Recent (and near-Future) Developments in Aerosol Modelling and Assimilation at NOAA

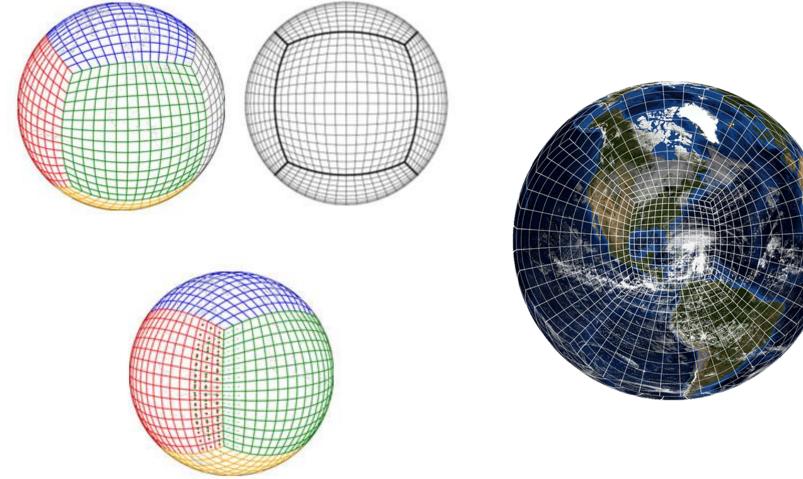
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Also with contributions from B. Scherllin-Pirscher (ZAMG), B. Johnson (JCSDA), A. da Silva (NASA/GMAO).

FV3 - the Future NOAA's Weather Model



from https://www.gfdl.noaa.gov/fv3/

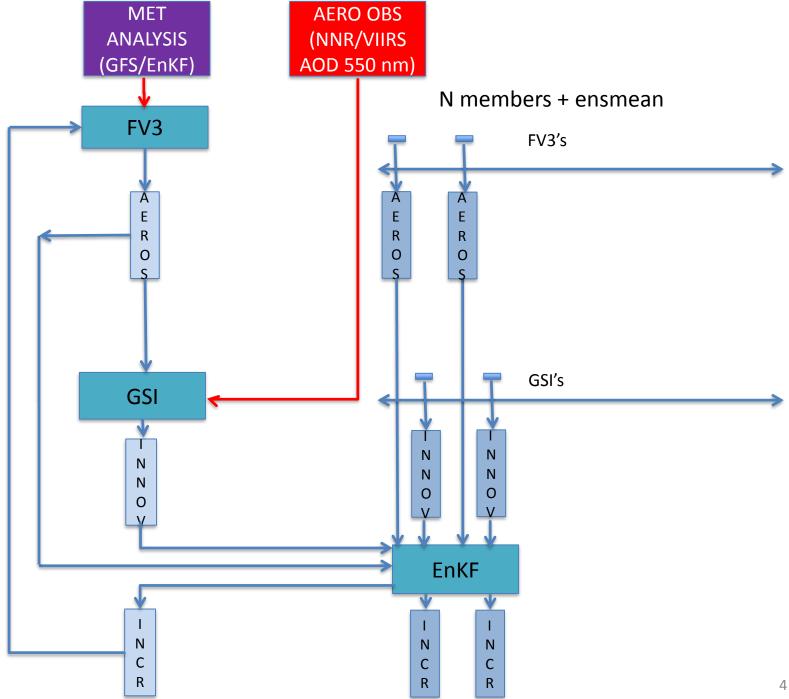
Developed by S.J. Lin et al. at GFDL. Finite Volume scheme with emphasis on mass/tracer conservation, over the years used in weather and climate models (notably GEOS)

GOCART and its on-line implementation in FV3

- Based on Chin, Ginoux et al.,
- 15 aerosol species: BC (hydrophobic/phillic), OC (hydrophobic/phillic), sulfate, five dust bins, four sea salt bins, plus unspecified P25.
- 3 gas species: SO₂, DMS, MSA plus climatological backgrounds of H₂O₂, OH, NO₃.
- Emissions:

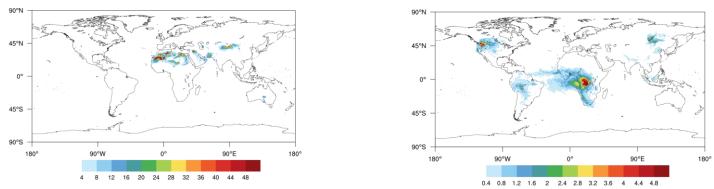
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- anthropogenic based on EDGAR-HTAP inventory:
 - flat, monthly, no temporal factors, 0.1 deg resolution,
 - BC, OC, sulfate, SO₂, PM_{2.5}, PM₁₀, other not relevant for GOCART: NO_x, NH₃, CO, NMVOC
- biomass burning and plume rise:
 - MODIS, about 4 km resolution, from CPTEC/Brasil, WRF-Chem,
- dust:
 - AFWA scheme (Jones et al.), erodibility data @ 0.75 deg, and sand/clay data @ 0.08 deg, from WRF-Chem,
- sea salt:
 - Gong et al., from NASA/NGAC.
- Chemistry: hydrophobic -> hydrophillic carbon by aging plus sulfate production applied on chemical time step (e.g. 30 mins).
- Physics (mostly GFS defaults with some exceptions due to tracers) applied on physical time step (e.g. 450 secs at ~ 50 km model):
 - mixing (PBL similarity based, non-local for heat, moisture though not tracers, required some additions including dry deposition and surface and plume emissions, implicit for numerical stability, ALL TRACERS), from GFS,
 - hygroscopic growth of some particles + gravitational settling (AEROSOLS), from NASA/NGAC,
 - Chikira-Sugiyama convective transport (ALL TRACERS) and scavenging (HYDROPHILLIC AEROSOLS), from GFS,
 - wet scavenging by resolved precipitation (HYDROPHILLIC AEROSOLS), from WRF-Chem,



Data Assimilation

- NASA's NNR AOD 550 nm (combines MODIS and AERONET) or VIIRS AOD 550 nm retrieval;
- Community Radiative Transfer Model CRTM (JCSDA);
- Gridpoint Statistical Interpolation (GSI, NCEP)
 - forward model on the Gaussian grid requires interpolation and reformatting C192 (NetCDF) $\leftarrow \rightarrow$ T382 (NEMSIO),
 - 6-hr cycle with 3-hr window and FGAT;
- Need for source (state) dependent model error:
 - Ensemble Kalman Filter (NCEP operational, Whitaker and Hamill, 2003):
 - 20 members,
 - currently only perturbations to meteorology;



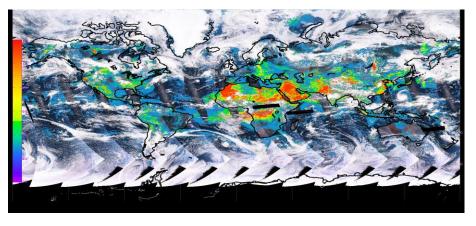
Model standard error deviation of mixing ratios [ug/kg] of fine dust (left) and secondary organic carbon (right) at the bottom level derived from month-long simulations in August 2015 using the NMC method (fcst_24hr-fcst_12hr).

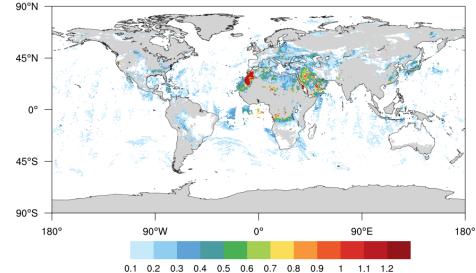
- Realistic for NRT:
 - 9-hr forecast on 96 processors on NOAA's Theia supercomputer less than 10 mins,
 - GSI/EnKF/interpolations in comparable time.

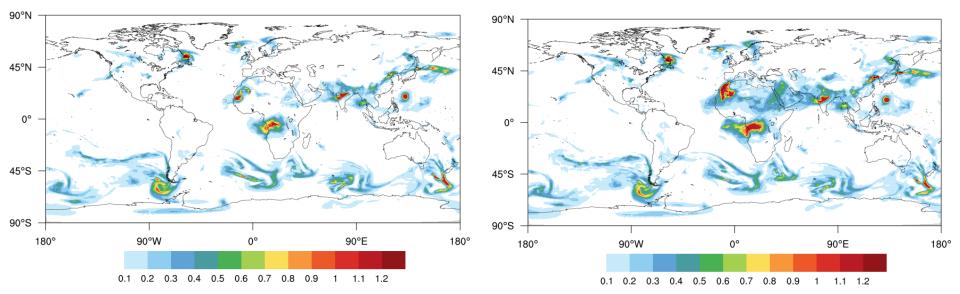
Example: AOD 550 nm 20150805

VIIRS

MODIS NNR







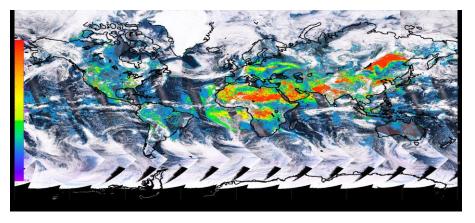
Free-run forecast 12 UTC

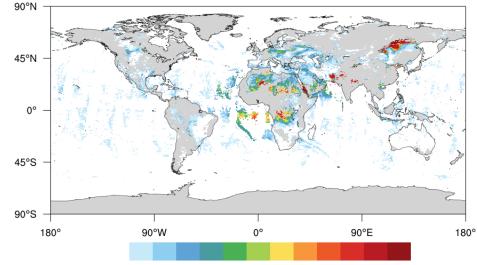
Analysis 12 UTC

Example: AOD 550 nm 20150810

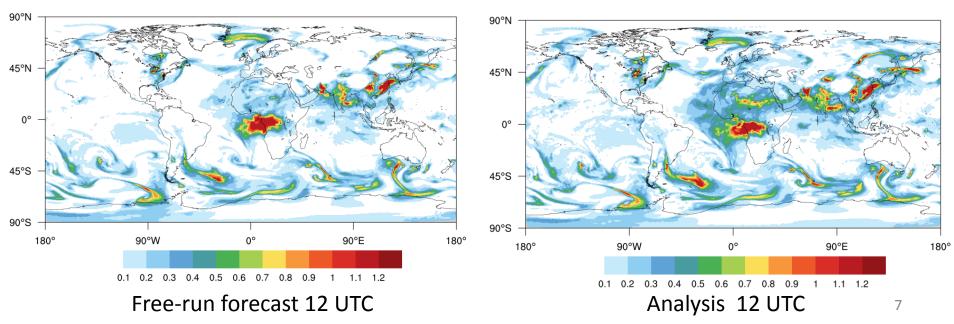
VIIRS

MODIS NNR

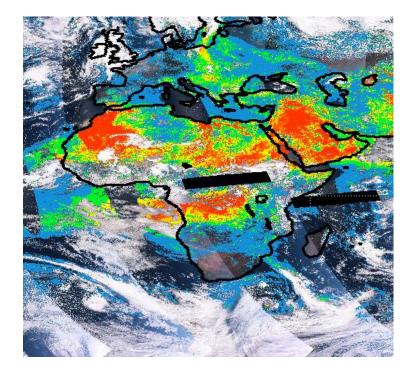


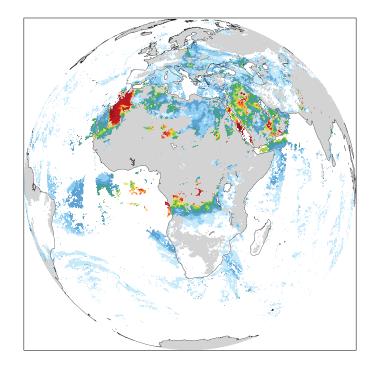


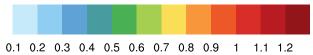
0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1 1.1 1.2



VIIRS vs. NNR 20150805



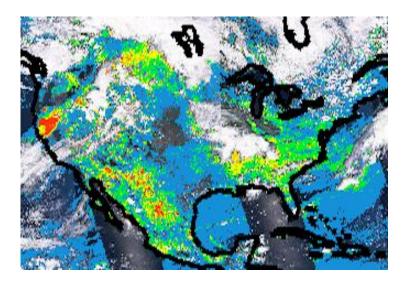


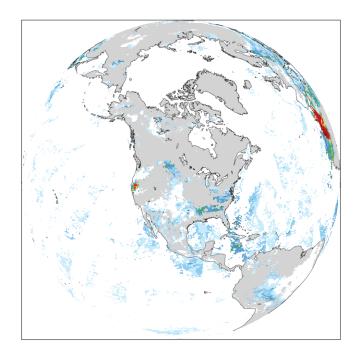


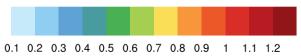
What is real?

VIIRS vs. NNR 20150805



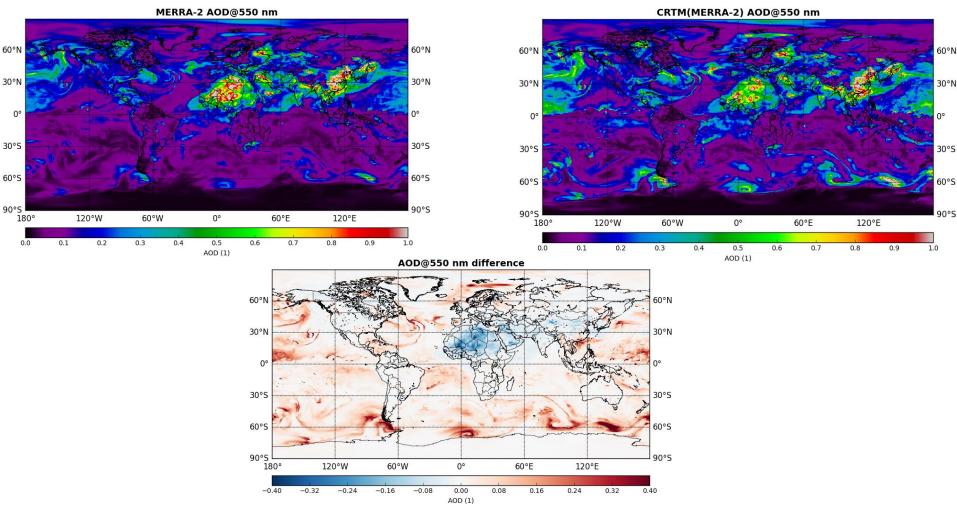






What is real?

MERRA -2 vs. CRTM(MERRA-2 species) 20100417



Possible differences:

- calculation of radii for sea-salt due to hygroscopic growth,
- non-spherical dust in MERRA-2.

EnKF and its application to AOD 550 nm assimilation

$$t(I) = \mathop{a}\limits^{n}_{i=1} \mathop{a}\limits^{ktop}_{k=1} E_{ext}(I, n_{r_i}, r_{eff_i}) \quad c_{ik} \quad r_{d_k} \quad d_k,$$

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

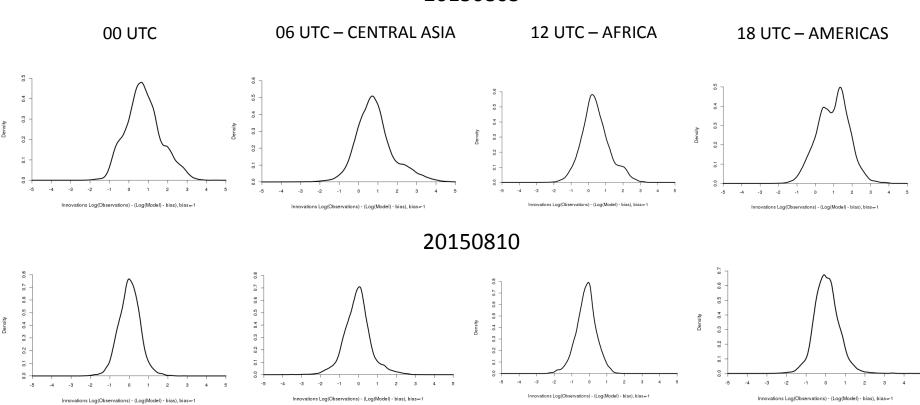
 $\Delta c_{ik} \sim \Delta \tau(\lambda)$ $\Delta c_{ik} = \mathbf{K} \times \left[(\tau_0(\lambda) - \tau_M(\lambda)) \right] = \mathbf{K} \times \Delta \tau(\lambda) \text{ and } \Delta \tau(\lambda) \sim \mathcal{N}(0, \sigma^2)$ 20150805 00 UTC 06 UTC - CENTRAL ASIA 12 UTC – AFRICA 18 UTC – AMERICAS 13 16 19 Density 6 8 10 -0.5 0.0 0.5 1.0 1.5 2.0 -0.5 0.0 0.5 1.0 1.5 2.0 -0.5 0.0 0.5 1.0 1.5 2.0 -0.5 0.0 0.5 1.0 1.5 2.0 Innovations Observations - Model Innovations Observations - Model Innovations Observations - Model Innovations Observations - Model 20150810 10 12 14 16 9 4 Density Density 0١ -0.5 0.0 0.5 1.0 1.5 2.0 1.0 1.5 2.0 -0.5 1.0 1.5 -0.5 -0.5 0.0 0.5 0.0 0.5 2.0 0.0 0.5 1.0 1.5 2.0 11 Innovations Observations - Model Innovations Observations - Model Innovations Observations - Model Innovations Observations - Model

EnKF and its application to AOD 550 nm assimilation

$$T = \log(\tau + B), \Delta T = \Delta \tau / (\tau + B)$$
$$\Delta c = K \times \Delta \tau = K \times \Delta T \times$$
$$\Delta c / (\tau + B) = K \times \Delta T, \text{ and } \Delta T \sim \mathcal{N}(0, \sigma^2)$$

(May be problematic for other moments ?)

20150805

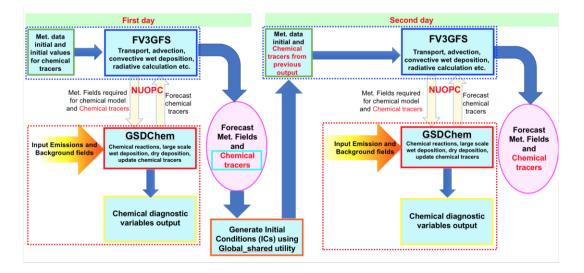


What are we doing now?

- Chemical model development
 - coupling aerosols/chemistry with meteorology via NUOPC interface;
 - various flavors of GOCART (incl. nitrate, brown carbon);
 - photochemical gas-phase mechanism RACM with GOCART;
 - RACM with secondary organic aerosols;
 - CMAQ.
- Data assimilation
 - addressing deficiencies of EnKF approach;
 - JEDI project;
 - enhancing aerosol radiative transfer model (CRTM):
 - flexible size distribution incl. variable modes, variance and mean,
 - flexible chemical composition,
 - non-spherical particle shapes,
 - coagulation (external vs. internal mixture),
 - UV;
 - aerosol reanalysis (joint with NASA/GMAO);
 - trace gases (CO, ...).

Chemical model development

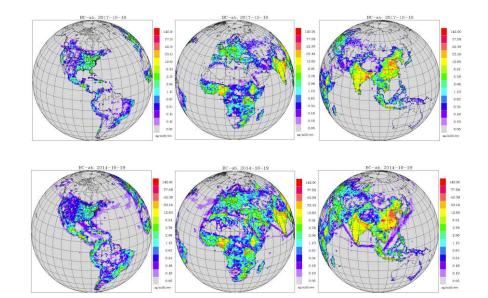
FV3-Chem coupled structure



Anthropogenic emission sources based on new emission inventories

Black Carbon HTAP 2010

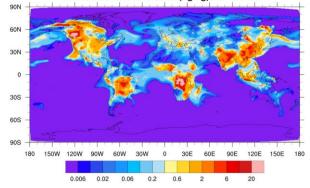
Black Carbon CEDS 2014



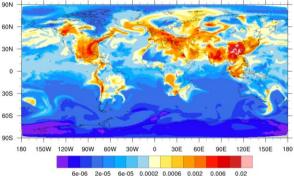
FV3-Chem

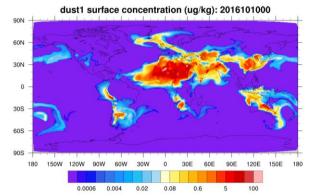
BC surface concentration (ug/kg): 2016101000 90N 60N 30N 0 30S 60S 905 180 150W 120W 90W 60W 120E 150E 180 30W 60E 90E 0 30E 0.002 0.006 0.02 0.06 0.2 0.6 2 8

OC surface concentration (ug/kg): 2016101000



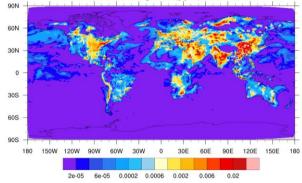
sulfate surface concentration (ppm): 2016101000





sea salt1 surface concentration (ug/kg): 2016101000 90N 60N 30N 0 305 60S 90S 180 150W 120W 90W 60W 30W 60E 90E 120E 150E 180 0 30E 1.8 2.4 2.8 3.2 3.6 4 4.4 4.8 5.5 6.5 1.4 1

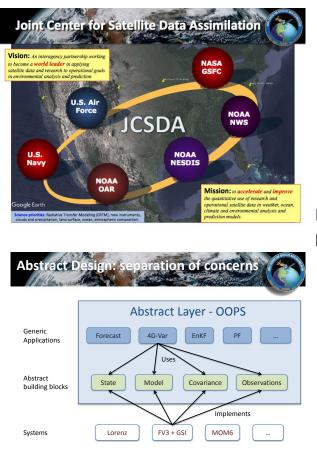
SO2 surface mixing ratio (ppm): 2016101000



Seven-day forecast at 2016101000

Data Assimilation

JEDI (Joint Effort for Data Assimilation Integration)



Abstract interfaces are the most important aspect of the design

- AOD operator coded using CRTM in UFO (United Forward Operator);
- CALIPSO and ground lidar backscatter (B. Scherllin-Pirscher, ZAMG, and B. Johnson, JCSDA);
- 3D/4D-EnsVar with FV3-GOCART available in a year (or sooner).

From T. Auligne's and Y. Tremolet's presentations at May 2018 JCSDA meeting