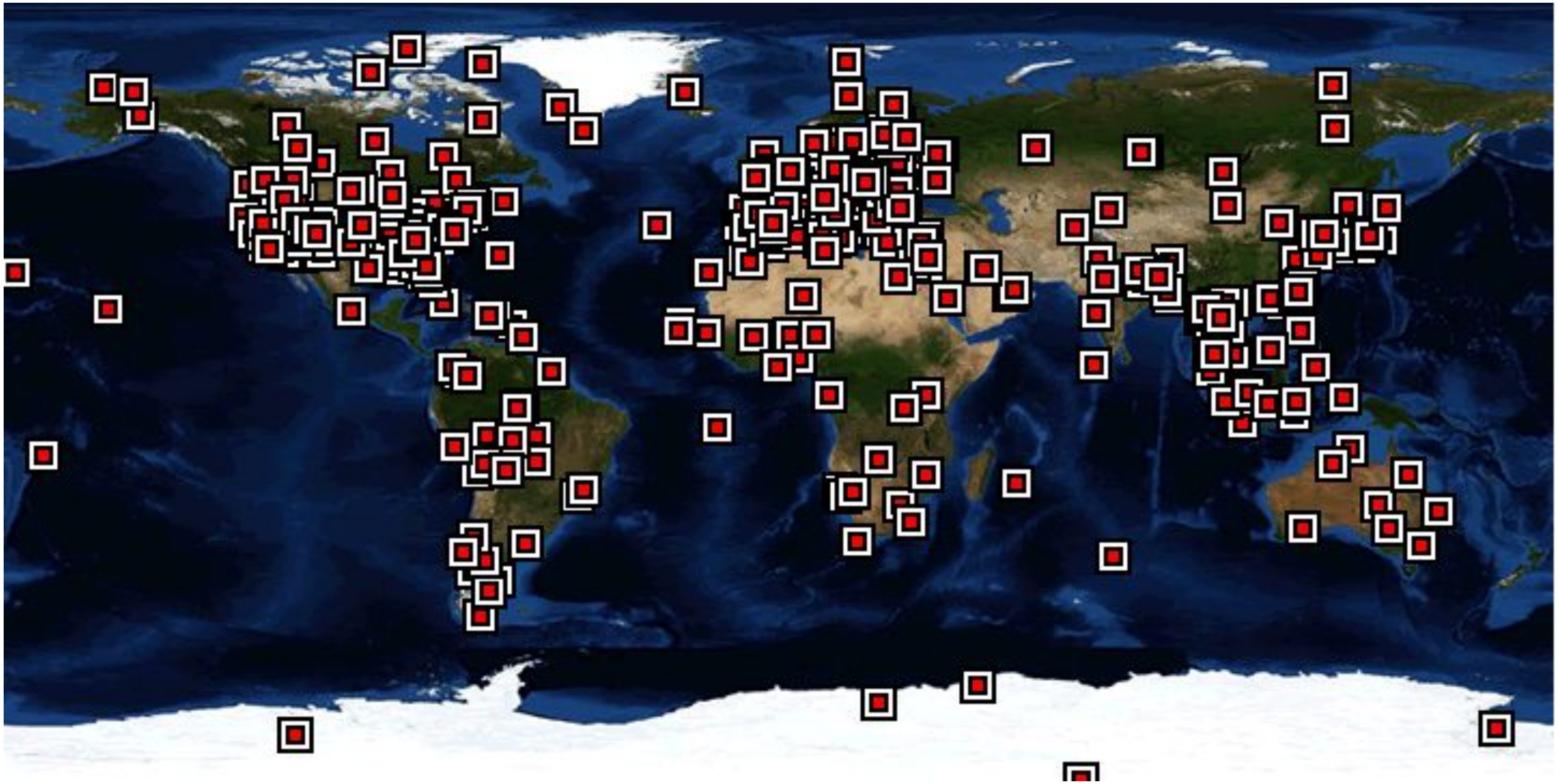
AOD@ 550 nm retrievals at 750 km resolution

AOD at 550 nm wavelength obtained using measurements at multiple wavelengths

Retrievals may differ significantly

Observations – space based

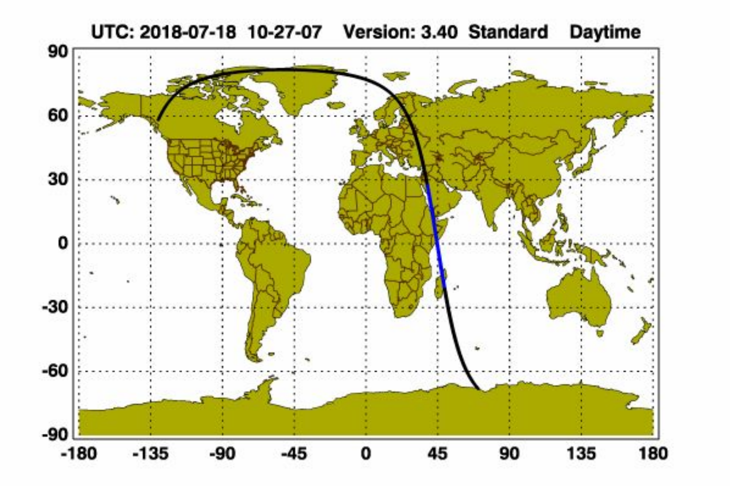
Aerosol Optical Depth

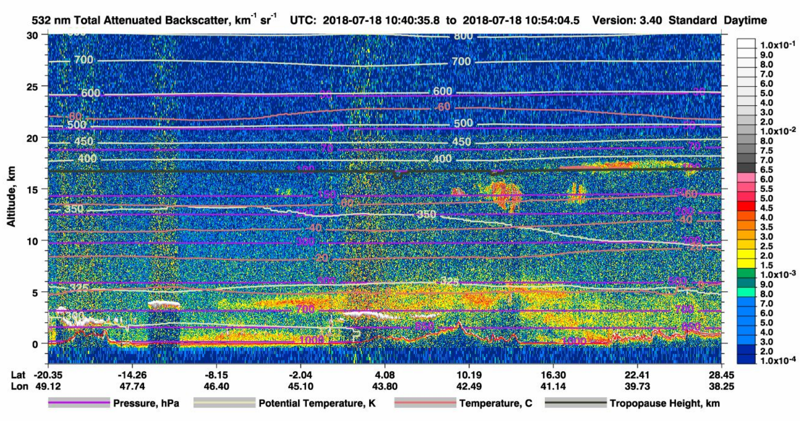


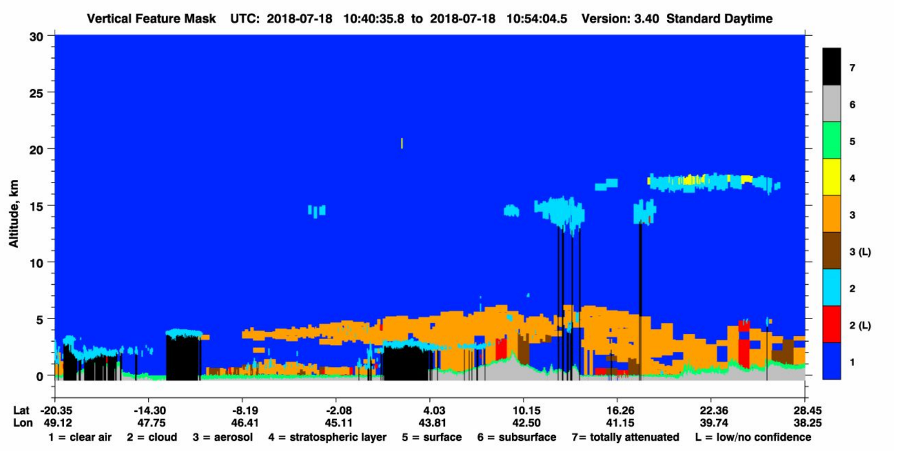
AERONET (UV: 340, 380 nm , VIS: 440, 500, 675 nm, IR: 870, 1020, 1640 nm)

Observations – space-based

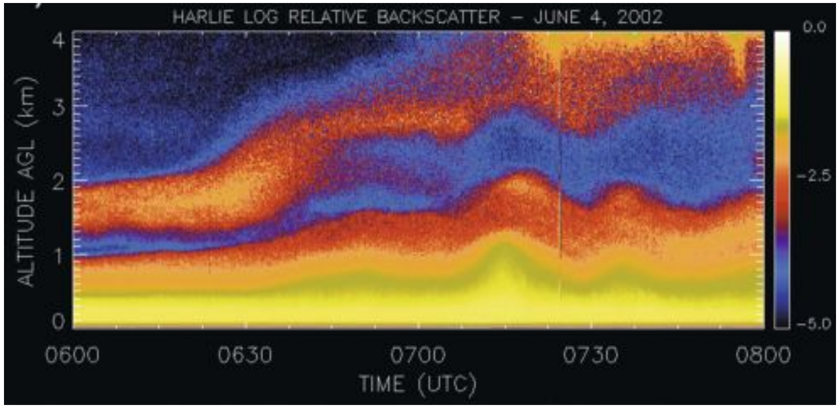
CALIPSO – satellite lidar





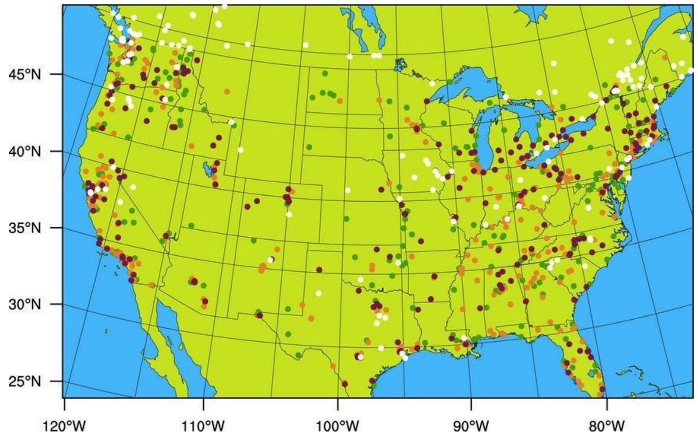


Observations – ground-based

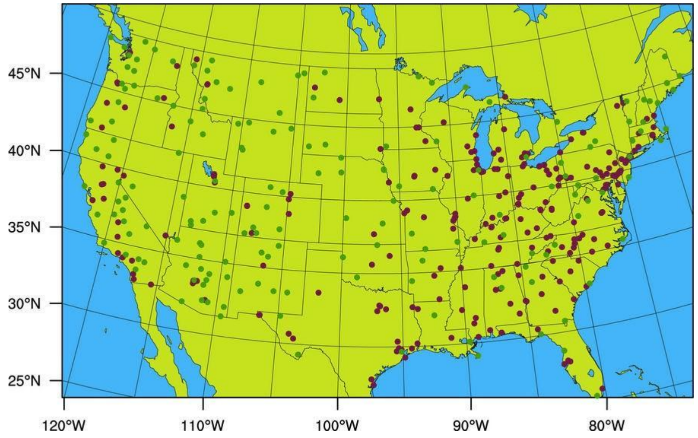


(from S. Koch et al., MWR, 2008, aerosol backscatter can be used to estimate boundary layer height)

HARLIE – a lidar
EARLINET lidar network over Europe



AIRNOW
Total aerosol mass PM2.5;
1-hr average available round the clock;
urban, suburban, rural sites, unknown;
suitable for r-t assimilation.



IMPROVE and STN
Aerosol species: SO4, OC, EC.;
24-hr averages available every three days;
limited value for assimilation.

Data Assimilation

- Purpose of Data Assimilation is to obtain an Optimal Estimation of the True State.
- Applications include forecasting and reanalysis.
- For aerosols (and chemical modeling in general) errors arise not only due to the initial conditions but also due to the boundary conditions (including emissions sources) and due to model/parameterization errors.
- Assimilation methods can be employed to improve emission sources such as for forest fires or to determine release of pollutants or radionuclides. Important application for Carbon Tracker to estimate fluxes of greenhouse gases.
- Application to model parameter estimation.
- The latter two applications require time dimension – 4D-Var or EnKF;
  a sought quantity becomes a control variable.
- In the following, we will only address improvements to the initial conditions.

Aerosol Data Assimilation – surface $PM_{2.5}$

Assimilation of hourly surface $PM_{2.5}$ observations with 3D-Var
(a regional WRF-Chem/GSI application)

$$J(\mathbf{x}) \equiv (\mathbf{x}-\mathbf{x_b})^T \mathbf{B}^{-1}(\mathbf{x}-\mathbf{x_b}) + (\mathbf{y}-H(\mathbf{x}))^T \mathbf{R}^{-1}(\mathbf{y}-H(\mathbf{x})).$$

b_{ij}=cov(e_i,e_j) are elements of background error covariance matrix **B**=[b_{ij}].
B is represented as $\mathbf{B}_z\mathbf{V}\mathbf{B}_x\mathbf{B}_y\mathbf{B}_y\mathbf{B}_x\mathbf{V}\mathbf{B}_z$, where **V** is the standard deviation of error and $\mathbf{B}_x\mathbf{B}_y\mathbf{B}_z$ are applications of recursive filters on correlation scales determined by analysis of covariances b_{ij}.
Background error statistics derived from differences in forecasts valid at the same time but issued at different times (e.g. with NMC method, forecasts 12 or 24 hours apart)

Observation operator **H** interpolates and sums individual aerosol species

$$PM_{2.5} = \rho_d\left[P_{2.5} + 1.375S + BC_1 + BC_2 + 1.8(OC_1 + OC_2) + D_1 + 0.286D_2 + SS_1 + 0.942SS_2\right],$$

$PM_{2.5}$ in GOCART is a sum aerosol species: unspecified P_{25}, sulfate S, hydrophobic and hydrophilic black carbon (BC_1, BC_2), hydrophobic and hydrophilic organic carbon (OC_1, and OC_2), fractions of five dust bins (D_1, D_2, D_3, D_4, and D_5), and fractions of four sea salt bins (SS_1, SS_2, SS_3, and SS_4).

Assume **R** to be diagonal; may include representativeness error based on character of measurement site.

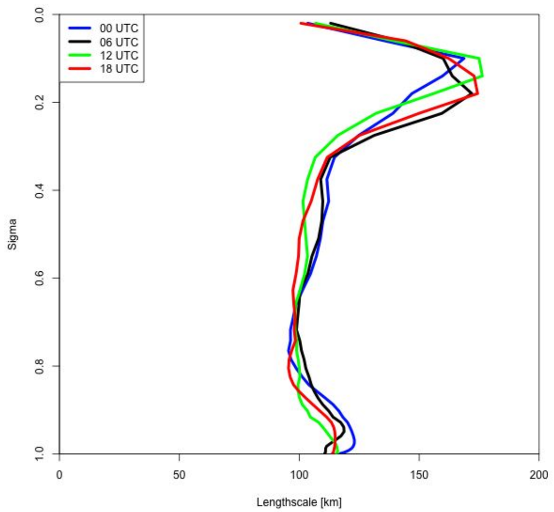
For other aerosol parameterizations with large number of species background error statistics may not be reliable. First, calculate increment of $PM_{2.5}$ ($\Delta PM_{2.5}$); then, $\Delta c_i = \Delta PM_{2.5} * c_i/c_{PM2.5}$ using a priori ratio of *i*-species mass to the total.

Aerosol Data Assimilation – surface $PM_{2.5}$

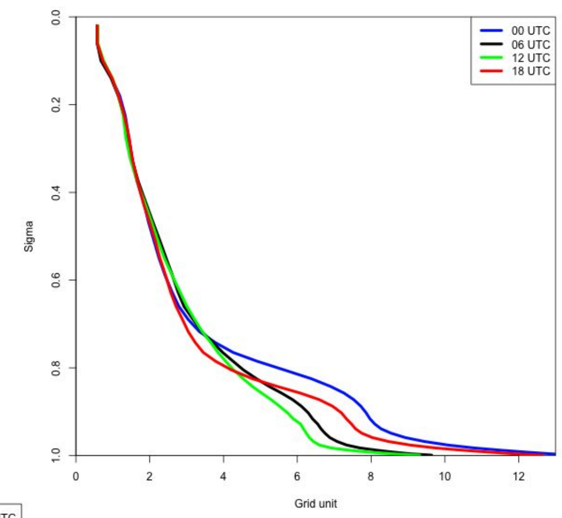
Example background error statistics for a 3D-Var application

- grid-resolution dependent
- latitude dependent
- season dependent

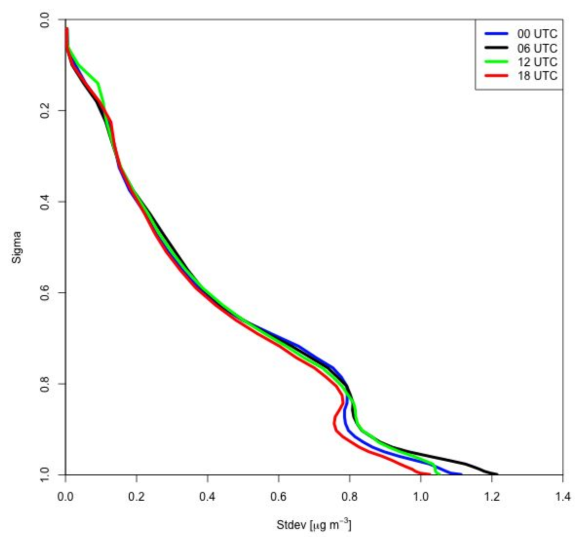
Horizontal lengthscales



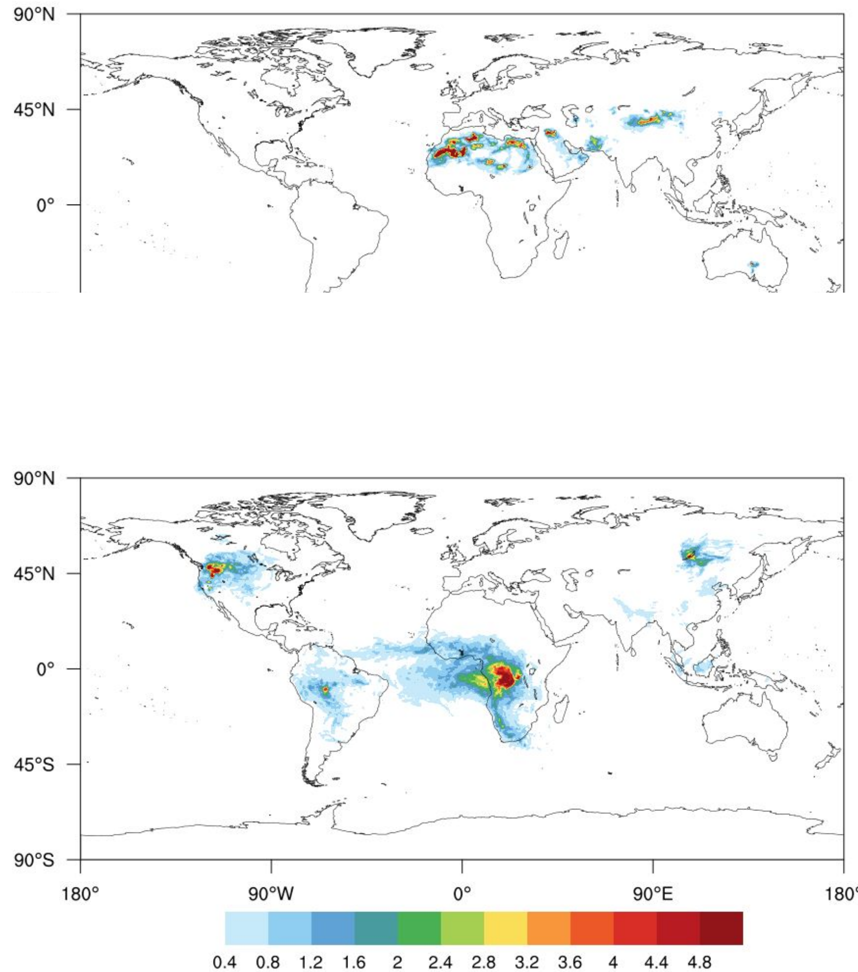
Vertical lengthscales



Standard deviations



Global model (background) error statistics



Model standard error deviation of mixing ratios [ug/kg] of fine dust (top) and secondary organic carbon (bottom) at the lowest level derived from month-long simulations in August 2015 with FV3-GOCART using the NMC method (fcst_24hr-fcst_12hr).

Error is source dependent and not zonal - standard 3D-Var hardly applicable.
Assimilation is state dependent.

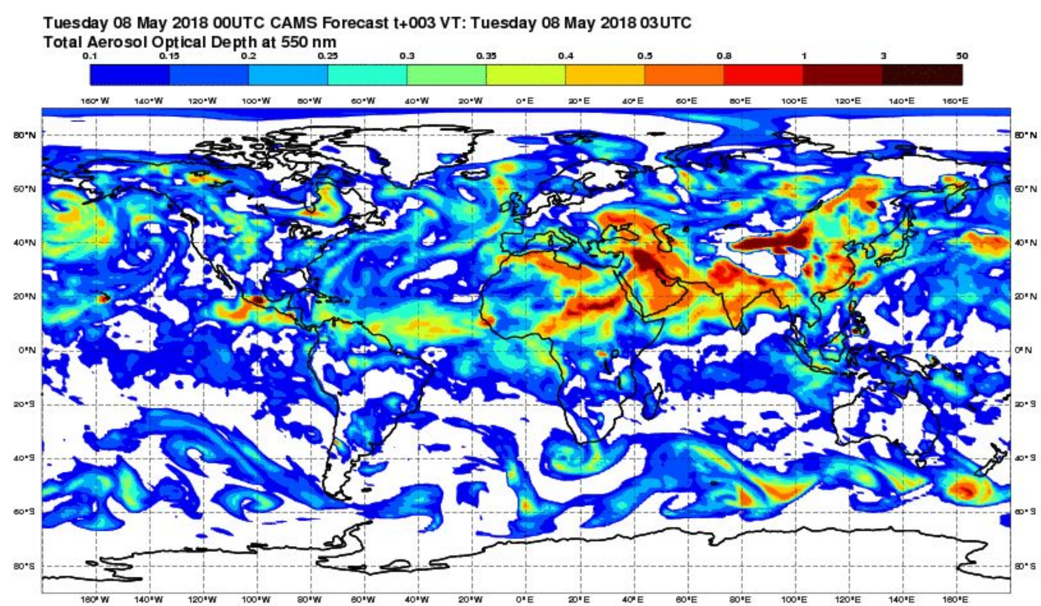
Aerosol Data Assimilation

Copernicus Atmosphere Monitoring System at ECMWF

- Aerosol parameterization similar to GOCART but has also multiple tracer gases.
- Algorithm based on 4D-Var with 12-hour window.

$$J(x) = \frac{1}{2}(x - x_b)^T B^{-1}(x - x_b) + \frac{1}{2}\sum_{k=0}^{K}(y_k - H_k(x_k))^T R^{-1}(y_k - H_k(x_k))$$

- Currently assimilate MODIS AOD 550 nm and recently VIIRS AOD 550 nm .
- Due to computational constraints control variable is total mixing ratio i.e. sum of all species/bins; then split to bins/species based on a priori ratio of a species mass to the total
- Available in real-time, available for lateral boundary conditions for regional models
- Reanalysis



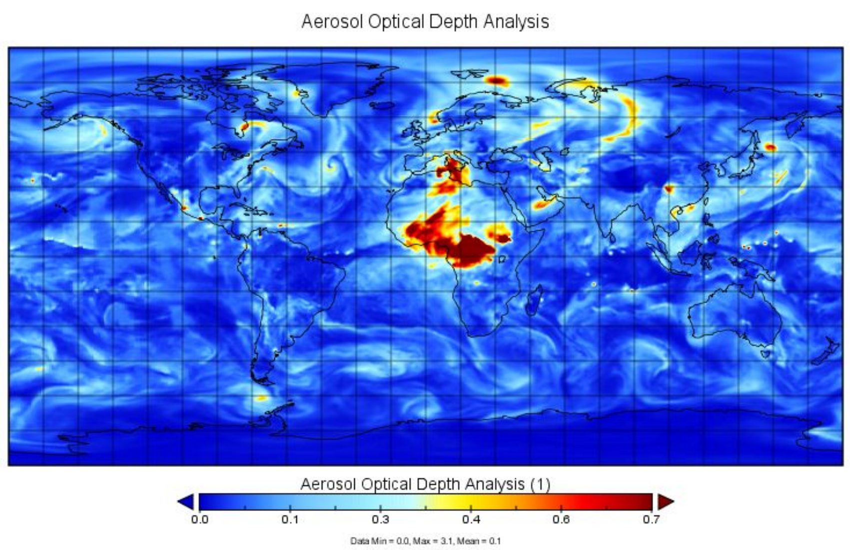
Aerosol Data Assimilation

GEOS and MERRA-2 at NASA/GMAO

- Aerosol parameterization based on GOCART.
- Algorithm based on Physical Space Statistical Analysis for AOD

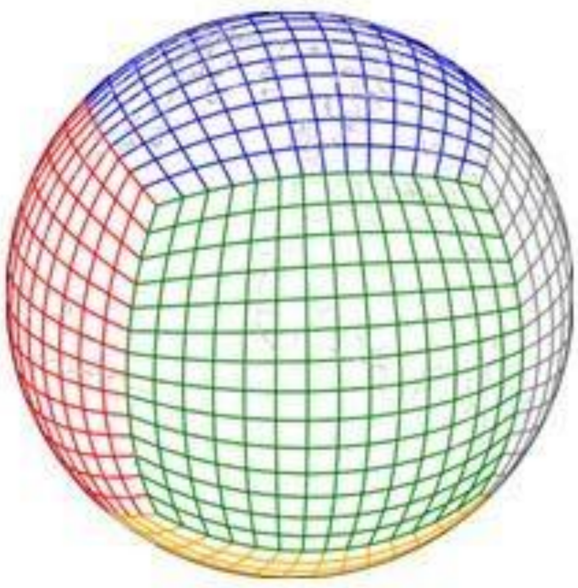
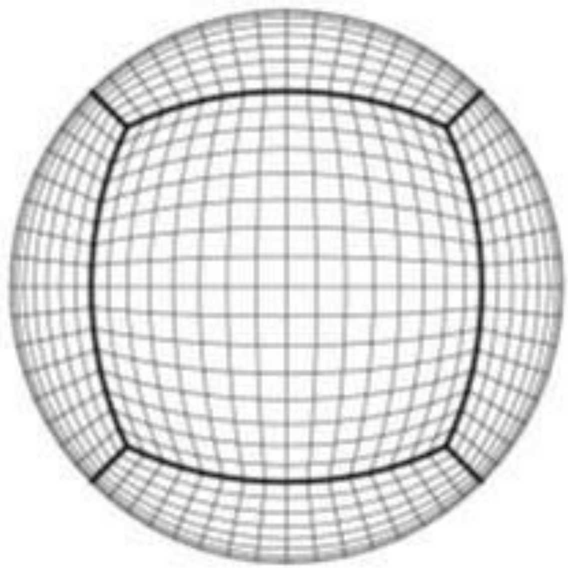
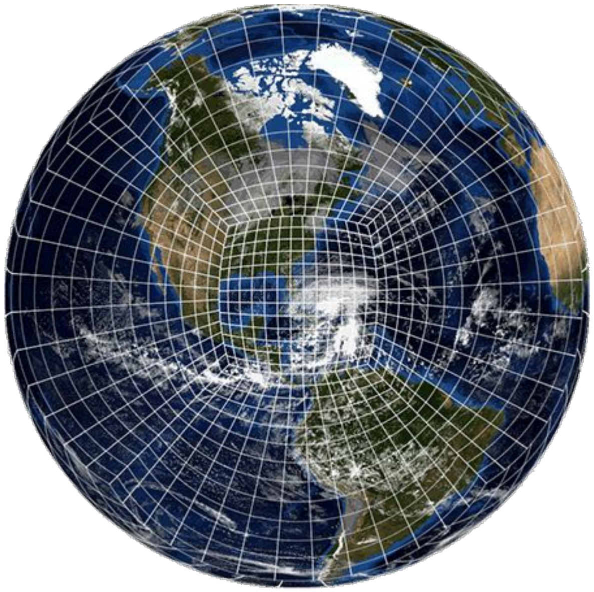
$$\delta\tau^a = HBH^T(HBH^T+R)^{-1}(\tau^o-Hx^f)$$
$$\delta x^a = BH^T(HBH^T)^{-1}\,\delta\tau^a$$

- *B* derived from ensemble of members with perturbed emissions
- Because of ~lognormal error distribution control variable is $log(\tau+\varepsilon)$
- Assimilate MODIS AOD 550 nm NNR
  - NNR - bias-corrected AOD derived from AVHRR and MODIS radiances calibrated with AERONET
- Reanalysis at 0.5 x 0.625 degree



Aerosol Modeling at NOAA

GEFS-Aerosols Operational Model

- FV3 dynamical core (cube-sphere);
- GOCART aerosol parameterization;
- Chemistry coupled with the core meteorological model via NUOPC interface;
- Meteorology from NOAA's 6-hourly ensemble analyses;
- DA at ~100km (C96) resolution.

A multi-agency research center to improve the use of satellite data for analyzing and predicting the weather, the ocean, the climate and the environment.

https://www.jcsda.org/jcsda-project-jedi

JEDI: Joint Effort for Data assimilation Integration – a collaborative effort led by JCSDA with participation of US gov't agencies, academy, and various institutions across the world. (*Not speaking on their behalf.)*

Flexible interfaces to

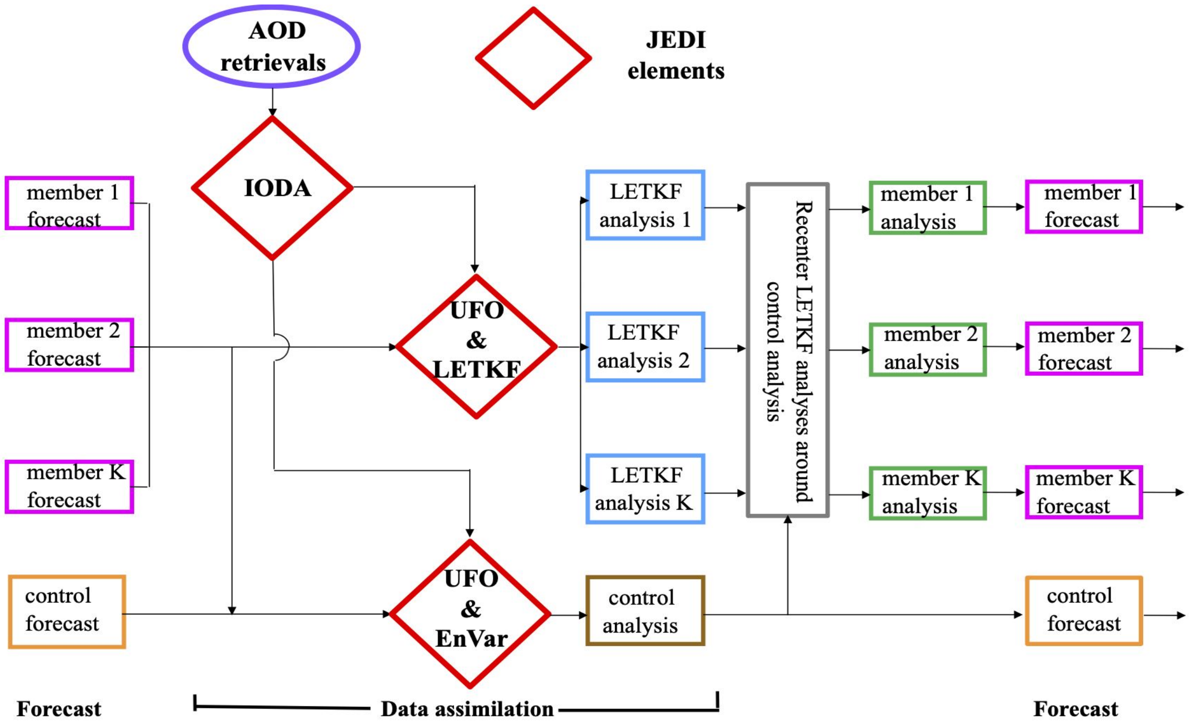
- Models incl. irregular grids
- Observation Formatting
- Forward Operators
- Assimilation algorithms on native model grids

Science and Operations

Education & Support

Aerosol Data Assimilation at NOAA

Ensemble-Based
Observations: VIIRS AOD 550 nm



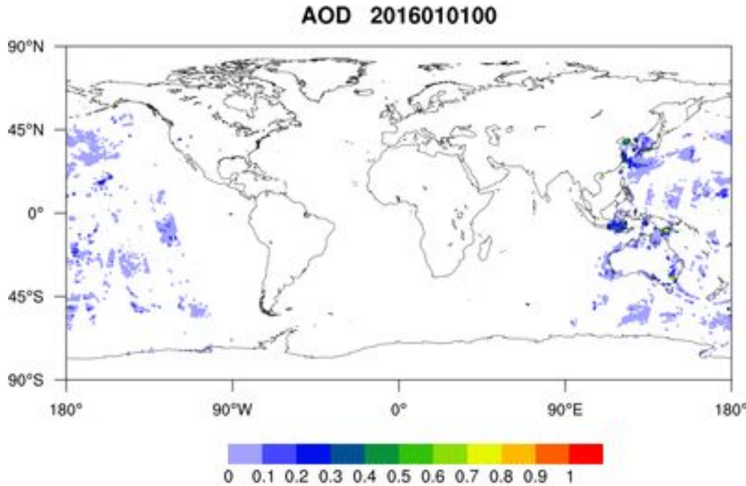
- **AOD**: Aerosol Optical Depth;
- **IODA**: Interface for Observation Data Access;
- **UFO**: Unified Forward Operator;
- **LETKF**: Local Ensemble Transform Kalman Filter
- **EnVar**: Ensemble-Variational solver.

Experimental aerosol data assimilation on native cubic sphere grid with 20/40 ensemble members at C96 (~100 km) resolution.
Running in near-real-time (VIIRS AOD) and for aerosol reanalysis (MODIS NNR AOD).
Meteorology not assimilated but incremented with ensemble analyses obtained separately.

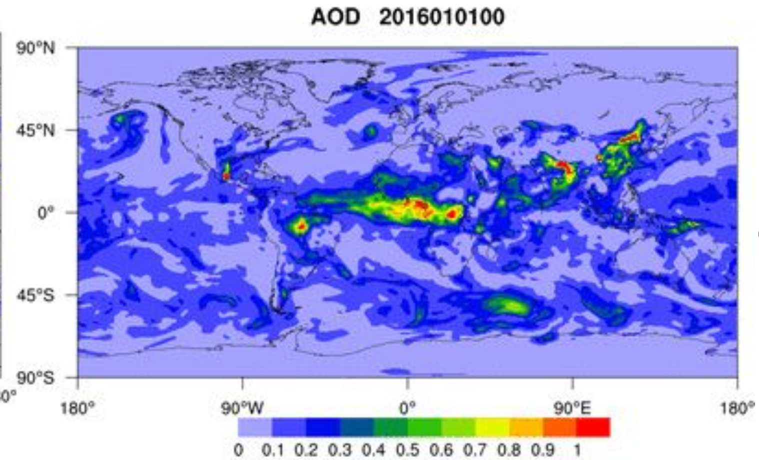
Comparison of Reanalyses

January – February 2016

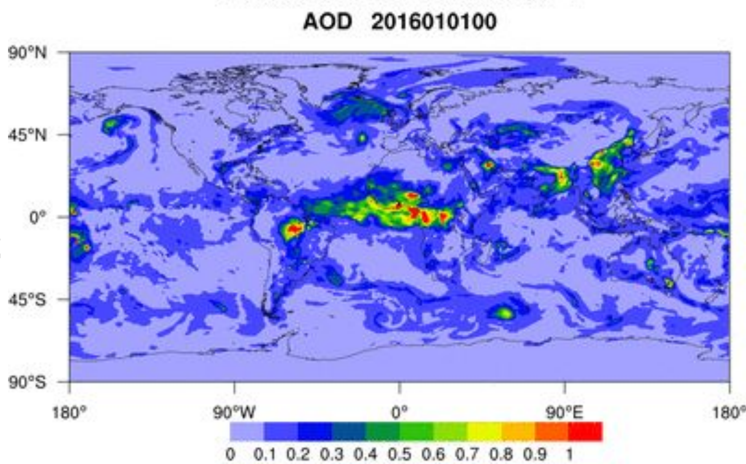
MODIS Aqua & Terra NNR retrievals



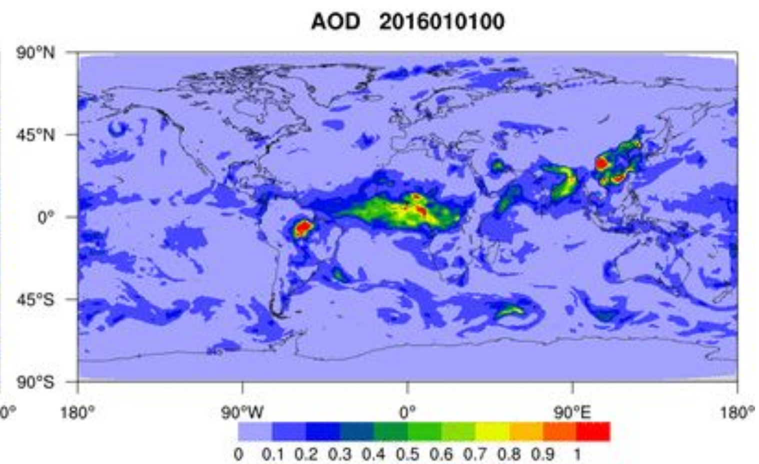
CAMSiRA



MERRA-2



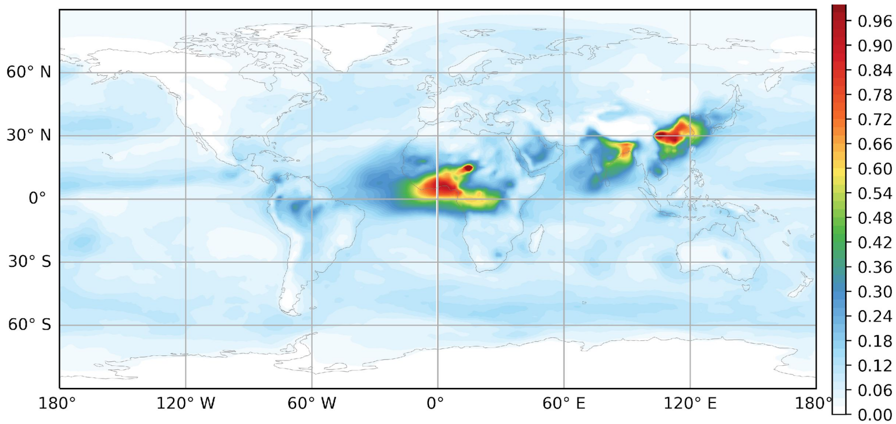
GEFS

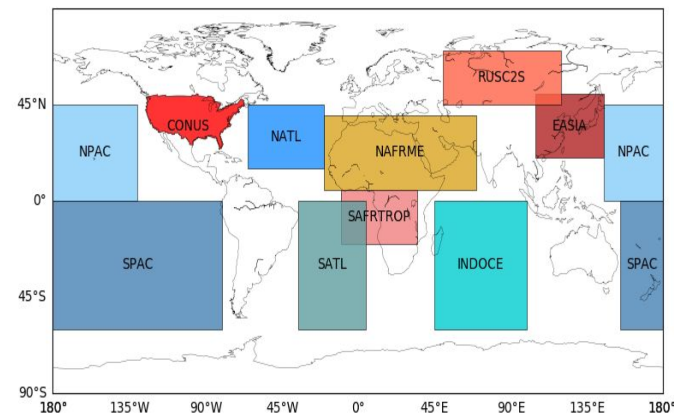


Comparison of Reanalyses

January 2016

AOD Monthly Mean





Carbonaceous Aerosols

Hydrophilic Hydrophobic

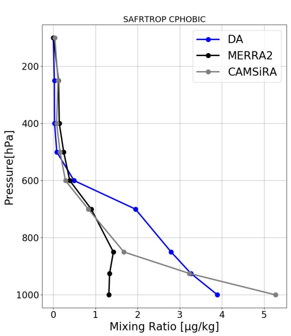
Dust

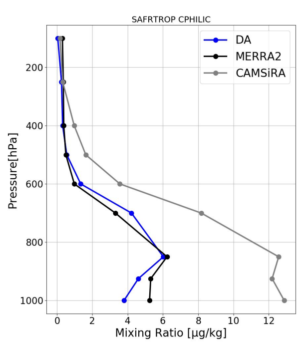
Sea salt

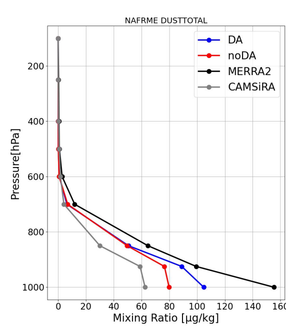
SAFRTROP

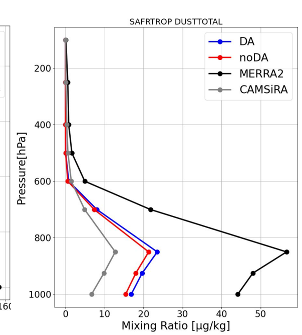
NARFME SAFRTROP

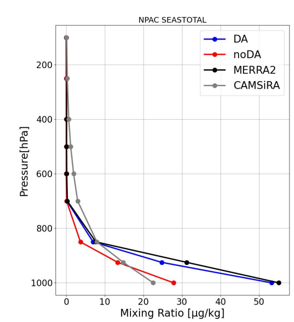
NPAC SPAC+SATL+INDOCE

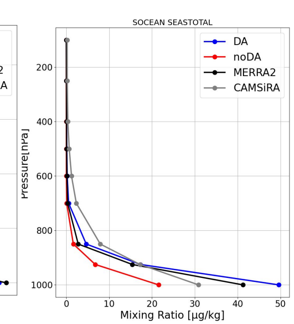








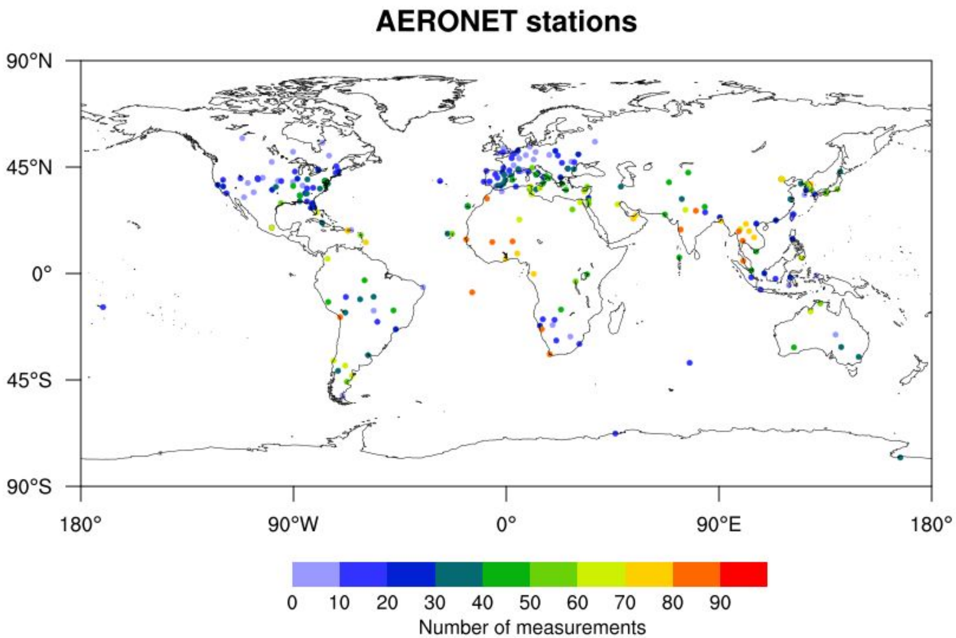




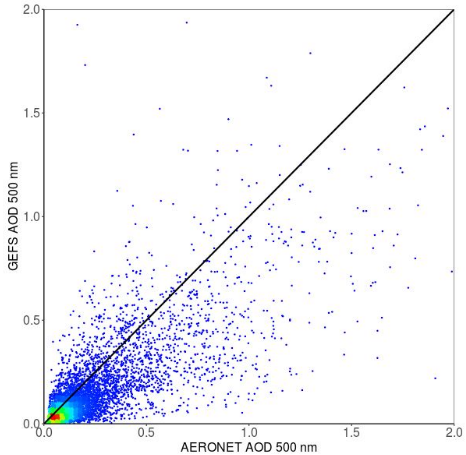
. AERONET

y 2016

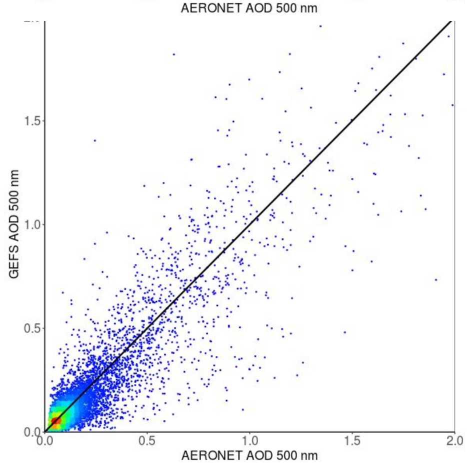
AOD 500 nm



noDA



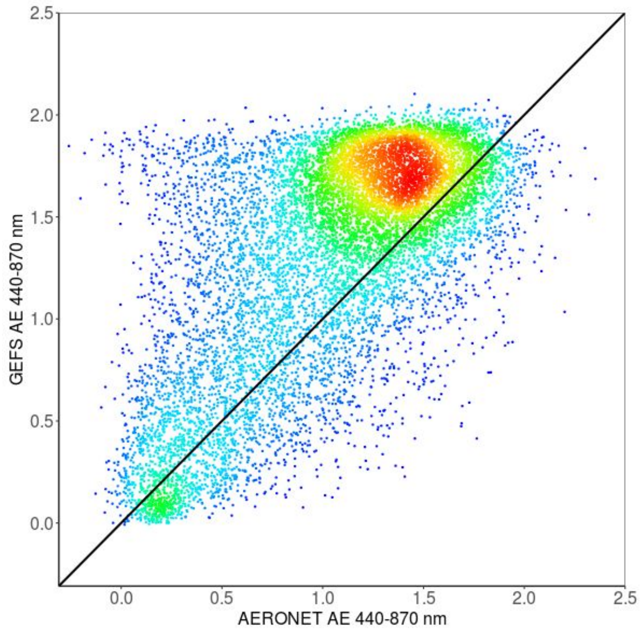
DA



GEFS Reanalysis vs. AERONET

January - February 2016

noDA

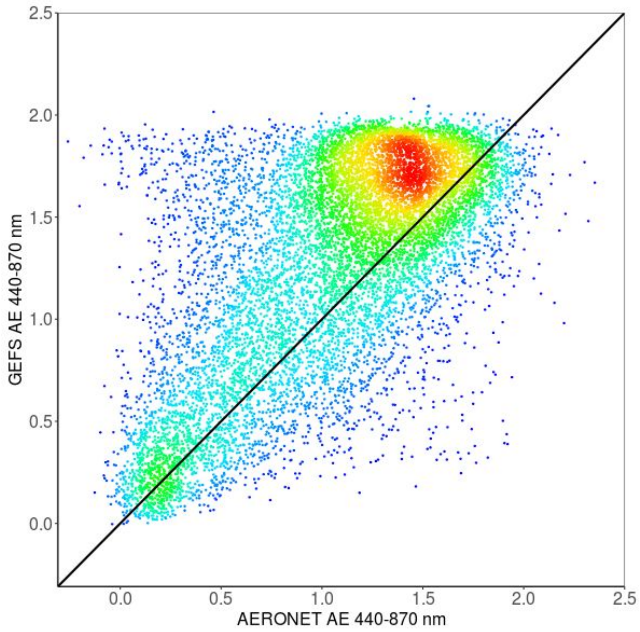


440 - 870 nm

Ångström Exponent

$$AE = -log[AOD(\lambda_1)/AOD(\lambda_2)]/log(\lambda_1/\lambda_2)$$

DA



Aerosol Data Assimilation

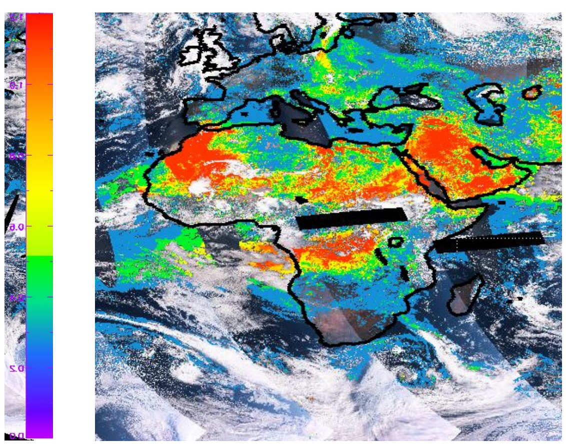
Fundamental problems

- Models quite inaccurate e.g. $PM_{2.5}$ forecasts usually hardly or do not beat persistence

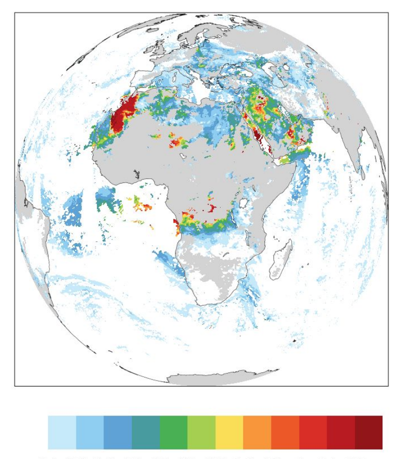
- Scarcity of observations of
    - Chemical composition
    - Size distribution
    - Vertical profiles

- Uncertainty of retrievals due to algorithm deficiencies and screening procedures

VIIRS



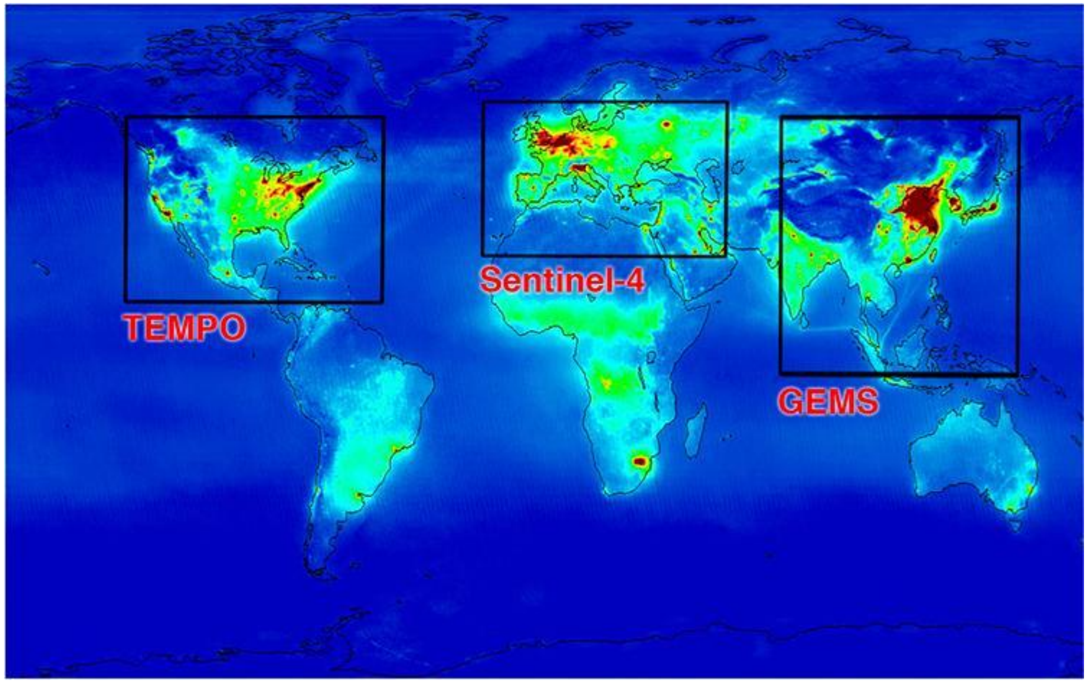
MODIS



Prospects for improving aerosol forecasting and analysis

New/recent satellites – assimilation and improvement of emission inventories and fire products

- Sentinel 5P (2017, polar orbiting)
- GEOS-5 ABI (2017, geostationary)
- TEMPO (Tropospheric Emissions: Monitoring Pollution, 2022), Sentinel 4 (2023), GEMS (2018), all geostationary



Global field missions for aerosol species e.g. ATom (Atmospheric Tomography) NASA

Thank you

Mariusz.Pagowski@noaa.gov