Science, Service, Stewardship

Advanced Air Quality Forecasting Capabilities Using NOAA's Unified Forecast System

Barry Baker, Lacey Holland, Youhua Tang, Patrick Campbell, Zach Moon, Wei-Ting Hung, Margaret Marvin, Beiming Tang, Wei Li, Irena Ivanova

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Office of Oceanic and Atmospheric Research (OAR)
NOAA Air Resources Laboratory (ARL)
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NOAA Air Resources Laboratory CM&E Group

Overview of the ARL modeling efforts

- *National Air Quality Forecast Capability - AQM*
  - Updates, emissions, innovation and science improvements
- *NOAA Emissions and eXchange Unified System (NEXUS)*
  - Emissions datasets and algorithms for NOAA AC models
- *Global Ensemble Forecast System (GEFS)-Aerosol*
  - Updates to global aerosol model – GEFSv12.3
- *UFS-Aerosol -> GEFSv13 – subseasonal-to-seasonal (S2S)*
  - UFS-based global aerosol model -> fully coupled ESM
- *Seasonal Forecast System - Seasonal 1 year forecasts*
  - Future UFS-based global ensemble forecast replacing CFS
- *RRFS-Smoke/Dust*
  - Aerosol-aware RRFS - with FENGSHA dust scheme and RAVE Fire
- *MELODIES-MONET*
  - Verification collaboration between NOAA ARL/CSL/GSL and NCAR
- *Configurable Atmospheric Chemistry (CATChem)*
  - New development of a unified chemistry component for all UFS Applications

Outline

Advancements to the Science and Emissions for the Future of NOAA's AQM
Patrick Campbell

Evaluation of NAQFC with Other Observations: A Study in Summer 2023
Youhua Tang

Path Forward for UFS based air composition forecasting: UFS-CMAQ, UFS-Aerosols, NEXUS and UFS-Chem
Barry Baker

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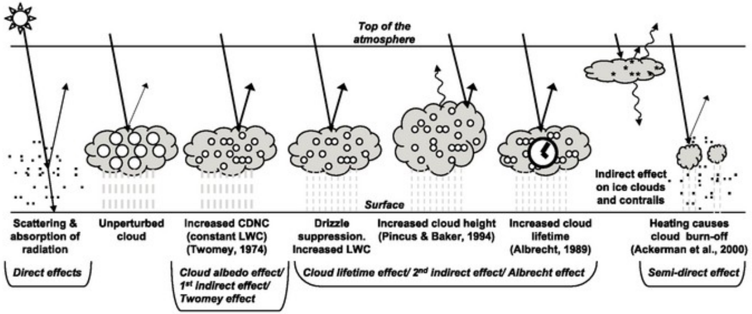
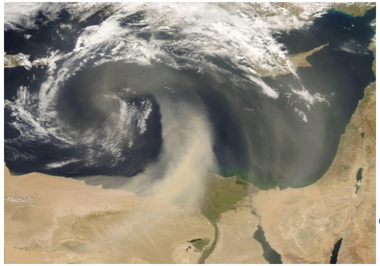
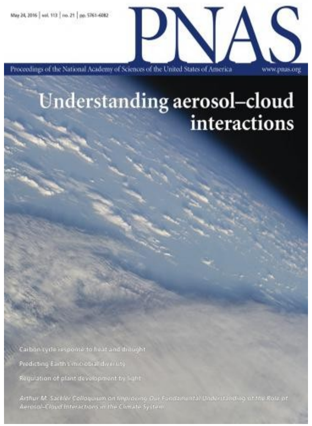
Outline

- *Current status of ARL R2O transitioning*
  - *AQM*
  - *RRFS*
  - *GEFSv13*
- *Updates to Biogenic Emissions*
- *Developments in dust modeling*
- *Wildfire spread*
- *CATChem - Configurable Atmospheric Chemistry Component in the UFS*
- *NEXUS updates*
- *MELODIES-MONET: New Capabilities*

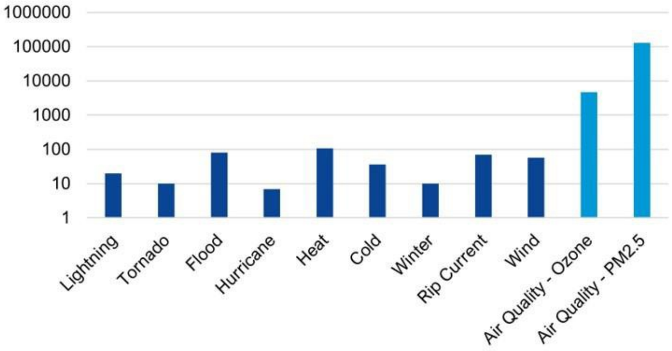
UFS Atmospheric Composition Modeling







Annual U.S. premature mortality



- Aerosols and trace gases alter the solar/terrestrial energy balance and cloud physics, affecting meteorology and climate on various timescales.
- Poor air quality has significant societal impacts, including degraded human health and visibility.
- NOAA has numerous legislative, interagency, and international mandates for its research and forecasts of atmospheric composition.

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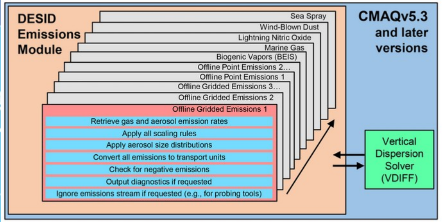
Preliminary Evaluation of Updated CMAQv5.4 in AQMv7 Ozone

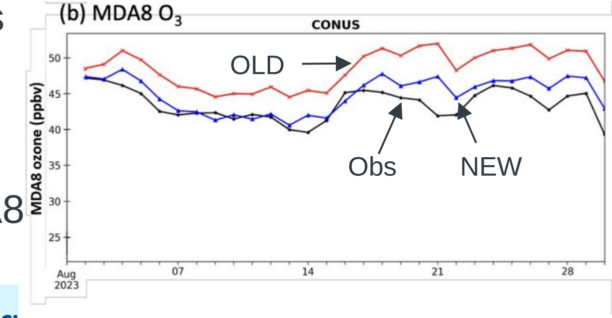


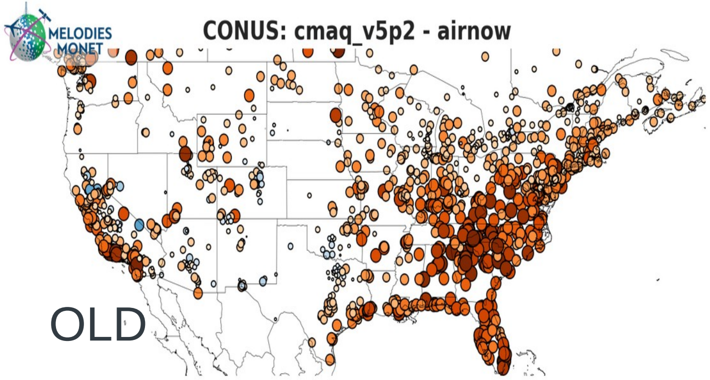
Inputs			DEP & Chem	Outputs
Environment variables		get_env_mod.f90 RUNTIME_VARS.F		
New namelists defined in aqm.rc		AE_cb6r5_ae7_aq.nml GC_cb6r5_ae7_aq.nml NR_cb6r5_ae7_aq.nml Species_Table_TR_0.nml CSQY_DATA_cb6r5_ae7_aq CMAQ_Control_DESID_cb6r5_ae7_aq.nml CMAQ_Control_DESID.nml CMAQ_Control_Misc.nml	VDIFF PHOT	O_3
Updated tables		field_table_aqm.FV3_GFS_v16 diag_table_aqm.FV3_GFS_v16	CLDPROC	ELMO controlled: PM25at PM25ac PM25co PM25 AOD
Meteorology		GRID_CRO_2D MET_CRO_2D MET_CRO_3D MET_DOT_3D OCEAN_1 LUFRAC (Gridded files are read through centralized IO & XTRACT3)	CHEM	
DESID controlled emission streams	Grid	GR_EMIS_001 (NEXUS)		Other species
	Point	STK_EMIS_001 (PT3D_FIRE) STK_EMIS_002 (PT3D_STKS)	AERO	
	Online	WB_DUST (Fengsha scheme) SEASPRAY		

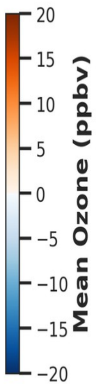
Summary of Changes

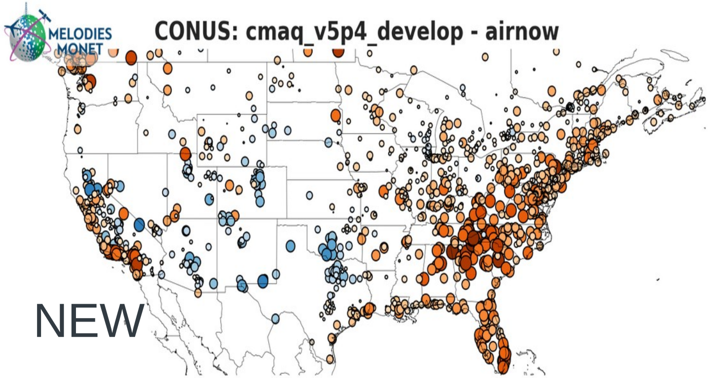
- New environment variable functions.
- New namelists, field and diag tables.
- Updated XTRACT3 function to use centralized IO
- Streamline emission sources for DESID module
- PM2.5 fraction and AOD are controlled through ELMO

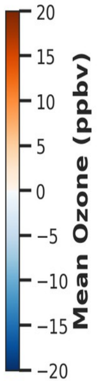
Large improvements in O3 forecasting, with improvements spatially and decreasing the MDA8 O3 bias drastically





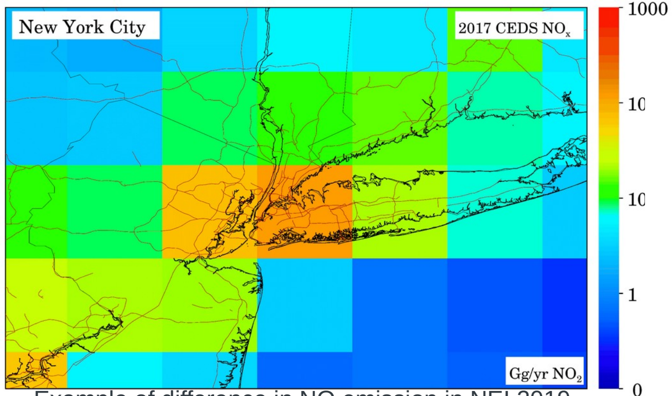






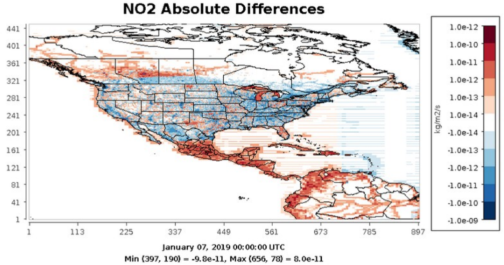
Updates to Emissions -> NEI Updates, New Diurnal Profiles, HTAPv3

NEMO High Resolution 1 km Emissions for 2019

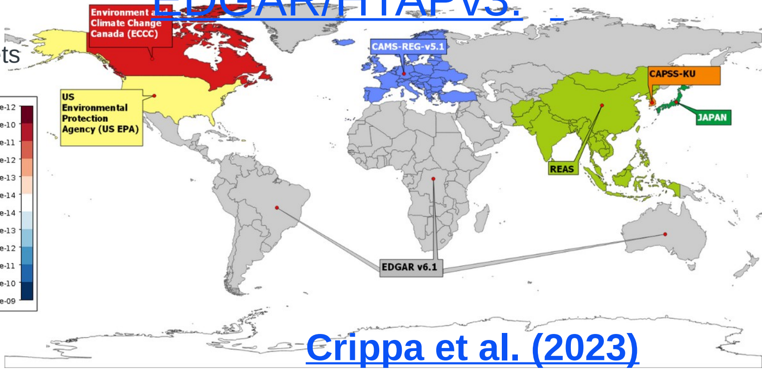


Example of difference in NO emission in NEI 2019

Applying Diurnal Profile to global datasets



[EDGAR/HTAPv3:](#)



[Crippa et al. (2023)](#)

January 5: Total NO Emissions differences (mt)

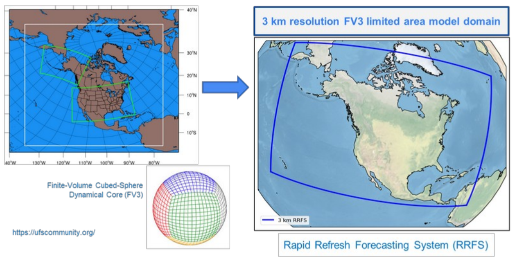
	Current (mt)	Updated (mt)	Percent Difference (%)
East	431	276	-36
West	192	114	-40
CONUS	624	390	-37

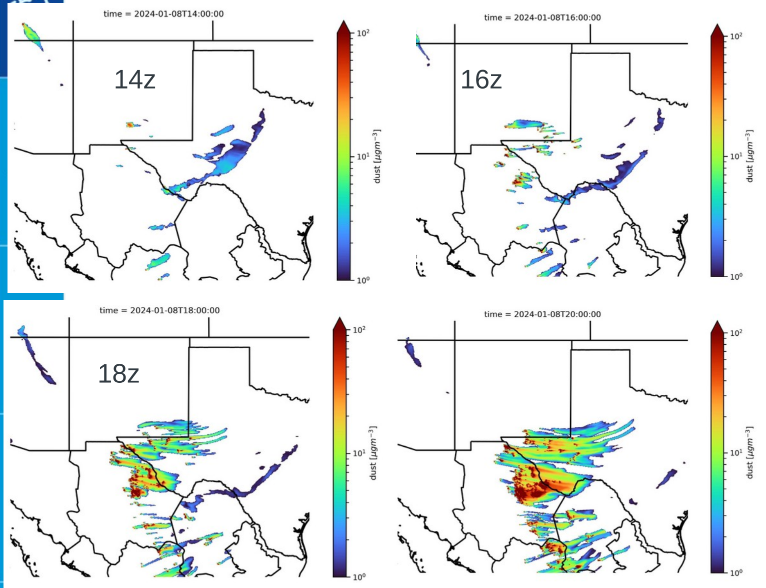
- NEI2016v1 → GMU/NEMO NEI2019 (Inside CONUS only)
- HTAPv2 2010 → HTAPv3 2018 (Outside CONUS)
- Global No Diurnal for major gas emissions → CAMS-TEMPO gridded weights (outside CONUS)

- HTAPv3 extends temporal coverage, sectoral breakdown and geographical coverage.
- Global mosaic of monthly air pollutant (SO2, NOx, CO, NMVOCs, NH3, **PM10, PM2.5**, BC, OC) emission gridmaps at 0.1x0.1 degree resolution.
- **Updates HTAP emissions from v2 (2010) -> v3 (2018)**

Rapid Refresh Forecast Model with Smoke and Dust

Transitioning of the RAP/HRRR-Smoke models to the FV3 dynamical core

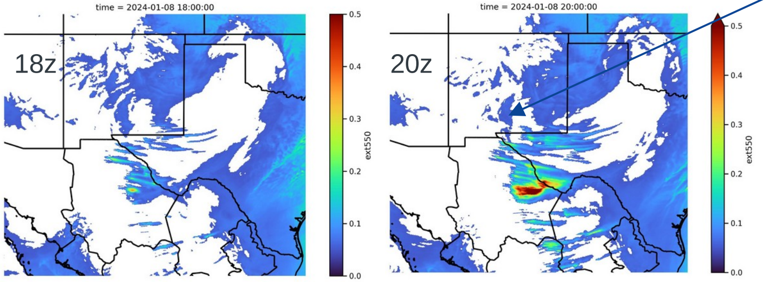




January 8th 2024

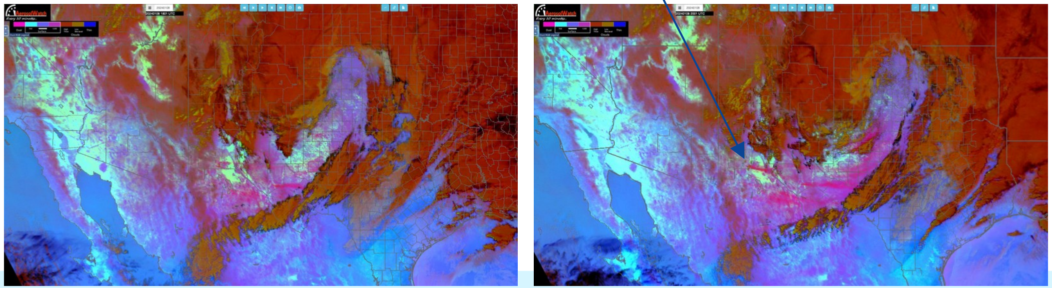
- Storm front pushed dust up over the Chihuahuan Desert blowing over multiple US Cities including El Paso and Odessa TX
- Overall the RRFS-SD system captured this event well
- Though a notable miss from southern NM which was responsible for the elevated PM in El Paso

RRFS-SD AOD 550nm



GOES DUST RGB

18z 20z

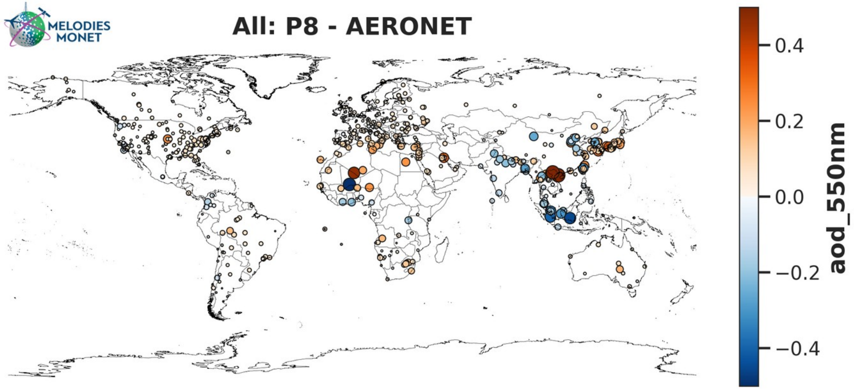


UFS-Aerosols: GEFSv13

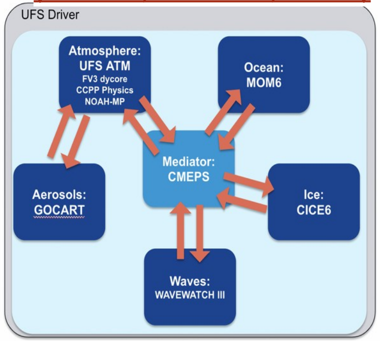
One NOAA Unified Forecast System (UFS) modeling applications currently in development is a coupled model for global predictions of weather to seasonal time scales, targeting NOAA/NCEP operational Medium Range (GFS v17), Subseasonal (GEFS v13), and Seasonal (SFSv1) forecasting systems.

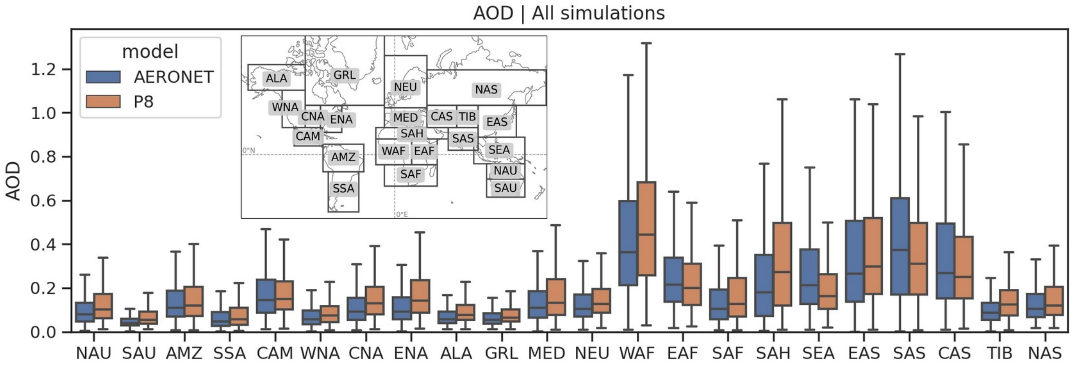
In the Global Coupled UFS development phase, discrete system prototypes were defined and evaluated within a fixed benchmark framework. Evaluation findings were used to inform subsequent development.

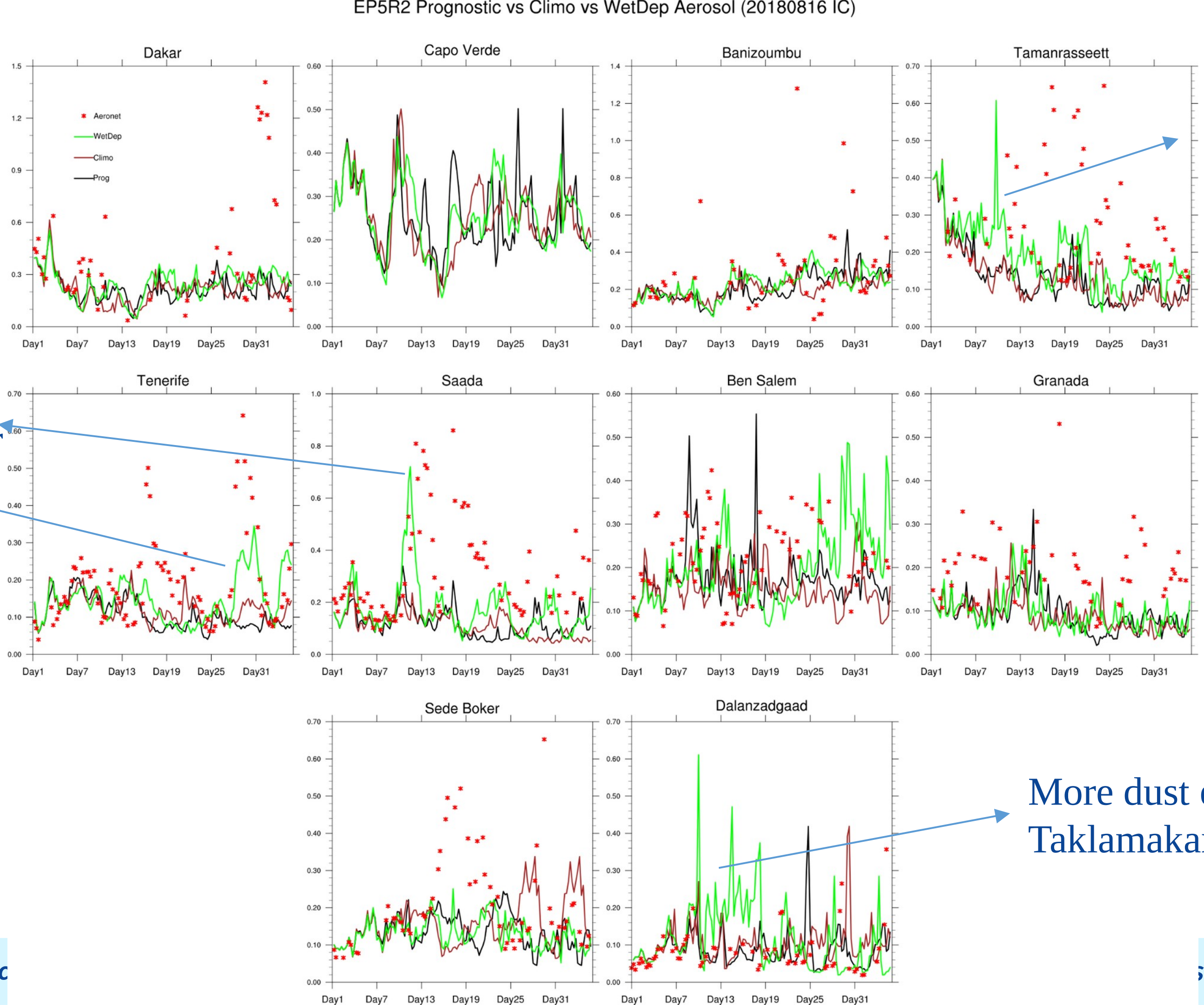
Prototype 8 (P8) is the last of these prototypes before tailored development for GFSv17/GEFSv13/SFSv1



Target configuration
(GFSv17, GEFSv13, SFSv1)





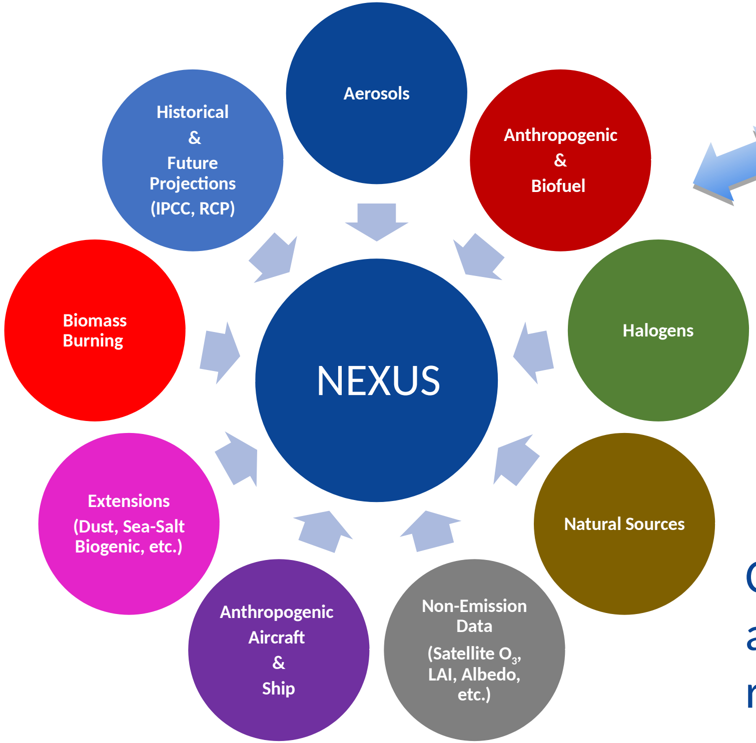


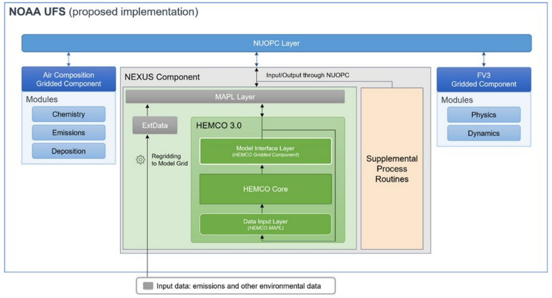
Improvement in dust emission over Sahara

Improvement in dust emission over Sahara

More dust emission from Taklamakan desert

NOAA Emissions and eXchange Unified System (NEXUS)





Barry Baker,
Patrick Campbell,
Daniel Tong and
Zach Moon (ARL)

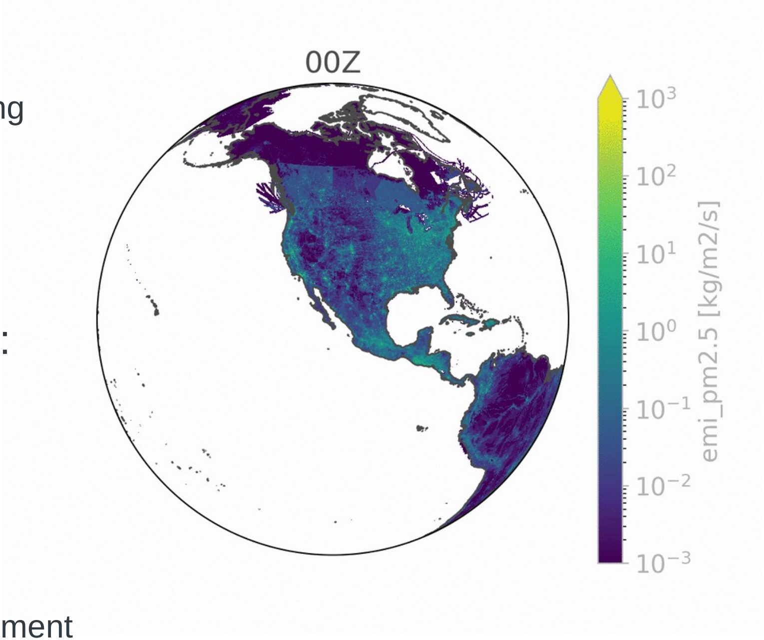
Community emissions processing system for UFS atmospheric composition models (both global and regional)- **Based on HEMCO (Lin et al. 2021)**

Collaborators: Harvard, NASA, NCAR

Lin et al. https://doi.org/10.5194/gmd-14-5487-2021

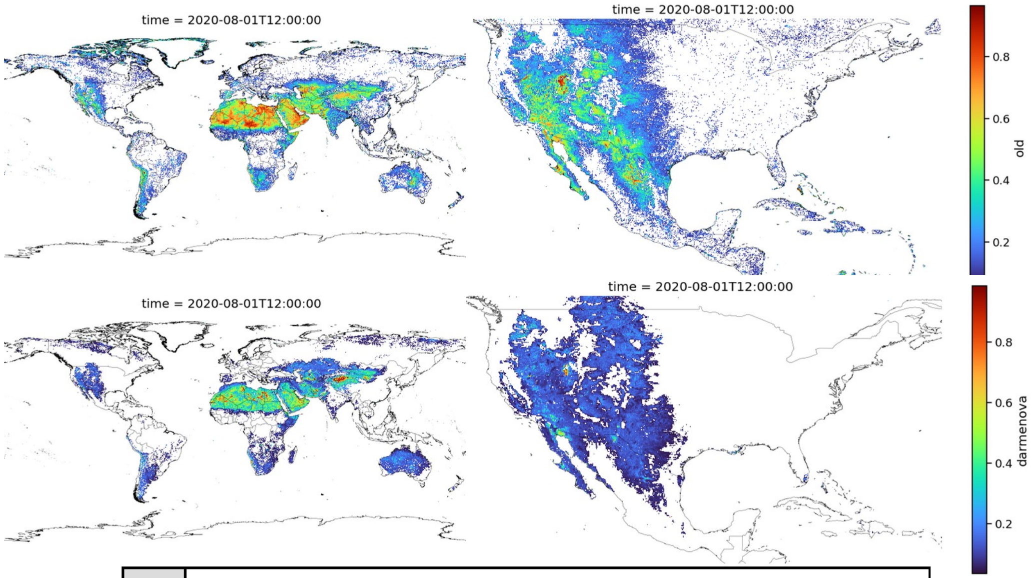
Future of NEXUS for the UFS-AQM and Beyond

- Initial NUOPC driver for standalone NEXUS has been created
  - Will replace the current standalone NEXUS
- Next steps:
  - (one-way) coupling to CDEPS via NUOPC
    - Data atmosphere will enable research and testing of long NEXUS simulations with emissions that depend on environmental parameters
  - two-way coupling to UFS-AQM via NUOPC
    - Ideal, science-wise
- Alternate biogenic emissions options in development:
  - (Current is HEMCO's MEGAN2.1 implementation)
  - Silva et al. (2020) (reduced-complexity "surrogate" version of MEGAN3)
  - Canopy-App Leaf-Scale BVOCs
- NEXUS-specific continuous integration in place
  - Currently only tests build, small-domain test cases in development



Dust Drag Partition development

Following [Marticorena et al. 2004](#) and [Laurent et al](#) a new drag partition is developed using VIIRS/MODIS for use in dust modeling. It combines the benefits of possible NRT satellite data with land surface model parameters (GVF/LAI) for inclusion into GEFS/RRFS-SD/AQM



1b — ***Drag partition correction R(λ)***

Double drag partition

$$R(\lambda) = \left(1-\sigma_V m_V \lambda_V\right)^{-0.5}\left(1+m_V \beta_V \lambda_V\right)^{-0.5}\left(1-\sigma_B m_B \frac{\lambda_B}{1-A_v}\right)^{-0.5}\left(1+m_B \beta_B \frac{\lambda_B}{1-A_v}\right)^{-0.5}$$

$\sigma_B = 1;\ m_B = 0.5;\ \beta_B = 90$ $\quad$ $\beta_v = 202;\ m_v = 0.16;\ \sigma_v = 1.45$

Required parameters: ***Roughness density***

Bare surface:

Option 1: $\lambda_B = \eta f_c$

Option 2: Marticorena et al. 2006

Vegetated surface:

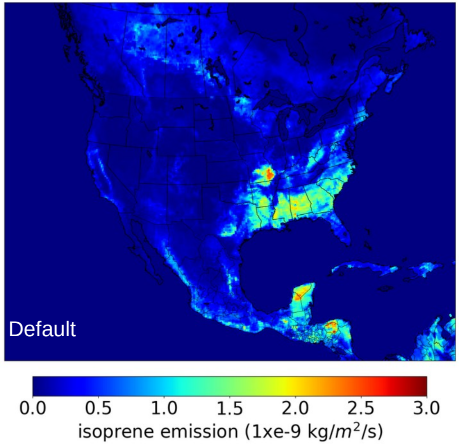
Option 1: $\lambda_v = -C_\lambda \ln(1-A_V)$

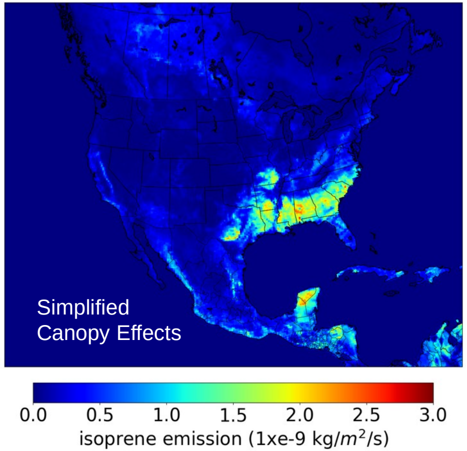
Option 2: $\lambda_v = Ae^{(a+b\times NDVI)}$

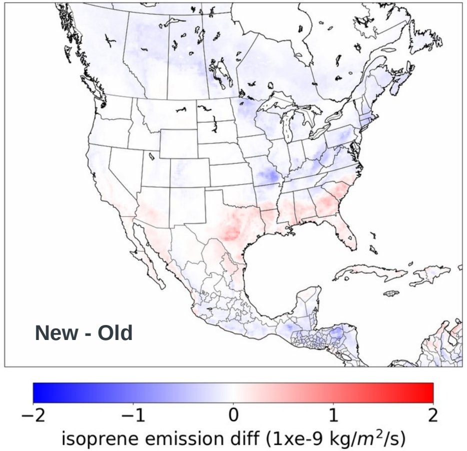
Improving the Biogenic Emissions for AQM and GEFS

With the decrease of anthropogenic emissions year after year biogenic emissions are becoming a larger source for ozone formation in comparison.

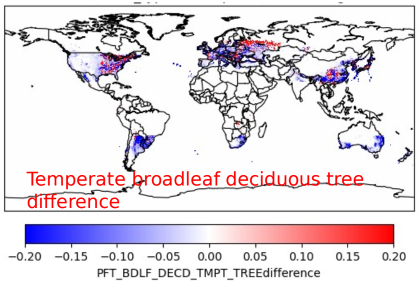
- Biogenic emissions are modified in AQMv7 from BEIS -> MEGANv2.1
- Update MEGANv2.1 with simplified canopy effects following [Silva et al. (2020)]
- New Canopy effects improves ozone distributions
- New canopy effects isoprene emissions with increased ISOP in the southeast US while decreases in the northern part of the domain

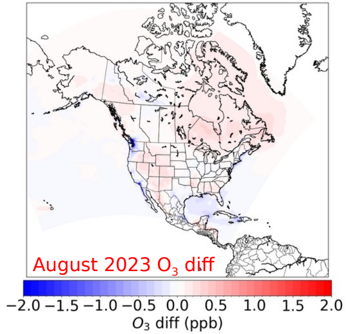


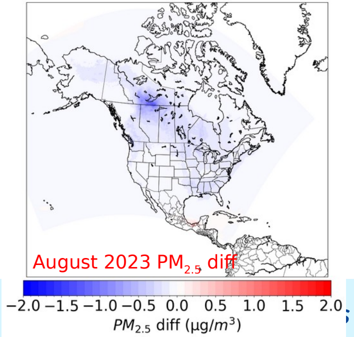




Improving the Biogenic Emissions for AQM and GEFS







Currently the plant functional types (PFTs) are static in MEGANv2.1 within NEXUS. This discounts land use change and so following Chen et al. (2022) using the IGBP class satellite observations and historical climate regimes.

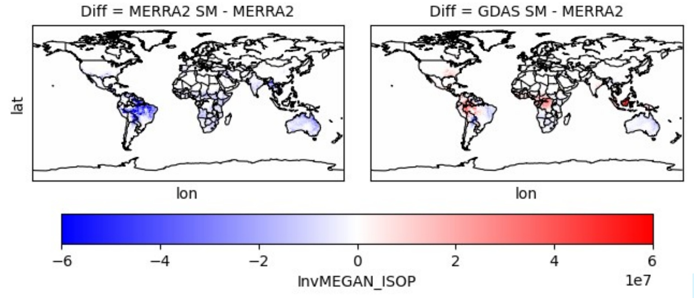
- PFTs have changed since 2001
- Minimal differences in ISOP but more differences in other species (APIN etc).
- New PFT method allows dynamic response and higher integration with UFS land models.
- Further research to better integrate with the land models including further integrating soil moisture vs GWETROOT

Preliminary forest-type PFT	Subdivided forest-type PFT	Climate rules
Broadleaf evergreen tree	Broadleaf evergreen tree, tropical	$T_c > 15.5°C$
Broadleaf evergreen tree	Broadleaf evergreen tree, temperate	$T_c \leq 15.5°C$
Broadleaf deciduous tree	Broadleaf deciduous tree, tropical	$T_c > 15.5°C$
Broadleaf deciduous tree	Broadleaf deciduous tree, temperate	$-15°C < T_c \leq 15.5°C$ and $GDD > 1200$
Broadleaf deciduous tree	Broadleaf deciduous tree, boreal	$T_c \leq -15°C$ or $GDD \leq 600$
Needleleaf evergreen tree	Needleleaf evergreen tree, temperate	$T_c > -19°C$ and $GDD > 600$
Needleleaf evergreen tree	Needleleaf evergreen tree, boreal	$T_c \leq -19°C$ or $GDD \leq 600$
Needleleaf deciduous tree	Needleleaf deciduous tree	None
Shrub	Broadleaf evergreen shrub, temperate	$T_c > -19°C$ and $GDD > 600$ and $P_{ann} > 520$ mm and $P_{win} > 2/3\ P_{ann}$
Shrub	Broadleaf deciduous shrub, temperate	$T_c > -19°C$ and $GDD > 600$ and ($P_{ann} \leq 520$ mm or $P_{win} \leq 2/3\ P_{ann}$)
Shrub	Broadleaf deciduous shrub, boreal	$T_c \leq -19°C$ or $GDD \leq 600$

Table 3. Subdivision rules for forest-type PFTs.

Preliminary grassland-type PFT	Subdivided grassland-type PFT	Climate rules
Grassland	C3 grass, arctic	$GDD < 400$
Grassland	C3 grass	$GDD \geq 400$ and ($T_w \leq 22°C$ or six months $P_{mon} \leq 25$ mm and for month $T_{mon} > 22°C$)
Grassland	C4 grass	$GDD \geq 400$ and $T_c \geq 22°C$ and driest month $P_{mon} > 25$ mm
Grassland	Mixed C3/C4 grass	Other grasslands that do not meet the above rules

Table 4. Subdivision rules for grassland-type PFT.



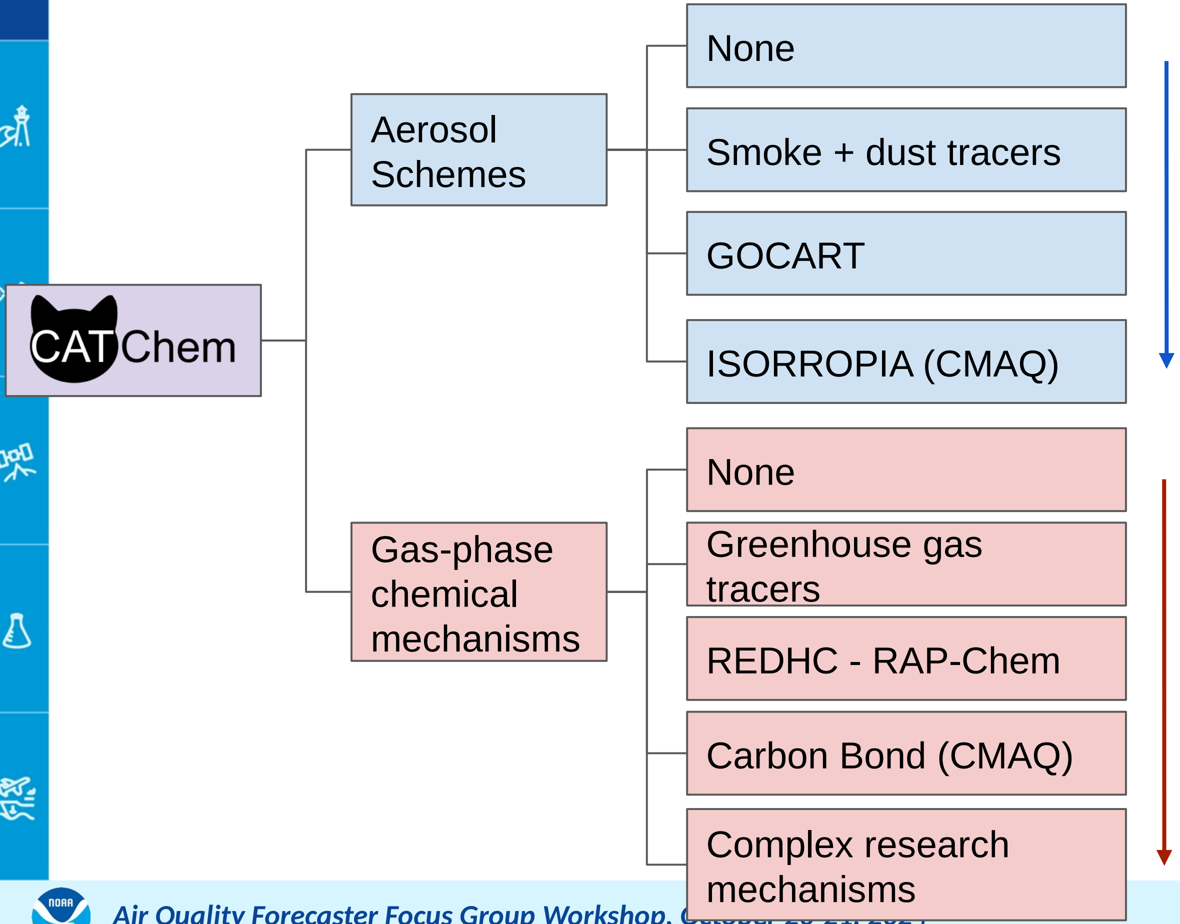
Current Structure of the UFS for Atmospheric Chemistry and Composition

Model	Chemistry Available	Application
RRFS-Smoke/Dust	Simplified Aerosols: Smoke + Dust tracers	Regional Wildfire Smoke Forecasts
UFS-Aerosols	Simplified Aerosols: GOCART	Global Weather Forecasts with aerosol feedbacks
UFS-AQM	Complex chemistry from CMAQ: Ozone and Aerosols	Regional Air Quality Forecasts
UFS-RAQMS	Simplified chemistry with data assimilation: Ozone and Aerosols	Global air quality forecasts

Problems:

- Chemistry-related code is duplicated across the UFS, which is not unified and time intensive to maintain
- The reliance on multiple externally developed models also limits expertise within NOAA
- We would like to add research capabilities for atmospheric composition and chemistry, but it is unclear how to do this with chemistry divided across so many models/applications

Development of CATChem

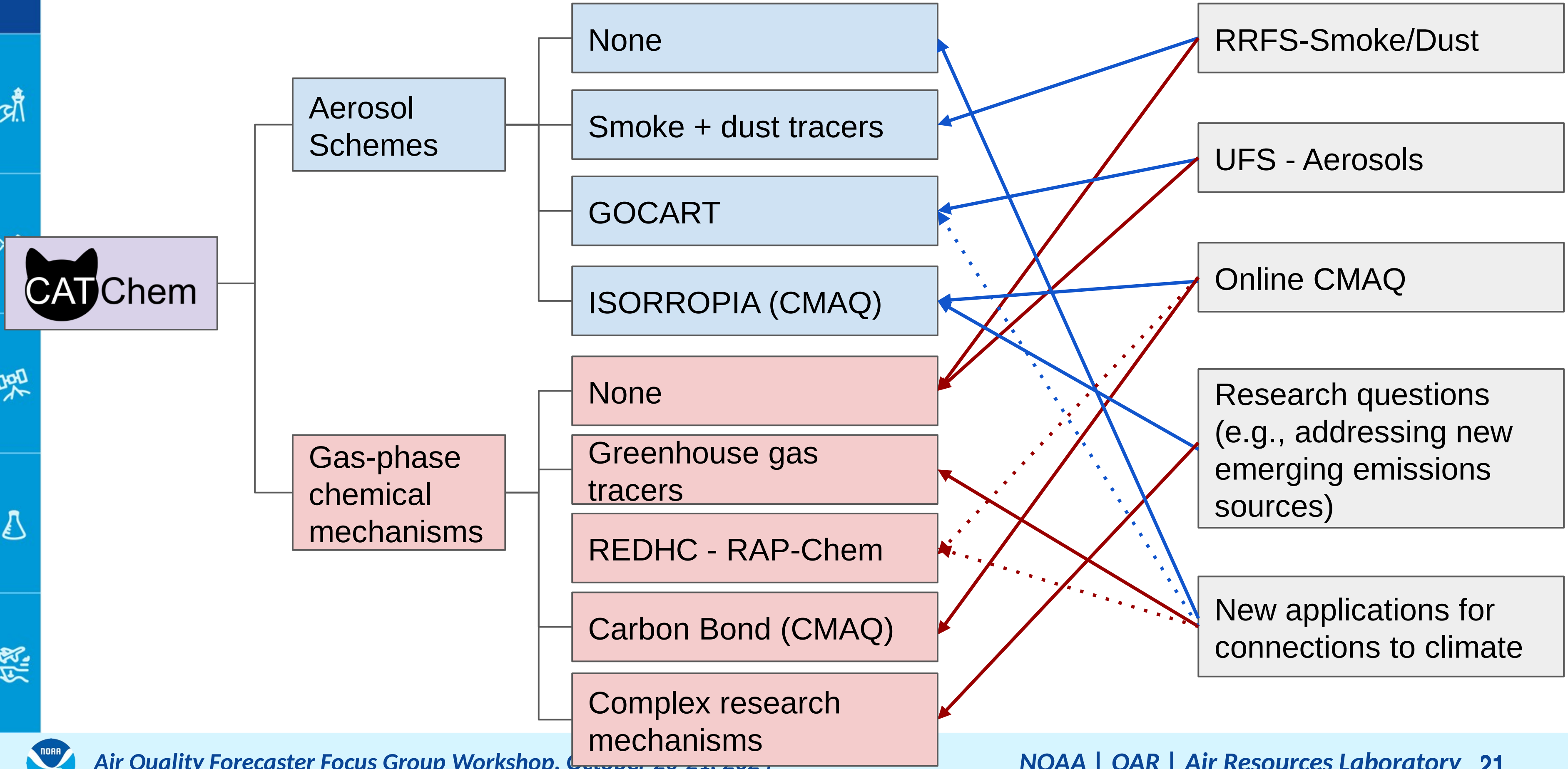


Increasing complexity & computational cost

UFS-Chem will be flexible and configurable where users can choose the aerosol scheme and the gas-phase chemical mechanism of the right complexity for their desired application or science question

Increasing complexity & computational cost

Options to use gas & aerosol chemistry of varying complexity



- MELODIES MONET is the model diagnostic/evaluation tool that uses the functionality already developed in [MONETIO](#) for reading in model/observation data and in [MONET](#) for analysis and plotting to quickly generate hundreds of plots and statistics through a easy to use interface
- Source code is publicly available:

  https://github.com/noaa-oar-arl/monet

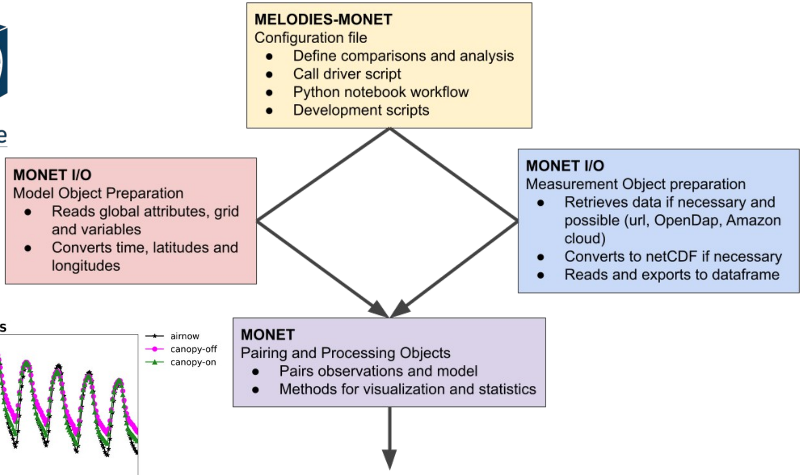
  https://github.com/noaa-oar-arl/monetio

  https://github.com/noaa-csl/melodies-monet
- User guide is on ReadTheDocs:

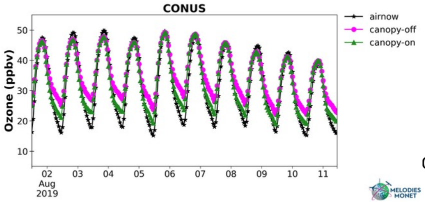
  https://monet-arl.readthedocs.io

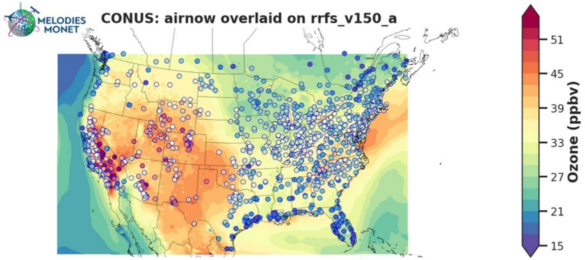
  https://monetio.readthedocs.io

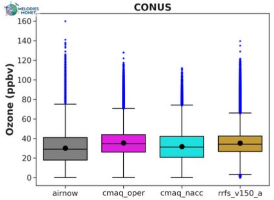
  https://melodies-monet.readthedocs.io

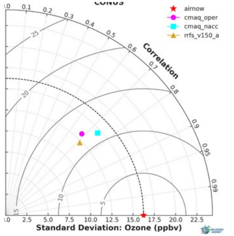


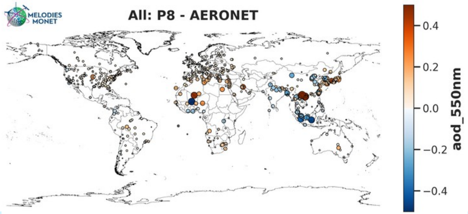
Capabilities to produce hundreds of plots for quick diagnostic assessments while also being flexible enough to produce publication quality plots

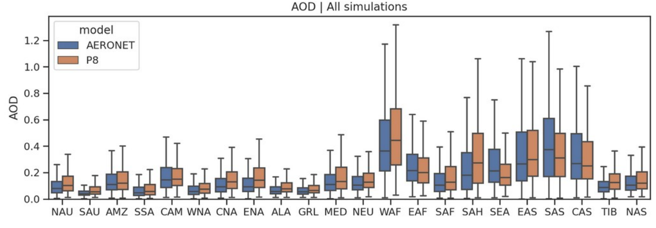






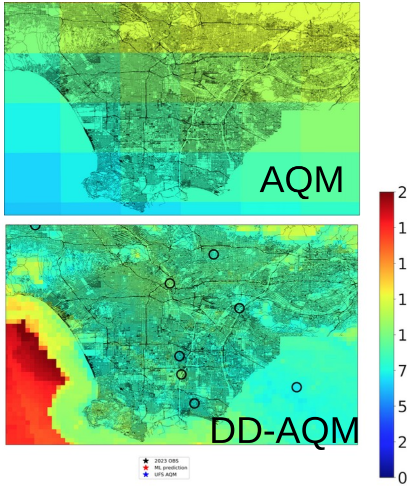


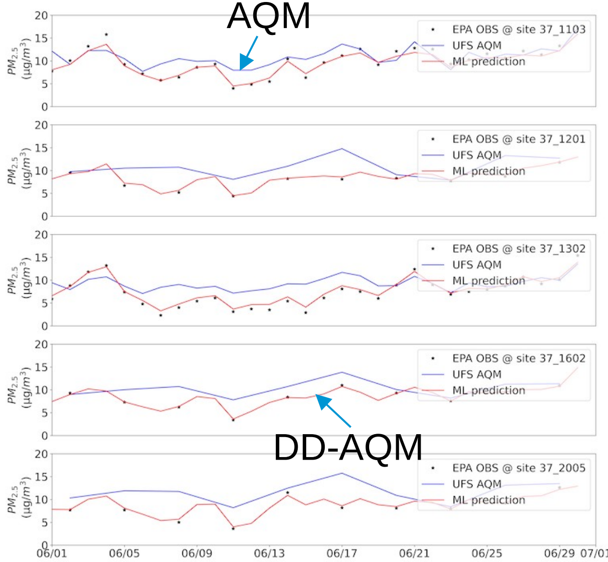


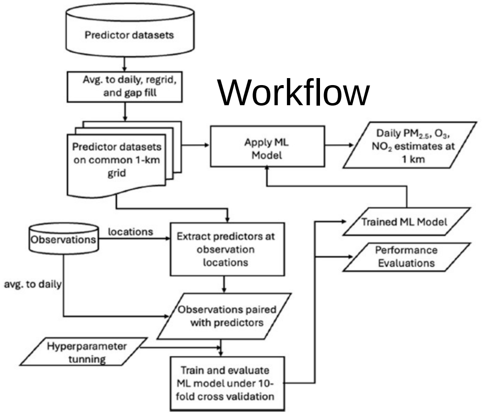


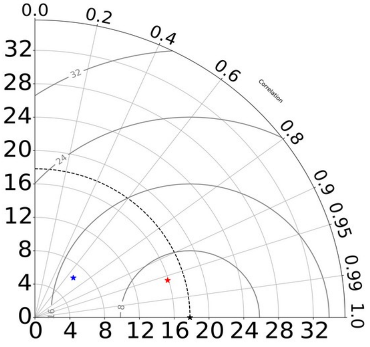
Dynamic Downscaling of UFS-AQM

We constantly hear that AQM is not high enough resolution but the model itself is extremely expensive and so we need to develop ways to create higher resolution forecasts in a timely manor. To do this we follow Tang et al. (2024). Preliminary results are showing impressive results but currently in a “reanalysis mode” not “forecast” mode





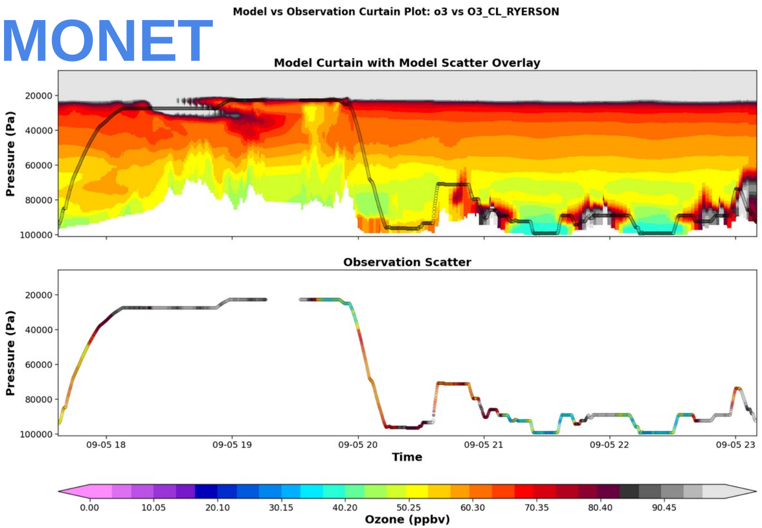




PM2.5	R	RMSE (µg/m³)	STD model (µg/m³)	STD obs (µg/m³)
ML model	0.96	5.03	15.84	17.82
Original UFS-AQM	0.68	15.32	6.48	17.82

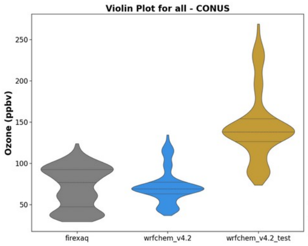
For more information see Tang et al. (2024) https://dc/10.1016/j.atmosenv.2024.120603

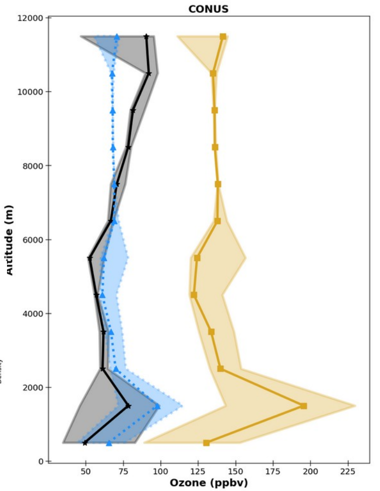
Adding new capabilities to Melodies-MONET



New Capabilities

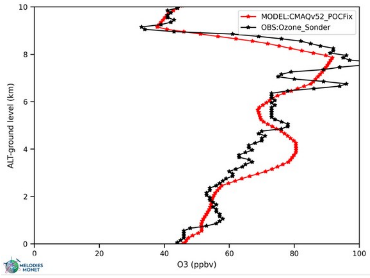
- Added capability to verify using aircraft data in MM
  - Curtain Plots
  - Vertical Profile Plotting
  - Violin Plots
  - Model vs Obs contour plots
- Added ability to do ozone sounder verification
  - Vertical plots
- Added the GEOMS reader to MONETIO to read Pandora and TOLNet data
- Added Methods to retrieve NESDIS VIIRS AOD/LAI/NDVI and AVHRR AOD
- Added NASA MODIS AOD
- Added TROPOMI





Future

- Adding TEMPO
- Support more NESDIS satellite observations
  - Expanded current GOES support in moneti in MM
- More vertical profiling including



08/29 @ Boulder, CO