NASA's High-Resolution GEOS Forecasting and Reanalysis Products: A unified Tool from Local to Global Scales

K. Emma Knowland

USRA/GESTAR

NASA Global Modeling and Assimilation Office (GMAO)

In collaboration with:

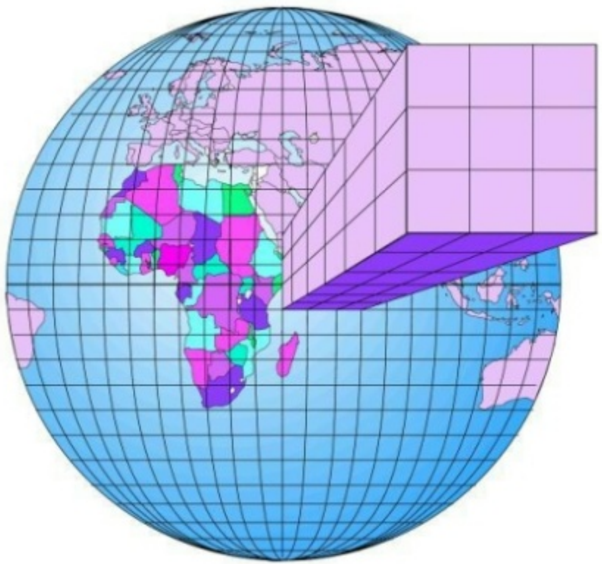
GMAO: Christoph Keller, Pamela Wales, Larry Coy, Kris Wargan, Lesley Ott, Steven Pawson

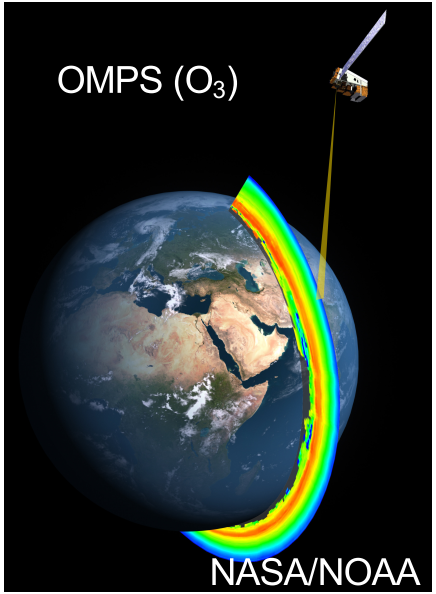
Atmospheric Chemistry and Dynamics Lab: Bryan Duncan, Sarah Strode, Junhua Liu, Julie Nicely, Dan Anderson, Eric Fleming

24 May 2021

NASA GMAO global meteorology and chemistry products

GEOS





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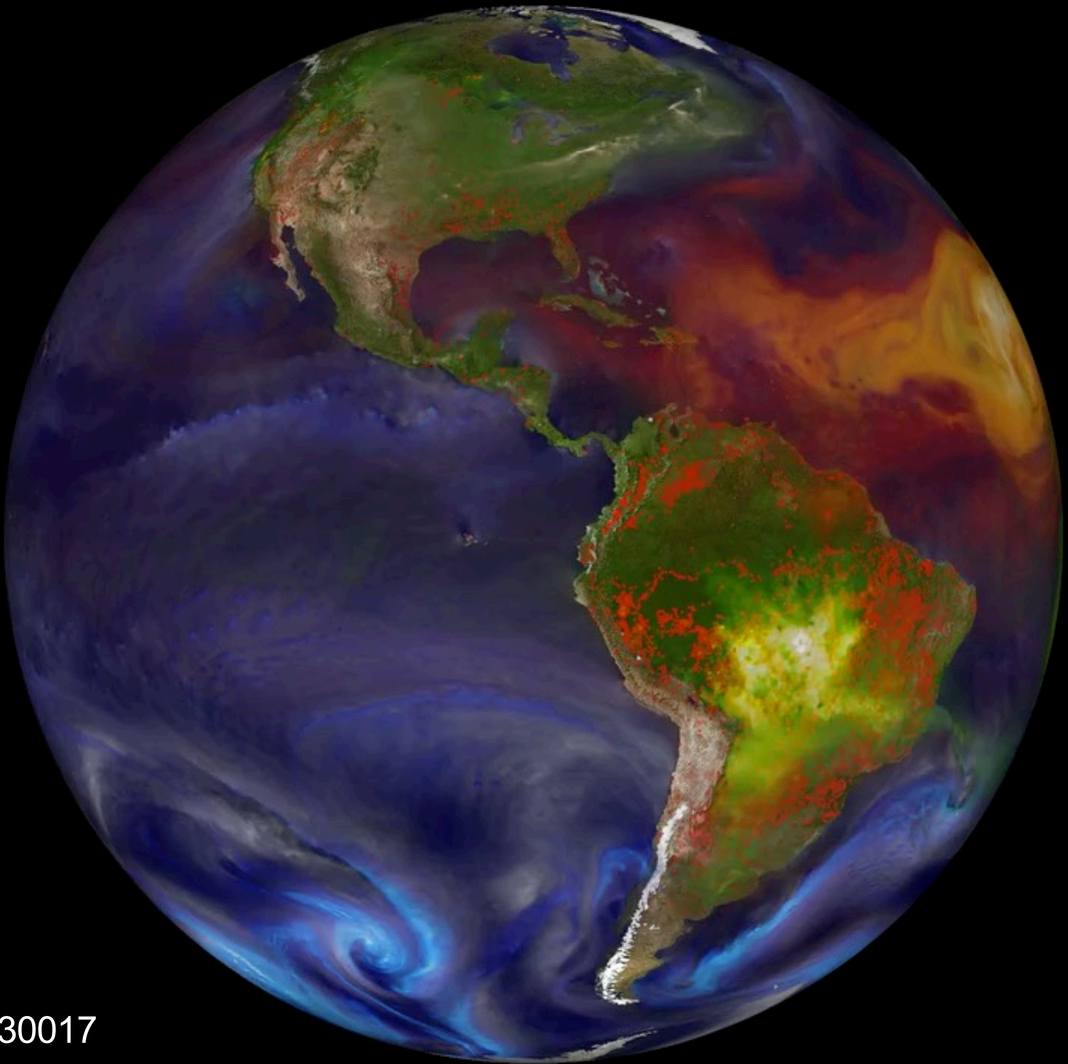
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov



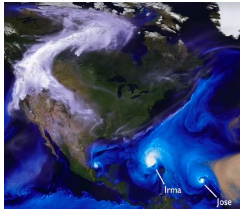
https://svs.gsfc.nasa.gov/30017

NASA GMAO global meteorology and chemistry products

GEOS

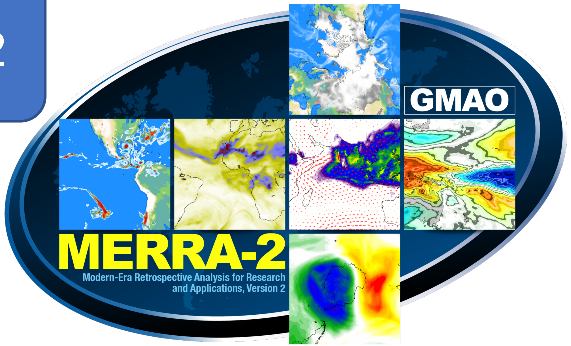
Forecasting

Reanalysis



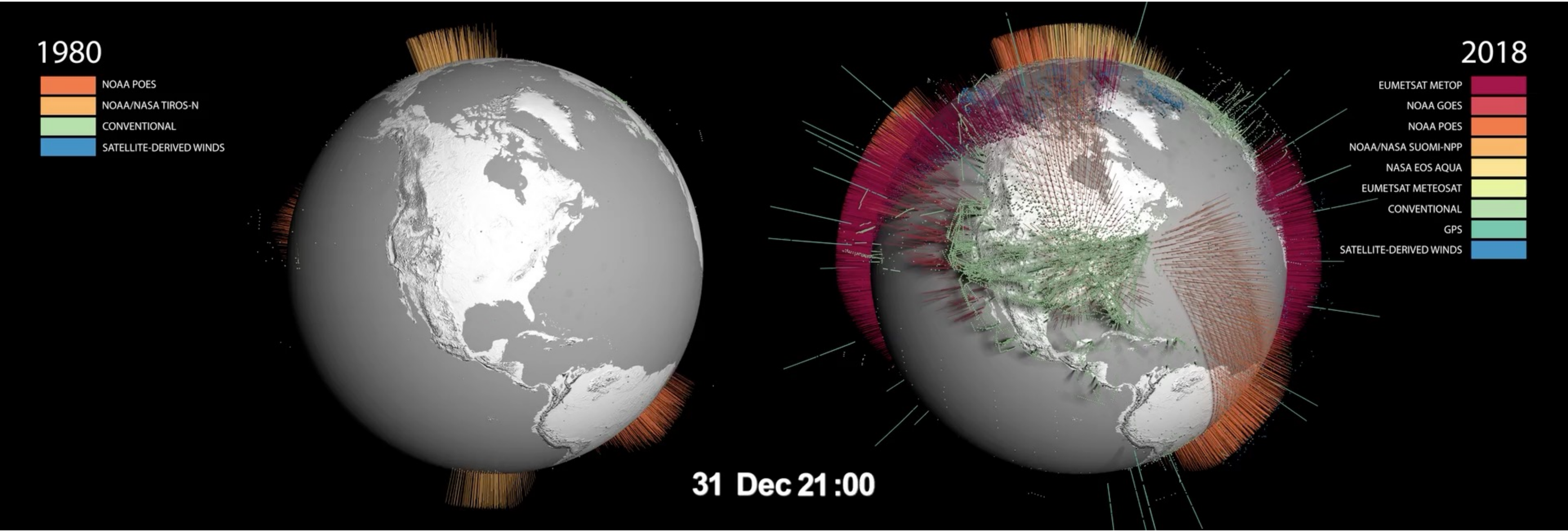
GEOS FP

MERRA-2



k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Changes to the observing system

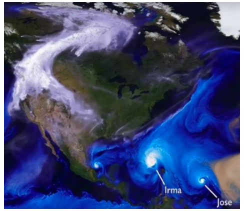


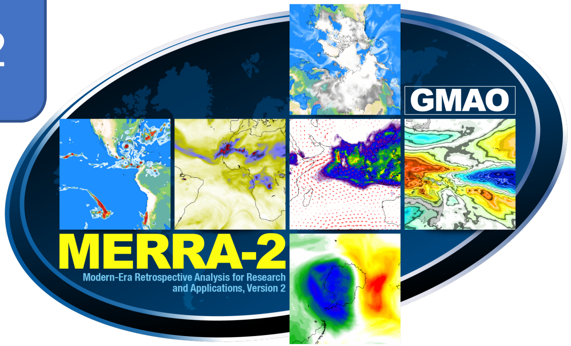
https://svs.gsfc.nasa.gov/4654

NASA GMAO global meteorology and chemistry products

GEOS

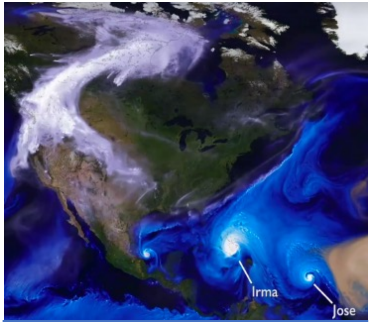
- Forecasting
  - GEOS FP
  - GEOS FP-IT
    - GEOS-CF
- Reanalysis
  - MERRA-2



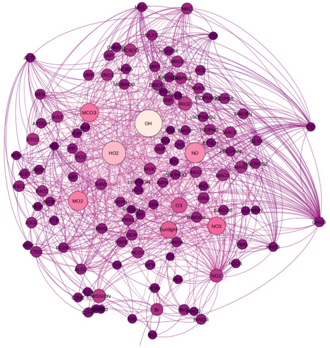


k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

GEOS Composition Forecast



GEOS NWP



GEOS-Chem

GEOS - CF

Version 12

Tropospheric and Stratospheric chemistry

- 250 Chemical Species
- 725 Chemical Reactions

https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

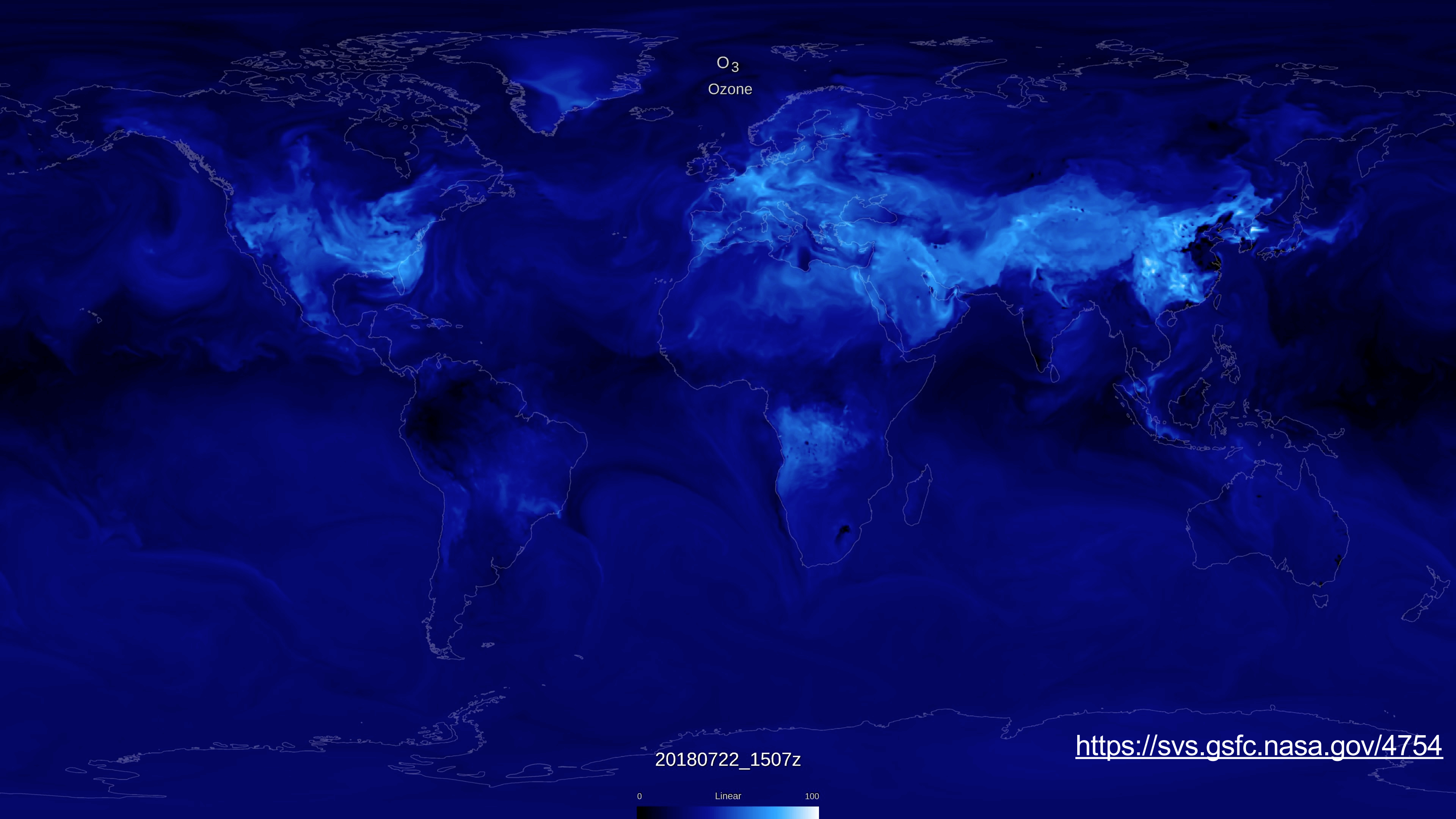
Summary of major GMAO products

System	Focus	Customers/Applications
GEOS-FP "weather prediction"	Impacts of NASA observations on NWP: forefront resolution and complexity	NASA Field Missions (weather, aerosols) Multiple Agencies: NOAA/FAA; NOAA field stations; NRL
GEOS-CF "air quality"	Pioneering global system for atmospheric composition using multiple NASA assets	Health/Air Quality studies (via NASA Applied Sciences) Multiple agencies: NIH, US Army Public Health Center, NOAA
GEOS-S2S "seasonal prediction"	Ensembles of coupled Earth System predictions, emphasizing NASA observations	National ensembles (NMME, SubX), drought/sea-ice prediction Multiple Agencies and international linkages
MERRA-2 "reanalysis"	Stable product for climate studies, emphasizing NASA data	Only current national reanalysis: USGCRP/NCA applications Interagency use: DoE, DoT, NOAA, …
GEOS-FPIT "mission support"	Stable, well validated, low-latency product for use by NASA instrument teams	More than 20 NASA Instrument Teams
GEOS-Nature Run "mission planning"	Complex Earth System simulations at fine resolution with obs. simulators	Planning for new space-based missions NOAA and broad community; DoE/Smithsonian; NSF

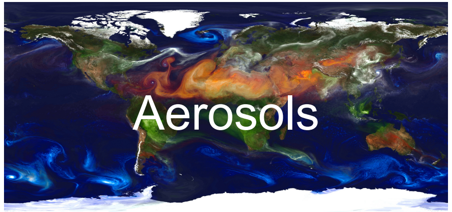
GMAO's current products that are documented both technically and through robust file specifications, well validated, and released to the broad community for research and applications

https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov


O_3
Ozone
20180722_1507z
0
Linear
100
https://svs.gsfc.nasa.gov/4754

Aerosol and Gas Phase Chemistry



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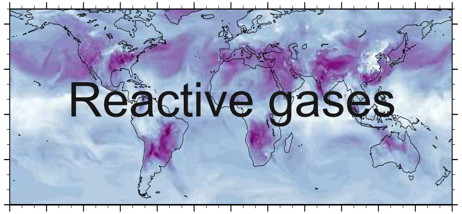


- Particulate matter:
  - Carbon
  - Sea salt
  - Dust
  - Sulfate
  - Nitrates
  - (Secondary Organics)

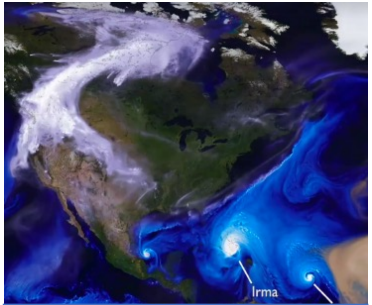
GOCART

- Ozone (O_3)
- Nitrogen dioxide (NO_2)
- Carbon monoxide (CO)
- Volatile organic compounds (VOCs):
  - Formaldehyde
  - Benzene / Toluene
  - And many more!

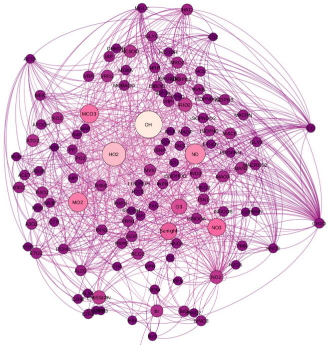
GEOS-Chem

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Daily composition forecast



GEOS NWP



GEOS - Chem

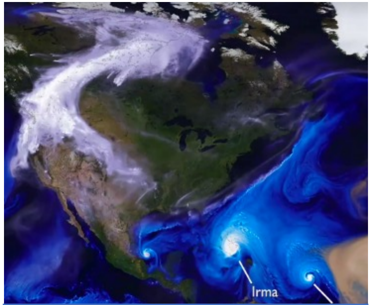
GEOS - CF

One **5-day forecast** per day

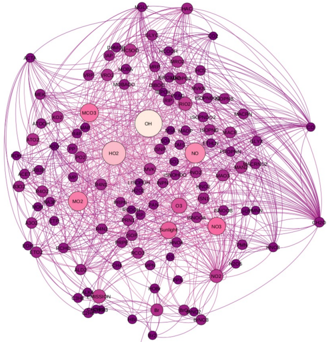
https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Daily composition forecast



GEOS NWP



GEOS - Chem

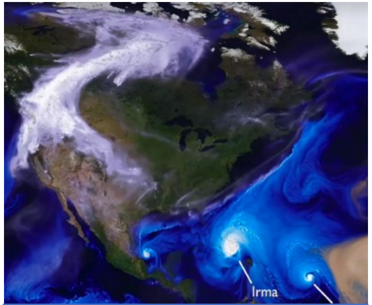
GEOS - CF

One **5-day forecast** per day

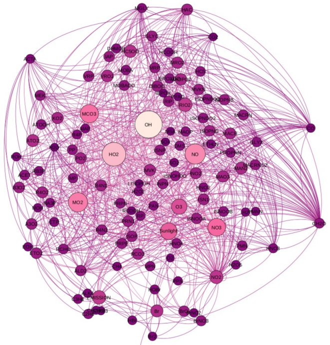
- ➢1-day meteorological replay "analysis"
- ➢5-day forecast

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Daily composition forecast



GEOS NWP



GEOS - Chem

GEOS - CF

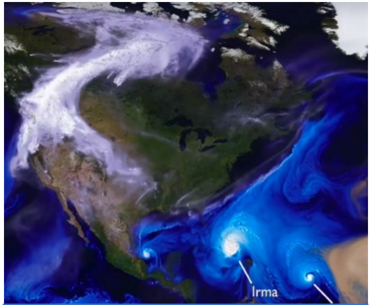
One **5-day forecast** per day

- ➢1-day replay
- ➢5-day forecast
- ➢c360 (0.25°, **~25x25 km^2**) resolution, 72 model layers

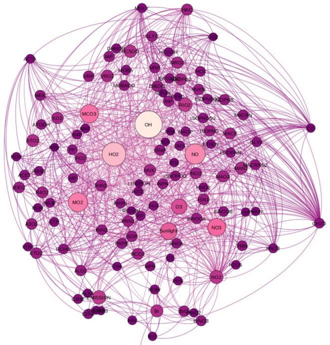
https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Daily composition forecast



GEOS NWP



GEOS - Chem

GEOS - CF

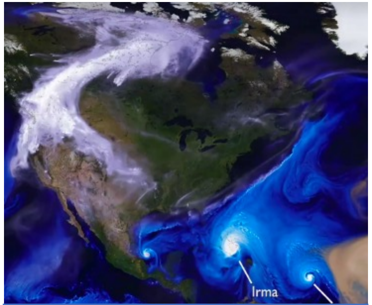
One **5-day forecast** per day

- 1-day replay
- 5-day forecast
- c360 (0.25°, **~25x25 km^2**) resolution, 72 model layers
- O_3, NO_x, VOCs, PM ...
- T, U, V, RH ....

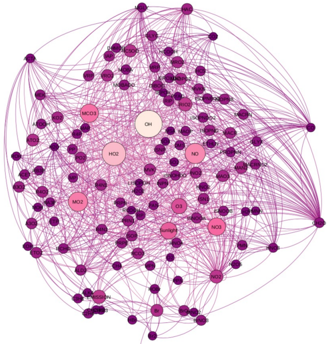
https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Daily composition forecast



GEOS NWP



GEOS - Chem

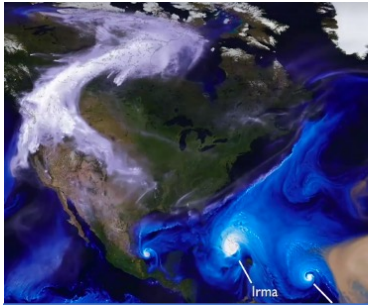
GEOS - CF

One **5-day forecast** per day

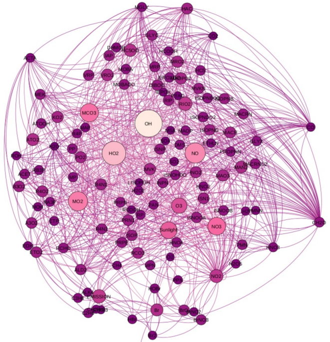
- 1-day replay
- 5-day forecast
- c360 (0.25°, ~25x25 km^2)
- **15 minute** "surface"
- **1-hour** average and instantaneous 2D & 3D

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Daily composition forecast



GEOS NWP



GEOS - Chem

GEOS - CF

One **5-day forecast** per day
- 1-day replay
- 5-day forecast
- c360 (0.25°, ~25x25 km^2)
- **Available since**
  1 January 2018 (replay)
  1 January 2019 (forecast)

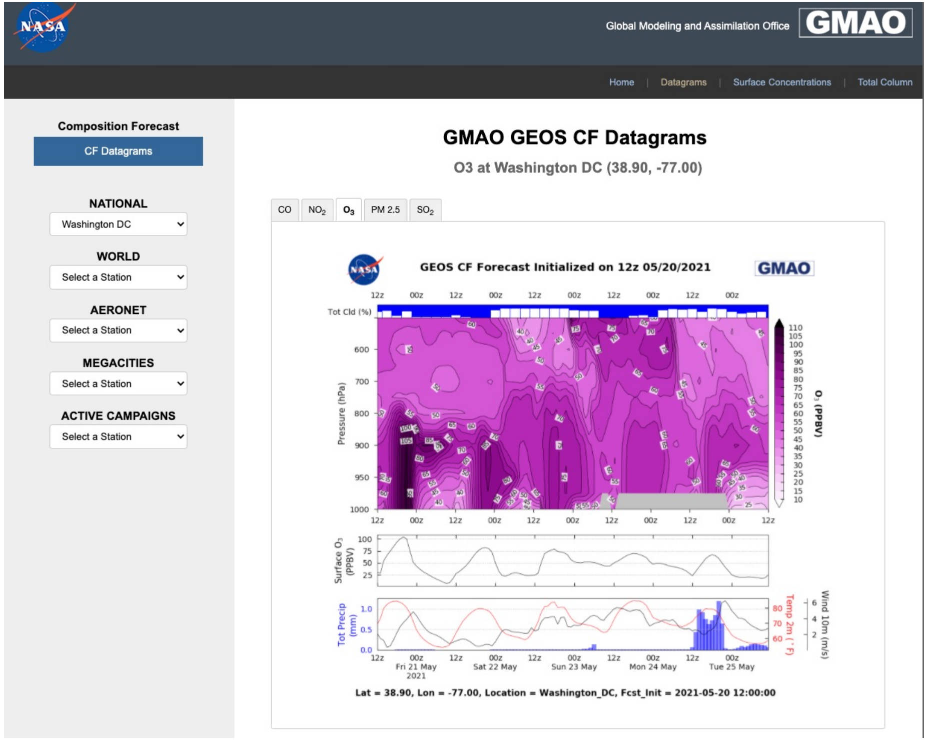
https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

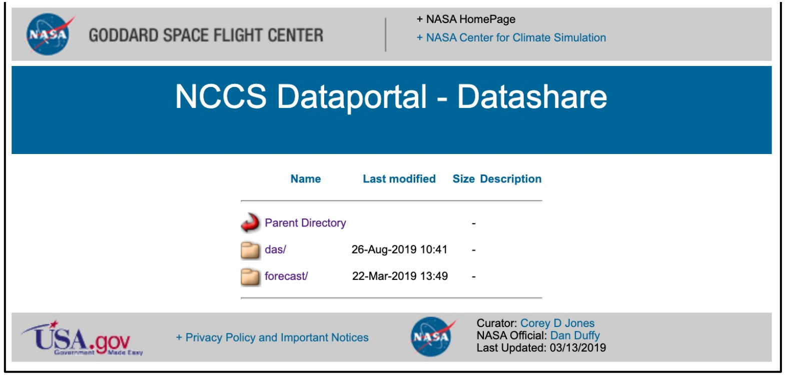
GEOS-CF are available online in near real-time

FLUID is a mobile-friendly website

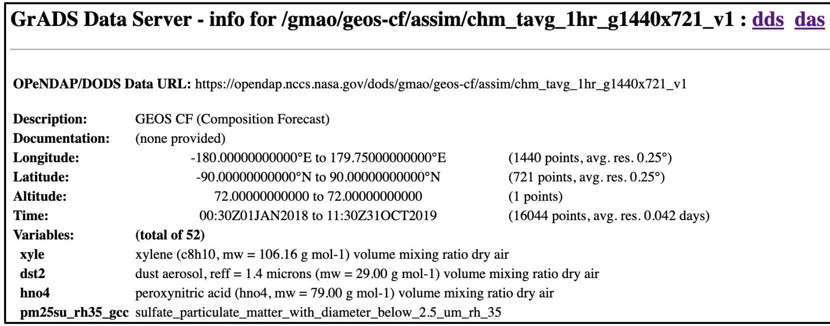
https://fluid.nccs.nasa.gov/cf/



https://portal.nccs.nasa.gov/datashare/gmao/geos-cf/v1/



https://opendap.nccs.nasa.gov/dods/gmao/geos-cf/



GrADS Data Server - info for /gmao/geos-cf/assim/chm_tavg_1hr_g1440x721_v1 : dds das

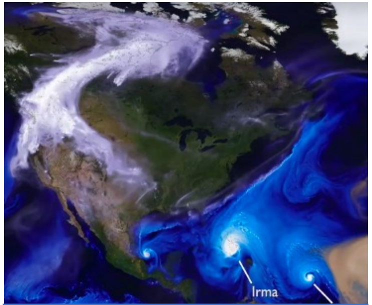
OPeNDAP/DODS Data URL: https://opendap.nccs.nasa.gov/dods/gmao/geos-cf/assim/chm_tavg_1hr_g1440x721_v1

Description:	GEOS CF (Composition Forecast)	
Documentation:	(none provided)	
Longitude:	-180.00000000000°E to 179.75000000000°E	(1440 points, avg. res. 0.25°)
Latitude:	-90.00000000000°N to 90.00000000000°N	(721 points, avg. res. 0.25°)
Altitude:	72.00000000000 to 72.00000000000	(1 points)
Time:	00:30Z01JAN2018 to 11:30Z31OCT2019	(16044 points, avg. res. 0.042 days)
Variables:	(total of 52)	
xyle	xylene (c8h10, mw = 106.16 g mol-1) volume mixing ratio dry air	
dst2	dust aerosol, reff = 1.4 microns (mw = 29.00 g mol-1) volume mixing ratio dry air	
hno4	peroxynitric acid (hno4, mw = 79.00 g mol-1) volume mixing ratio dry air	
pm25su_rh35_gcc	sulfate_particulate_matter_with_diameter_below_2.5_um_rh_35	

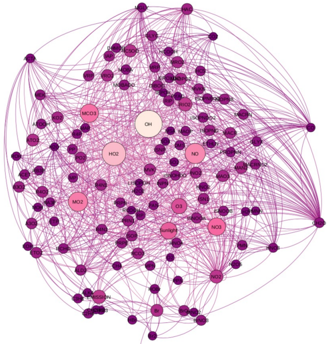
https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Daily composition forecast



GEOS NWP



GEOS - Chem

GEOS - CF

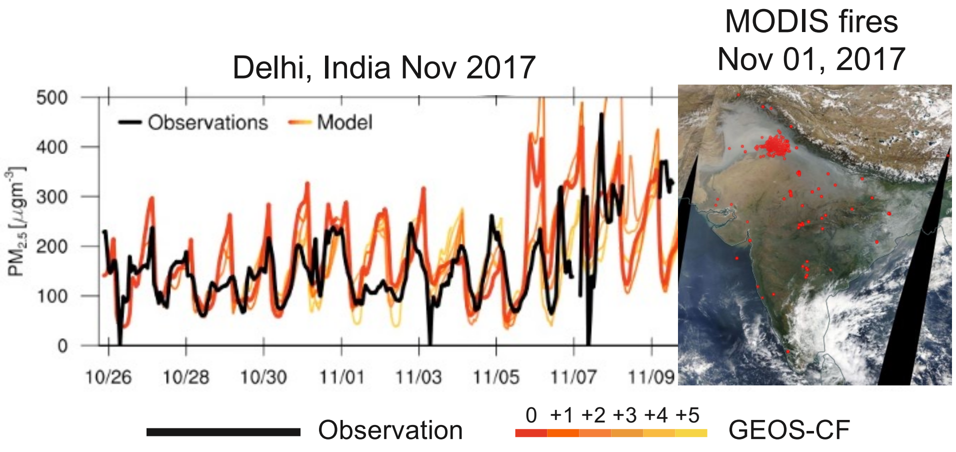
- Currently **no <u>direct</u>** data **assimilation of constituents** in GEOS-CF

https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

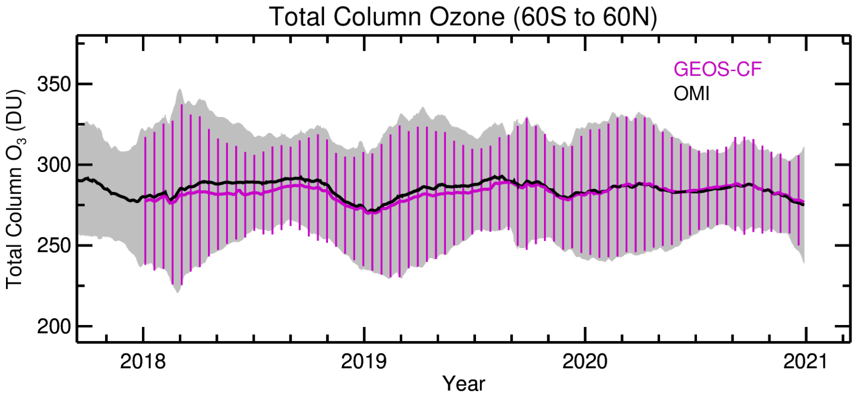
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Near-real time updates from satellite data

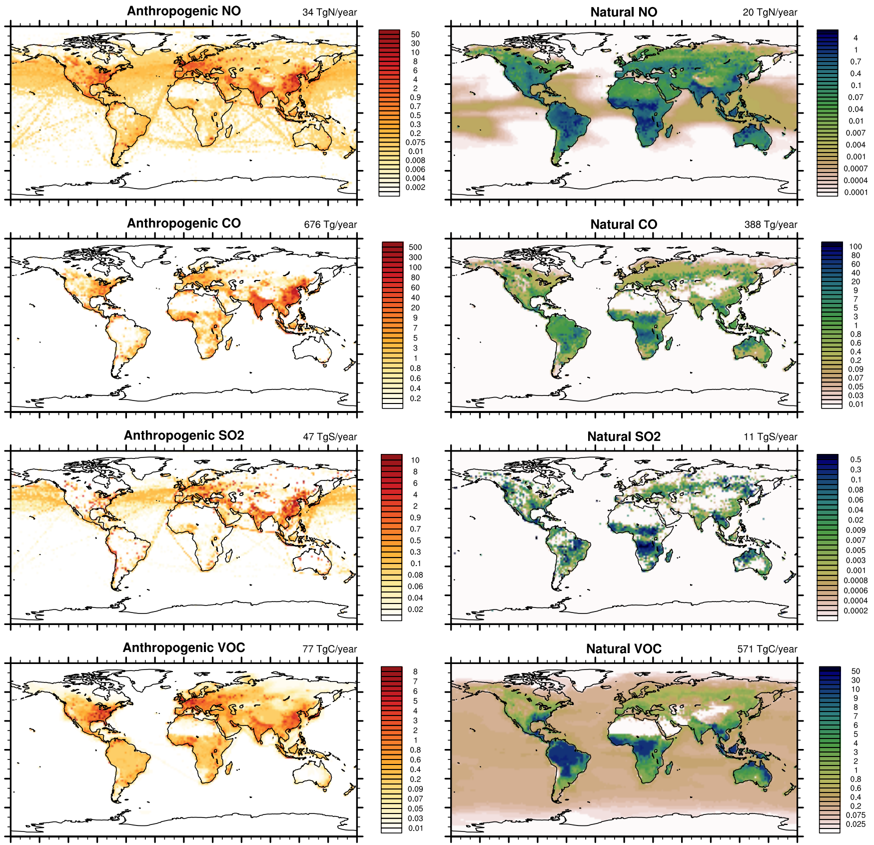
- Biomass burning emissions from near-real time QFED v2.5



- GEOS-CF Stratospheric O_3 is weakly nudged to the GEOS FP assimilated O_3



GEOS-Chem emissions



Anthropogenic: HTAP, RETRO, DICE (Africa), AEIC (aircraft)

Biomass burning: QFED NRT

Biogenic: Megan 2.1

Lightning: online (Murray et al., 2012)

Soil NOx: online (Hudman et al. 2012)

Dust: online (Zender et al. 2003)

Sea salt: online (Jaegle et al., 2011)

Ocean: online: sea salt, DMS, acetone, acetaldehyde, HOI, I_2

Prescribed: CFCs, VSLS, CH_4, CO_2

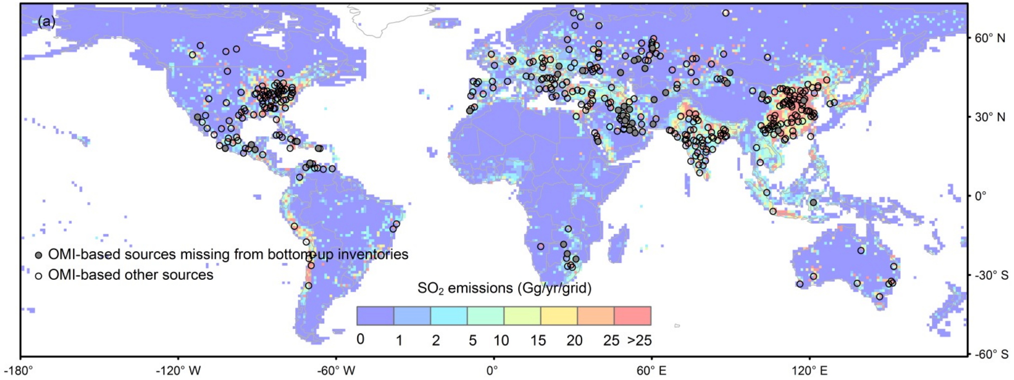
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Year-to-year emissions changes

Emissions:

- Annual gridded scale factors based on satellite data are applied to the emissions of CO (Oda et al., 2017) and SO_2 (Liu et al., 2018).
- "Business-as-usual" assumed for 2020 and 2021

SO_2 emissions in the OMI-HTAP inventory

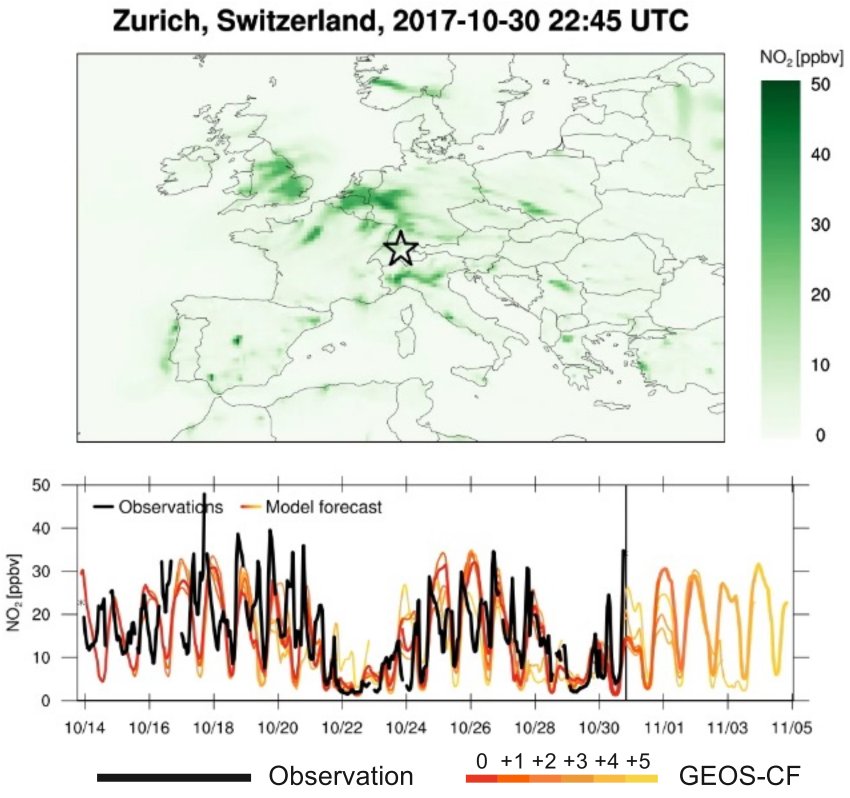


A new emission inventory, OMI-HTAP, combines OMI-based SO_2 emissions for large sources and the bottom-up inventory, HTAP, for smaller sources.

Liu, F., et al., *Atmos. Chem. Phys., 18*, 2018

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Daily variations of emissions

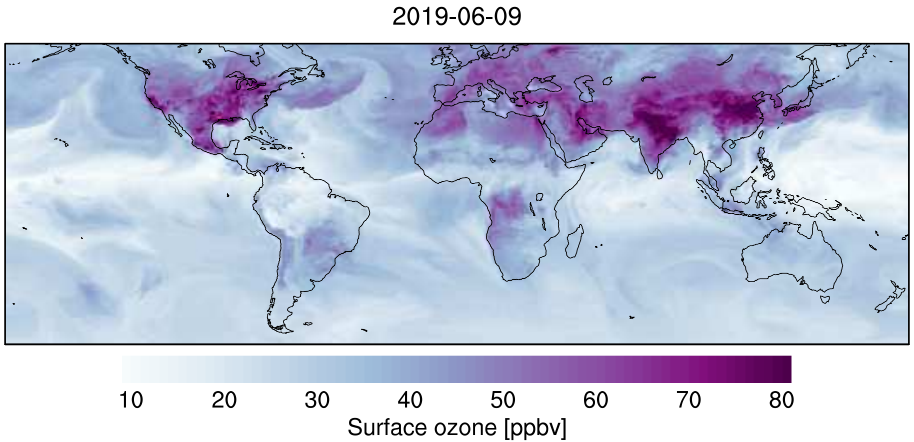


- Scale factors applied to emissions for diurnal and weekly variations
- These are clearly beneficial for surface NO_2 analyses and forecasts
- Shown for Zurich - weather and diurnal/weekly signals are prominent
- Surface observations obtained through emerging connection to OpenAQ (openaq.org)

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

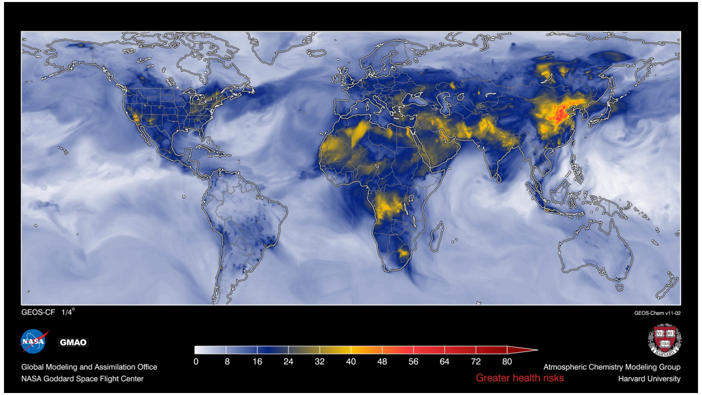
Air quality and health applications

- ➢ **How good is the model?**



Optimize model predictions

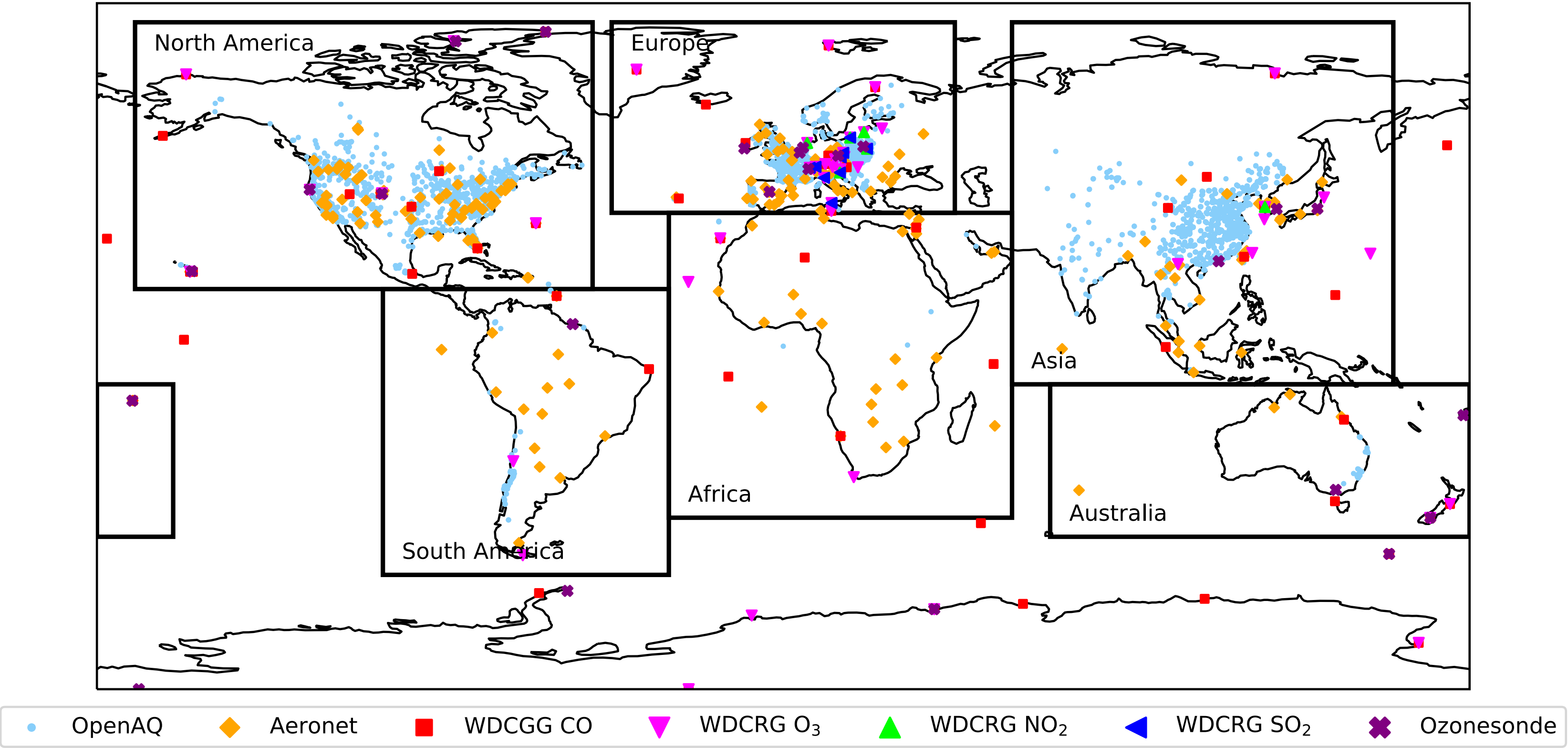
- ➢ **How bad is the air pollution?**



Global exposure assessment

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

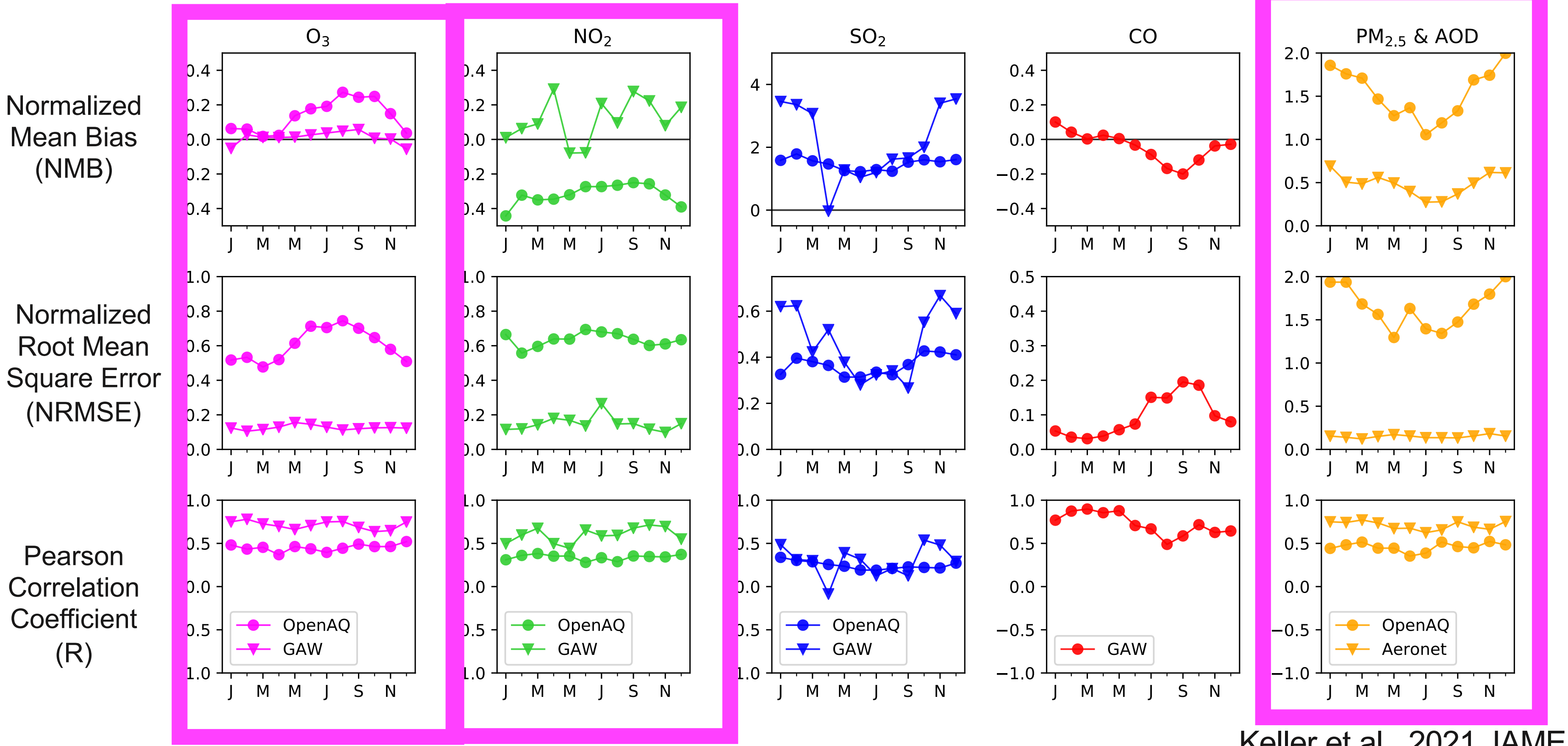
Observations for evaluation



Keller et al., 2021 JAMES

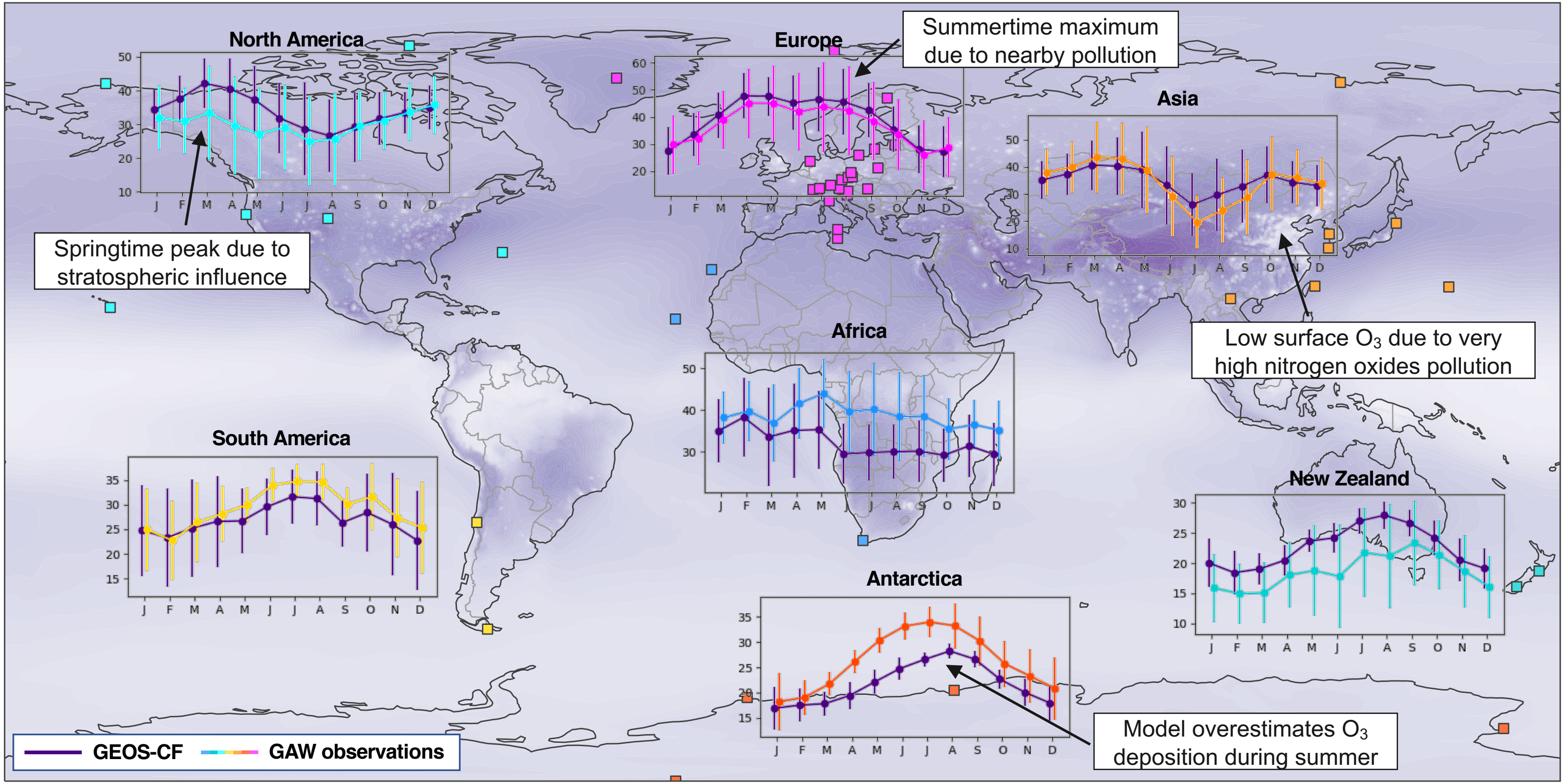
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Global surface comparisons - monthly



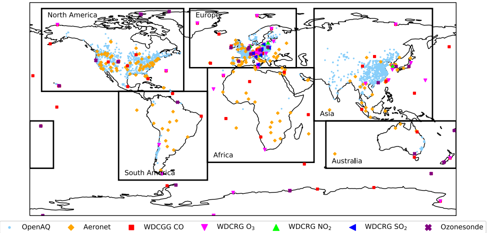
Keller et al., 2021 JAMES

GEOS-CF surface ozone compares well against background observations from the Global Atmospheric Watch (GAW) network

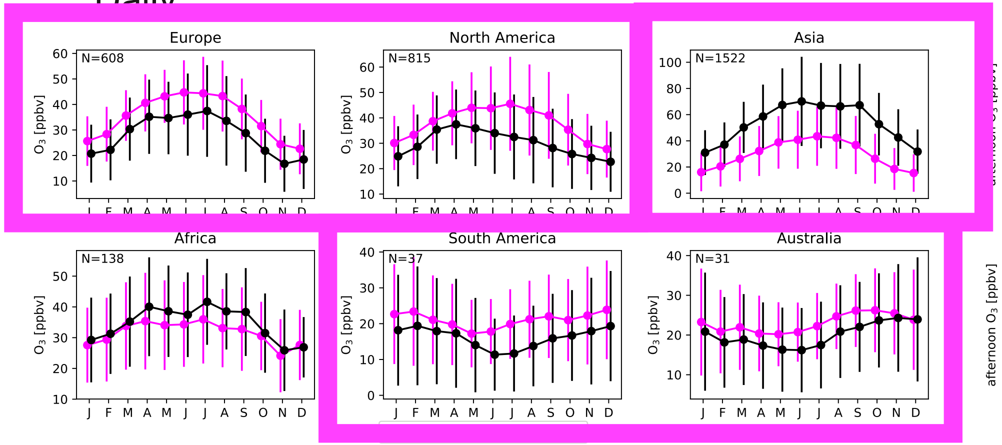


k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

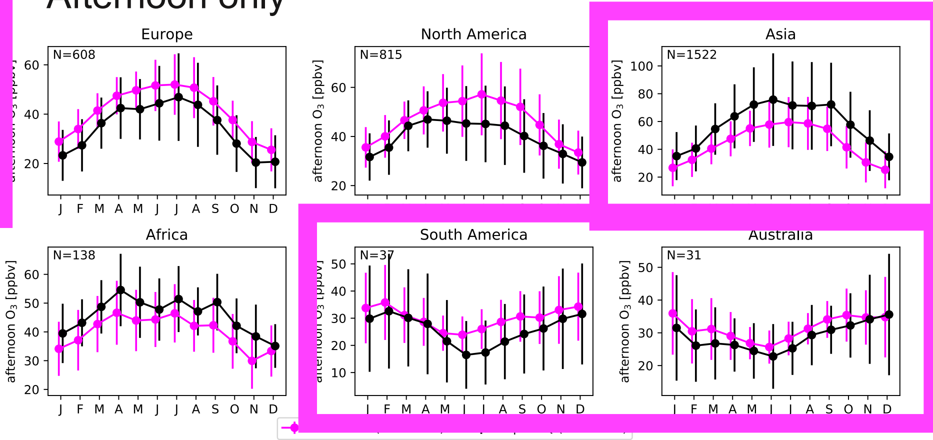
Surface O_3 (OpenAQ sites only)



Daily



Afternoon only



- GEOS-CF captures the overall seasonal cycle in the six regions, but generally overestimates in Europe, North & South America and Australia, while underestimating in Asia and Africa.
- In polluted regions, such as Asia, the bias is reduced when focusing on peak photochemical production period. GEOS-CF still has a bias over US during summer and fall, a known GEOS-Chem issue (Travis et al., 2016;2019; Hu et al., 2018).

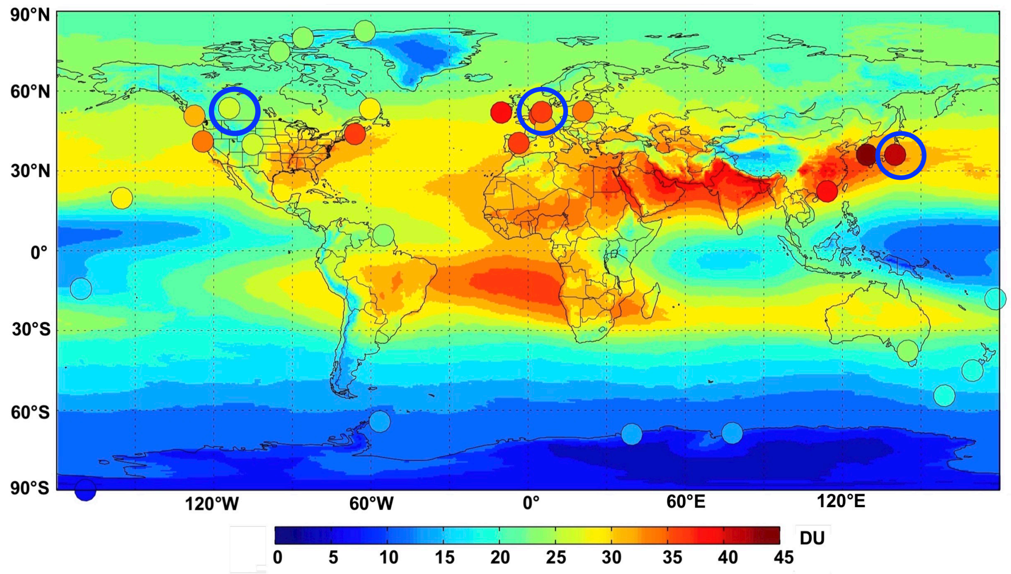
■ Observations ■ GEOS-CF

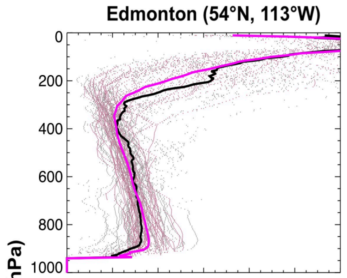
Keller et al., 2021 JAMES

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

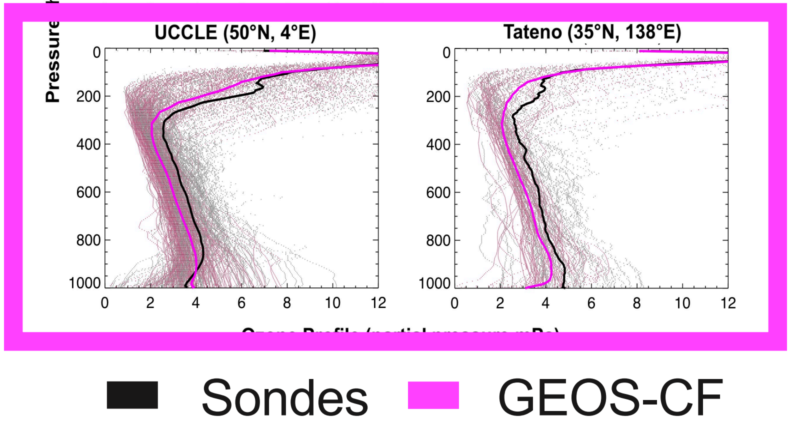
GEOS-CF captures the observed ozone spatial distribution and profile shapes shown by ozonesondes

2018 Tropospheric O_3 column (TOC): GEOS-CF and sondes





GEOS-CF in general captures the observed ozonesonde profile shapes, as seen at these three stations.



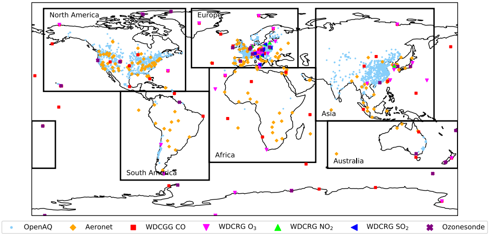
- GEOS-CF captures the overall spatial distribution of ozonesonde TOC, but with underestimates over polluted regions (e.g. sites over eastern US, Europe, east Asia).

Figures courtesy of Junhua Liu

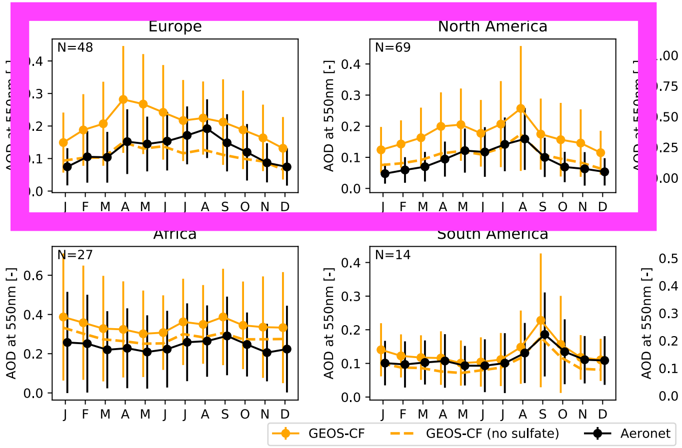
Thin lines: daily profiles in 2018
Thick lines: annual means

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

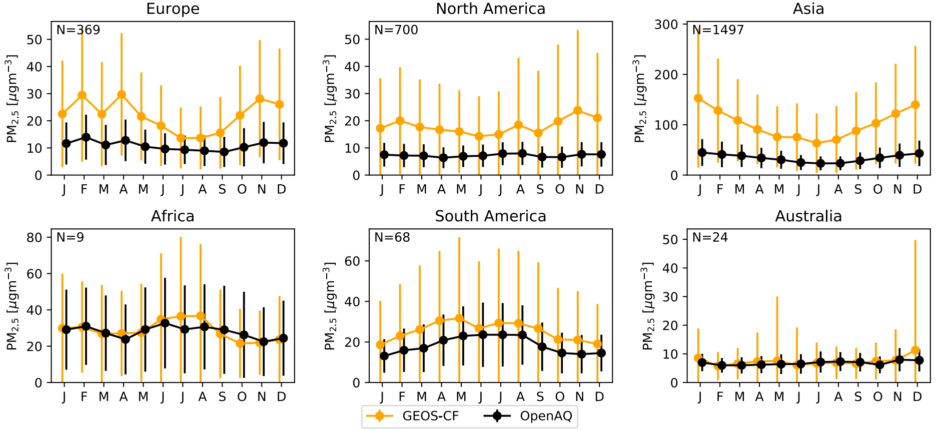
GEOS-CF generally overestimates aerosols (AOD and $PM_{2.5}$)



AOD from Aeronet network



PM2.5 from OpenAQ database



- GEOS-CF overestimates AOD 550 nm at most Aeronet sites. This is likely due to the overestimation of sulfates in the model.
- Similarly, GEOS-CF $PM_{2.5}$ is overestimated in Europe, North America, Asia and South America.

Observations GEOS-CF

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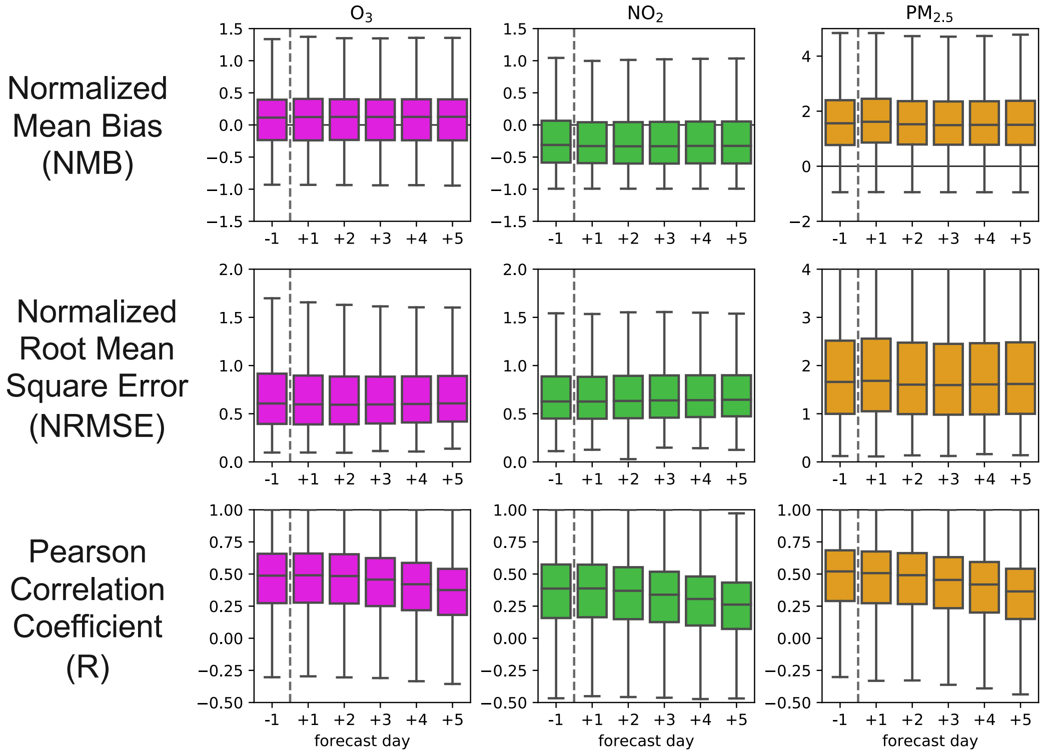
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

GEOS CF Forecast skill (GAW and OpenAQ)



- Little variation in the skill scores out to 5 days
- Correlation tends to decrease after day 2 and this is likely due to changes in the meteorological forecast and biomass burning emissions.

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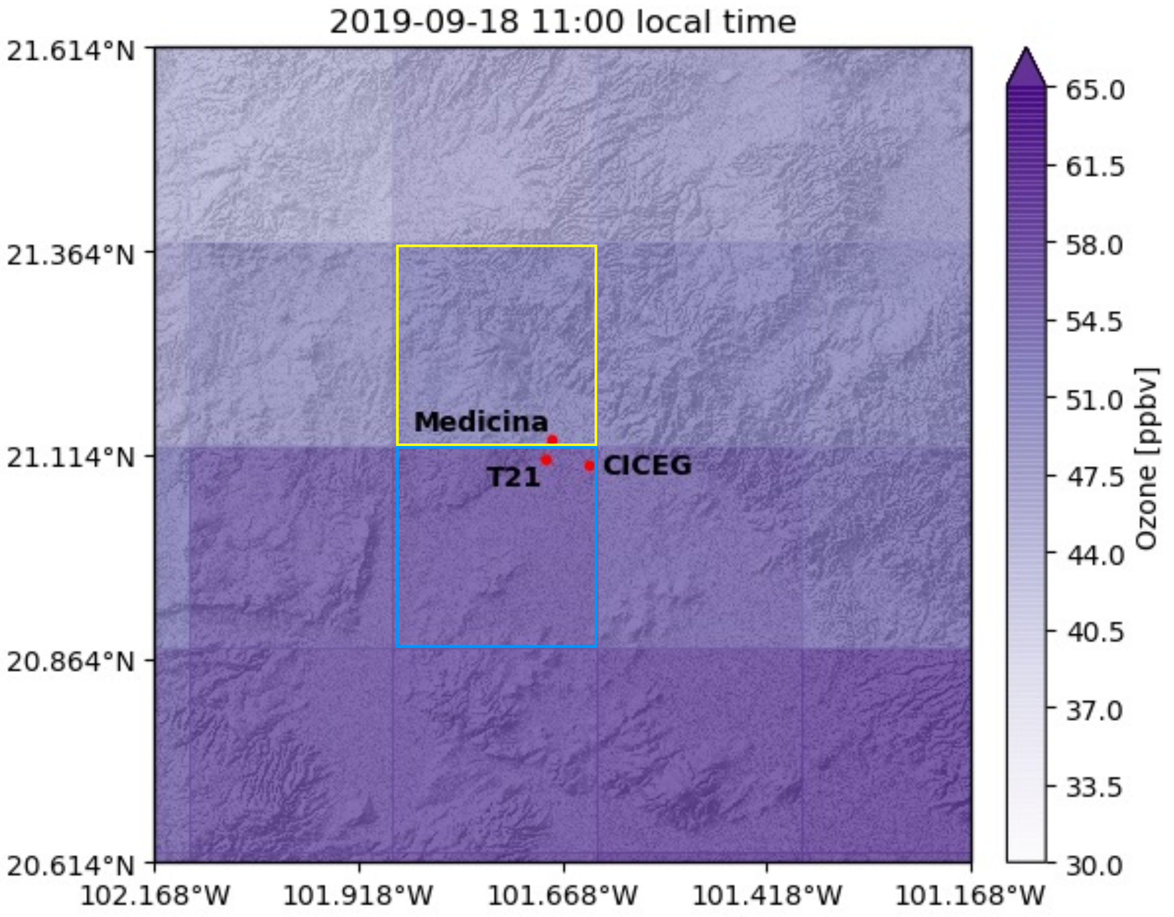
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov



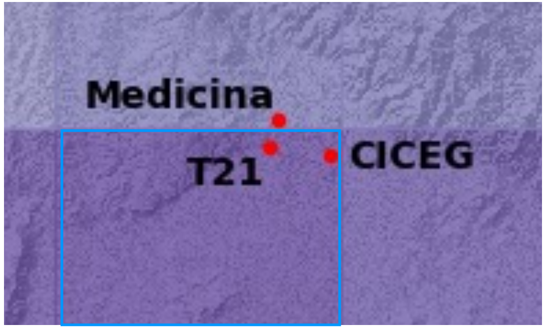
Improve local forecasts using statistical bias correction

3 monitoring stations in Leon, Mexico

- 1 in one grid box
- 2 share a grid box
- Difficult terrain within each grid box

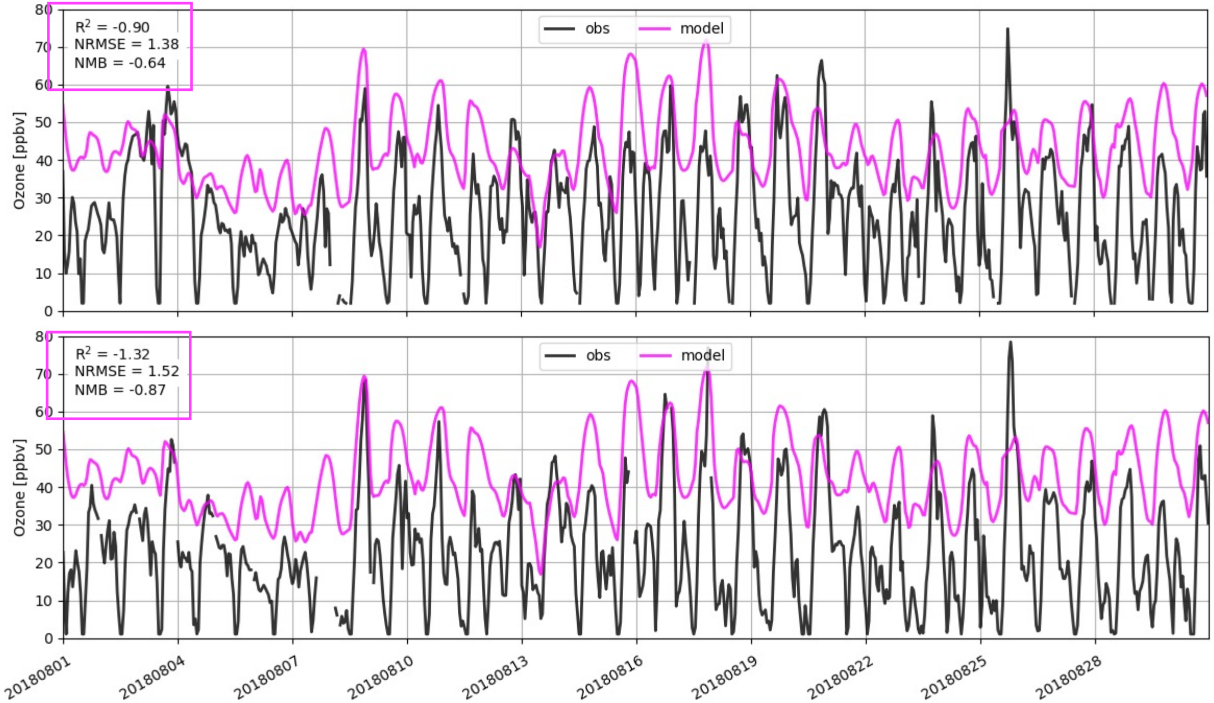
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Improve local forecasts using statistical bias correction



Two observation sites in the same grid box

- ➢ GEOS-CF generally over-estimates



Observations Model

Use machine learning to correct for small scale variability and/or model biases

Inputs

- Meteorology (10 vars)
- Chemistry (42 vars)
- ~~Emissions~~ (not used)
- Calendar (4 vars)

ML →

Output

Local concentration adjustment

- Algorithm: gradient boosted decision trees (XGBoost)
- Train separate algorithm for each site

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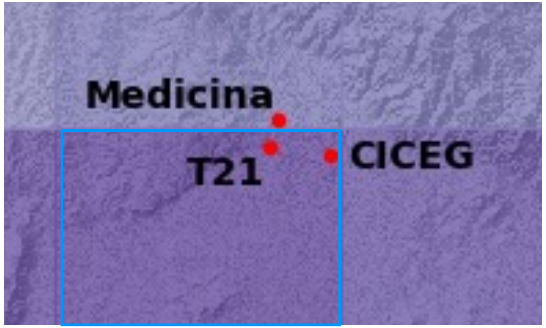
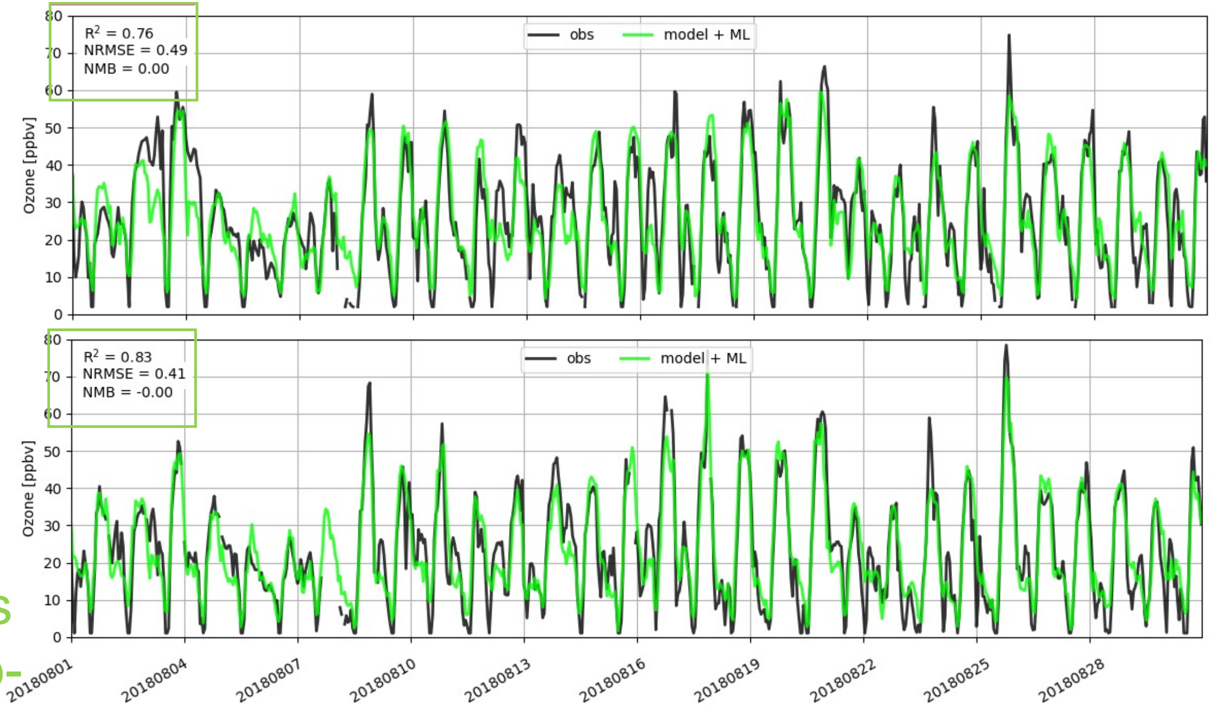
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Improve local forecasts using statistical bias correction





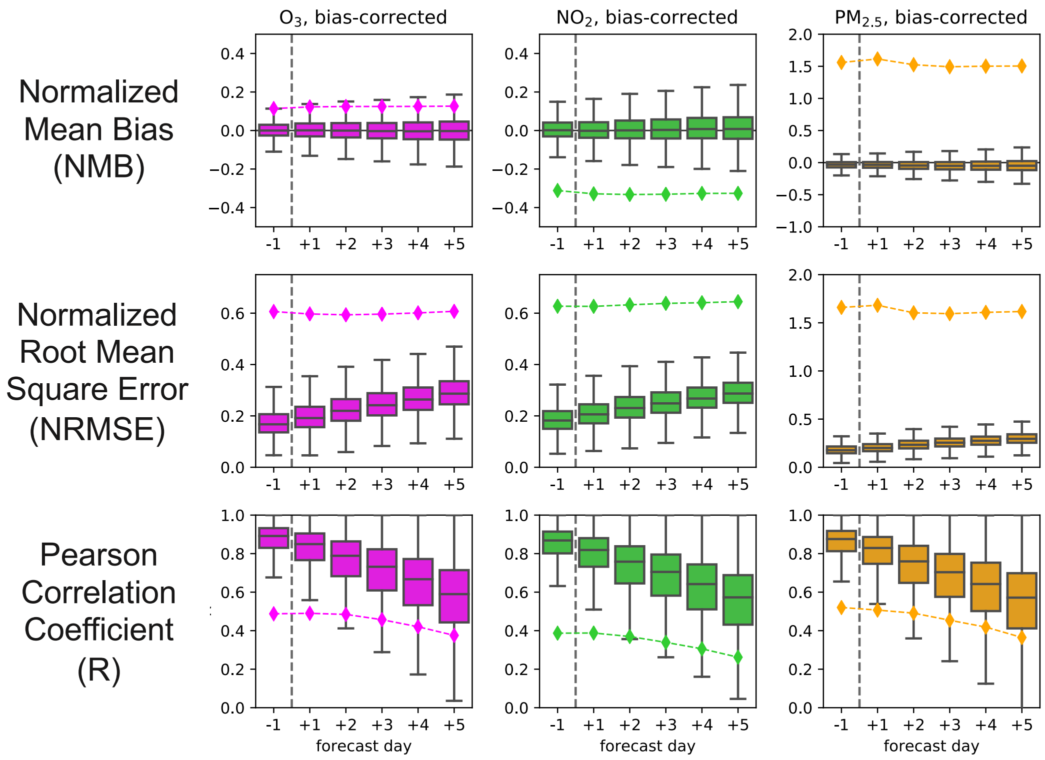
Two observation sites in the same grid box

- GEOS-CF+ML captures diurnal variability at sub-grid scale

Observations Model + ML

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

GEOS CF Forecast skill



- ✓ Using a Machine Learning (ML) algorithm to calculate bias-correction term for each monitoring site can drastically improve the forecast skill at the individual locations

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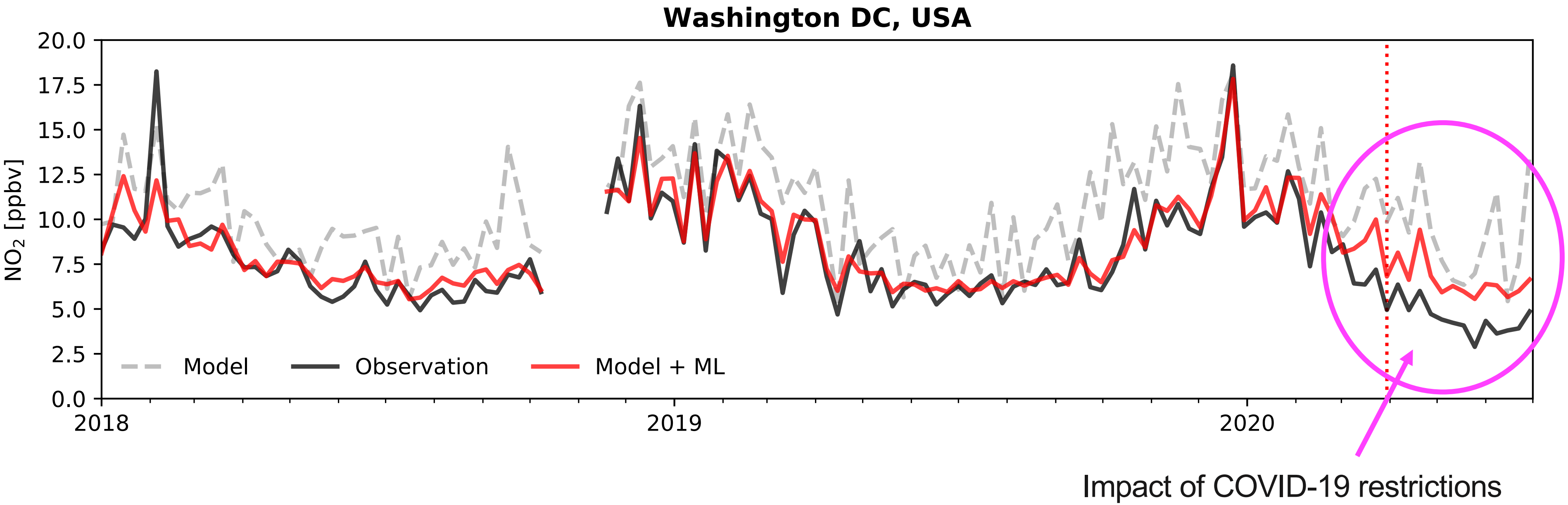
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

New application of the GEOS-CF ML algorithm



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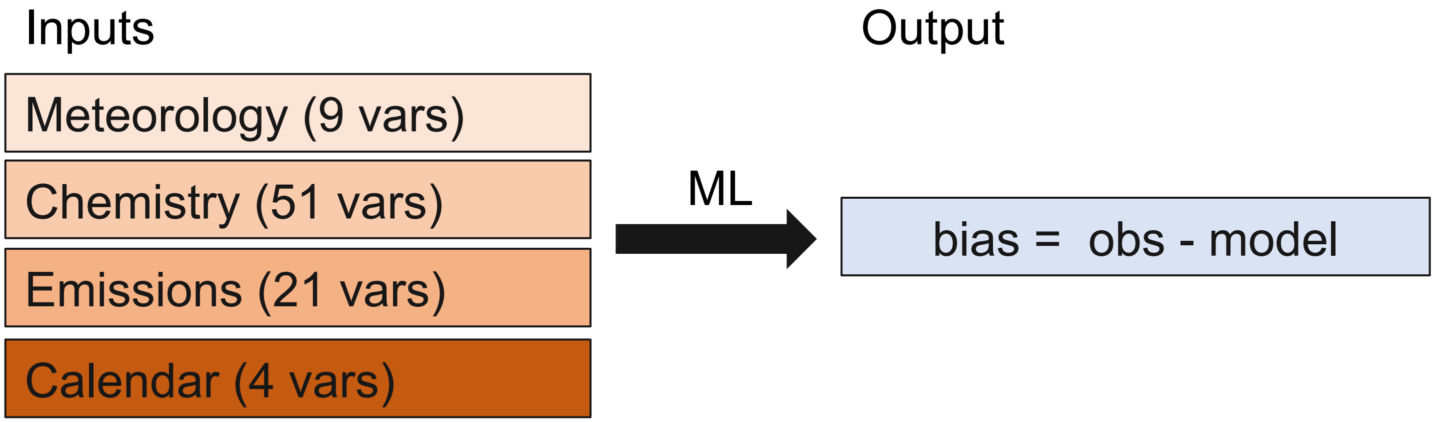
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Apply bias-correction to model output using machine learning (using historical observation-model comparisons)



- Algorithm: gradient boosted decision trees (XGBoost)
- Training: 2018-2019 (8-fold cross validation)

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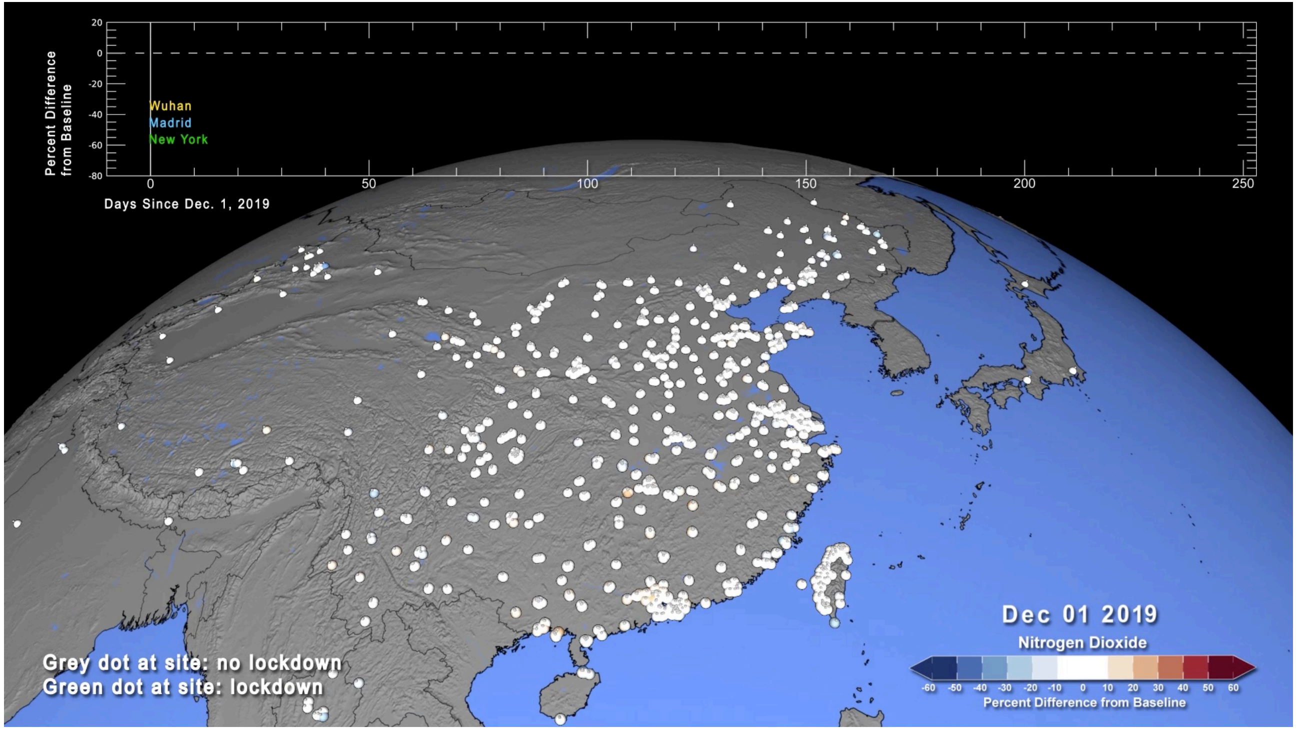
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Apply analysis to 5756 sites worldwide

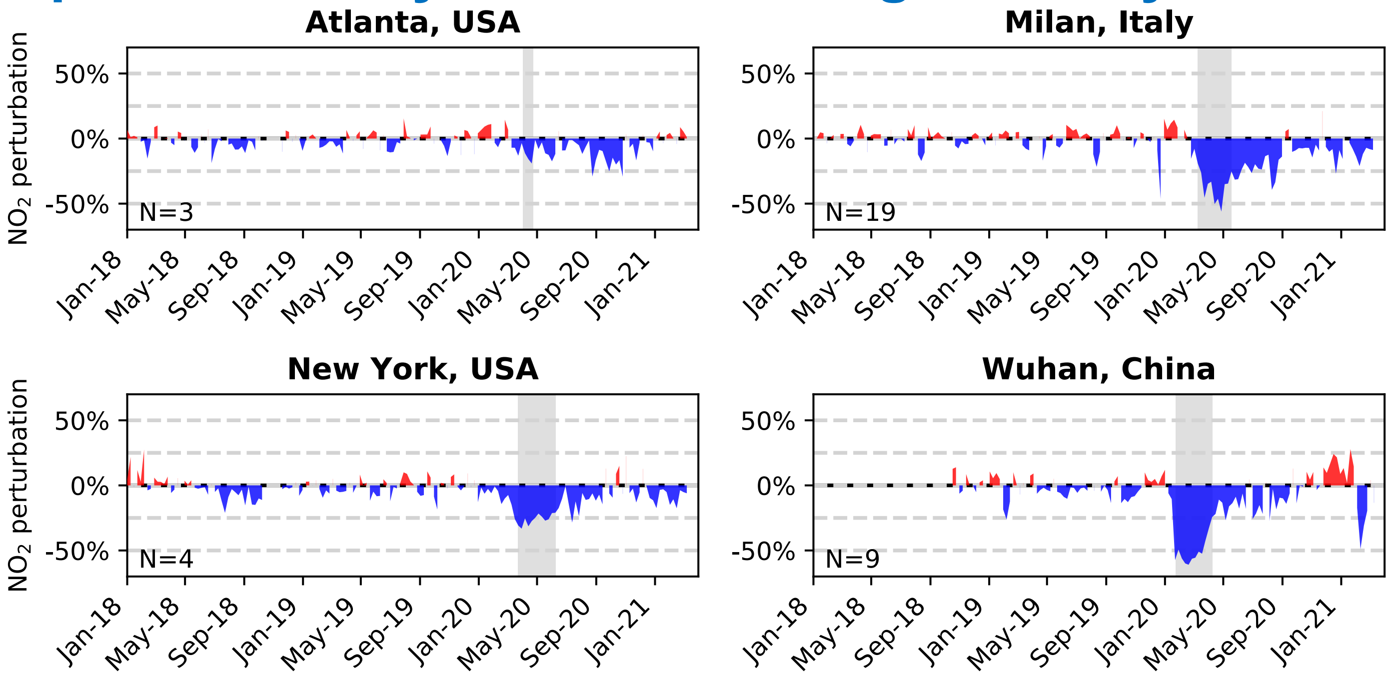


https://svs.gsfc.nasa.gov/13753 https://svs.gsfc.nasa.gov/4872

https://www.nasa.gov/feature/goddard/2020/nasa-model-reveals-how-much-covid-related-pollution-levels-deviated-from-the-norm

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Observation-model differences indicate city-wide NO_2 declines of up to 50% early on and a halting recovery since then



Updated through March 16, 2021

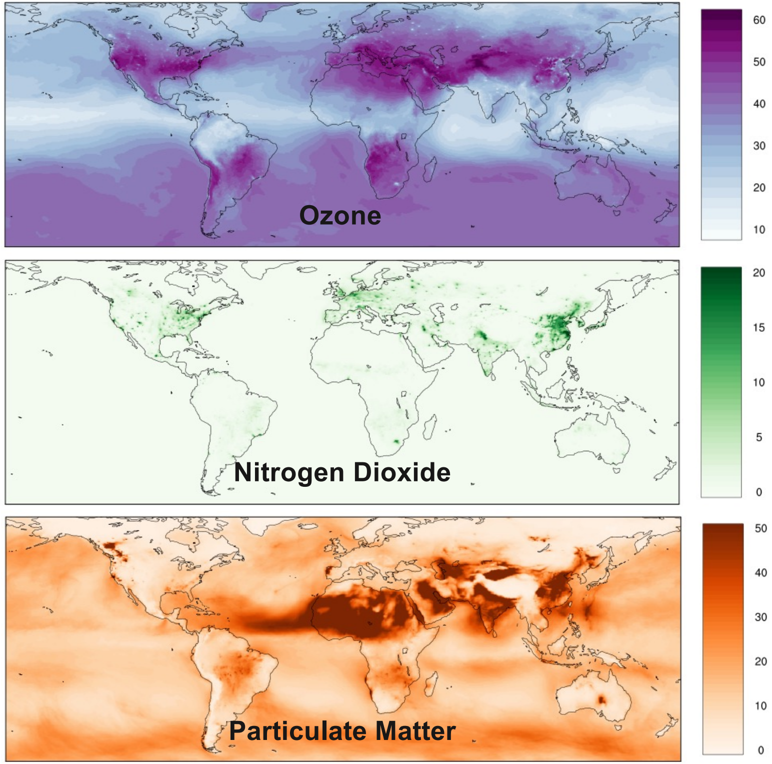
Keller et al., 2021 ACP

https://www.nasa.gov/feature/goddard/2020/nasa-model-reveals-how-much-covid-related-pollution-levels-deviated-from-the-norm

https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

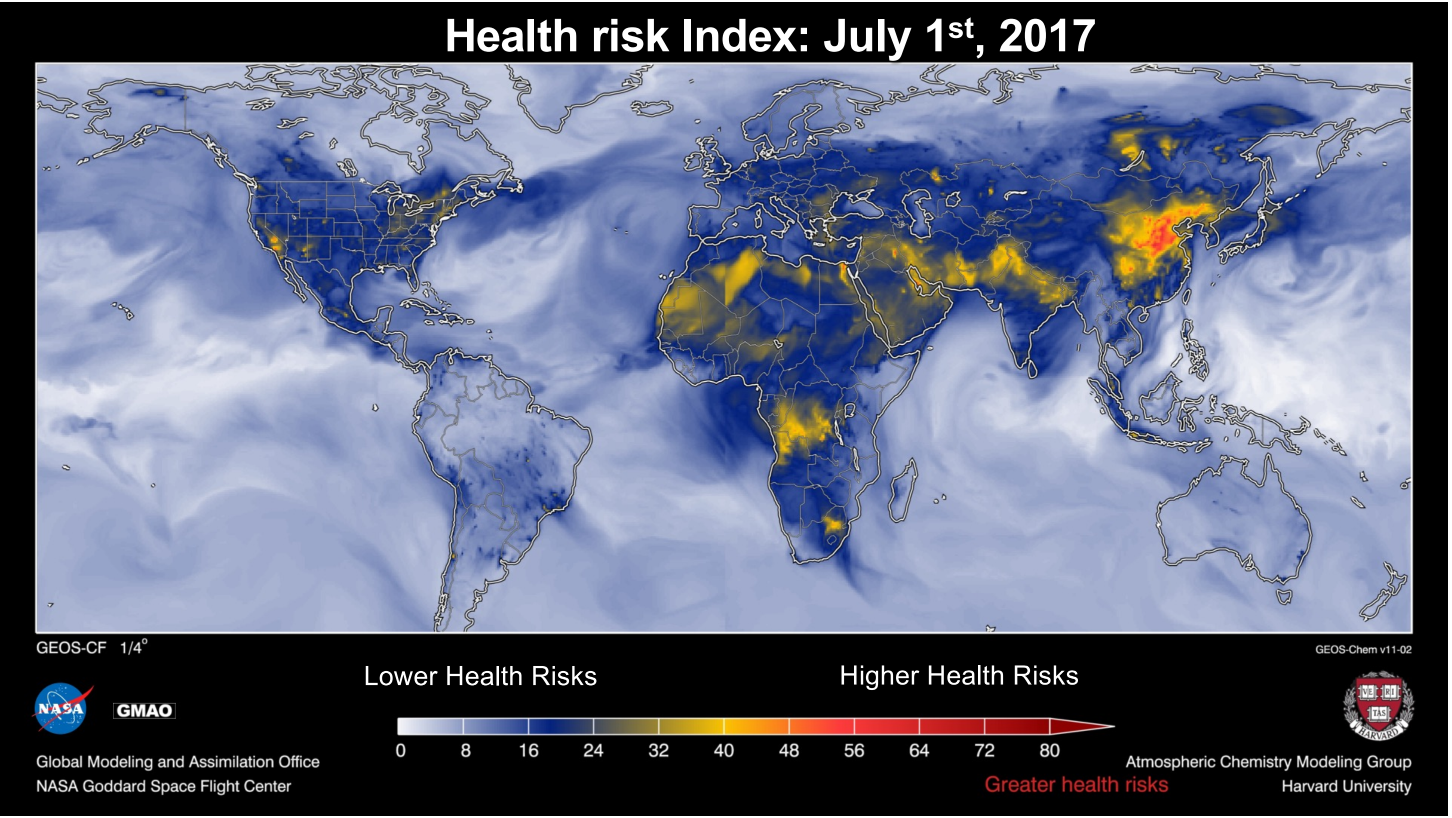
Forecast Application: Multi-pollutant Health Risk Index



- O_3 influences Background levels
- NO_2 is Short-lived
- Extreme gradients
- $PM_{2.5}$ driver of spatial gradients

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Forecast Application: Multi-pollutant Health Risk Index



Multi-pollutant index, developed by Kevin Cromar and NYU team (Gladson et al. *in prep*)

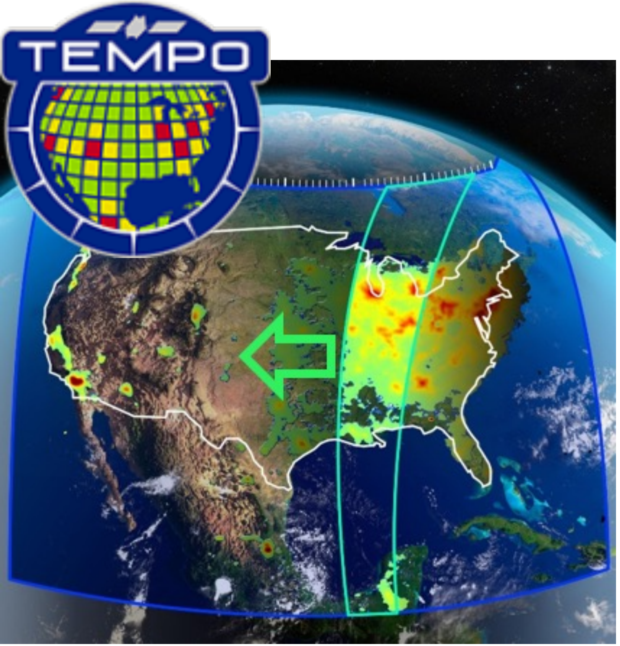
- Maximum daily 8-hour average (MDA8) O_3
- 24-hour-average NO_2
- 24-hour-average $PM_{2.5}$

Daily *atmospheric composition* forecast

GEOS - CF

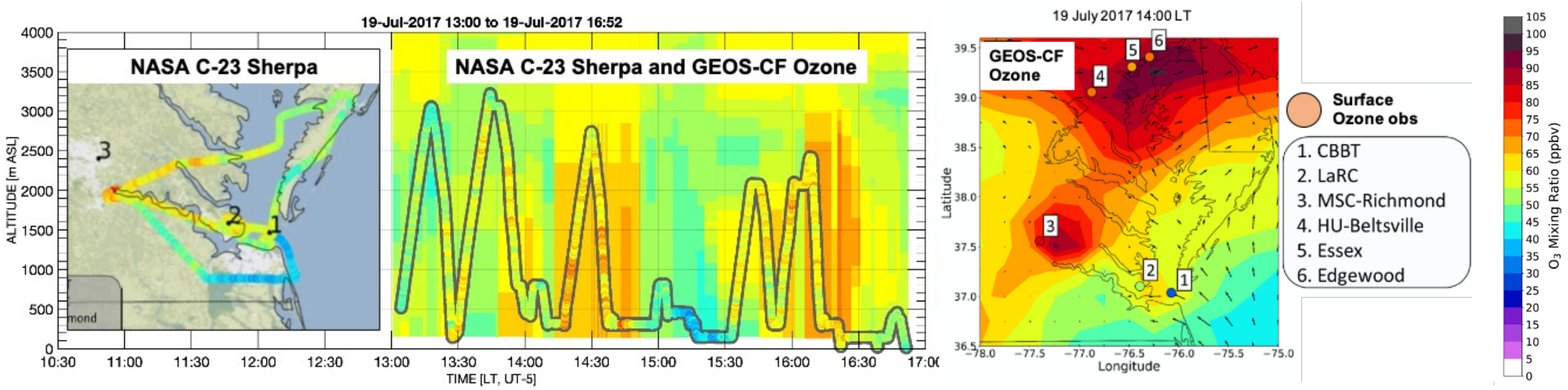
A realistic stratosphere in GEOS-CF is essential to support a broad range of NASA applications, including:

- Satellite retrievals of trace gases
- Airborne campaigns
- Stratosphere-troposphere exchange



k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

GEOS-CF evaluation with NASA's OWLETS campaign observations



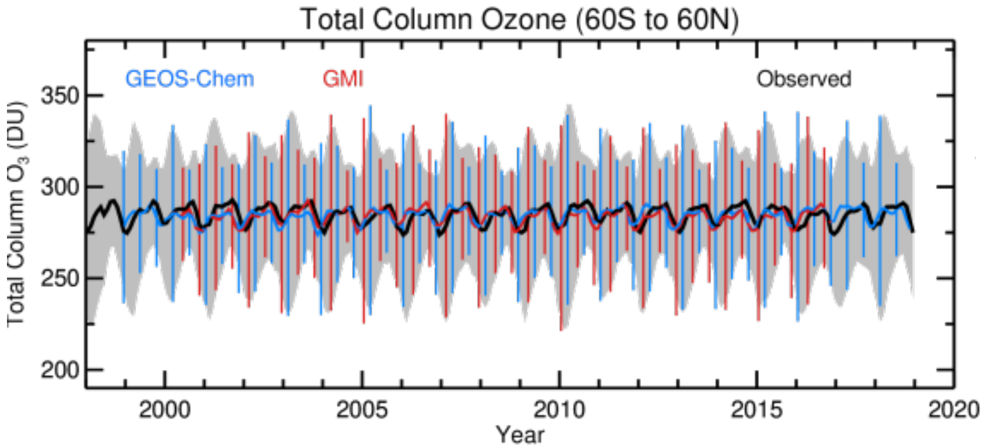
Dacic et al. (2020) used the GEOS-CF simulated ozone to put the OWLETS observations in 'the big picture', using the combined meteorology and chemistry to represent the synoptic conditions that lead to the observed ozone exceedances at surface observation sites.

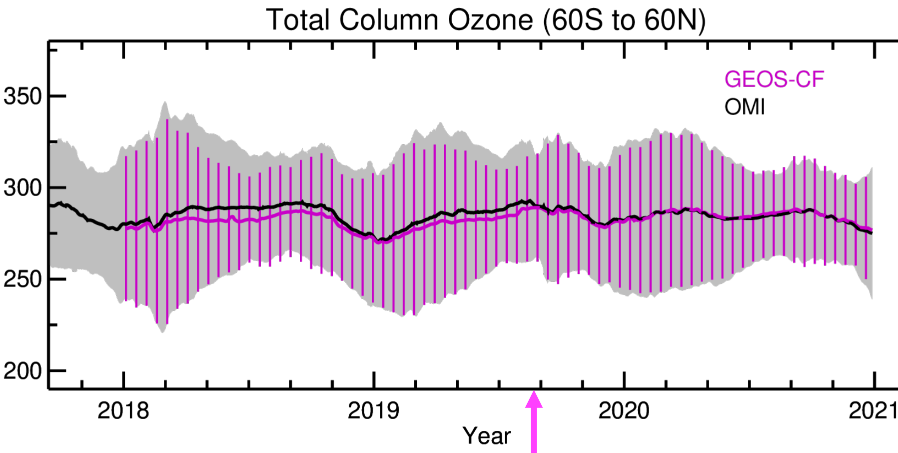
From where the model and the observations diverged, we learned where there are missing local marine emission sources and errors in the boundary layer chemical and dynamical processes in the model over the Chesapeake Bay.

Dacic, N. et al., 2020, Atmos. Environ. "Evaluation of NASA's high-resolution global composition simulations: Understanding a pollution event in the Chesapeake Bay during the summer 2017 OWLETS campaign"

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Stratospheric Composition Evaluation





Updates were made to GEOS-Chem in GEOS-CF based on experience from the GSFC Chemistry Climate Modeling (CCM) group with GMI

Figure courtesy of Pam Wales

Knowland et al., 2021 in prep

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

GEOS-CF has realistic stratospheric ozone forecasts

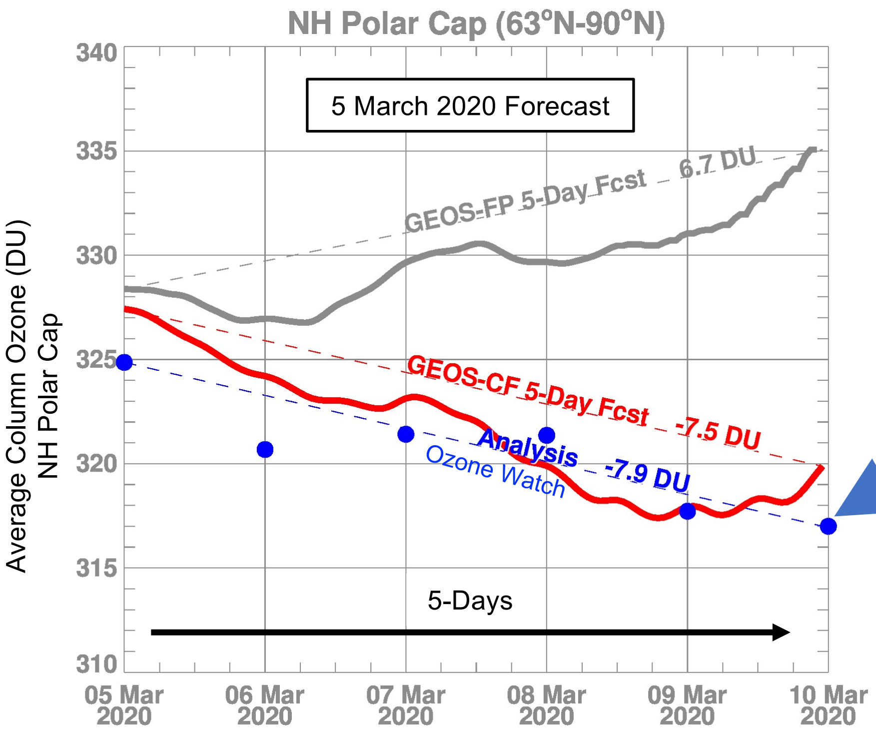
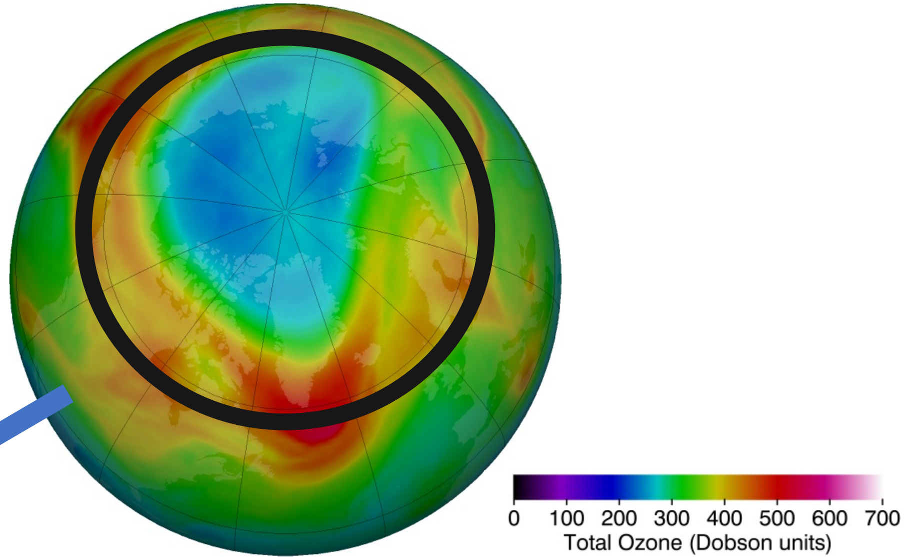


Figure courtesy of Larry Coy



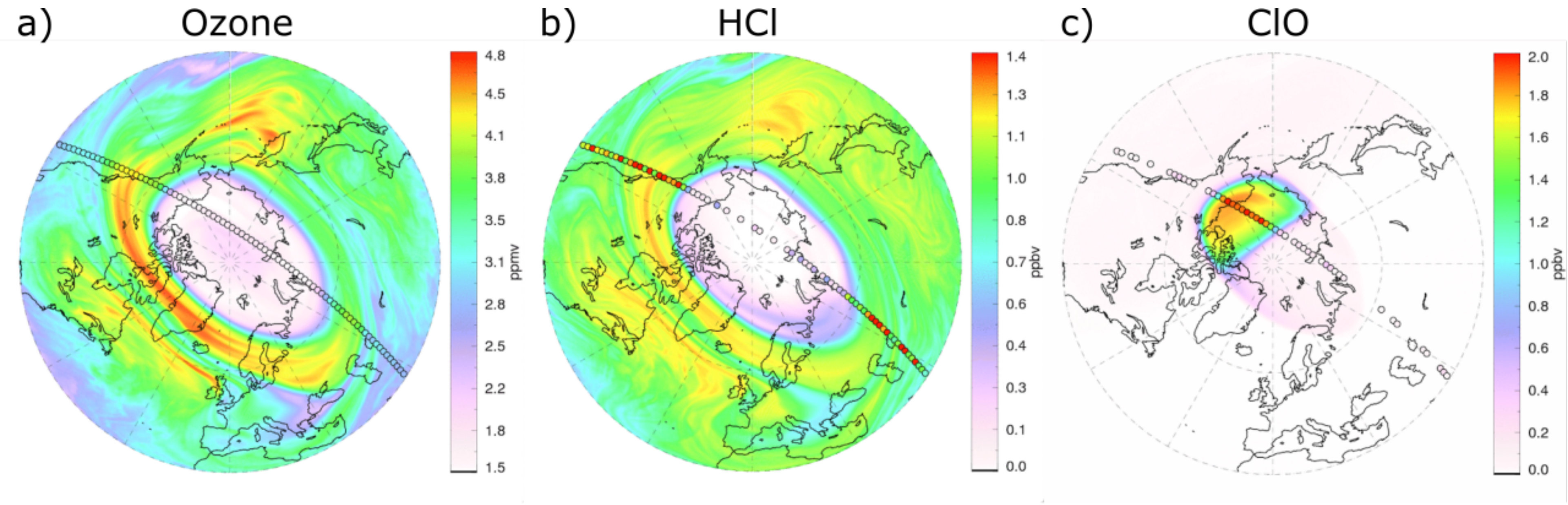
March 10, 2020: Ozonewatch.gsfc.nasa.gov

The GEOS-CF with stratospheric chemistry is responsible for the improved ozone forecasts adding realistic near-real-time stratospheric ozone forecasting capability to the NASA GMAO.

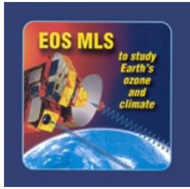
Knowland et al., 2021 in prep

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Evaluation GEOS-CF against MLS at 45 hPa



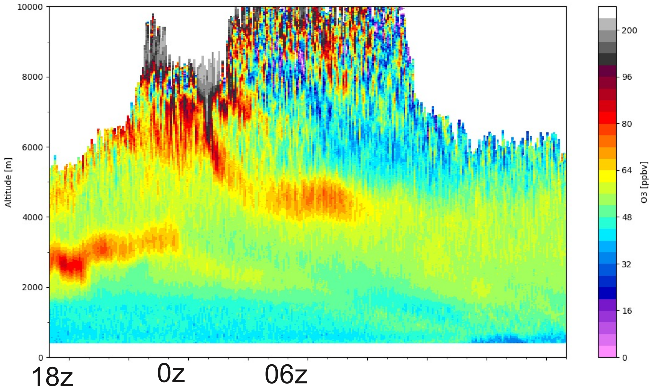
Figures courtesy of Kris Wargan



Knowland et al., 2021 in prep

Stratosphere Troposphere Exchange

NASA LaRC Feb 13-14, 2019

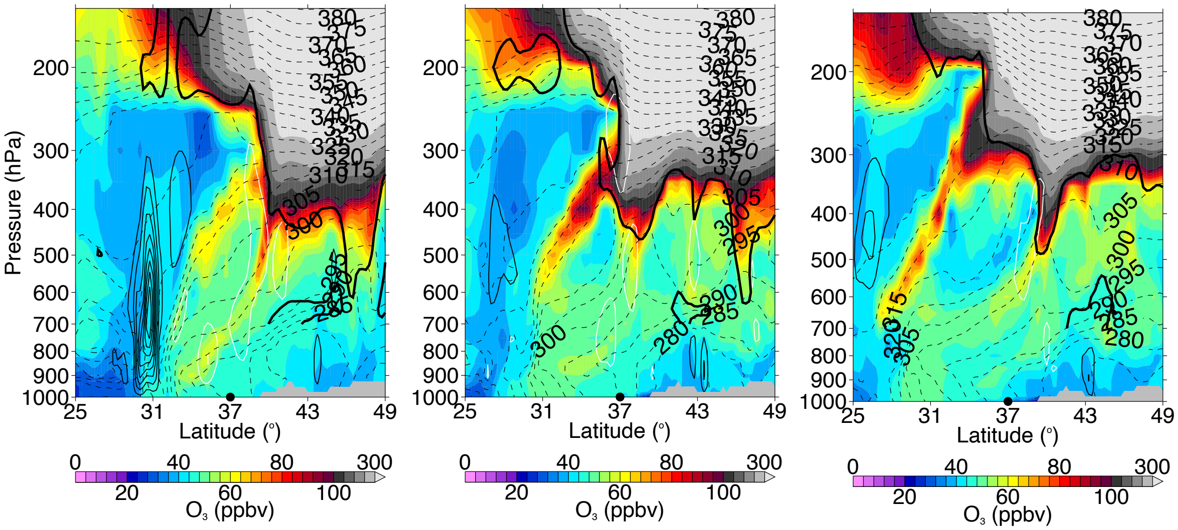


LMOL lidar plot courtesy of G. Gronoff

GEOS-CF
Feb 13, 2019 18z

Feb 14, 2019 00z

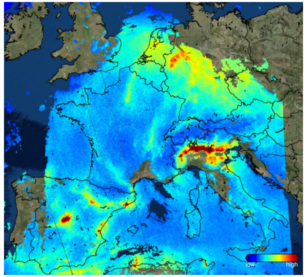
Feb 14, 2019 06z

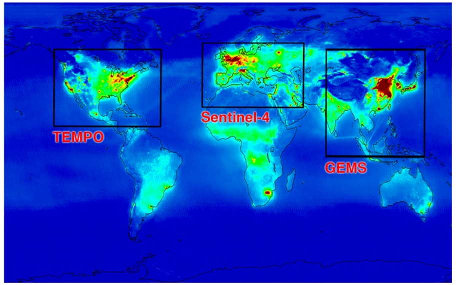


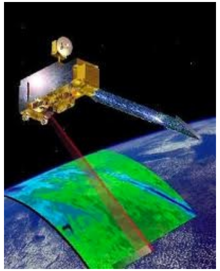
Case study of stratospheric Intrusion above Hampton, Virginia: lidar-observation and modeling analysis
Gronoff et al., Accepted to Atmospheric Environment

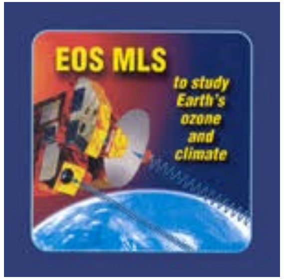
Planned upgrades for GEOS-CF

- Model update to GEOS-Chem v13.0
  - Improvements to ozone deposition
  - Updates to NO_3 washout ⇢ likely reduce PM2.5 bias
- CEDS emission inventory (latest release through 2019)
- Constituent Data Assimilation System (CoDAS)
  - Multi-constituent assimilation with O_3, CO, NO_2
  - Satellite-based emission scale factors





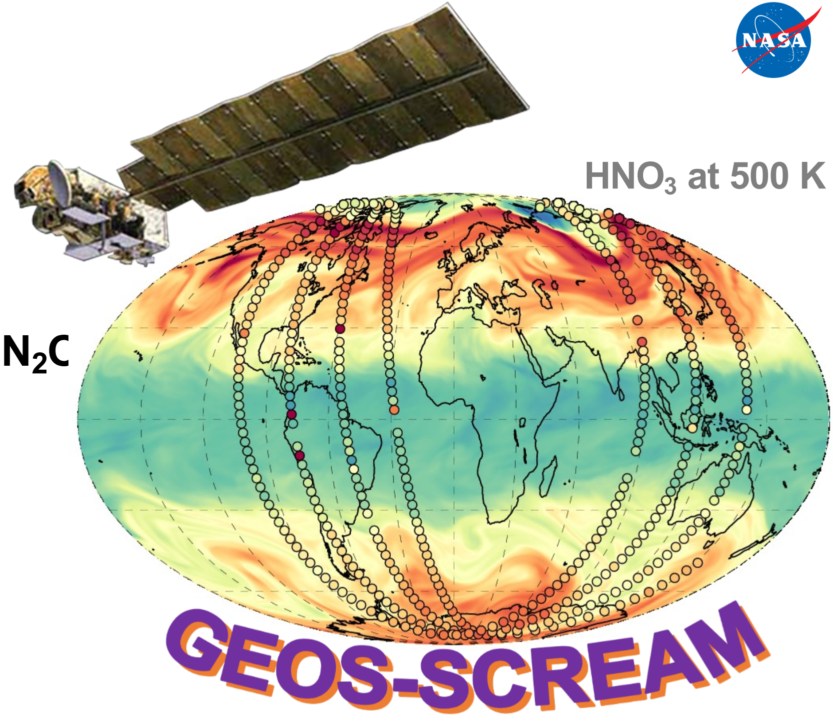




k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

GEOS Stratospheric Composition Reanalysis with Aura MLS (GEOS-SCREAM)

Kris Wargan, Brad Weir, Gloria L. Manney, Stephen E. Cohn, Nathaniel J. Livesey and JPL colleagues



- ❑ Assimilating MLS v4.2 **ozone, H_2O, HCl, HNO_3,** & **N_2O** and **total ozone** from OMI
- ❑ Replay to MERRA-2
- ❑ GEOS "StratChem" stratospheric-only chemistry
- ❑ Period: September 2004 – December 2020+

✓ Close agreement with ACE-FTS and GLORIA data and the BRAM2 reanalysis

➢ GMAO Reanalysis of the 21st Century (R21C, ~2022) with chemistry

Wargan, K., Weir, B., Manney, G. L., Cohn, S. E., & Livesey, N. J. (2020). The anomalous 2019 Antarctic ozone hole in the GEOS Constituent Data Assimilation System with MLS observations. *Journal of Geophysical Research: Atmospheres*, 125, e2020JD033335. https://doi.org/10.1029/2020JD033335

Summary of GEOS-CF Status

- GEOS-CF daily global composition forecasts at 25km resolution are generated in near-real time:
  - High-resolution replay segments are available since January 2018
    - ✓ Model realisticly captures global distribution of the major pollutants, though aerosols and SO2 are biased high, when compared against surface observations, ozonesondes and satellite.
    - ✓ Due to grid-box size, model skill is typically worse for the urban sites (OpenAQ) than the background sites (GAW)
  - Forecasts accessible via data servers for two weeks, or since January
    - ✓ Forecast skill is improved using ML algorithm in post-processing step.
    - ✓ Now have realistic stratospheric ozone 5-day forecasts
- Emerging applications users, including:
  - NASA field missions (SCOAPE, FIREX-AQ, ACT-America, TRACER-AQ)
  - Daily alerts sent to NASA TOLNet lidar teams (Matt Johnson, NASA Ames)
  - TEMPO a priori for trace gas product

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Thank you!

Referred

Keller, C. A., Knowland, K. E., Duncan, B. N., Liu, J., Anderson, D. C., Das, S., et al. (2021). Description of the NASA GEOS composition forecast modeling system GEOS-CF v1.0. *Journal of Advances in Modeling Earth Systems*, 13, e2020MS002413. https://doi.org/10.1029/2020MS002413

Johnson, M. S., Strawbridge, K., Knowland, K. E., Keller, C., and Travis, M. (2021), Long-range transport of Siberian biomass burning emissions to North America during FIREX-AQ, *Atmos. Environ.*, 252, https://doi.org/10.1016/j.atmosenv.2021.118241.

Keller, C. A., Evans, M. J., Knowland, K. E., Hasenkopf, C. A., Modekurty, S., Lucchesi, R. A., Oda, T., Franca, B. B., Mandarino, F. C., Díaz Suárez, M. V., Ryan, R. G., Fakes, L. H., and Pawson, S. (2021), Global impact of COVID-19 restrictions on the surface concentrations of nitrogen dioxide and ozone, *Atmos. Chem. Phys.*, 21, 3555–3592, https://doi.org/10.5194/acp-21-3555-2021.

Dacic, N., Sullivan, J. T., Knowland, K. E., Wolfe, G. M., Oman, L. D., Berkoff, T. A., and Gronoff, G. P. (2020), Evaluation of NASA's high-resolution global composition simulations: Understanding a pollution event in the Chesapeake Bay during the summer 2017 OWLETS campaign, *Atmospheric Environment*, 117133, https://doi.org/10.1016/j.atmosenv.2019.117133.

Non-Refereed

Knowland, K. E., Keller, C. A. and Lucchesi, R. A. (2020), "File Specification for GEOS-CF Products." *GMAO Office Note No. 17 (Version 1.1), 37pp, available from http://gmao.gsfc.nasa.gov/pubs/office_notes*

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov