

EMC, PSL,



# UFS-R2O Progress & Year 3 Plan Atmospheric Composition Development Cross Cutting Team

## 6&7 December 2021



UFS-R2O Project - Year 3 Review: Dec 6&7, 2021

https://vlab.noaa.gov/web/ufs-r2o/



### **Atmospheric Composition - Description and Goal**



**Project Scope:** Improved representation of aerosol distribution and initial inclusion of aerosol-radiation interactions on S2S timescales for GEFSv13

### Team:

- OAR/GSL: Grell, Sun, L Zhang\*, Montuoro\*, Pagowski\*, Huang\*
- OAR/ARL: <u>Saylor</u>, Baker\*, Campbell\*, Tong\*
- OAR/CSL: Frost, He\*, Wang\*, McKeen\*, Schwantes\*
- NESDIS/STAR: Kondragunta, X Zhang\*, Hughes\*
- NWS/NCEP/EMC: <u>Stajner</u>, Montuoro\*, Pan\*, McQueen, Bhattacharjee\*, Tangborn\*, Cheng\*, Martin\*

Subproject Leads, Subproject PI's, \*NOAA Affiliated Scientists

The UFS R2O Atmospheric Composition subproject team **builds on the strong collaboration that developed GEFS-Aerosols**, which has been producing 120-hr global aerosol forecasts 4 times per day operationally at NCEP since September 2020.





Milestones and Deliverables	End Date	Health
Model upgrades to produce a NUOPC-compliant coupled	06/30/22	On Track
atmosphere-aerosol application with aerosol-radiation interactions		
Global aerosol emissions processing system based on HEMCO for GEFS	06/30/22	On Track
v13		
Biomass burning emissions for S2S timescales for GEFS v13	06/30/22	At Risk
Quality control and bias correction procedures for AOD data	06/30/22	On Track
assimilation for GEFS v13		
Assist AOD data assimilation system development with focus on	06/30/22	On Track
improved representation of aerosol species and vertical profiles for		
GEFS v13		



### **Atmospheric Composition - Major Accomplishments (1)**



### Model infrastructure upgrades

- Developed UFS-Aerosols, a fully NUOPC-compliant coupled atmosphere-aerosol application in the UFS framework
- UFS-Aerosols uses latest version of NASA's GOCART aerosol model and integrates NASA's MAPL coupler
- Global CROW workflow was extended to include aerosols in UFS-Aerosols
- Successfully operating UFS-Aerosols on Orion, Hera and WCOSS
- Now testing, tuning and evaluating UFS-Aerosols in atmosphere-only and in Prototype simulations that couple UFS-Aerosols to atmosphere, ocean, sea ice and wave models

### **Aerosol-radiation interactions**

- Evaluated aerosol-radiation feedbacks with CCPP coupling of predictive aerosols to physics
- Identified and corrected errors in Unified Post-Processor calculation of aerosol optical depth (AOD), including in the currently operational GEFS-Aerosols runs
- Evaluated NASA look-up tables relating aerosol mass & speciation to optical properties
- Continuing evaluations of aerosol-radiation feedbacks at MRW/S2S scales with UFS-Aerosols



### **Atmospheric Composition - Major Accomplishments (2)**



### Emissions

- Updated, tuned and evaluated Fengsha dust scheme, an improved description of global dust sources that is not available in NASA's GOCART aerosol model
- Developed NEXUS anthropogenic emissions processing system based on HEMCO
- Updated anthropogenic emissions inventories to more recent years and evaluated them
- Prepared and evaluated biomass burning emissions for retrospective and real-time simulation periods at different grid resolutions

### Aerosol Data Assimilation (ADA)

- Compiled ADA error statistics for satellite AOD using AERONET remote sensing observations
- Evaluated ADA aerosol speciation and vertical profiles with unique aircraft field dataset
- Developing JEDI-based assimilation system for satellite AOD (through in-kind support)
- Included JEDI ADA in prototype workflow (through in-kind support)
- Compared skill of ADA to forecasts without ADA and NASA MERRA-2 reanalysis (through in-kind support)
- Implemented near-real-time ensemble-variational ADA (through in-kind support)

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## AC Results: Coupled Prognostic Aerosol Simulations (Leads: GSL, EMC, ARL)



### Coupled Prototype 7.1: FV3GFSv16 + MOM6 + CICE6 + WW3 + UFS-Aerosols Prognostic Aerosol Component

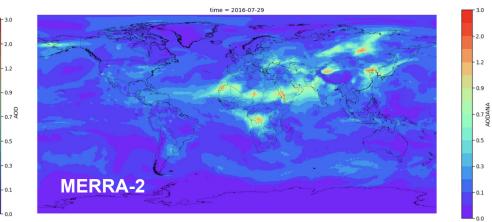
- GOCART aerosols from NASA repository, fully NUOPC compliant, in UFS authoritative repository
- Built through NOAA collaboration with NASA; extends MAPL infrastructure
- Initialize on: 1/1/13, 3/1/13, 7/1/13, 10/1/13, 1/1/16, 3/1/16, 5/1/16, 7/1/16, 10/1/16, 1/1/18, 3/1/18
- C384L127. Aerosol ICs = MERRA-2 reanalysis.
- 31-day integration free run (achievable within 8 hrs of wall clock time)
- Aerosol-radiation interactions not enabled currently, but will be after testing and tuning completed.

Results shown below compare **UFS-Aerosols free forecasts of AOD at week 4** (from 7/1/16 start) to MERRA-2 reanalysis.

- These are free runs, so some drift is expected relative to reanalysis.
- Nonetheless, predictive aerosol simulation looks remarkably similar to reanalysis. Tuning, which remains to be done, • will only improve these results.

- 0.9

UES





# AC Results: Aerosol-Radiation Interactions (Lead: GSL)

Coupled Prototype 6+: FV3GFSv16 + MOM6 + CICE6 + WW3 + CCPP-Aerosols Prognostic Aerosol Component

- Aerosols based on GEFS-Aerosol, with GOCART aerosol scheme coupled to physics via CCPP
- Carried out as part of <u>Working Group on Numerical</u> <u>Experimentation (WGNE)</u> S2S experiments
- Initialize on 1 May & 1 Sept, 2003-2019.
- C384L64. Aerosol ICs = 30-day no-cycling cold run with zero aerosol to start.
- 32-day integration free run (per WGNE protocol; P6+ CCPP-Aero can run ~2 months w/in 8 hrs wall clock time)
- Aerosol-radiation interactions enabled

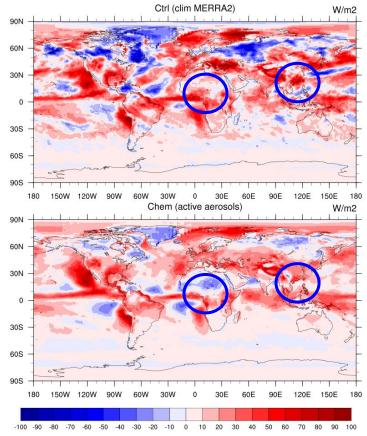
Results shown at right demonstrate the bias in mean downward surface shortwave flux relative to observations from NASA's Clouds and the Earth's Radiant Energy System (CERES) satellite.

- Top plot: Control run using NASA's MERRA-2 aerosol climatology
- Bottom plot: Chemistry run using CCPP-coupled predictive aerosols
- In blue circled areas with high aerosol loadings, warmer biases in the control runs are reduced in the chemistry runs

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# AC Results: Anthropogenic Emissions (Lead: ARL)



Results show decrease in bias over Eastern Asia with CEDS2019 (preliminary) versus CEDS2014 for Sep 2019 - Feb 2020.

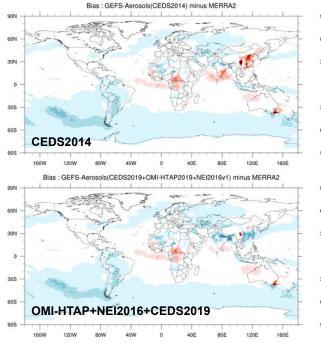
A parallel simulation using a combined emissions dataset of CEDS2019 (preliminary)+ OMI-HTAP + NEI2016 shows similar results.

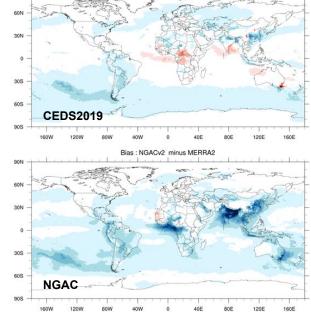
Increased correlation vs AERONET for SON and DJF.

# If results hold, a CEDS2019-based dataset could be recommended for use operationally in GEFS-Aerosol.

Analysis shows overall decrease in SO<sub>2</sub> emissions between CEDS2014 and CEDS2019, mainly in industrial, waste and shipping sectors.

#### Total AOD (550 nm) Day 1 Forecast Bias vs MERRA-2 12/1/19-2/29/20





Bias : GEFS-Aerosols(CEDS2019)

-0.45 -0.4 -0.35 -0.3 -0.25 -0.2 -0.15 -0.1 -0.05 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45



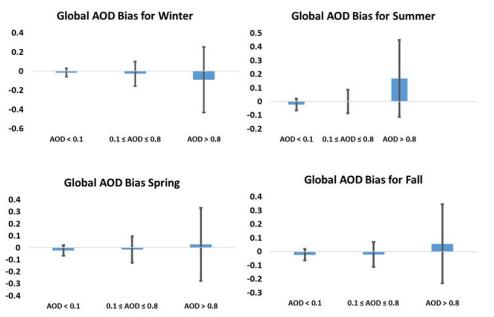
# AC Results: Error Statistics for Assimilation of Satellite AOD (Lead: STAR)



- Evaluation of Suomi NPP VIIRS aerosol optical depth (AOD) using 2017 – 2020 AERONET data as reference was completed.
- Bias and standard deviation of bias for three different AOD ranges (as required by JPSS Level 1 Requirements Document) were estimated. The sample size is large enough for the estimates to be statistically valid.
- Powerpoint slides with tables for different regions was provided to the DA team via email. At right is example of the global AOD biases for different seasons.



Bias and standard deviation of bias for the globe and several different regions of the globe (East CONUS, West CONUS, South America, Europe, Central Africa, South Africa, India, and China) were computed using a network of sun photometers (NASA AERONET data).

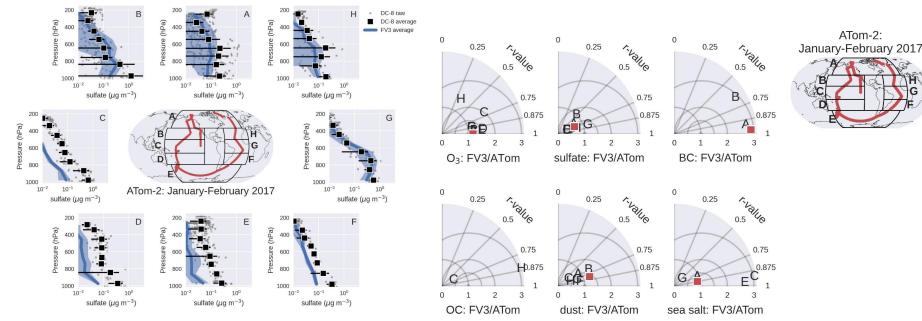




## **AC Results: Evaluations with Aircraft Aerosol Data** (Lead: CSL)



ATom-2:



Observations of aerosol speciation and vertical profiles were collected by aircraft in the

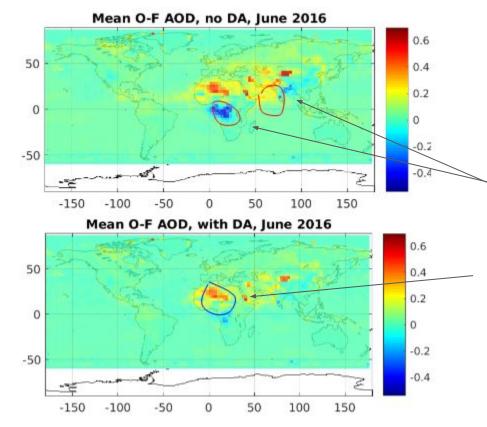
Atmospheric Tomography (ATom) campaign in 2016 -2018.

The same evaluation and statistical analysis is available for all four ATom deployments (ATom-1 thru ATom-4). These evaluations will be critical information for aerosol data assimilation efforts.



# AC Results: Assimilation of Aerosol Optical Depth (Lead: EMC)





# EMC assimilated aerosol optical depth (AOD) for June 2016:

One month data assimilation (DA) cycling experiment is compared to control model run (without DA). DA reduces biases in the system.

Assimilation of MODIS AOD observations reduces forecast overestimates in Western Africa and underestimates in the Arabian Sea (red circled regions in upper plot).

AOD underestimation in Northern Africa shows a smaller reduction (blue circle), likely due to higher observation errors over high albedo desert regions. This is an area of current research focus.

The time period chosen is a spinup to the first ATom deployment in July-August 2016 to coordinate DA system evaluation with speciated vertically resolved ATom data.

## AC Results: Global Aerosol Data Assimilation System (Lead: GSL)

NASA's MERRA-2

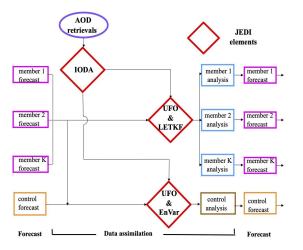
135\*W 90\*W

AOD MERRA2 Reana

# **UFSR20**

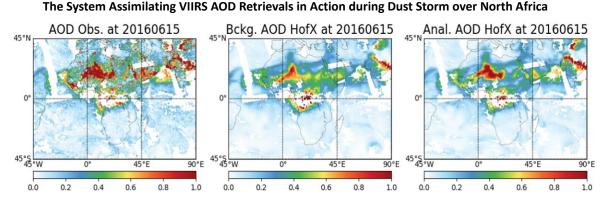
## JEDI-based system imbedded in a workflow for real-time application and reanalysis

- Observations: satellite retrievals of 550-nm Aerosol Optical Depth;
- Model: GEFS-Aerosol;
- Assimilation: Hybrid Variational Ensemble Kalman Filter.

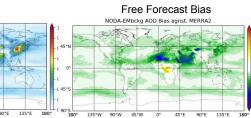


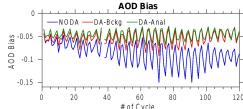
- AOD: Aerosol Optical Depth;
- JEDI: Joint Effort for Data assimilation Integration;
- IODA: Interface for Observation Data Access;
- UFO: Unified Forward Operator;
- LETKF: Local Ensemble Transform Kalman Filter;
- EnVar: Ensemble-Variational solver.

#### NWS/OSTI & OAR/WPO: NGGPS - HFIP - Week 3&4 - JTTI - EPIC

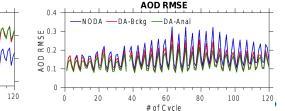


#### **Evaluation Statistics for June 2016**





#### Reanalysis Bias ENVAR-Cbckg AOD Bias agnst. MFRRA2 0.60 - 0.45 0.45 0.30 0.30 0.15 0.15 0.00 0.00 -0.15 -0.15 -0.30 -0.30 -0.45 -0.45 135°W 90°W 45\*W 45°E 90°F 135°E 180





### **Atmospheric Composition - Major Challenges**



- Upgrades to Physics components require close attention from the AC subproject, given the tight coupling between aerosols and physics.
- More work lies ahead to seamlessly blend biomass burning predictions with climatological descriptions of fire emissions.
- Numerous issues with aerosol DA require additional effort, including:
  - Adequately translating AOD, a single integrated quantity, into credible adjustments to speciated aerosol spatial distributions;
  - Accurately relating the forward AOD operator to modeled aerosol properties.
- Additional compute resources have been needed throughout the project. Orion should help to ease this burden, although instabilities in Orion are currently causing difficulties.
- Need to improve computational performance of UFS-Aerosols in coupled prototype simulations in order to consistently complete 35-day simulations within 8 hrs of wall clock time. Solving instability issues on Orion and assigning more nodes to atmosphere calculation should help solve this challenge.
- Workflow complexity made upgrades to include aerosols difficult and time consuming.
- Most aerosol DA work was carried out through in-kind support. We are seeking direct support for ADA efforts in Year 3.

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### **Atmospheric Composition - Work Plan for Year 3**



Tasks	Lead FMCs	Dependencies	Impact if not funded
Test and evaluate aerosol	GSL, EMC	Physics,	Inconsistent approach to direct and
coupling with radiation and		Infrastructure	indirect aerosol impacts on meteorology
microphysics			
Enhance accuracy and timeliness	ARL, GSL, STAR	Physics, Marine,	Unrealistic simulations of aerosol
of aerosol and precursor		Infrastructure	distributions and aerosol impacts on
emissions and distributions			meteorology
Atmospheric composition model	EMC, CSL, ARL	Verification &	Inability to demonstrate improved
integration, testing and		Post-Processing,	performance of predictive aerosols
evaluation		Infrastructure	
Advance AOD assimilation	EMC, GSL,	Data Assimilation,	Unrealistic simulations of aerosol
	JCSDA	Infrastructure	distributions and impacts on meteorology
Develop RRFS-CMAQ	EMC, ARL, GSL,	DSUP, FY22 WSUP	Inconsistent global and regional
development for RRFSv2	CSL, PSL	projects	approaches to atmospheric composition
Prepare for constraints of aerosol	CSL, EMC, ARL	Data availability	Unrealized opportunities for evaluation
and trace gas distributions from			and improvement of UFS Atmospheric
additional satellite data			Composition component



### **Atmospheric Composition - Compute Requirements**



- Hera: at least 500K core hours
- Orion: 1M core hours
- WCOSS: at least 500K core hours



### **Atmospheric Composition: Possible in-kind efforts**



- FY19 Disaster Supplement WF-1, WF-2, WF-3
- FY22 Wildfire Supplemental
- WPO JTTI proposals
- OSTI FY22 proposals?



### **Atmospheric Composition - Summary & Closing Remarks**



- Atmospheric Composition (AC) is a fundamental part of the Earth System. Atmospheric composition prediction should be included in UFS forecasts at all scales.
- Prognostic aerosols are now included in fully coupled UFS R2O MRW/S2S simulations, a key goal of the AC subproject that could lead to a major advance in NOAA's operational predictions.
- The AC subproject's work builds on existing strong collaborations and evaluated model components that have demonstrated operational performance.
- The performance of the coupled model prognostic aerosol MRW/S2S forecasts relative to the use of aerosol climatologies is now being evaluated, in order to demonstrate the value of the additional expense to predict aerosol distributions and impacts.
- More discussion and extensive coordination is needed to understand how proposed new UFS-R2O project structure will advance global and regional UFS atmospheric composition development. UFS-R2O Project - Year 3 Review: Dec 6&7, 2021