

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

K. Emma Knowland

Morgan State University/GESTAR-II

NASA Global Modeling and Assimilation Office (GMAO)

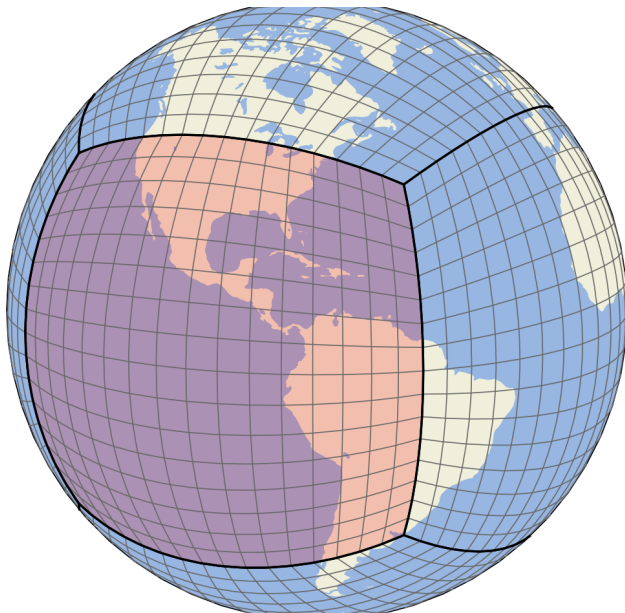
In collaboration with:

Christoph Keller, Pamela Wales, Larry Coy, Carl Malings, Kris Wargan, Callum Wayman, Brad Weir, Stephen Cohn, Lesley Ott, Steven Pawson

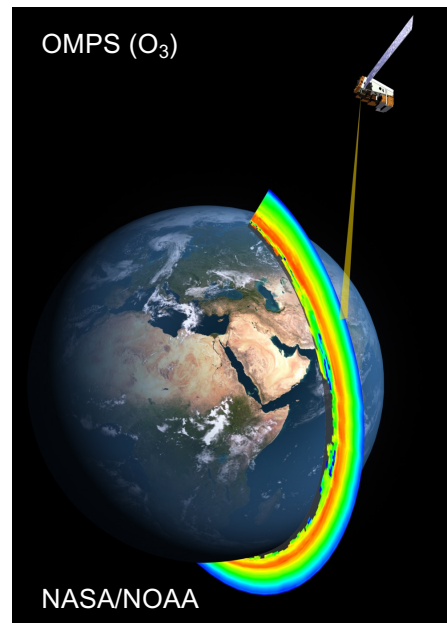
16 September 2022

NASA GMAO global meteorology and chemistry products

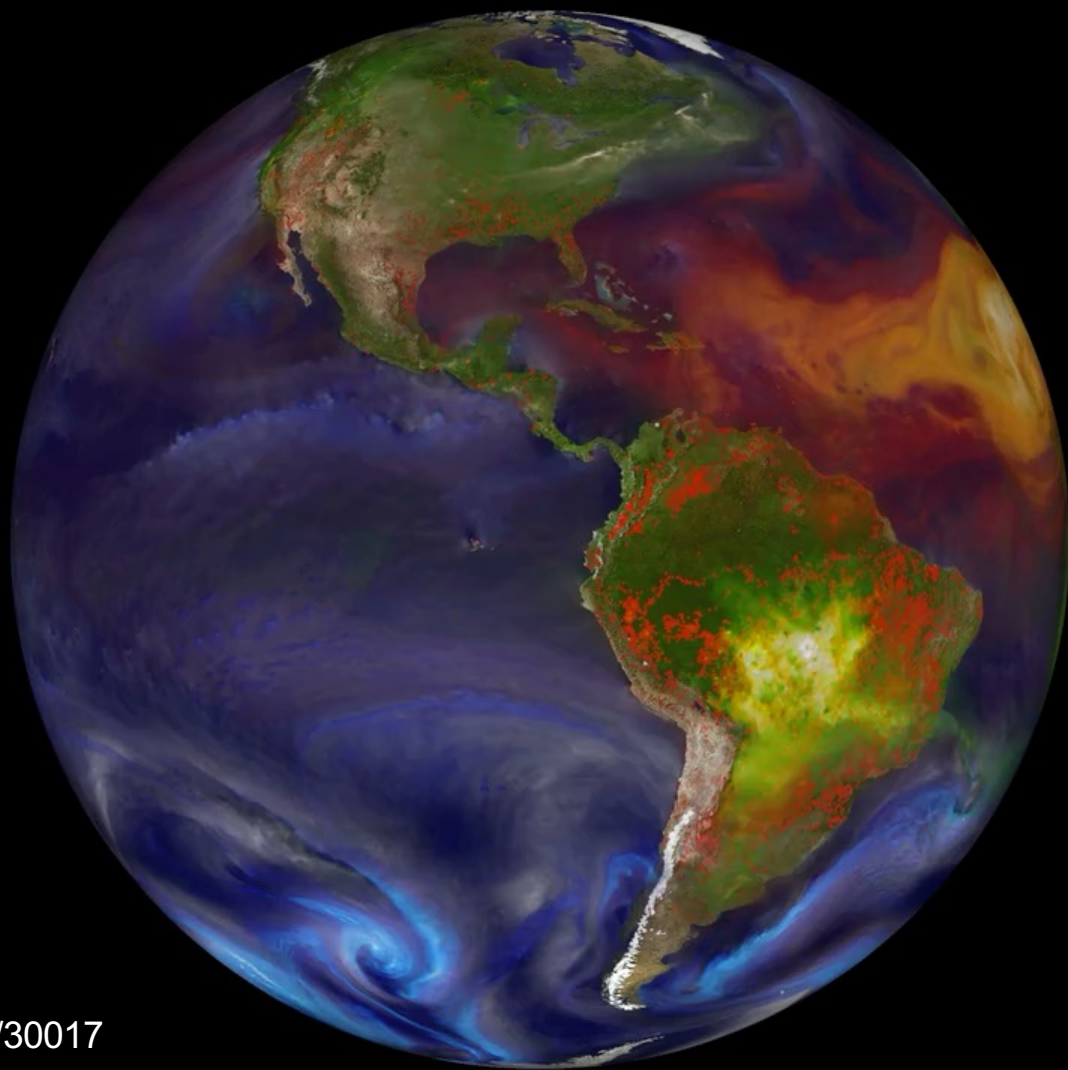
GEOS



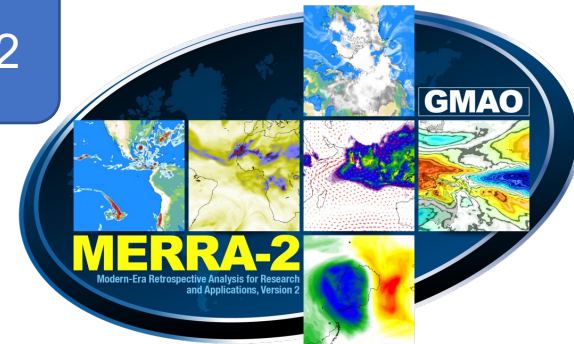
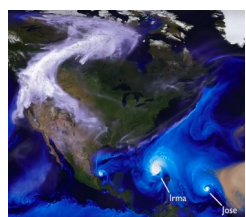
Bindle et al., 2021 GMD



www.nasa.gov



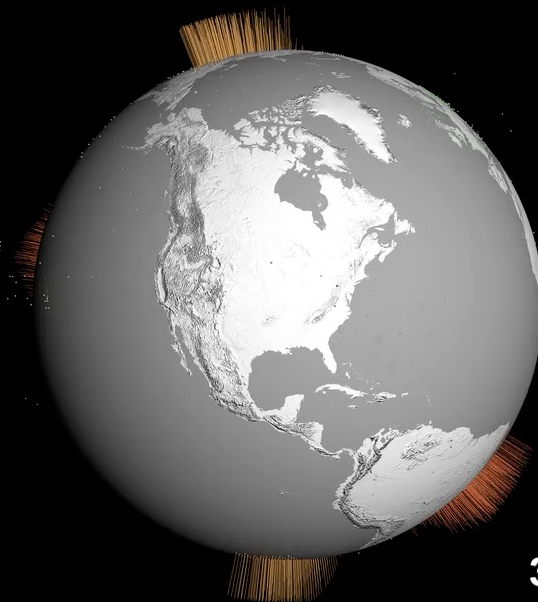
NASA GMAO global meteorology and chemistry products



Changes to the observing system

1980

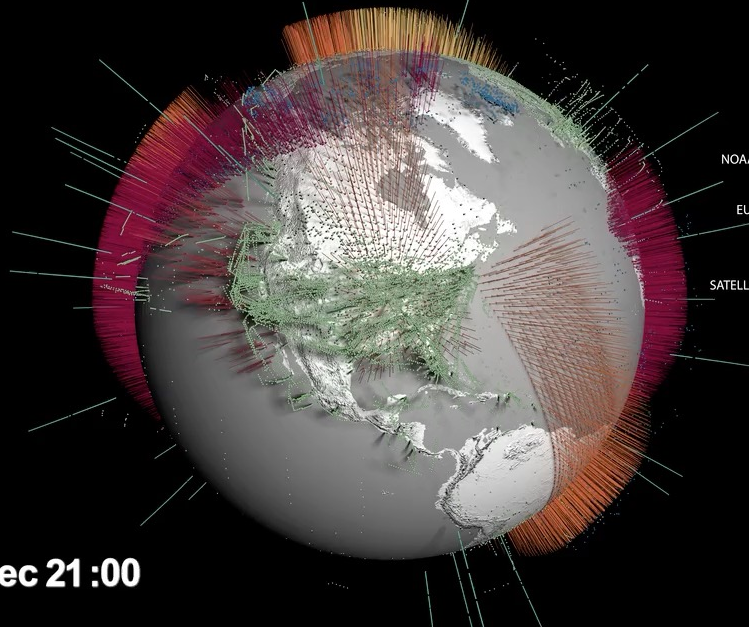
- NOAA POES
- NOAA/NASA TIROS-N
- CONVENTIONAL
- SATELLITE-DERIVED WINDS



31 Dec 21:00

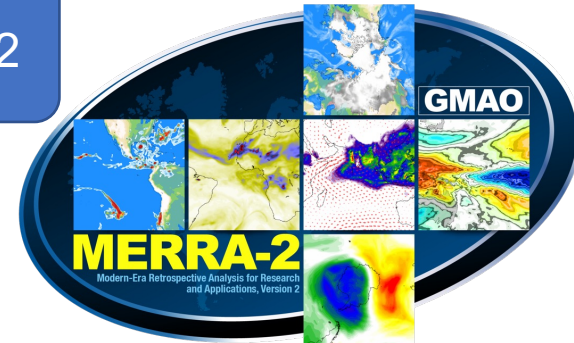
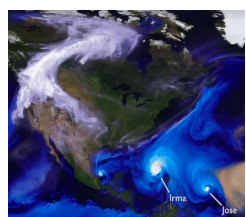
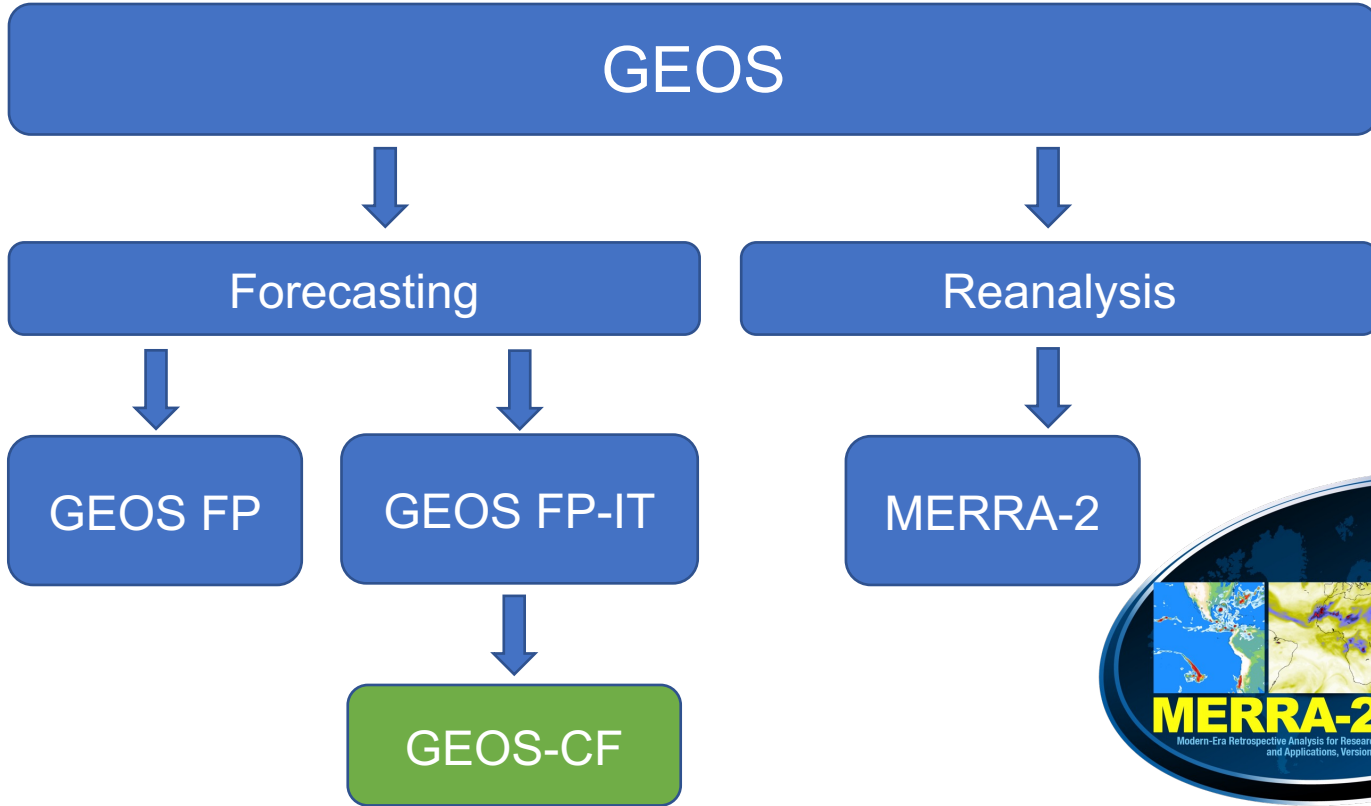
2018

- EUMETSAT METOP
- NOAA GOES
- NOAA POES
- NOAA/NASA SUOMI-NPP
- NASA EOS AQUA
- EUMETSAT METEOSAT
- CONVENTIONAL
- GPS
- SATELLITE-DERIVED WINDS

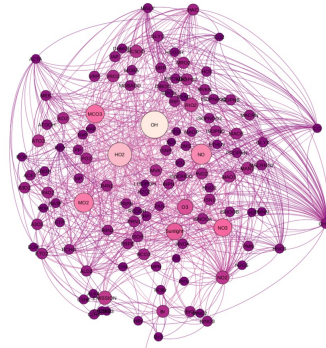
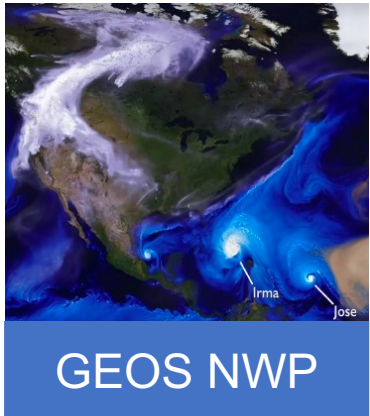


<https://svs.gsfc.nasa.gov/4654>

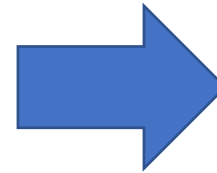
NASA GMAO global meteorology and chemistry products



GEOS Composition Forecast



GEOS-Chem



GEOS - CF

Version 12

Tropospheric and Stratospheric chemistry

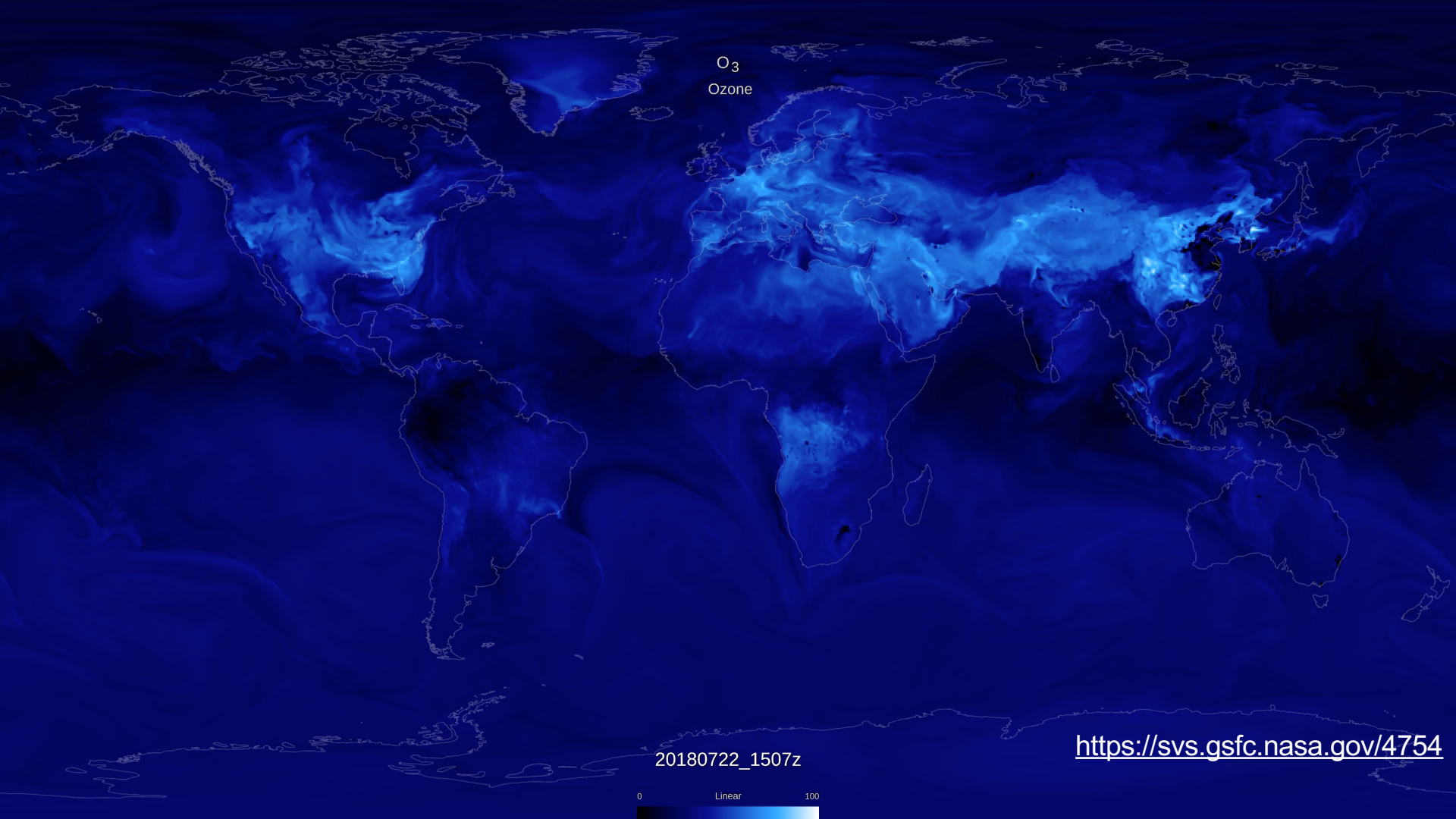
- 250 Chemical Species
- 725 Chemical Reactions



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



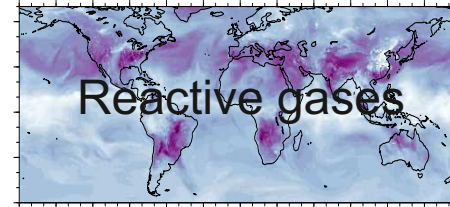
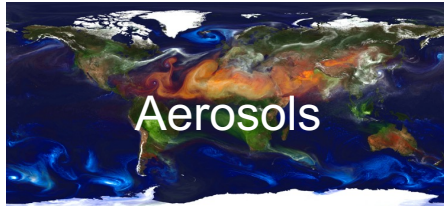
O₃
Ozone

20180722_1507z

<https://svs.gsfc.nasa.gov/4754>

0 Linear 100

Aerosol and Gas Phase Chemistry



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

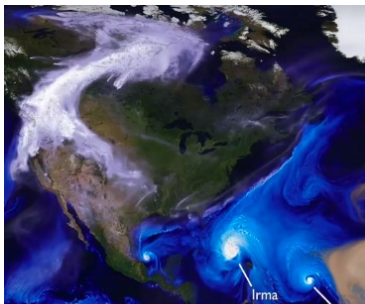
GOCART

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

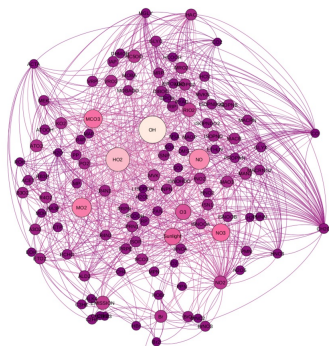
GEOS-Chem



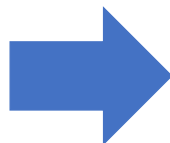
Daily composition forecast



GEOS NWP



GEOS - Chem

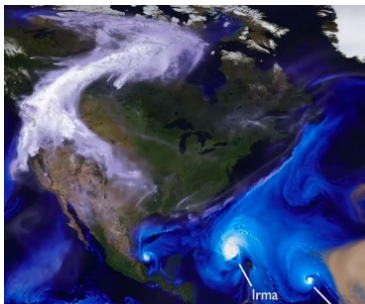


GEOS - CF

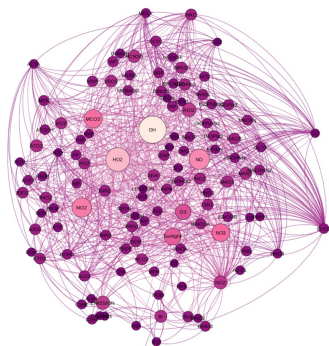
One **5-day forecast** per day



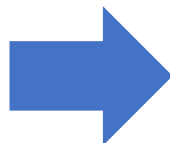
Daily composition forecast



GEOS NWP



GEOS - Chem

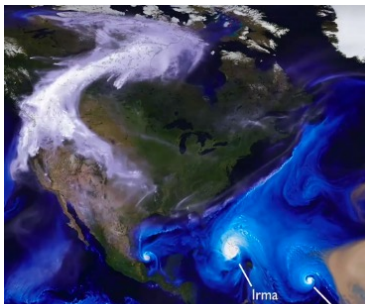


GEOS - CF

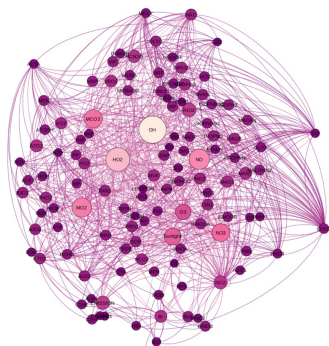
One **5-day forecast** per day

- 1-day meteorological replay
“analysis”
- 5-day forecast

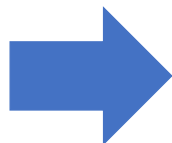
Daily composition forecast



GEOS NWP



GEOS - Chem

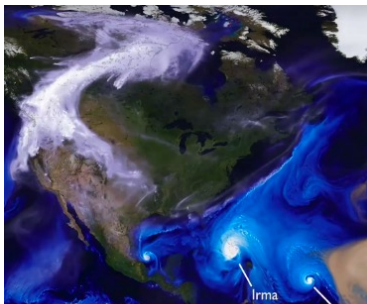


GEOS - CF

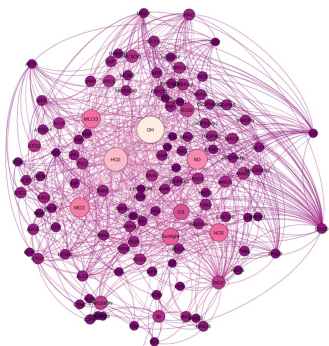
One **5-day forecast** per day

- 1-day replay
- 5-day forecast
- c360 (0.25° , $\sim 25 \times 25 \text{ km}^2$) resolution, 72 model layers

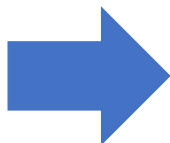
Daily composition forecast



GEOS NWP



GEOS - Chem

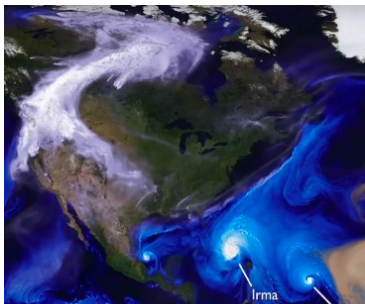


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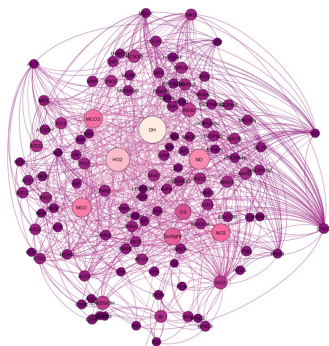
One **5-day forecast** per day

- 1-day replay
- 5-day forecast
- c360 (0.25° , **$\sim 25 \times 25 \text{ km}^2$**) resolution, 72 model layers
- O_3 , NO_x , VOCs, PM ...
- T, U, V, RH

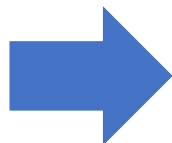
Daily composition forecast



GEOS NWP



GEOS - Chem

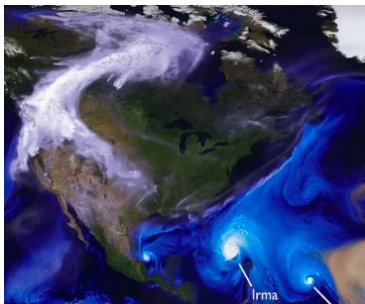


GEOS - CF

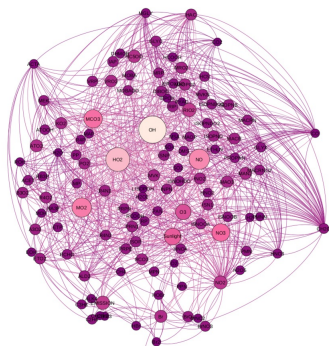
One **5-day forecast** per day

- 1-day replay
- 5-day forecast
- c360 (0.25° , $\sim 25 \times 25 \text{ km}^2$)
- **15 minute** “surface”
- **1-hour** average and instantaneous 2D & 3D

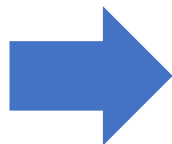
Daily composition forecast



GEOS NWP



GEOS - Chem



GEOS - CF

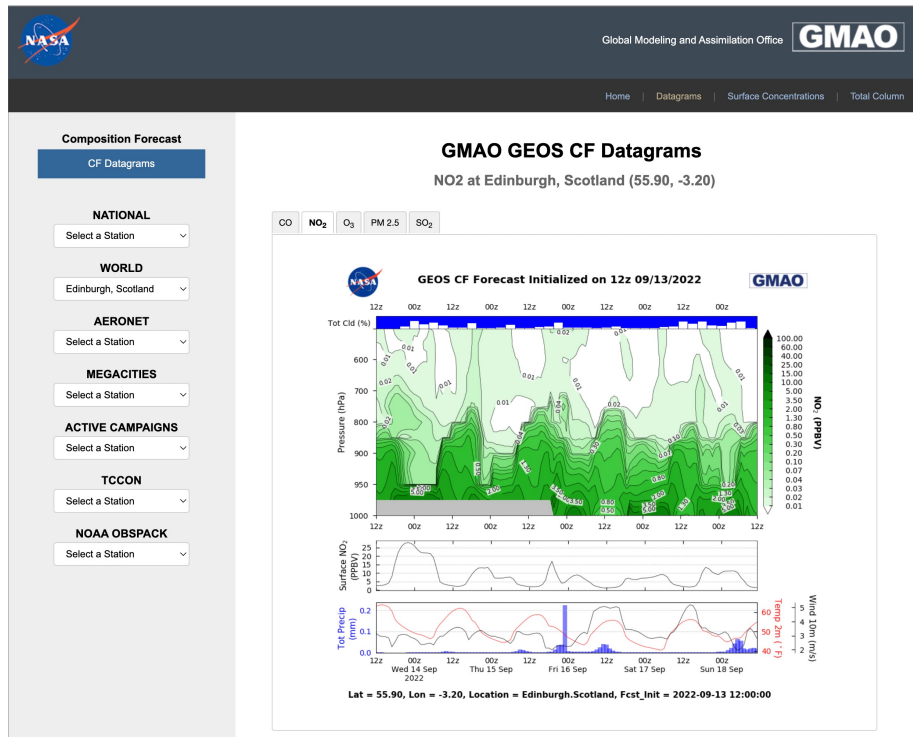
One **5-day forecast** per day

- 1-day replay
- 5-day forecast
- c360 (0.25° , $\sim 25 \times 25 \text{ km}^2$)
- **Available since**
 - 1 January 2018** (replay)
 - 1 January 2019** (forecast)

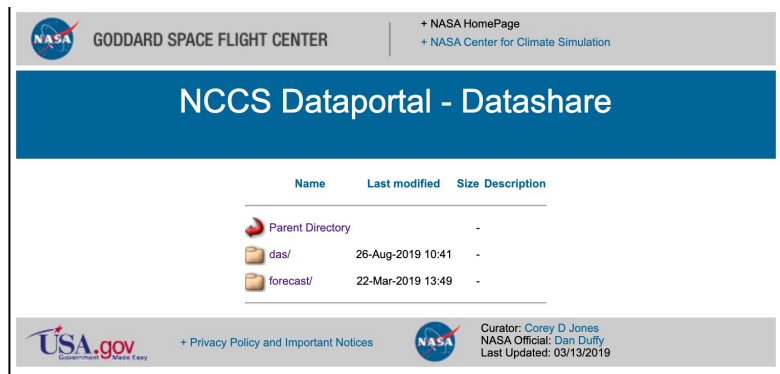
GEOS-CF are available online in near real-time

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

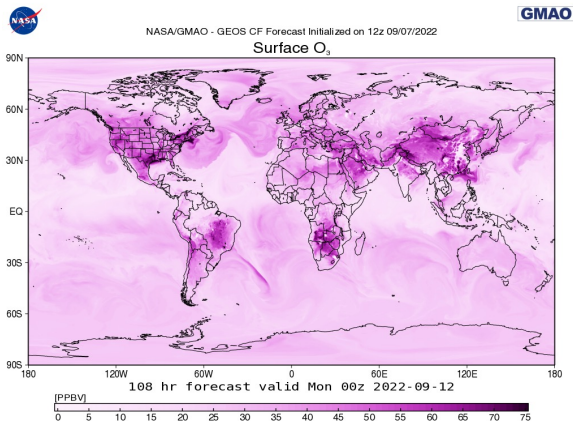
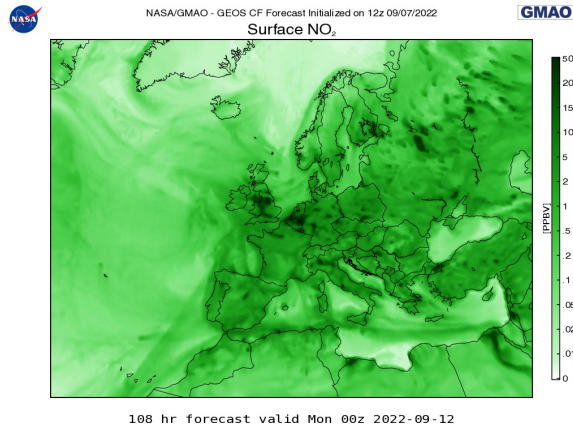
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Latitude: -90.000000000000°N to 90.000000000000°N (721 points, avg. res. 0.25°)
Altitude: 72.000000000000 to 72.000000000000 (1 points)
Time: 00:30Z01JAN2018 to 11:30Z31OCT2019 (16044 points, avg. res. 0.042 days)
Variables: (total of 52)
xyle xylene (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 peroxyntic 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

GEOS-CF output is available online in near real-time



Fluid is a mobile-friendly website

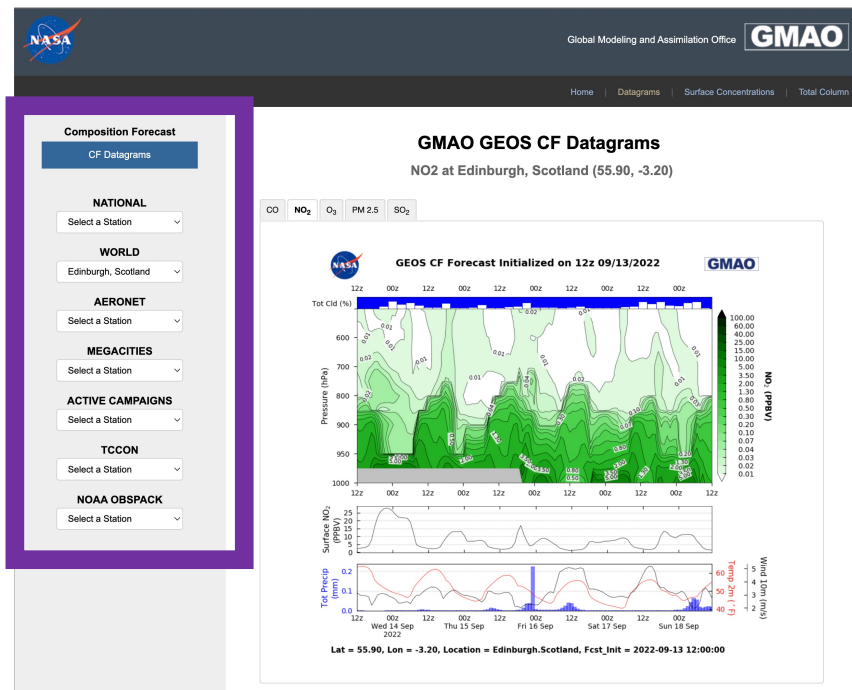
<https://fluid.nccs.nasa.gov/cf/>



GEOS-CF output is 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/>

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forecast/	22-Mar-2019 13:49	-	-

USA.gov | Privacy Policy and Important Notices | Curator: Corey D Jones, NASA Official: Dan Duffy, Last Updated: 03/13/2019

<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](#)

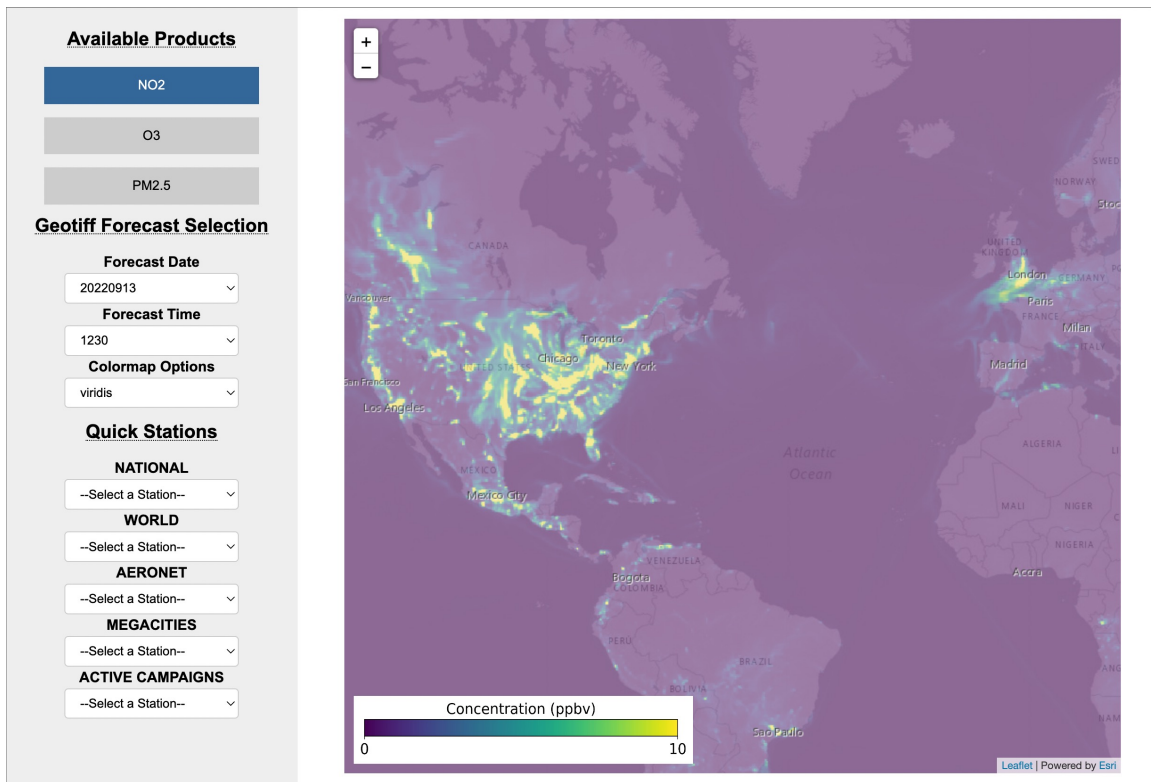
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pm25su_rh35_gcc sulfate_particulate_matter_with_diameter_below_2.5_um_rh_35

GEOS-CF output is available online in near real-time

On-demand Forecast Imagery with cf_map tool

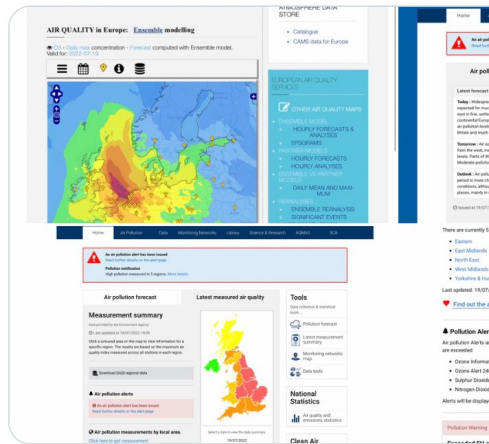
https://fluid.nccs.nasa.gov/cf_map/





Clean Air in London
@CleanAirLondon

Towards the end of 7-long-days, w
to @LondonAir @MayorofLondon 1
ozone #AirPollution alert and the i
@CopernicusECMWF @Copernicu
predicting the #PollutionBomb clip
England today. Thank you



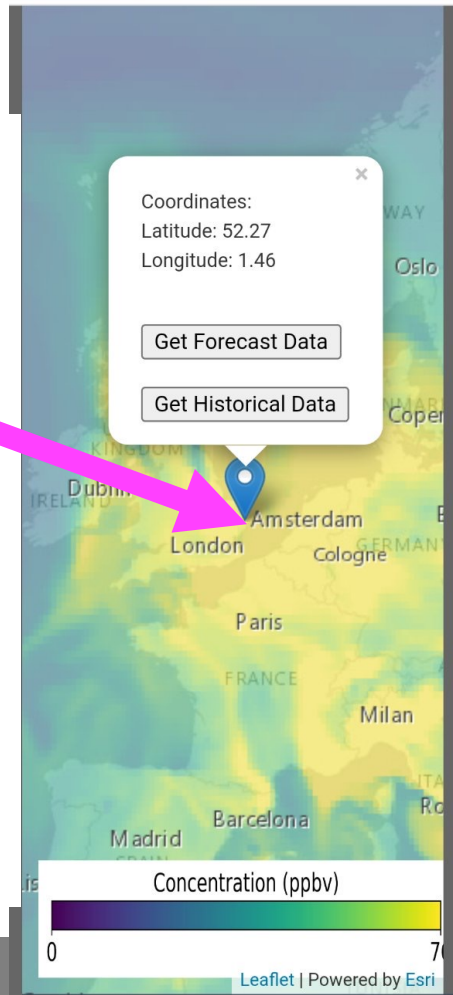
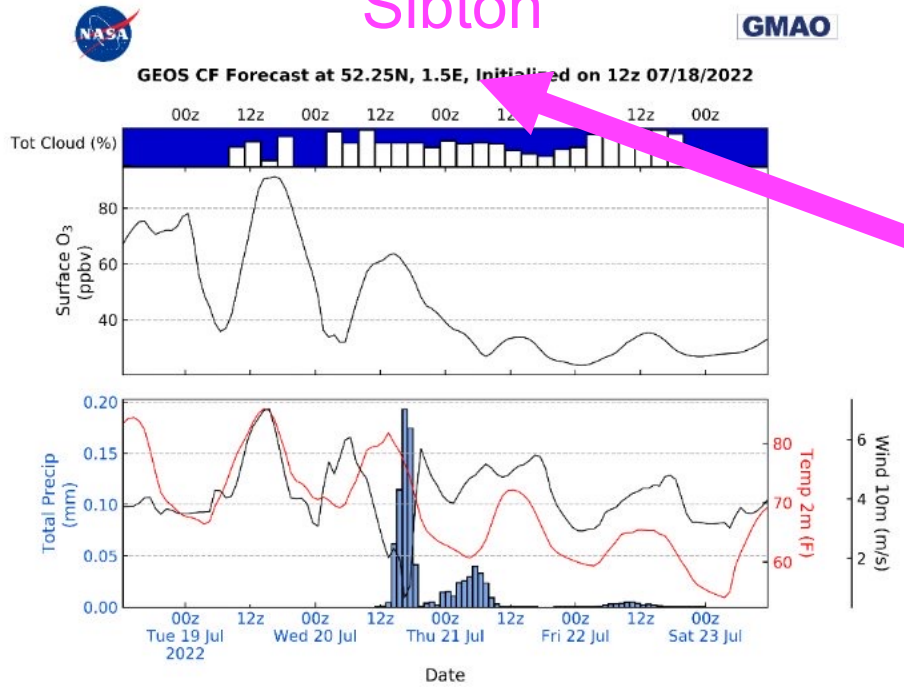
8:41 PM · Jul 19, 2022 · Twitter for iPad

4 Retweets 1 Quote Tweet 6 Likes



Global Modeling and Assimilation Office
gmao.gsfc.nasa.gov

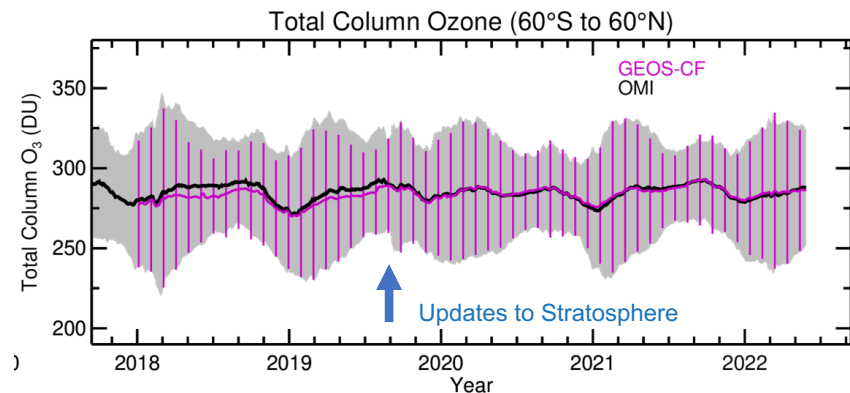
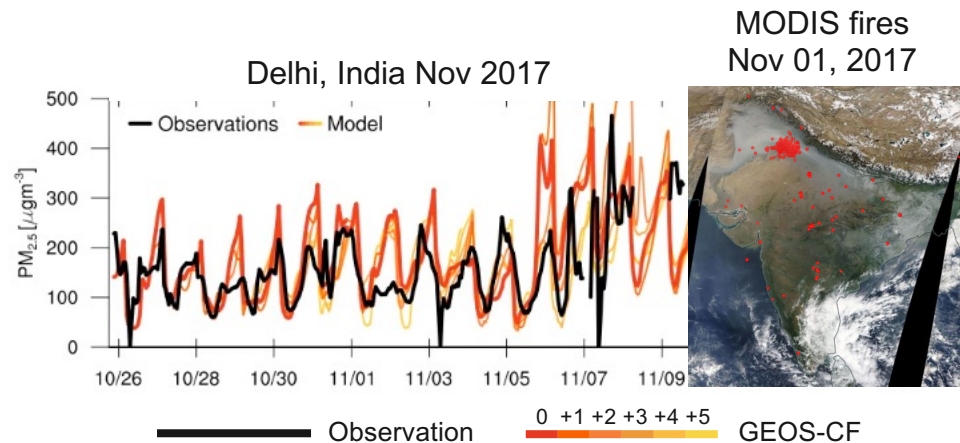
Sibton



Near-real time updates from satellite data

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

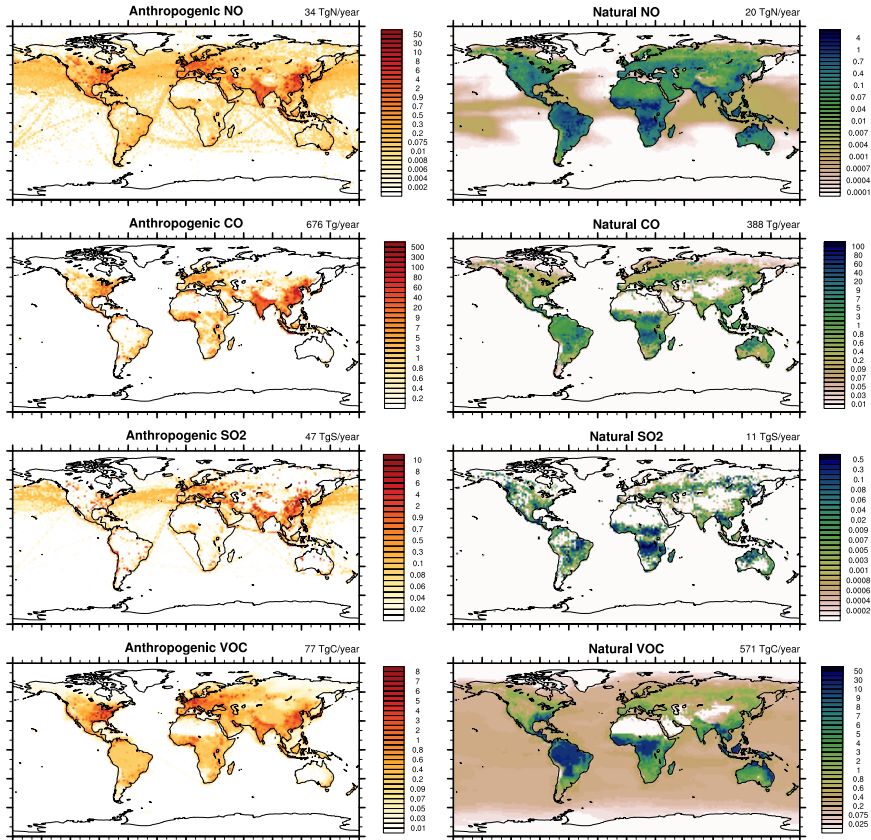
- GEOS-CF Stratospheric O_3 is weakly nudged to the GEOS FP assimilated O_3



Knowland et al., 2022,
JAMES

Currently developing direct data assimilation of tropospheric constituents into GEOS

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 NO_x: online (Hudman et al. 2012)

Dust: online (Zender et al. 2003)

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

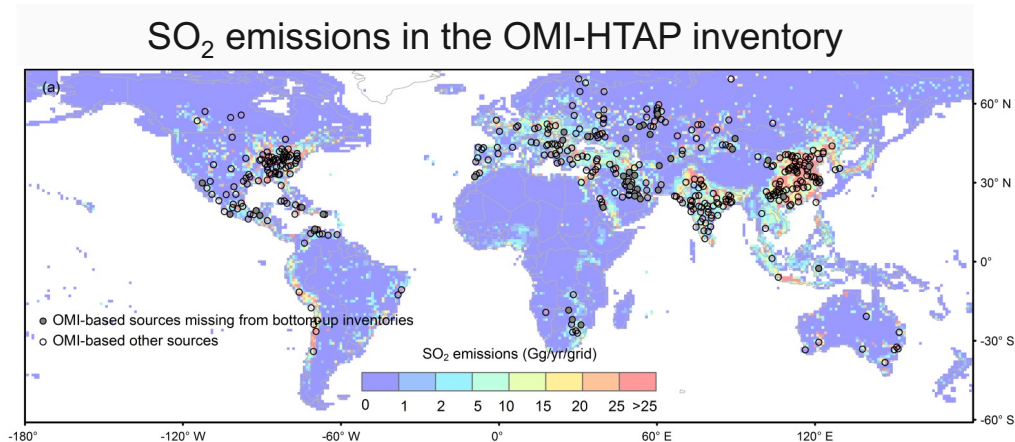
Ocean: online: sea salt, DMS, acetone, acetaldehyde, HOI, I₂

Prescribed: CFCs, VSLs, CH₄, CO₂

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 SO₂ (Liu et al., 2018).
- “Business-as-usual” assumed for 2020 and 2021

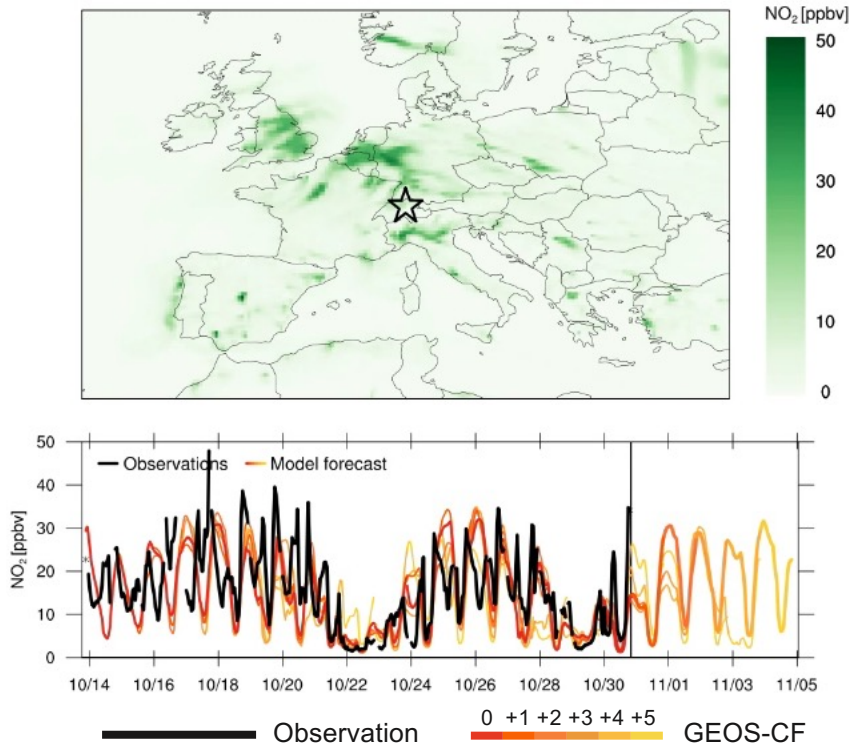


A new emission inventory, OMI-HTAP, combines OMI-based SO₂ emissions for large sources and the bottom-up inventory, HTAP, for smaller sources.

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

Daily variations of emissions

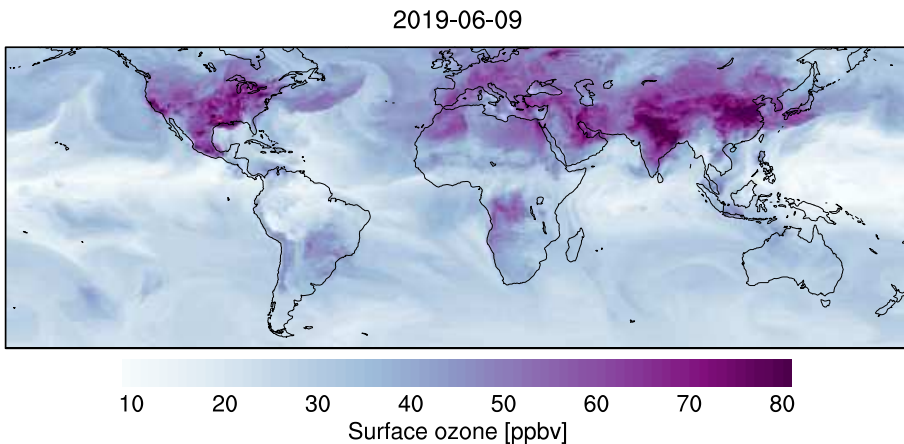
Zurich, Switzerland, 2017-10-30 22:45 UTC



- Scale factors applied to emissions for diurnal and weekly variations
- These are clearly beneficial for surface NO₂ analyses and forecasts
- Shown for Zurich - weather and diurnal/weekly signals are prominent
- Surface observations obtained through emerging connection to OpenAQ (openaq.org)

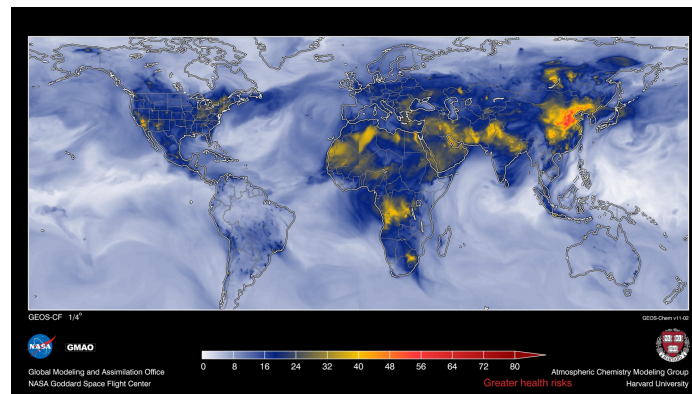
Air quality and health applications

➤ How good is the model?



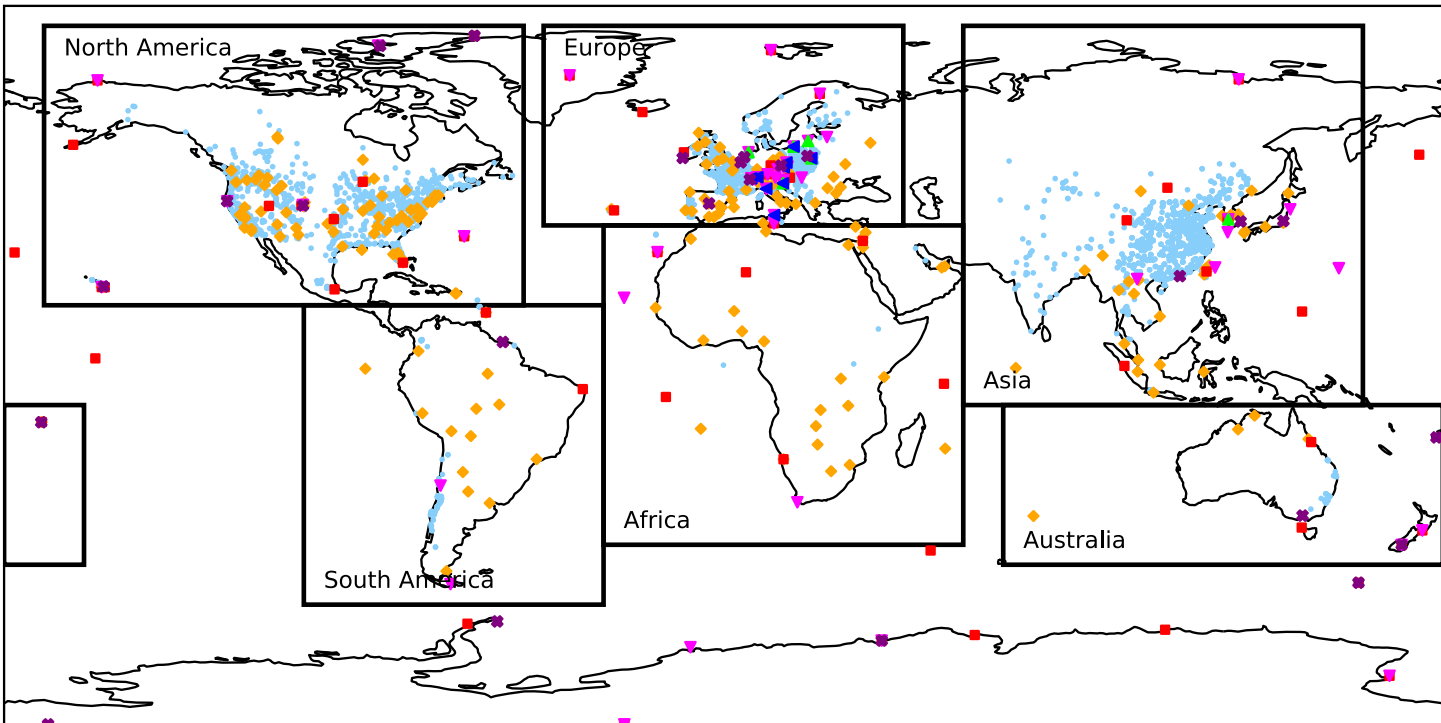
Optimize model predictions

➤ How bad is the air pollution?



Global exposure assessment

Observations for evaluation

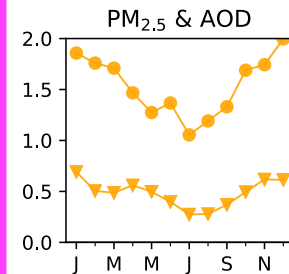
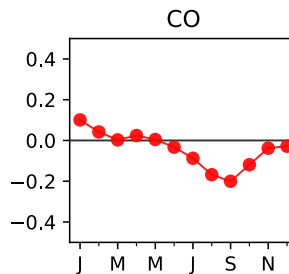
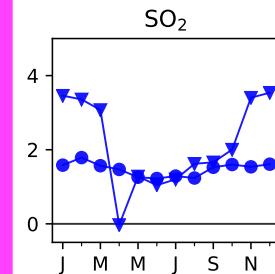
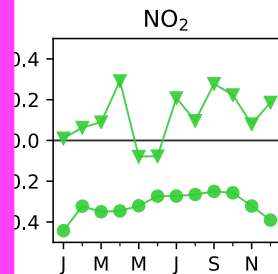
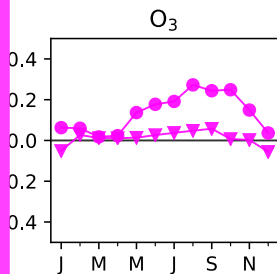


● OpenAQ
 ◆ Aeronet
 ■ WDCGG CO
 ▼ WDCRG O₃
 ▲ WDCRG NO₂
 ◄ WDCRG SO₂
 ✱ Ozonesonde

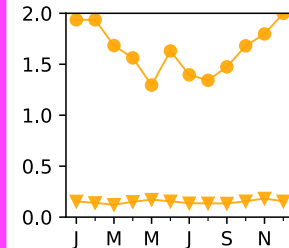
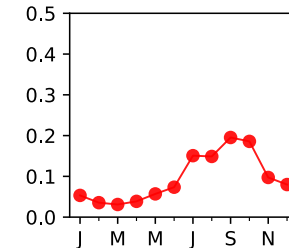
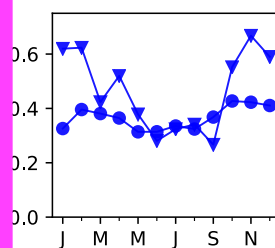
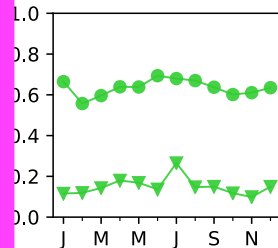
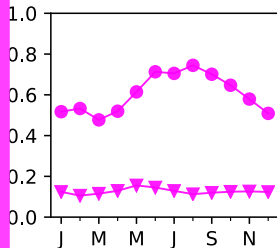
Keller et al., 2021 JAMES

Global surface comparisons - monthly

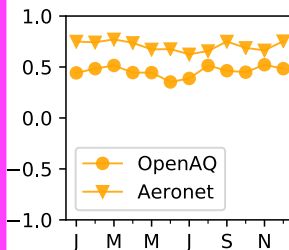
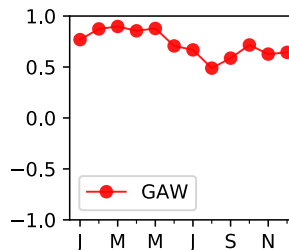
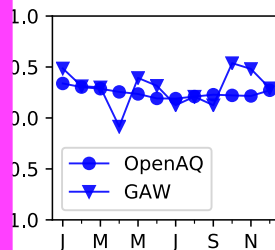
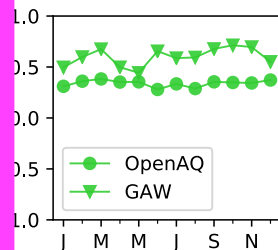
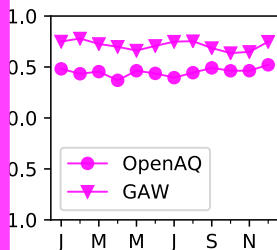
Normalized
Mean Bias
(NMB)



Normalized
Root Mean
Square Error
(NRMSE)

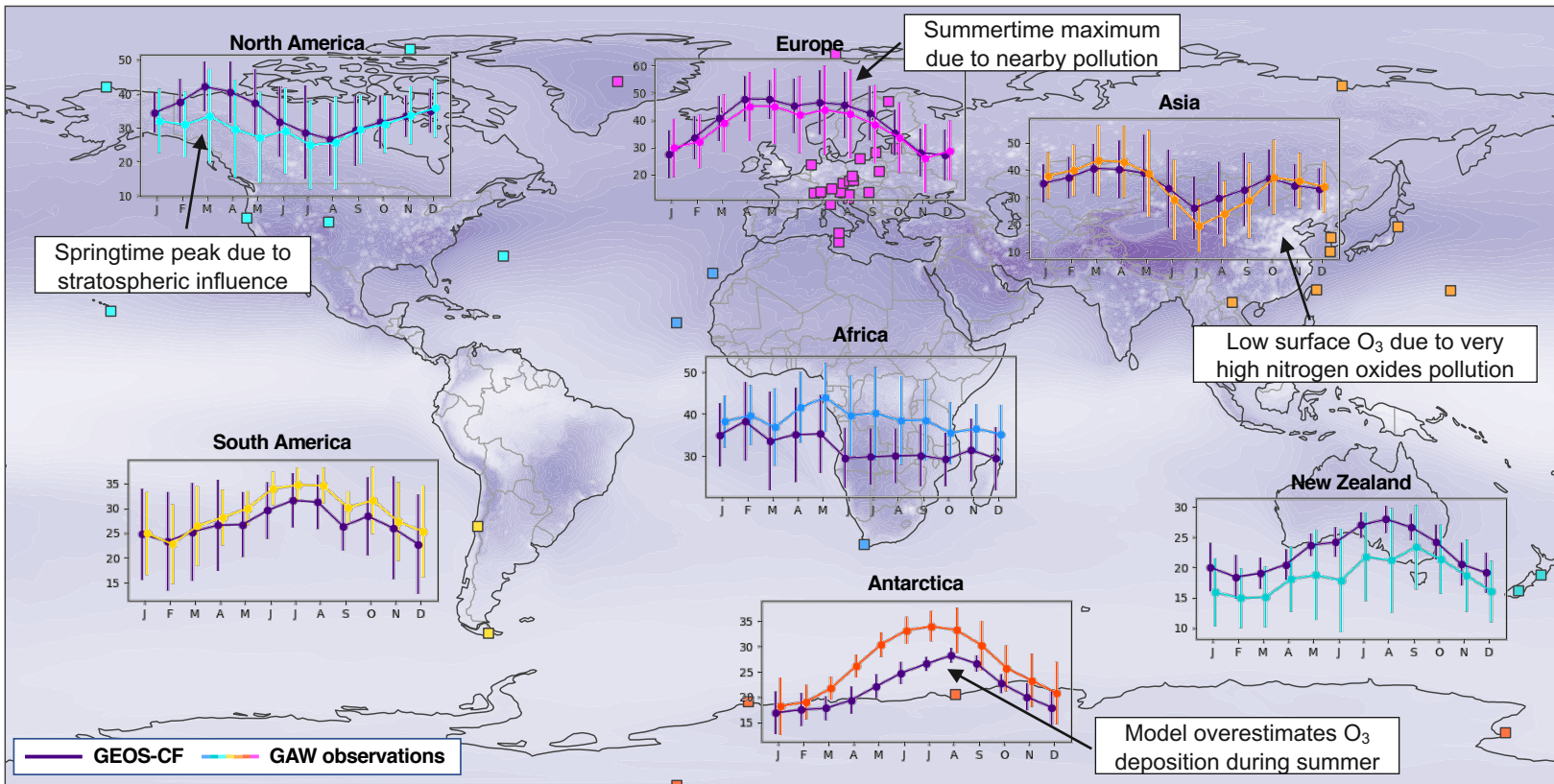


Pearson
Correlation
Coefficient
(R)



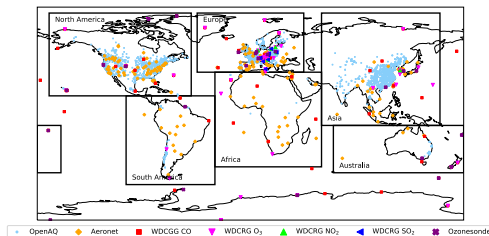
Keller et al., 2021 JAMES

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

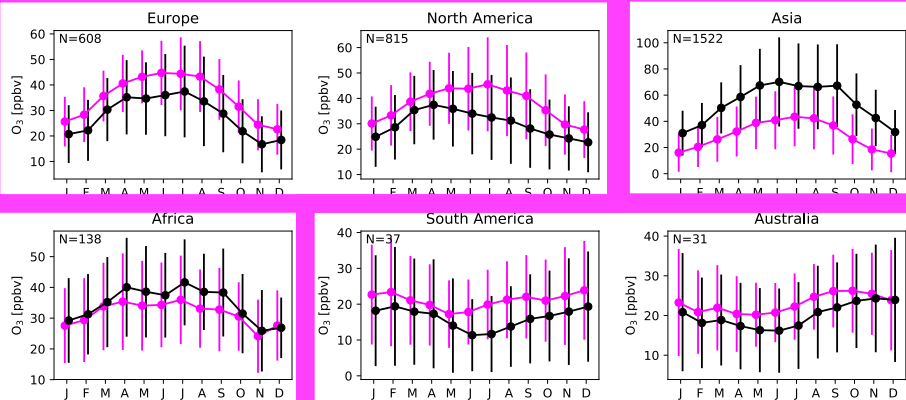




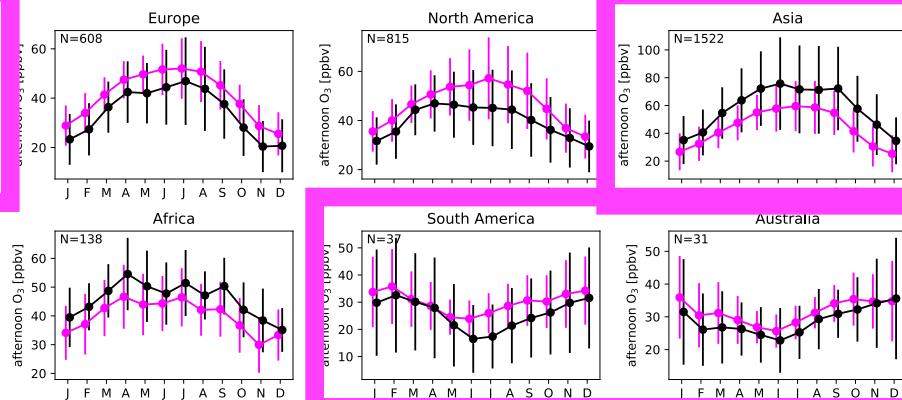
Surface O₃ (OpenAQ sites only)



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.

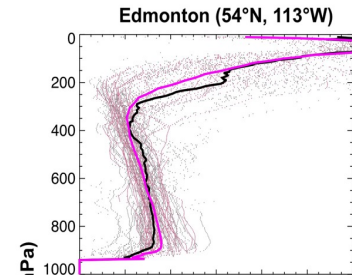
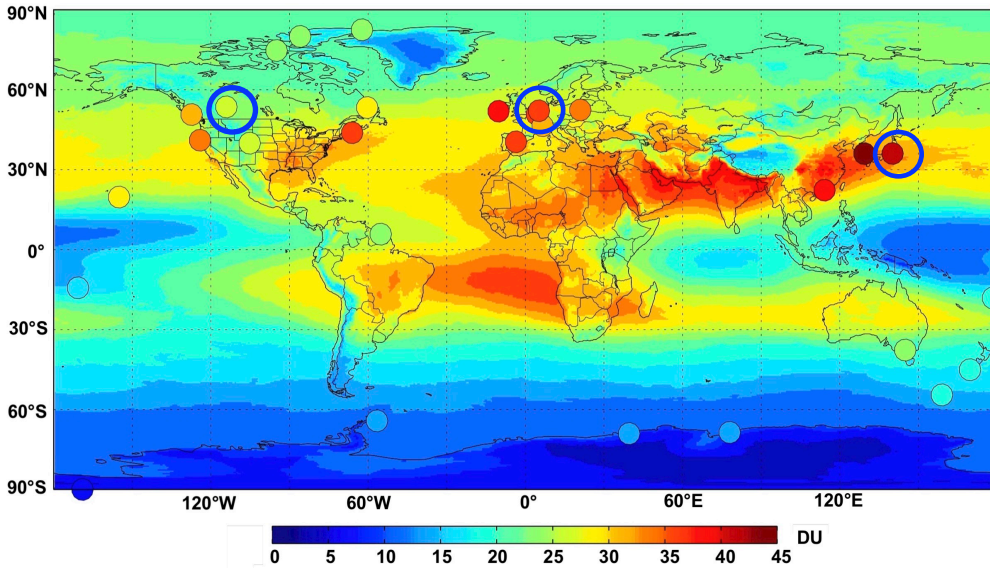
- In polluted regions, such as Asia, the bias is reduced when focusing on peak photochemical production period. GEOS-CF still has a bias over US during summer and fall, a known GEOS-Chem issue (Travis et al., 2016;2019; Hu et al., 2018).

■ Observations ■ GEOS-CF

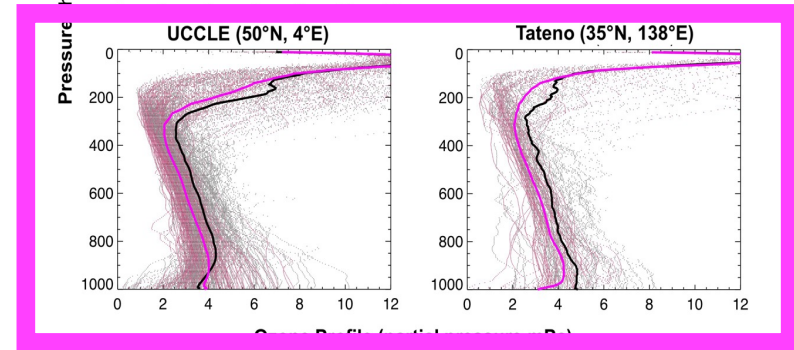
Keller et al., 2021 JAMES

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

2018 Tropospheric O₃ column (TOC): GEOS-CF and sondes



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



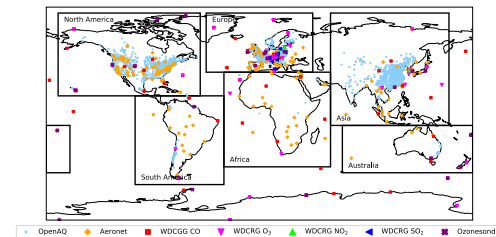
■ Sondes ■ GEOS-CF

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

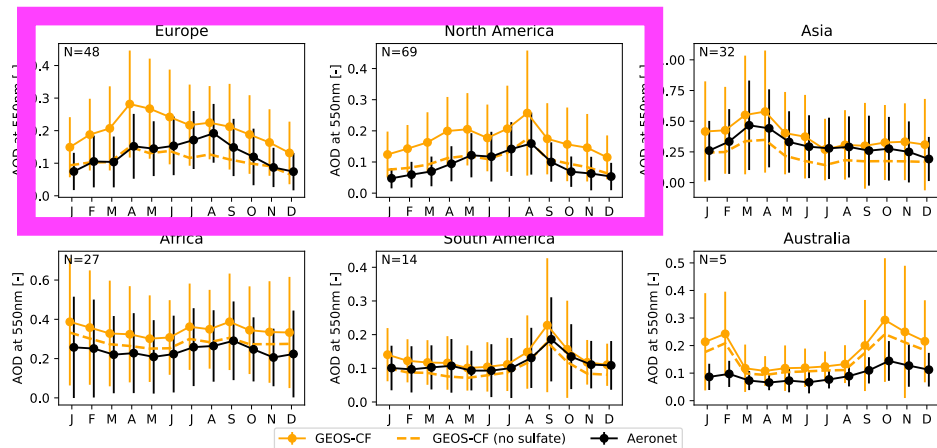
- GEOS-CF captures the overall spatial distribution of ozonesonde TOC, but with underestimates over polluted regions (e.g. sites over eastern US, Europe, east Asia).

Figures courtesy of Junhua Liu

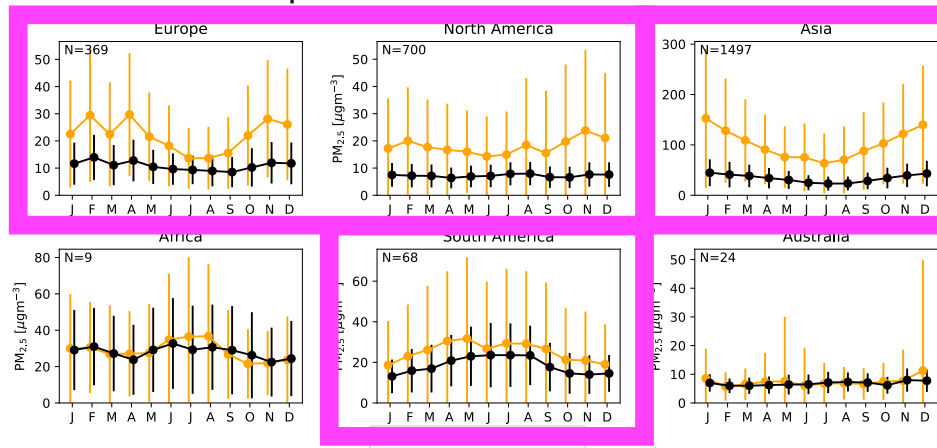
GEOS-CF generally overestimates aerosols (AOD and PM_{2.5})



AOD from Aeronet network



PM_{2.5} from OpenAQ database



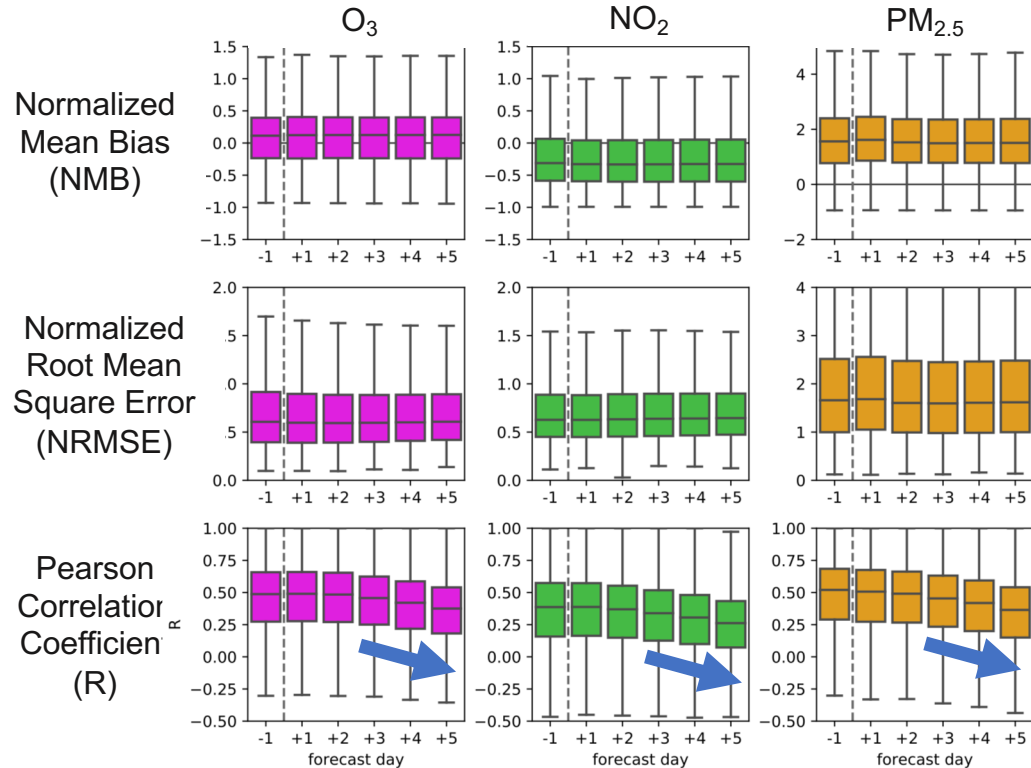
- GEOS-CF overestimates AOD 550 nm at most Aeronet sites. This is likely due to the overestimation of sulfates in the model.

- Similarly, GEOS-CF PM_{2.5} is overestimated in Europe, North America, Asia and South America.

■ Observations ■ GEOS-CF

Keller et al., 2021 JAMES

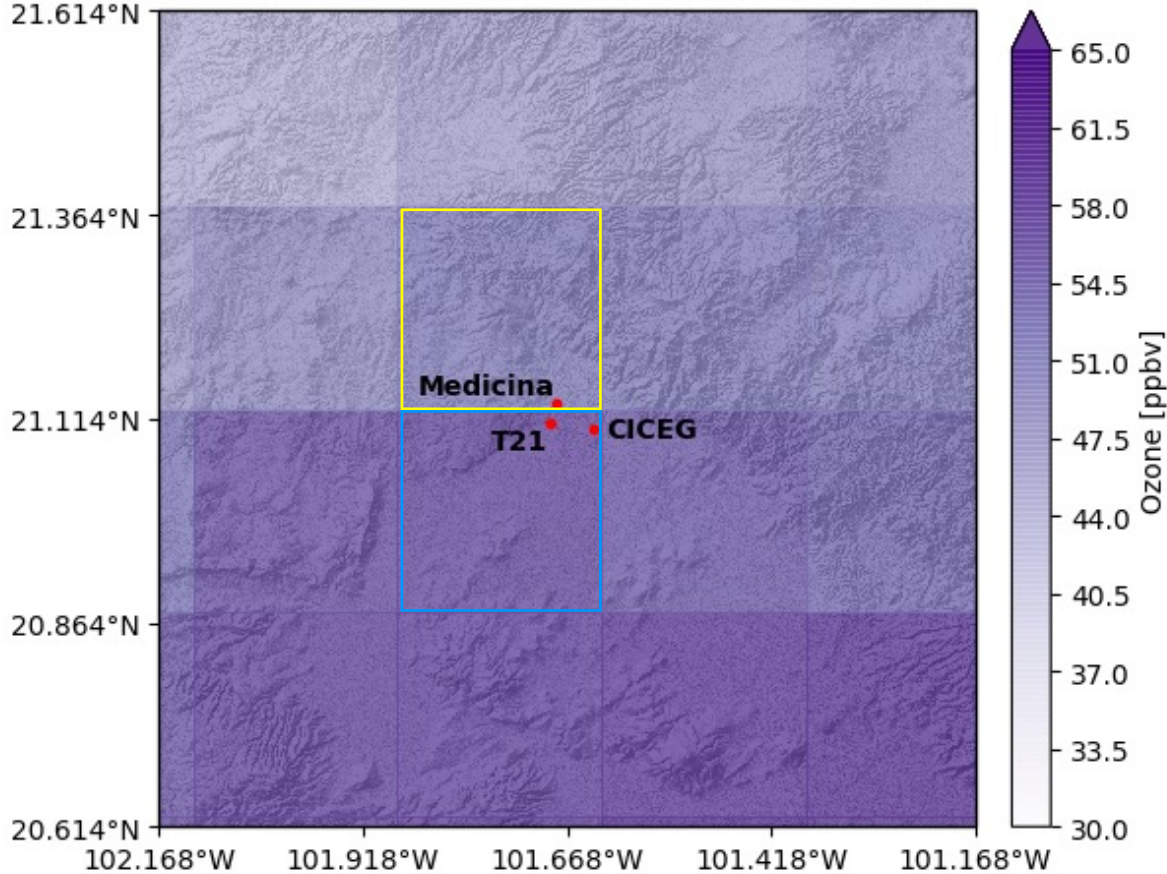
GEOS CF Forecast skill (GAW and OpenAQ)



- 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.

Keller et al., 2021 JAMES

2019-09-18 11:00 local time

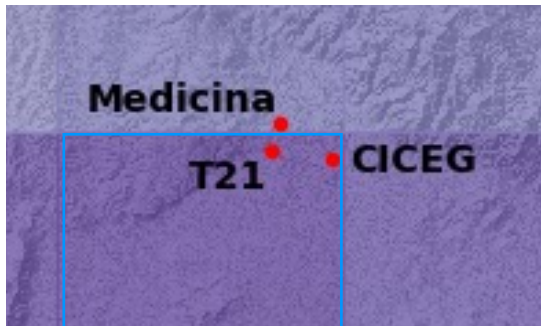


Improve local forecasts using statistical bias correction

3 monitoring stations in Leon, Mexico

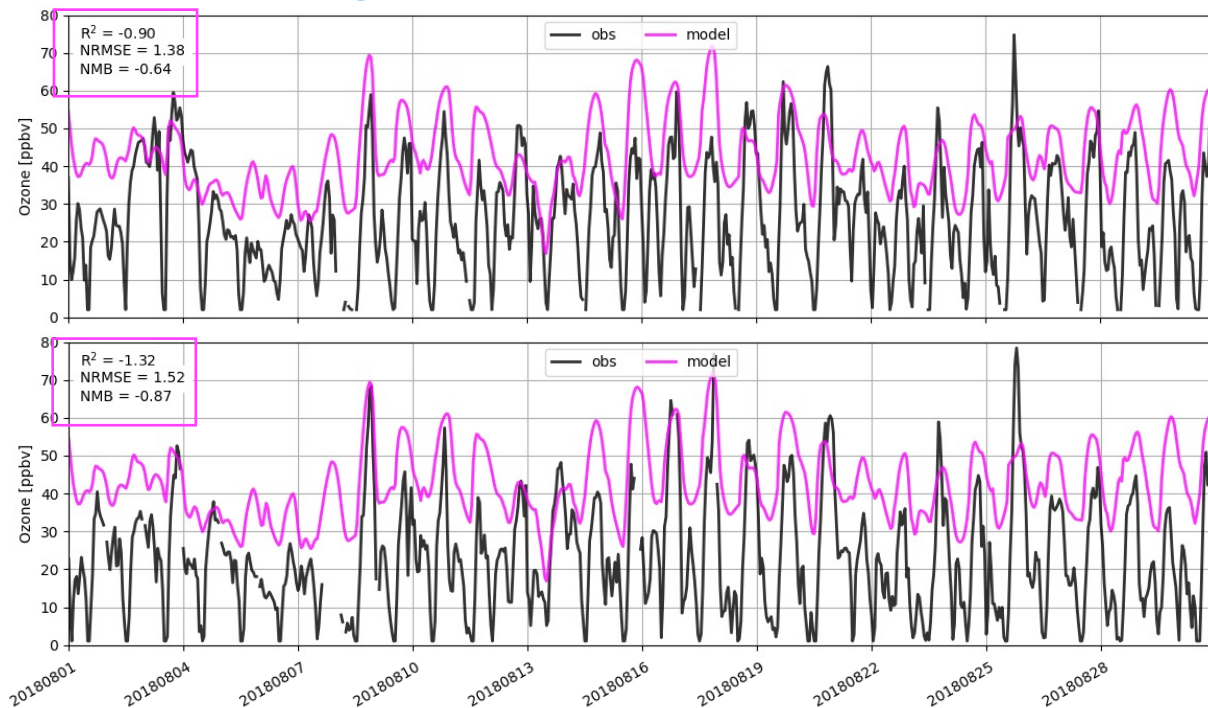
- 1 in one grid box
- 2 share a grid box
- Difficult terrain within each grid box

Improve local forecasts using statistical bias correction



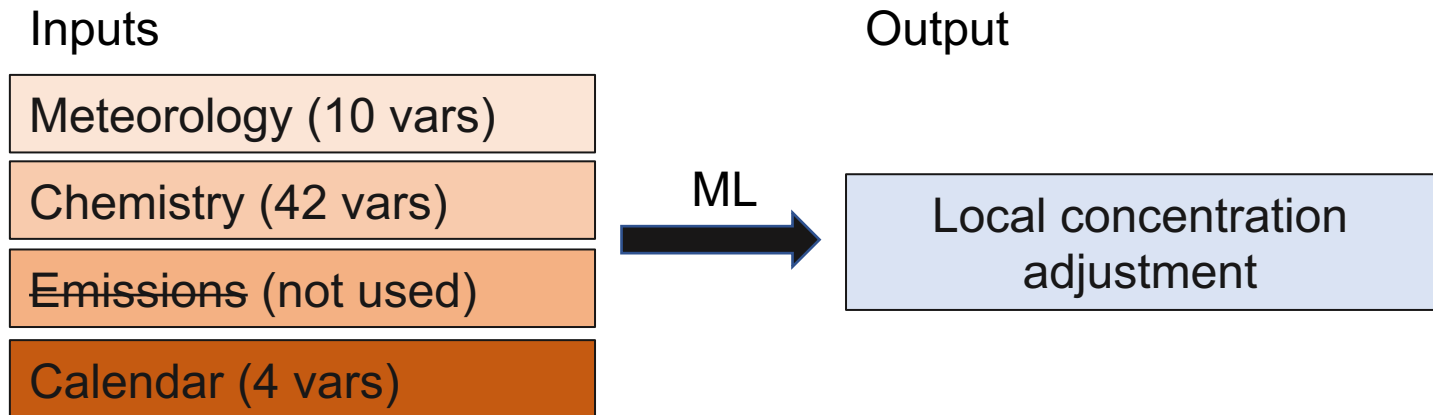
Two observation sites in the same grid box

- GEOS-CF generally overestimates



Observations Model

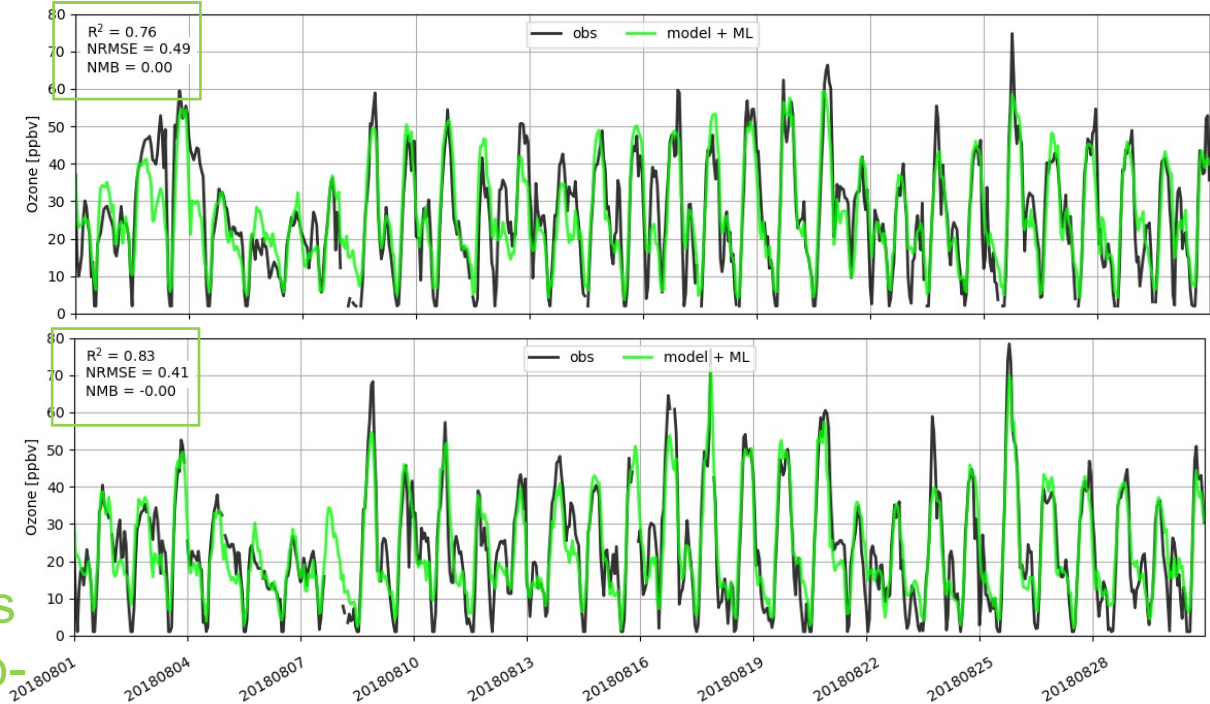
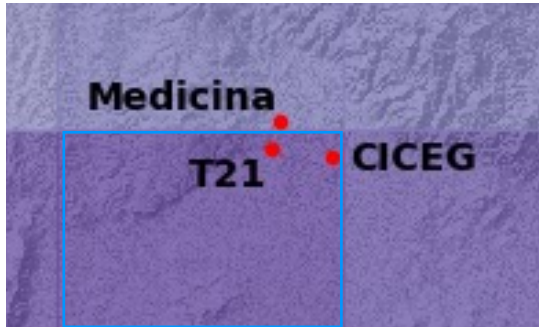
Use machine learning to correct for small scale variability and/or model biases



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

Keller et al., 2021 ACP

Improve local forecasts using statistical bias correction

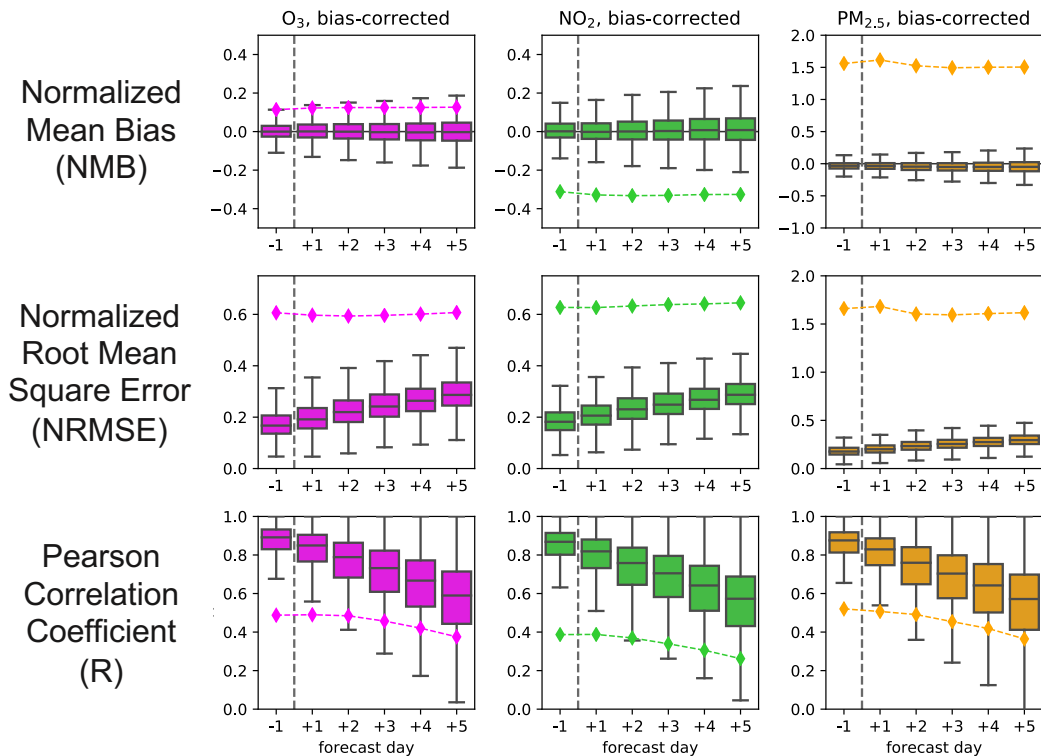


Two observation sites in the same grid box

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

Observations **Model + ML**

GEOS CF Forecast skill



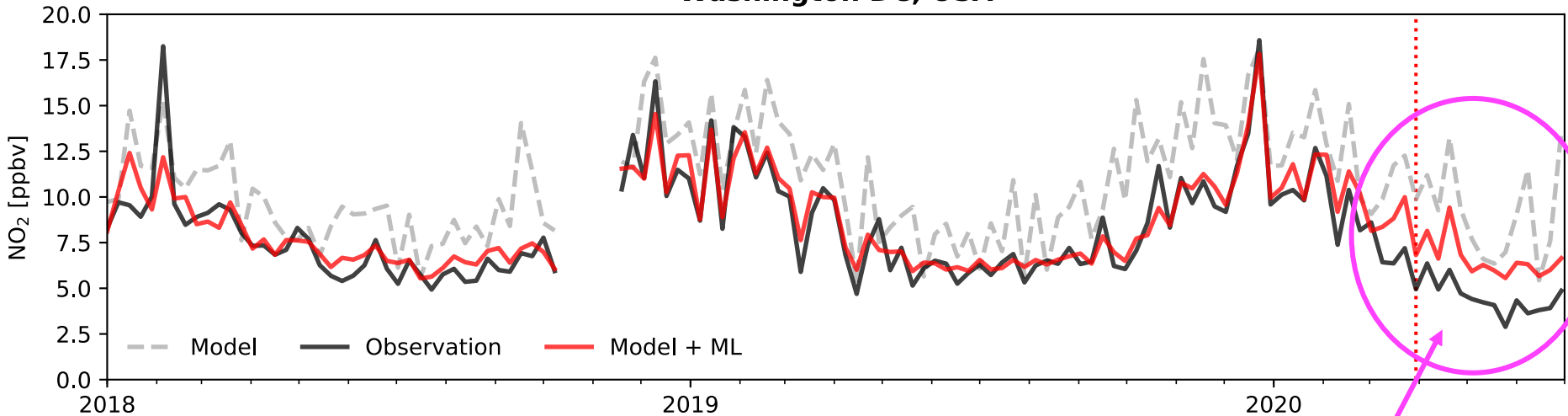
- ✓ Using a Machine Learning (ML) algorithm to calculate bias-correction term for each monitoring site can drastically improve the forecast skill at the individual locations

Keller et al., 2021 JAMES



New application of the GEOS-CF ML algorithm

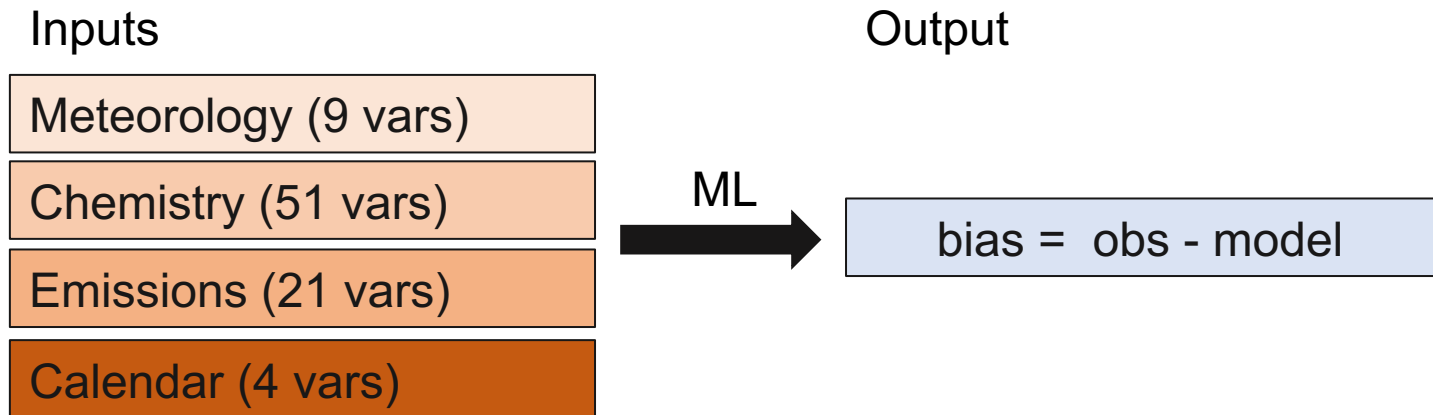
Washington DC, USA



Impact of COVID-19 restrictions

Keller et al., 2021 ACP

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

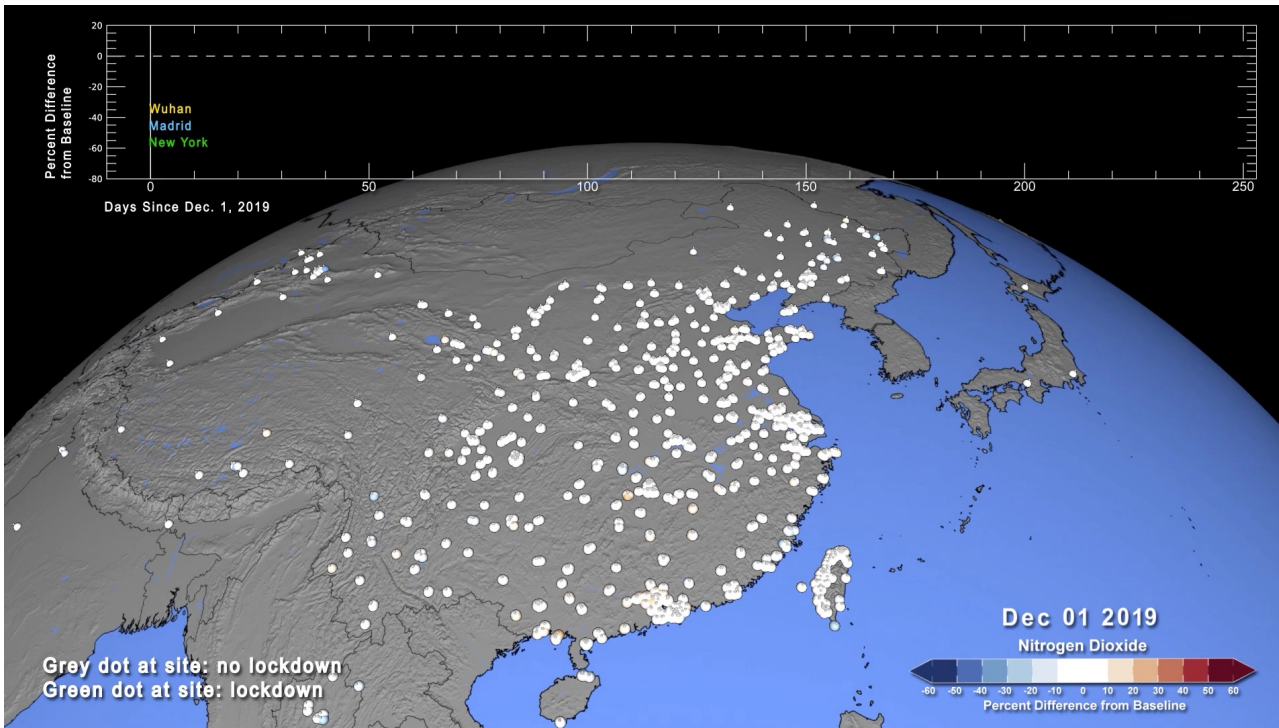


- Algorithm: gradient boosted decision trees (XGBoost)
- Training: 2018-2019 (8-fold cross validation)

Keller et al., 2021 ACP



Apply analysis to 5756 sites worldwide



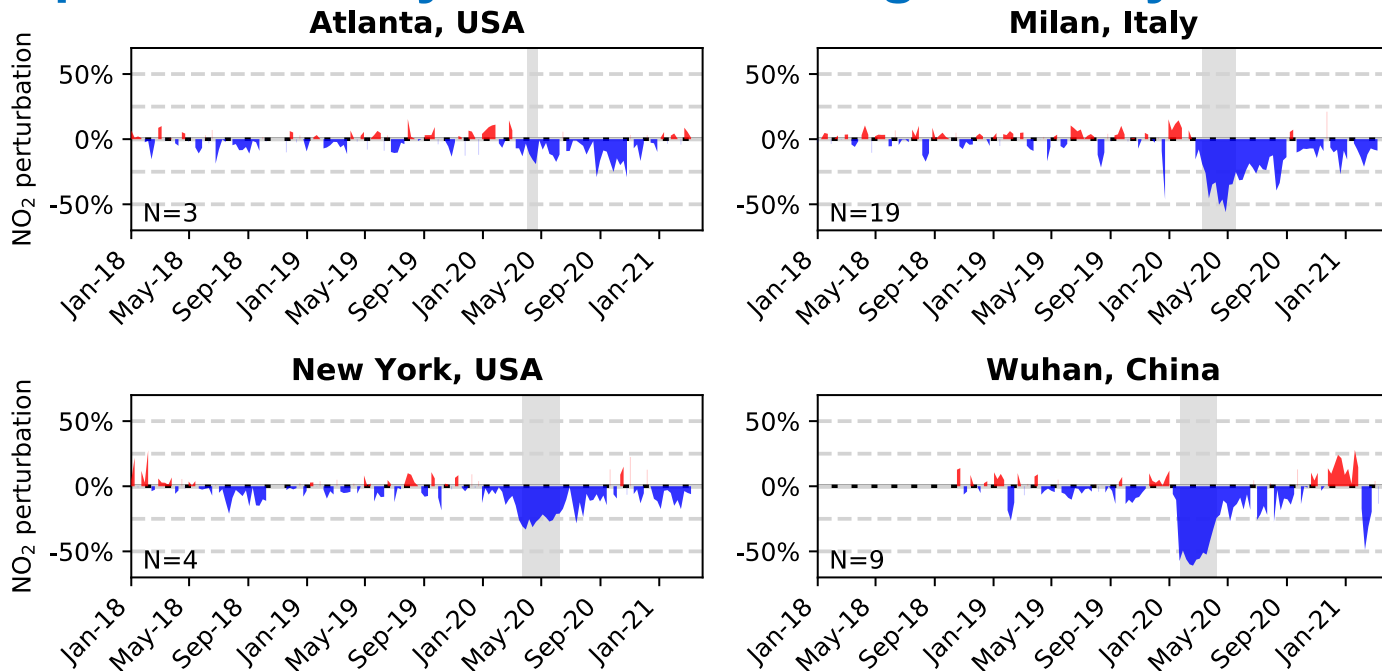
<https://svs.gsfc.nasa.gov/13753>

<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>



Observation-model differences indicate city-wide NO₂ 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>

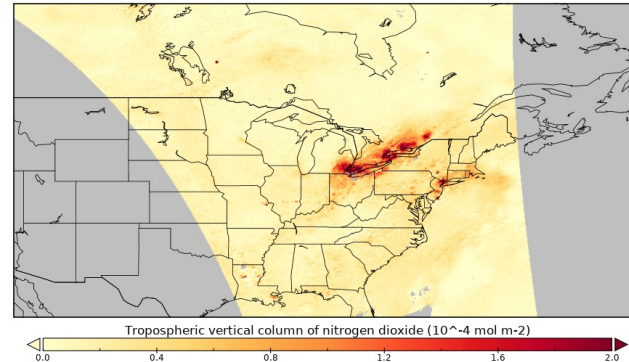
Multiple Sources of Air Quality Data

regulatory monitoring

- + accurate
- expensive
- ? representativity

form the "backbone" of the monitoring system, but insufficient alone

Copernicus TROPOMI Nitrogen Dioxide Product (Orbit #9397)



satellite retrievals

- + global coverage
- low time resolution
- column-integrated

good coverage and frequency, but need to be related to the ground-level situation

low-cost monitoring

- + relatively inexpensive
- + dense/remote deployment
- greater noise and bias

calibration is an open issue, but leveraging network density can offset some of these shortcomings



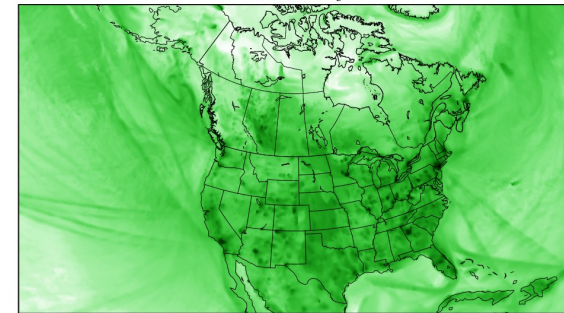
simulation models

- + global coverage
- + forecasting
- limited resolution

The best tool for prediction, but need the support of other data sources for accuracy

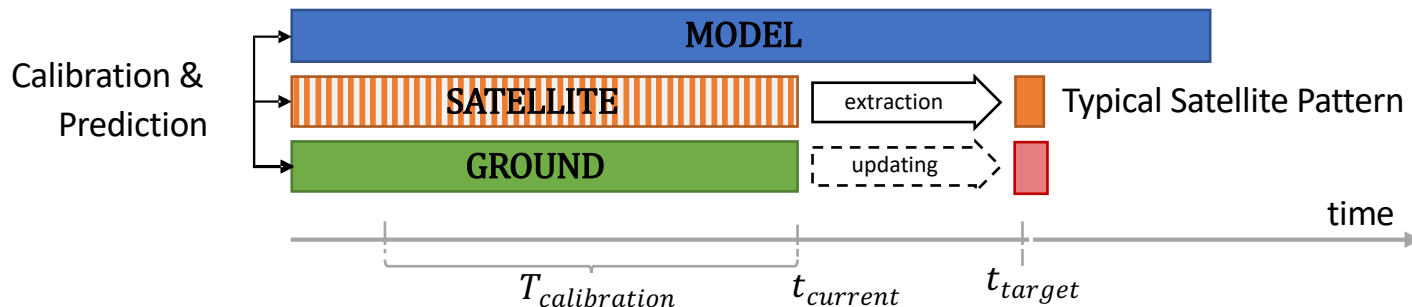


NASA/GMAO - GEOS CF Forecast Initialized on 12z 07/07/2020
Surface NO_2

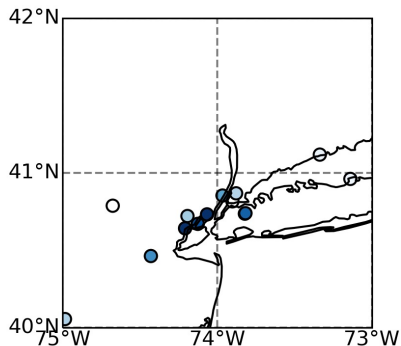


GMAO

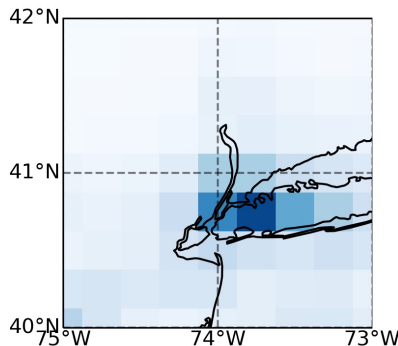
Data Fusion method for city-scale AQ forecasts



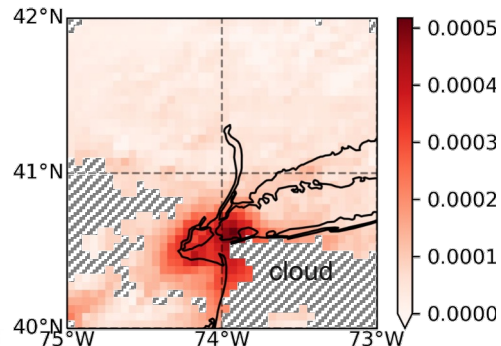
Ground Data (US EPA)



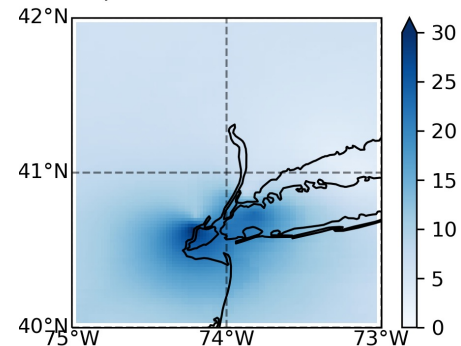
Model (GEOS-CF)



Satellite (TROPOMI)

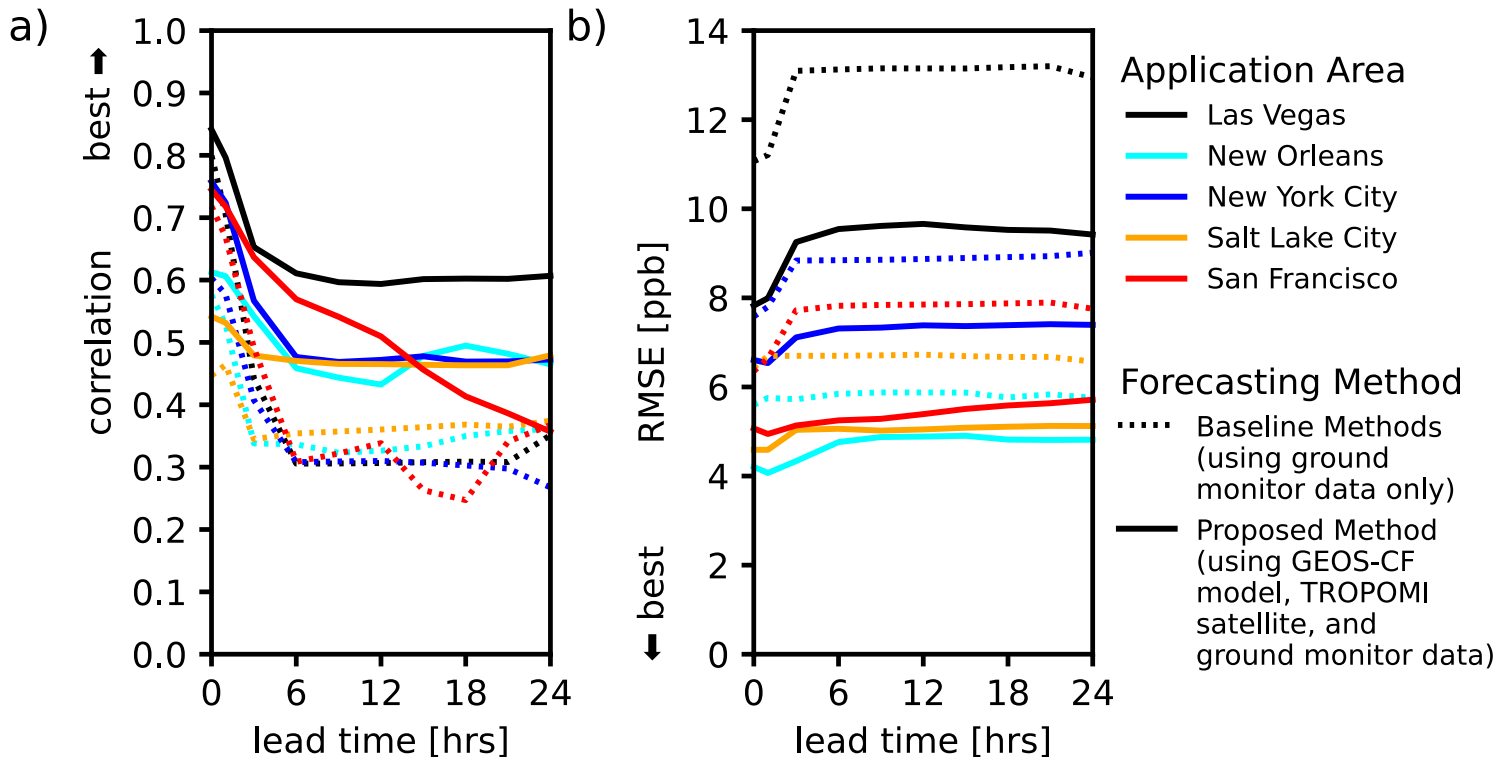


Forecast (Proposed Method)



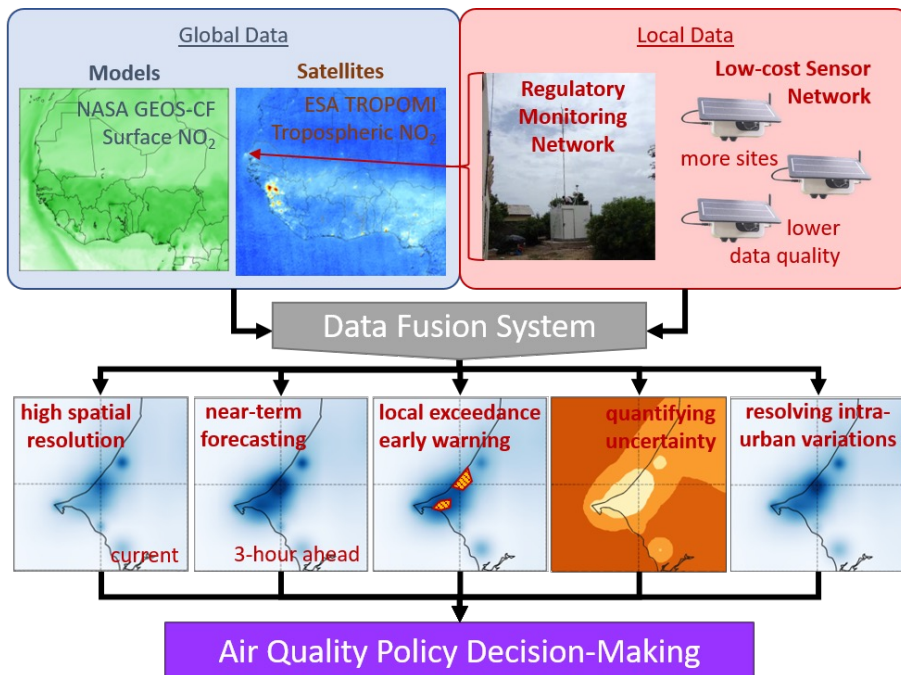
Malings et al., 2021 ESS

Data Fusion method for city-scale AQ forecasts



Malings et al., 2021 ESS

Ongoing & Future Work



NASA Earth Science Applications: Health and Air Quality

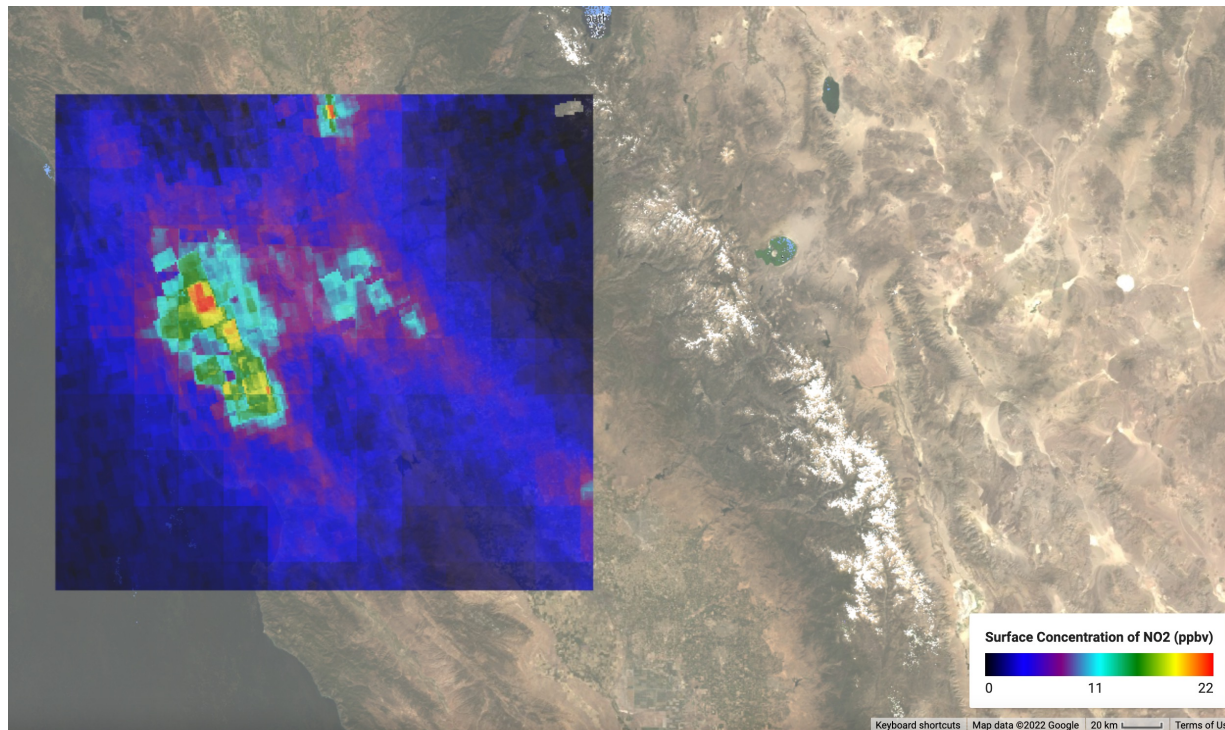
Supporting local government public health and air quality decision-making with a sub-city scale air quality forecasting system from data fusion of models, satellite, in situ measurements, and low-cost sensors.

Cities: Dakar, **Senegal**
Rio de Janeiro, **Brazil**
Charleston, Denver, Boulder, Gulfport,
Portland, **USA**

Co-Investigators: Sonoma Technology, Inc.

Collaborators: US EPA
UN Environment Programme
Clarity Movement, Co.
Columbia University, WUSTL

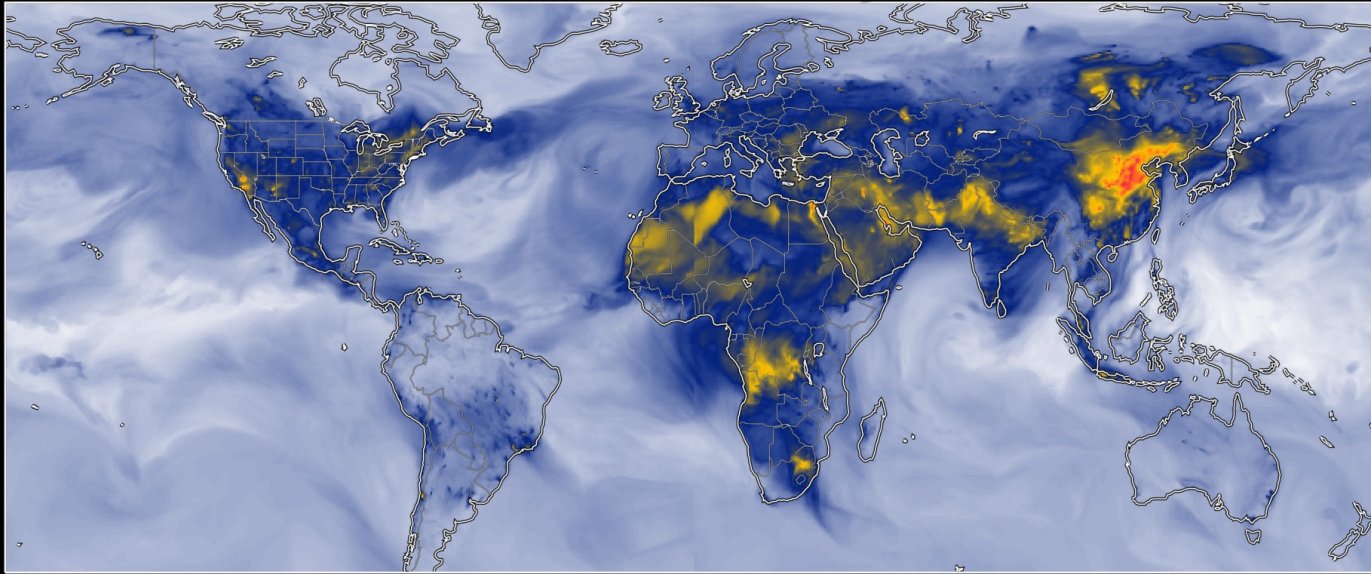
Work started on GEE with GEOS-CF to downscale NO_2



Figures courtesy of Callum Wayman

Forecast Application: Multi-pollutant Health Risk Index

Health risk Index: July 1st, 2017



GEOS-CF 1/4°

GEOS-Chem v11-02

Lower Health Risks

Higher Health Risks



Greater health risks



Global Modeling and Assimilation Office
NASA Goddard Space Flight Center

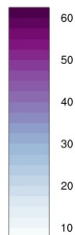
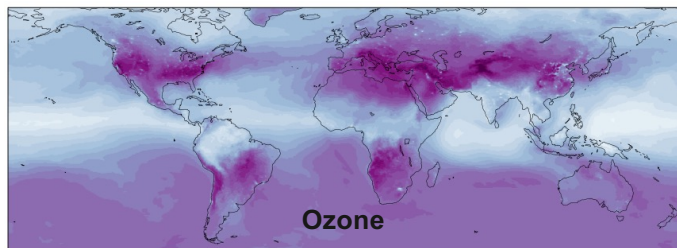


Atmospheric Chemistry Modeling Group
Harvard University

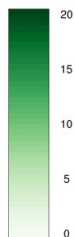
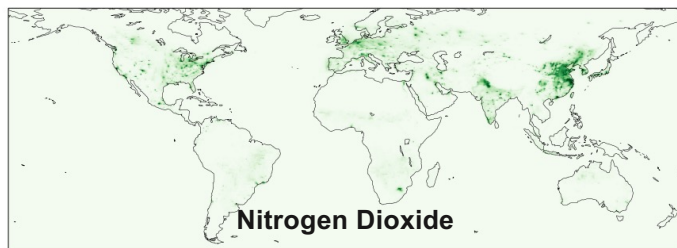
Multi-pollutant index, developed by Kevin Cromar and NYU team (Gladson et al. *in prep*)

- Maximum daily 8-hour average (MDA8) O₃
- 24-hour-average NO₂
- 24-hour-average PM_{2.5}

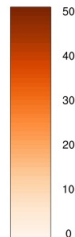
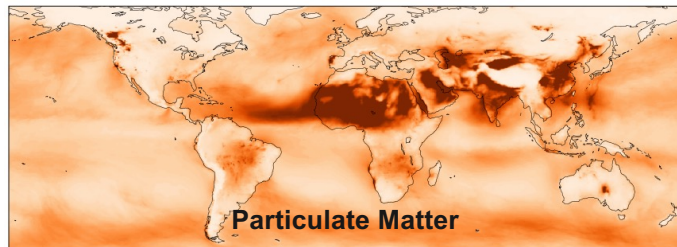
Forecast Application: Multi-pollutant Health Risk Index



- **O₃ influences Background levels**



- **NO₂ is Short-lived**
- **Extreme gradients**



- **PM_{2.5} driver of spatial gradients**

WMO Air Quality and Climate Bulletin No. 2 - September 2022

Growing air pollution hazards from wildfires

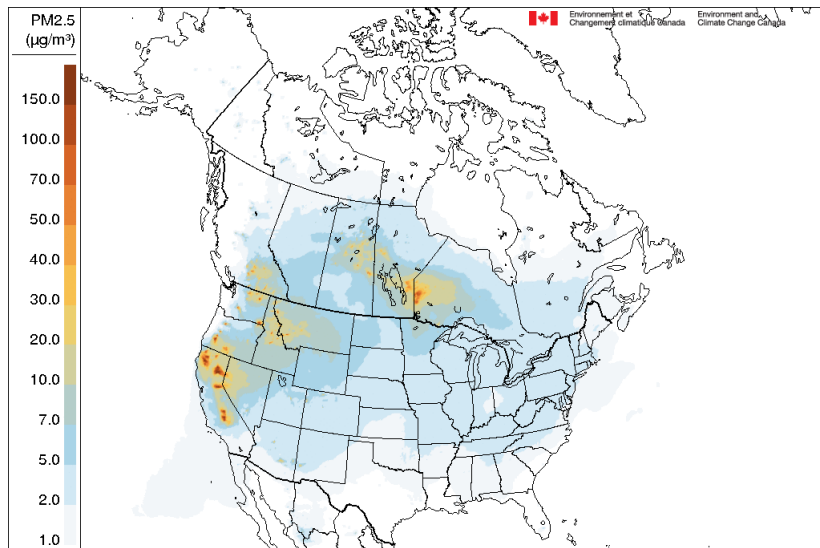
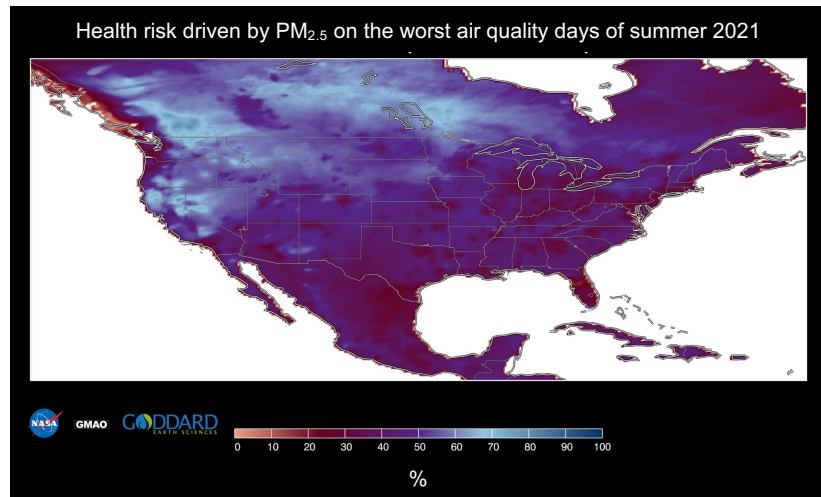


Figure 2: Seasonal (May-Sept mean) fire-PM_{2.5} contribution to total forecasted surface PM_{2.5} concentrations (µg/m³) for 2021 over North America.



The extreme PM_{2.5} concentrations are largely driven by wildfire emissions and are primarily responsible for the highest adverse health risks in parts of Western and Northern North America.

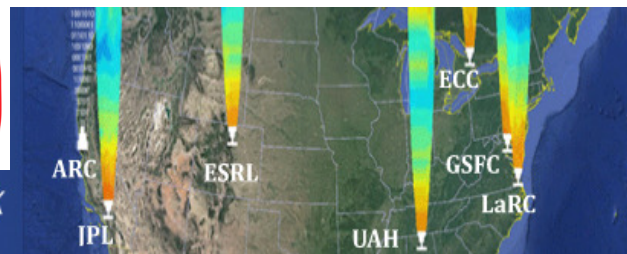
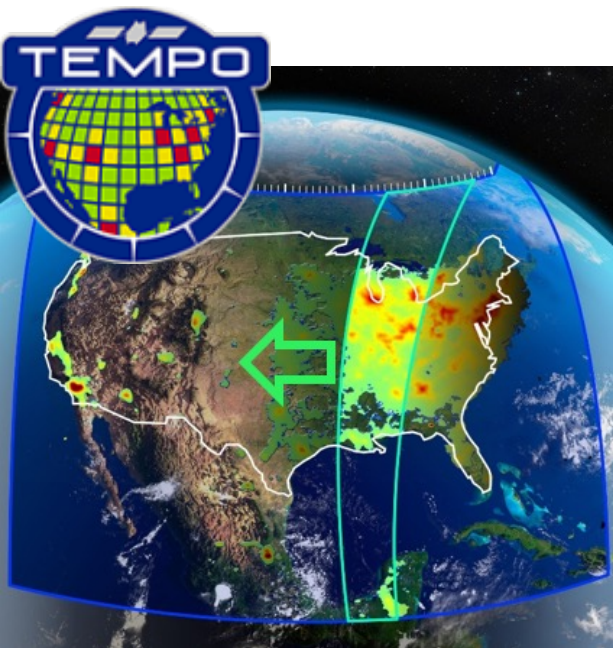
https://public.wmo.int/en/our-mandate/focus-areas/environment/air_quality/wmo-air-quality-and-climate-bulletin-no.2

Daily atmospheric composition forecast

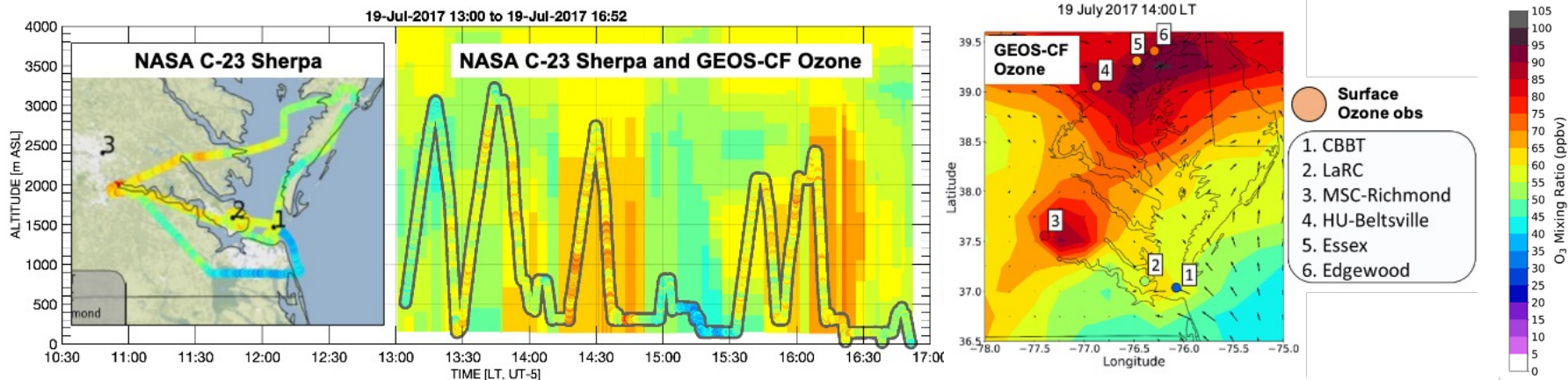
GEOS - CF

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



GEOS-CF evaluation with NASA's OWLETS campaign observations

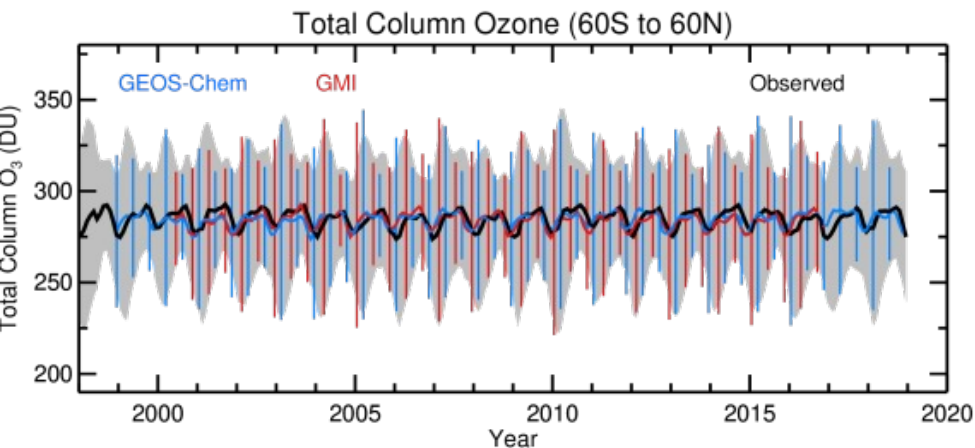


Dacic et al. (2020) used the GEOS-CF simulated ozone to put the OWLETS observations in 'the big picture', using the combined meteorology and chemistry to represent the synoptic conditions that lead to the observed ozone exceedances at surface observation sites.

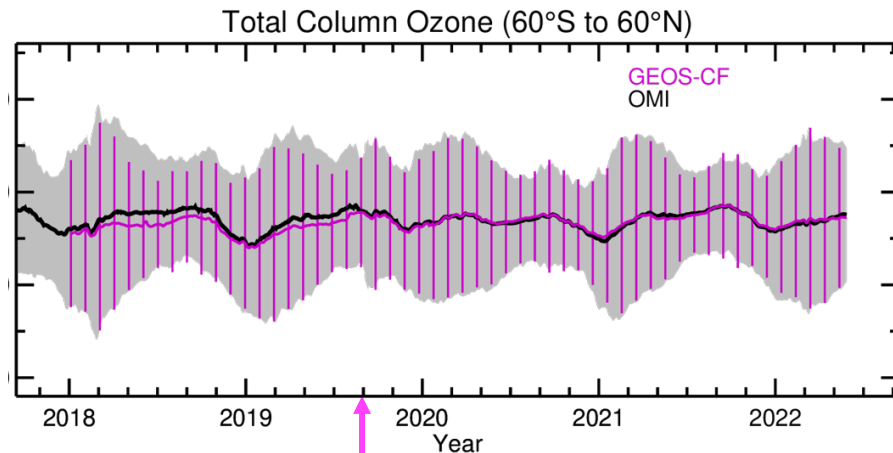
From where the model and the observations diverged, we learned where there are missing local marine emission sources and errors in the boundary layer chemical and dynamical processes in the model over the Chesapeake Bay.

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"

Stratospheric Composition Evaluation



GEOS-Chem non-polar TCO agrees well with GMI simulated TCO and the observable TCO range

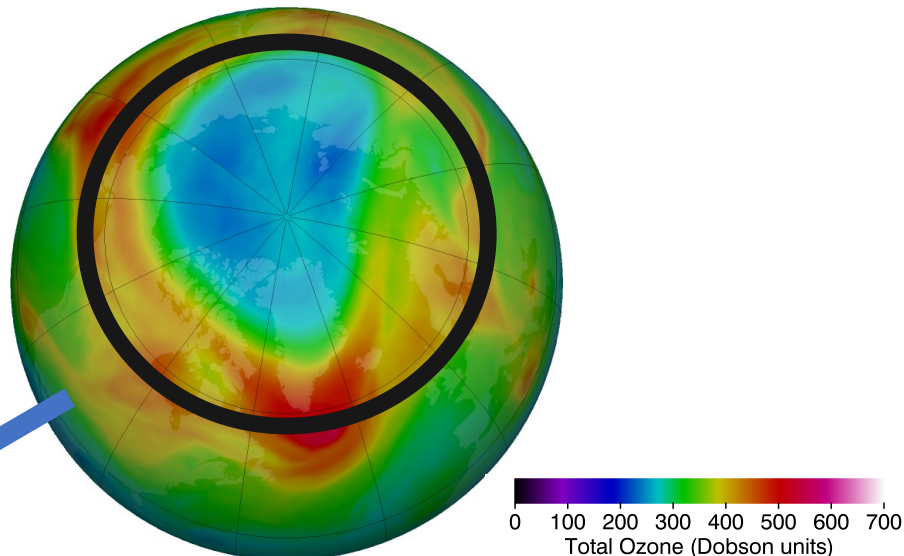
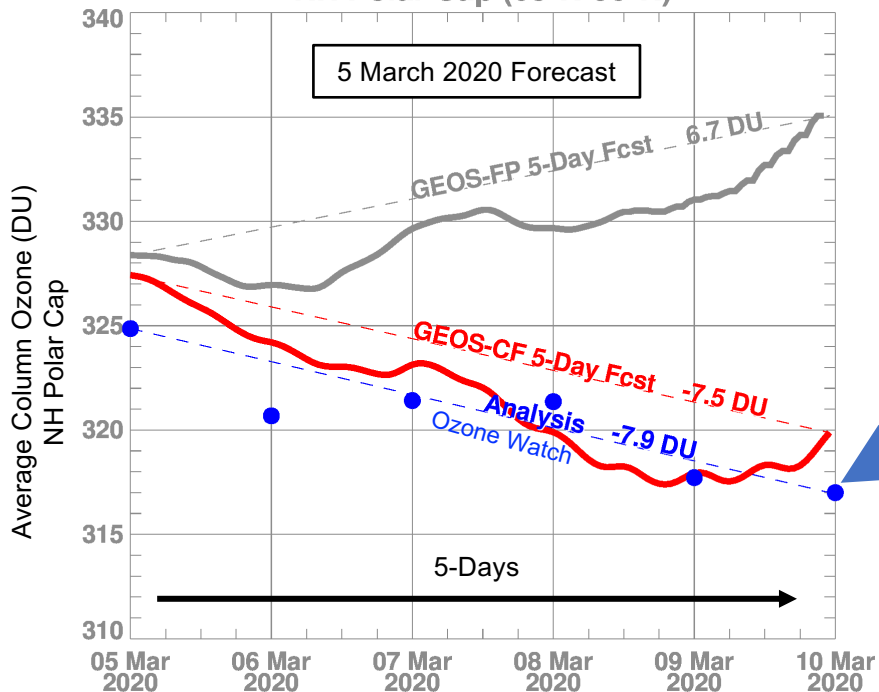


Updates were applied to GEOS-CF stratospheric mechanism on July 31, 2019, which improved the treatment of halogen and nitrogen families

Knowland et al., 2022, JAMES

GEOS-CF has realistic stratospheric ozone forecasts

NH Polar Cap (63°N-90°N)



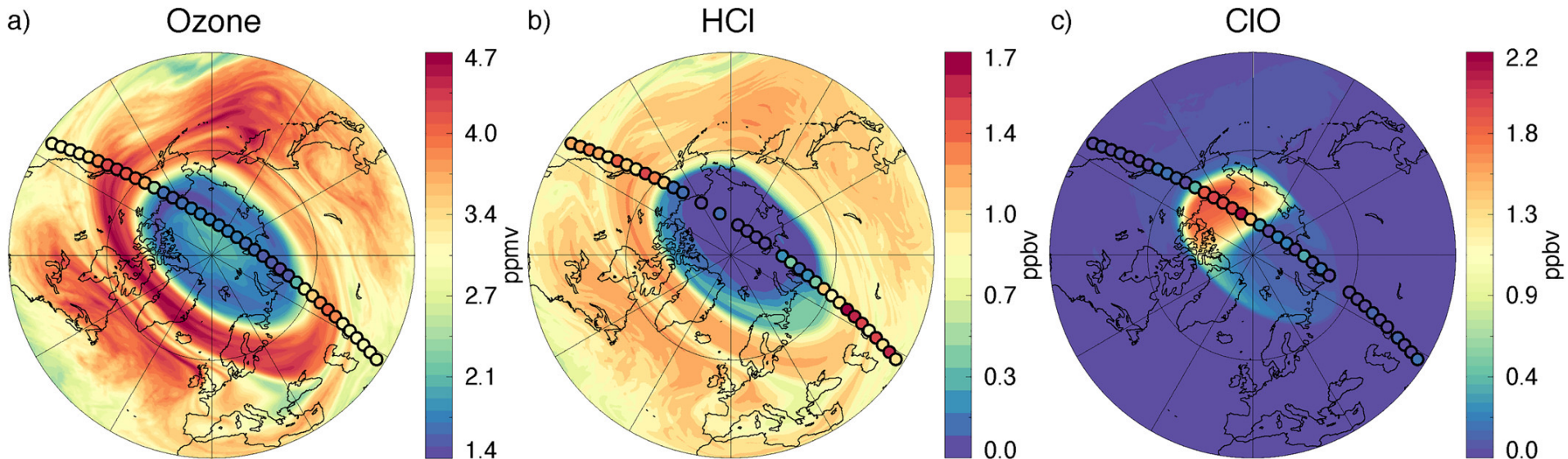
March 10, 2020: [Ozonewatch.gsfc.nasa.gov](https://ozonewatch.gsfc.nasa.gov)

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., 2022, JAMES

Evaluation GEOS-CF against MLS at 45 hPa

29 February 2020 at 22:00 UTC



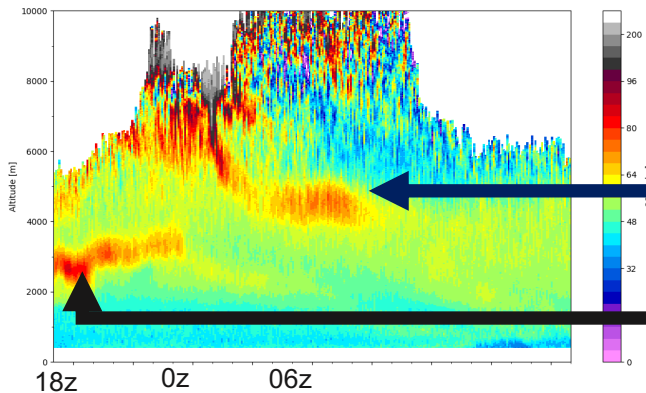
Within the vortex, HCl is expected to be converted into reactive chlorine (e.g., ClO), with high concentrations within the sunlight portion.

Knowland et al., 2022, JAMES



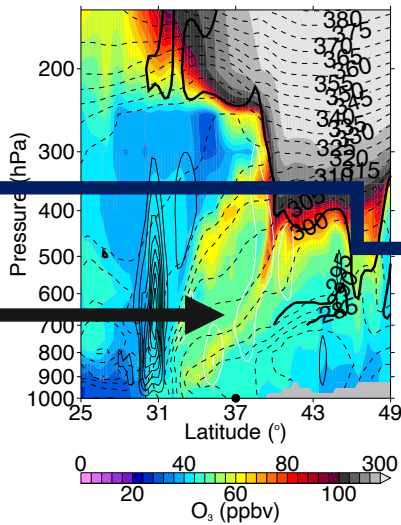
Stratosphere Troposphere Exchange

NASA LaRC Feb 13-14, 2019

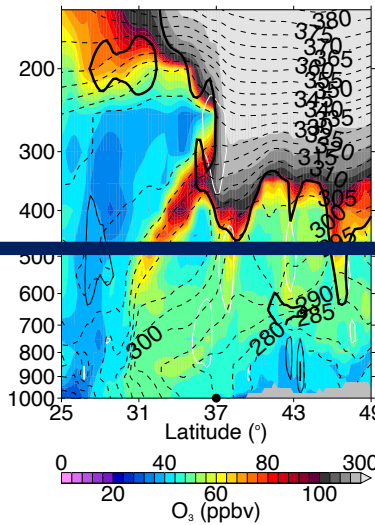


LMOL lidar plot courtesy of G. Gronoff

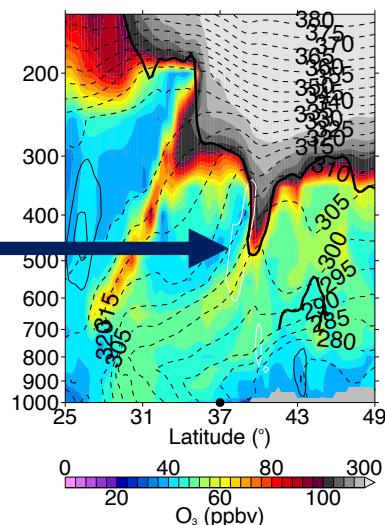
GEOS-CF
Feb 13, 2019 18z



Feb 14, 2019 00z

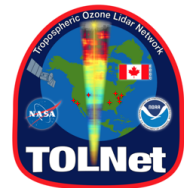


Feb 14, 2019 06z



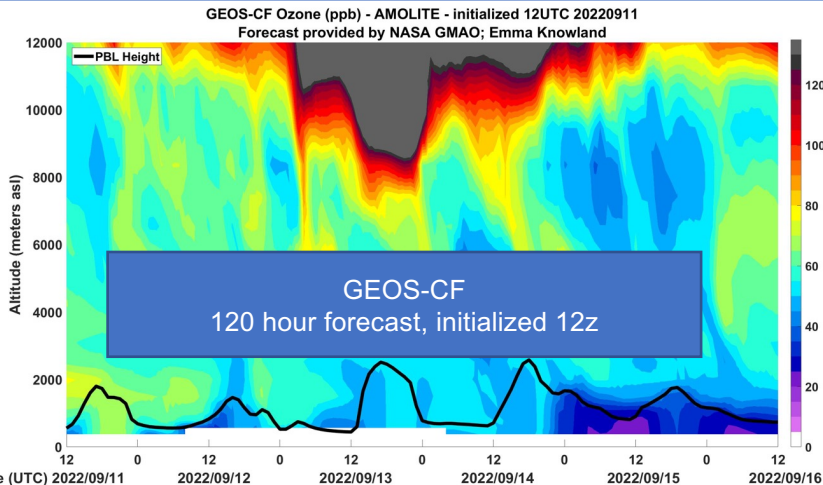
High ozone observed in the troposphere on February 13th and 14th of 2019 at LaRC have stratospheric origin, as indicated by the GEOS-CF curtain plots

Gronoff, G., Berkoff, T., Knowland, K. E., et al. "Case study of stratospheric Intrusion above Hampton, Virginia: lidar-observation and modeling analysis." *Atmos. Environ.*, 2021, DOI: 10.1016/j.atmosenv.2021.118498

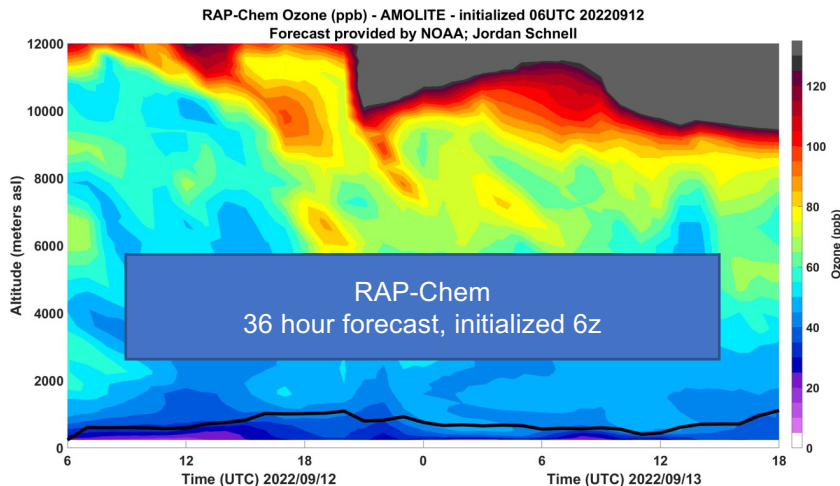
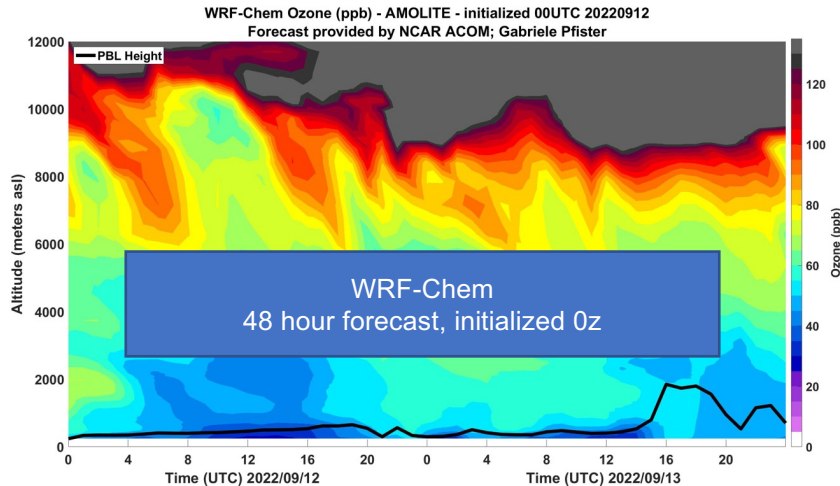
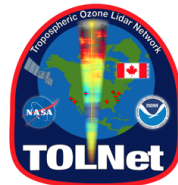


Daily alerts to TOLNet Lidar teams sent by Matt Johnson, NASA AMES

GEOS - CF

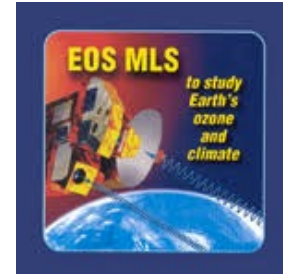
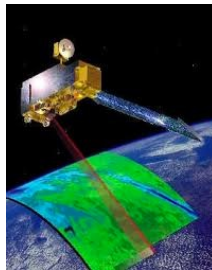
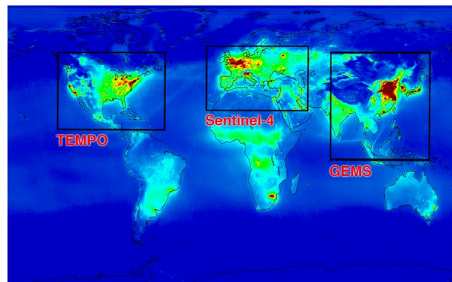
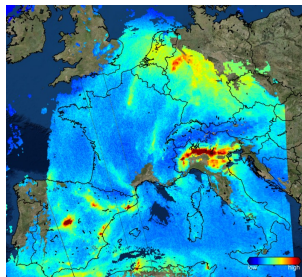


Tailored email alert system using three forecast models provides operators with confidence/uncertainty in predicted features



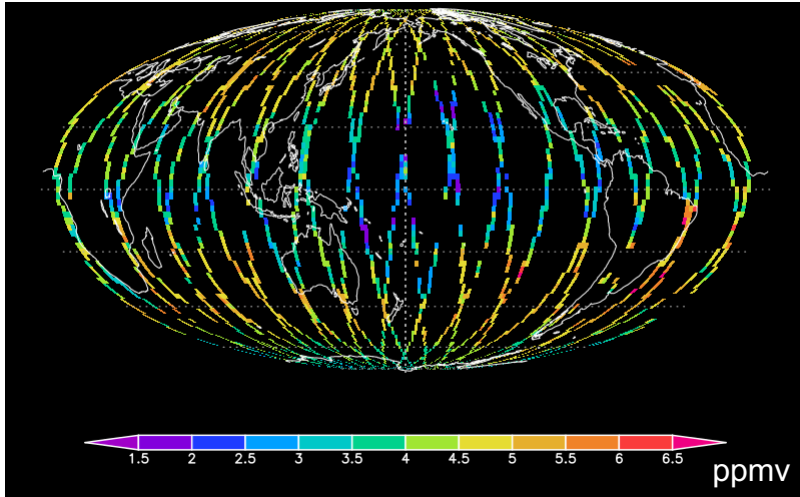
Planned upgrades for GEOS-CF

- Model update to GEOS-Chem v14
 - Improvements to ozone deposition
 - Updates to NO_3 washout \rightarrow likely reduce $\text{PM}_{2.5}$ bias
- GEOS AGCM update
- CEDS emission inventory (latest release through 2019)
- Constituent Data Assimilation System (CoDAS)
 - Multi-constituent assimilation with O_3 , CO , NO_2 , SO_2

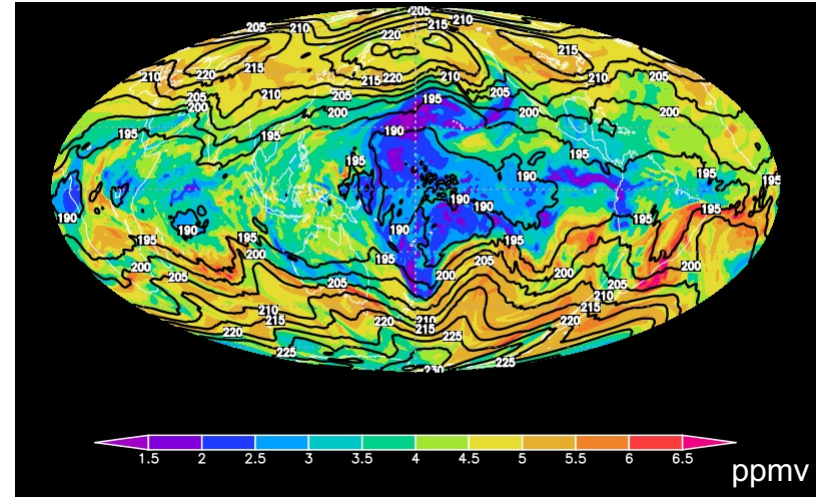


Constituent data assimilation

MLS water vapor at 100 hPa, 2 Jan 2016



Assimilated MLS water vapor and MERRA-2 temperature at 100 hPa, 2 Jan 2016



Data assimilation is a Bayesian method of combining and propagating information from observations in space and time using the governing equations and error estimates.

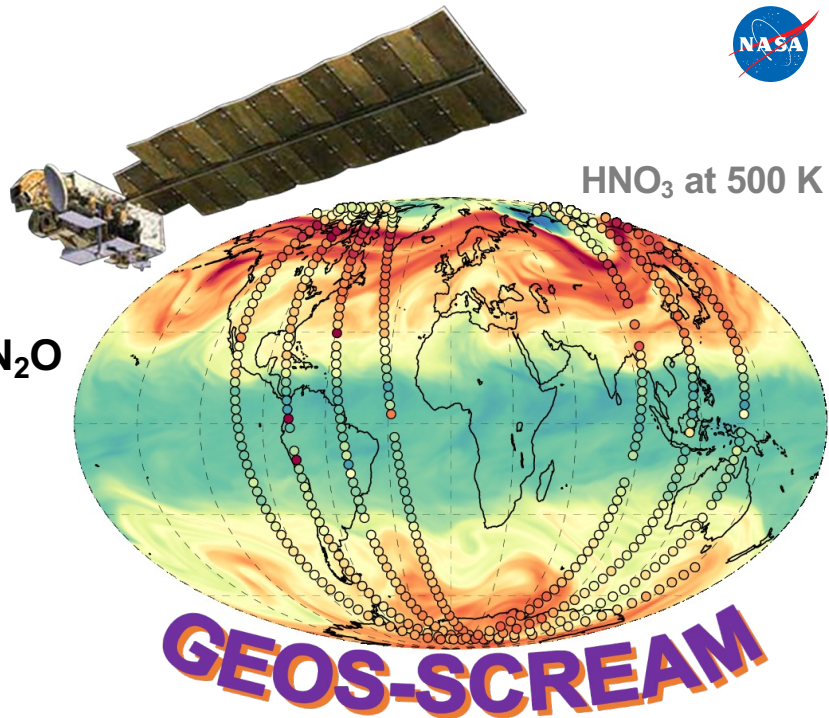
Figures courtesy of Kris Wargan

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**, **H₂O**, **HCl**, **HNO₃**, & **N₂O**
and **total ozone** from OMI
- ❑ Replay to MERRA-2
- ❑ GEOS “StratChem” stratospheric-only chemistry
- ❑ Period: September 2004 – December 2020+

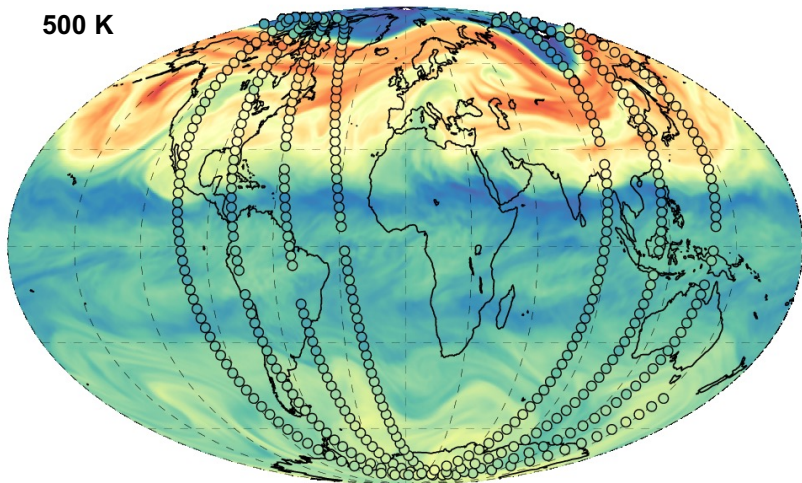
- ✓ Close agreement with ACE-FTS and GLORIA data and the BRAM2 reanalysis
- GMAO Reanalysis of the 21st Century (R21C, ~2022) with chemistry



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>

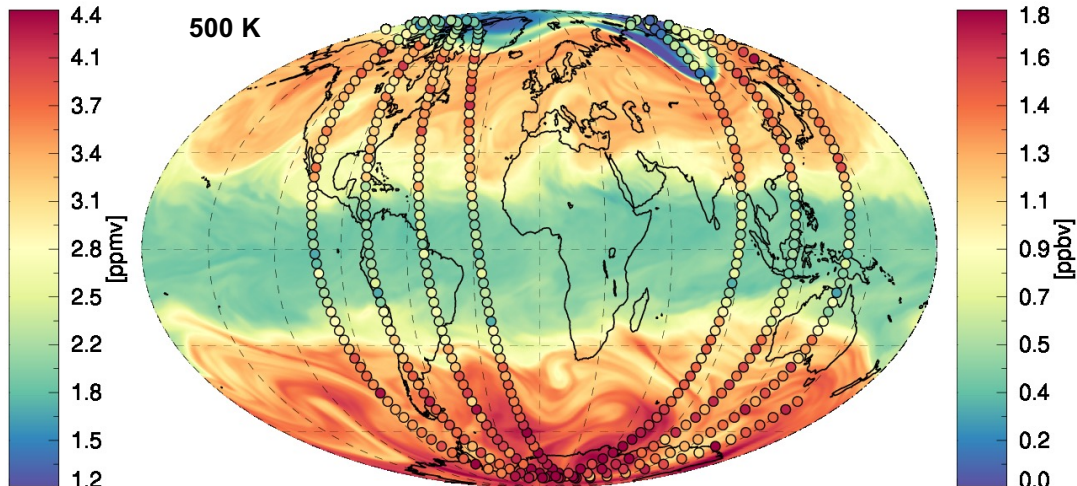
Analysis O₃, 2011-03-18 : 18 UTC

500 K



Analysis HCl, 2011-03-18 : 18 UTC

500 K



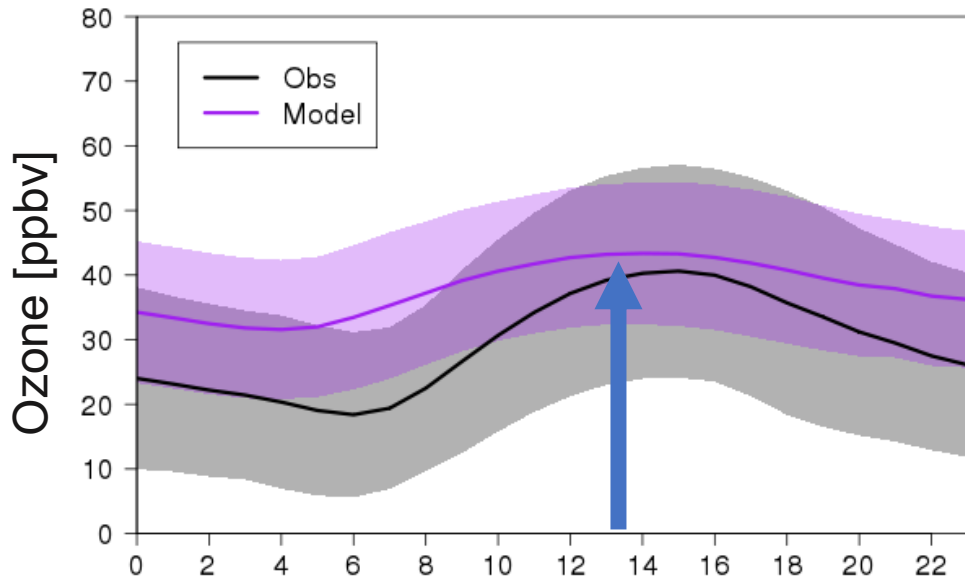
Maps of assimilated ozone and HCl and MLS observations (circles)

Close agreement between the constituent fields and assimilated MLS data.
Note dynamically driven features at mid- and high latitudes, and areas of depleted ozone and low HCl within the polar vortex.

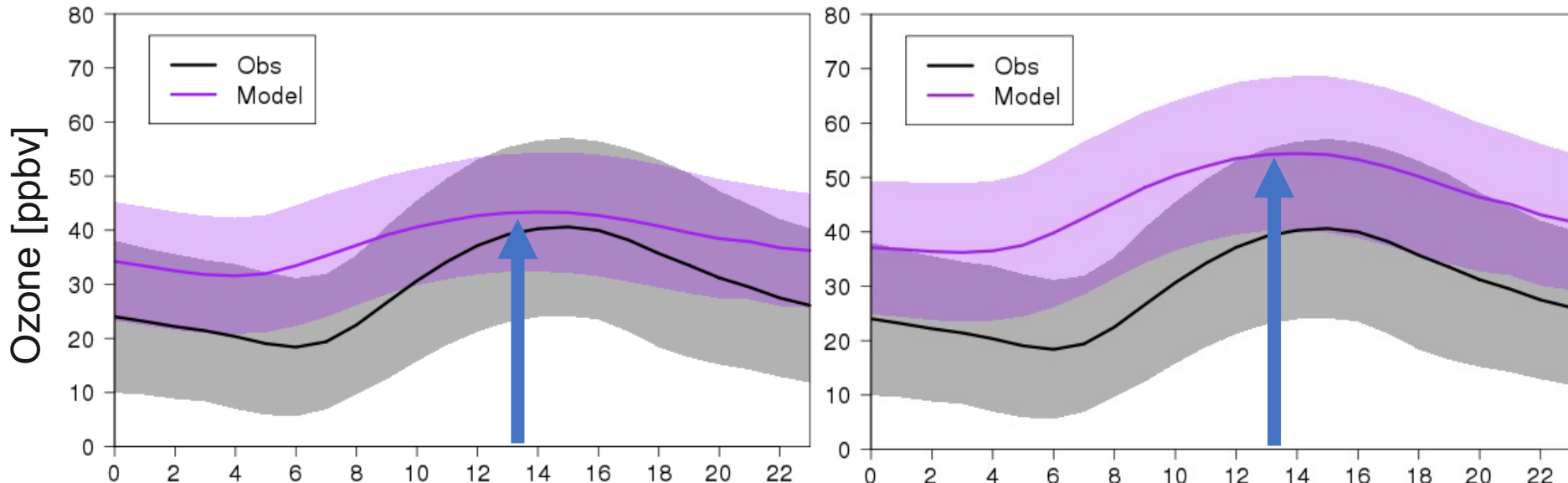
Figures courtesy of Kris Wargan

Assimilation of NO_x and CO exacerbates tropospheric ozone bias

Control (no assimilation)



With multi-species assimilation



➤ Improved diurnal cycle, most likely due to improved afternoon NO_2



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 realistically 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



Referred

Knowland, K. E., C. A. Keller, P. A. Wales, et al. (2022). NASA GEOS Composition Forecast Modeling System GEOS-CF v1.0: Stratospheric composition. *Journal of Advances in Modeling Earth Systems*, 14, e2021MS002852. <https://doi.org/10.1029/2021MS002852>

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>

Gladson, L. A., K. R. Cromar, M. Ghazipura, et al. (2022). Communicating respiratory health risk among children using a global air quality index. *Environment International*, 159: 107023 [10.1016/j.envint.2021.107023]

Bi, J., K. E. Knowland, C. A. Keller, and Y. Liu. 2022. "Combining Machine Learning and Numerical Simulation for High-Resolution PM2.5 Concentration Forecast." *Environmental Science & Technology*, 56 (3): 1544-1556 [10.1021/acs.est.1c05578]

Duncan, B. N., C. A. Malings, K. E. Knowland, et al. 2021. "Augmenting the Standard Operating Procedures of Health and Air Quality Stakeholders With NASA Resources." *GeoHealth*, 5 (9): [10.1029/2021gh000451]

Lee, J. D., F. A. Squires, T. Sherwen, et al. 2021. "Ozone production and precursor emission from wildfires in Africa." *Environmental Science: Atmospheres*, (Accepted) [10.1039/d1ea00041a]

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Malings, C., K. E. Knowland, C. A. Keller, and S. E. Cohn. 2021. "Sub-City Scale Hourly Air Quality Forecasting by Combining Models, Satellite Observations, and Ground Measurements." *Earth and Space Science*, 8 (7): [10.1029/2021ea001743]

Johnson, M. S., K. Strawbridge, K. E. Knowland, C. Keller, and M. Travis. 2021. "Long-range transport of Siberian biomass burning emissions to North America during FIREX-AQ." *Atmospheric Environment*, 252: 118241 [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. (2022), "File Specification for GEOS-CF Products." *GMAO Office Note No. 17 (Version 1.2)*, 54pp, available from http://gmao.gsfc.nasa.gov/pubs/office_notes

Long-range transport of Siberian biomass burning emissions to North America during FIREX-AQ campaign

- GEOS-CF and satellite observations characterized the long-range transport pathway of Siberian smoke over the AMOLITE location during FIREX-AQ.
- The long-range transport agreed with the timing of aerosol and ozone lamina measured by AMOLITE.
- GEOS-CF, AMOLITE, and in situ data suggest that while surface air quality impacts in western Canada were small, there were significant free tropospheric ozone (>20 ppb) and aerosol ($>30 \mu\text{g m}^{-3}$) enhancements.

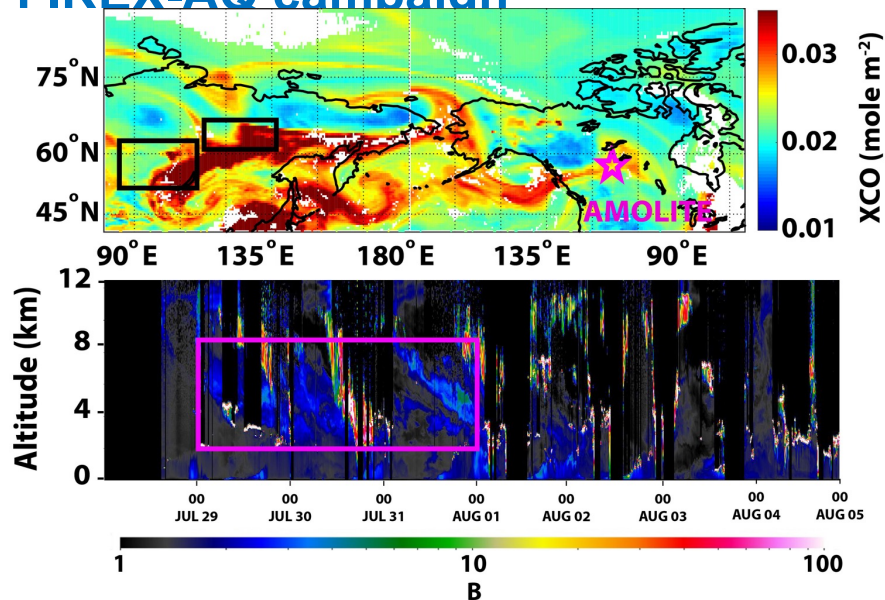


Figure 1. **GEOS-CF** XCO (mole m^{-2}) on July 29, 2019 (top) and AMOLITE aerosol backscatter ratio (B) between July 28 and August 5, 2019 (bottom). The magenta star and box highlight the location of **AMOLITE** and the large aerosol lamina observed by the system, respectively.

Johnson, M. S., Strawbridge, K., Knowland, K. E., et al., "Long-range transport of Siberian biomass burning emissions to North America during FIREX-AQ." *Atmos. Environ.*, 2021. DOI: 10.1016/j.atmosenv.2021.118241

TEMPO specific collection: “sat_inst_1hr_r721x361_v72”

Regional Chemistry and Meteorology Diagnostics to support TEMPO satellite

Frequency: *hourly instantaneous from 00:00 UTC*

Spatial Grid: *3D, model-level, subset region of full horizontal resolution*

Dimensions: *longitude=721, latitude=361, every 0.25°*

longitude: 0° to -180°

latitude: 0° to 90°

vertical level: 72 layers

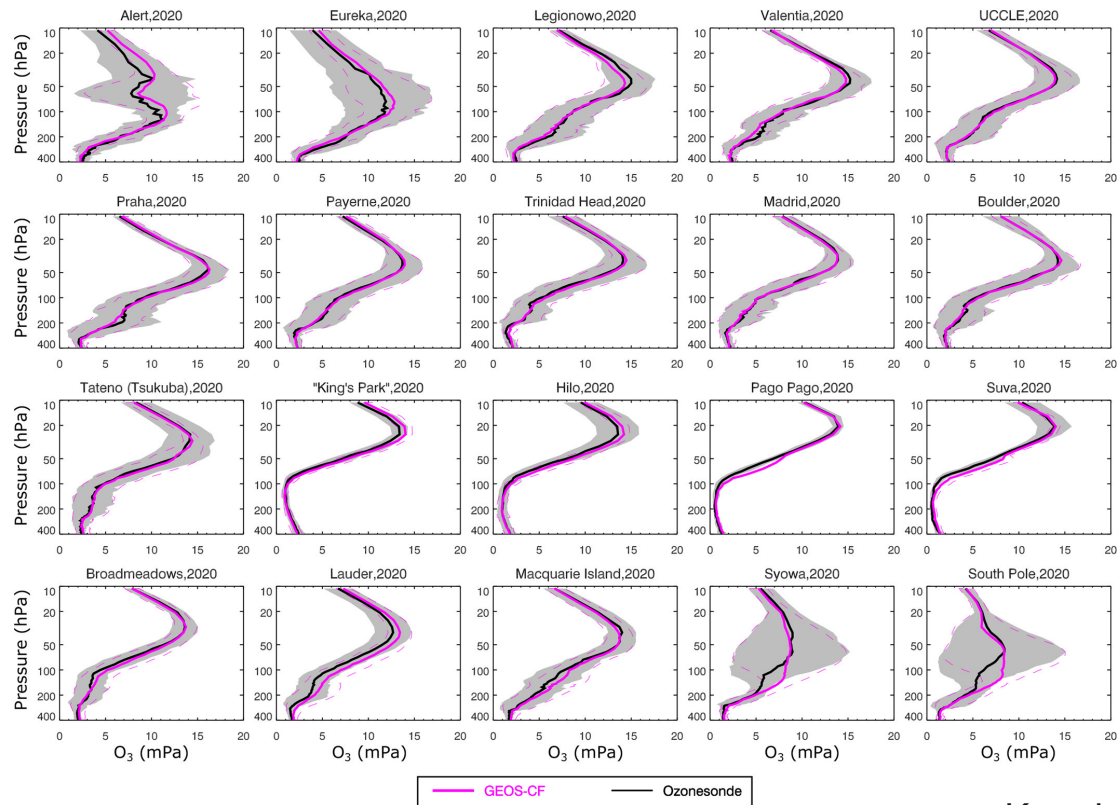
Granule Size: *~258 MB per file*

Start date: 00 UTC 1 January 2022

Mode: *Replay only; Forecasts available based on mission requirements*

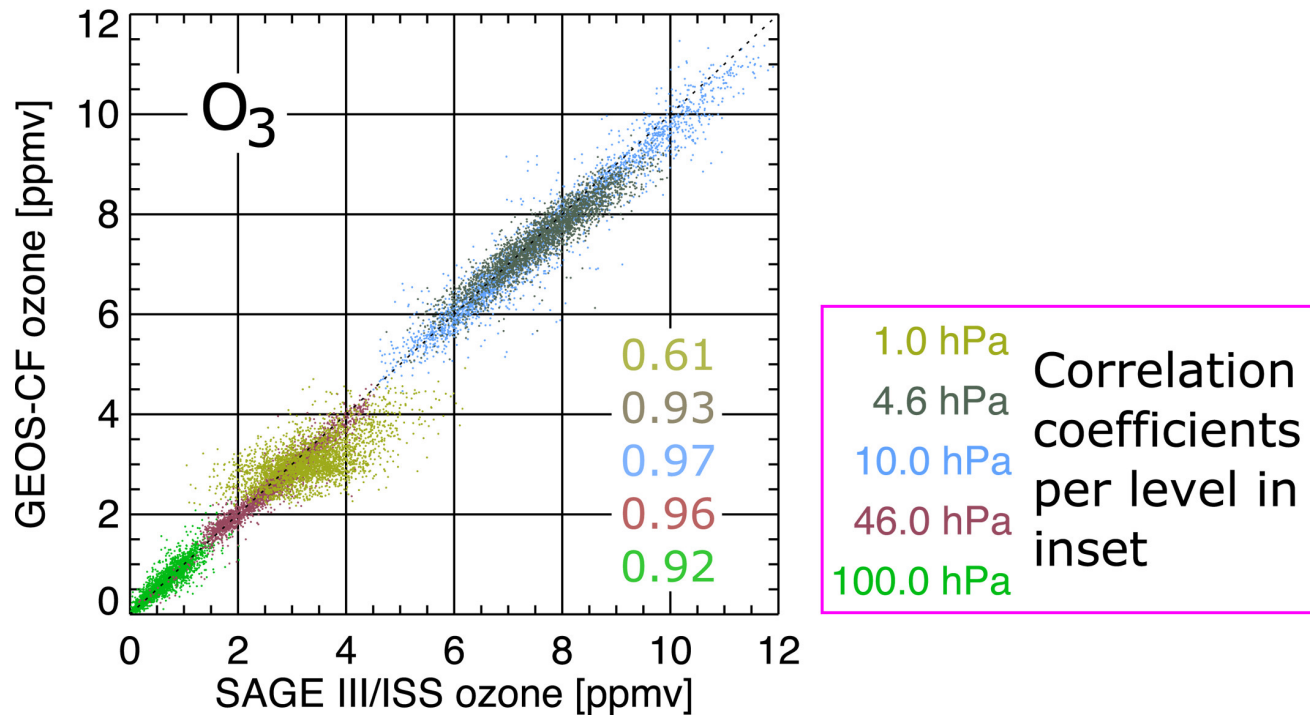
Knowland et al., 2022. "File Specification for GEOS-CF Products." *GMAO Office Note No. 17 (Version 1.2), available from http://gmao.gsfc.nasa.gov/pubs/office_notes*

Name	Dim	Description	Units
BrO	tzyx	Bromine monoxide (BrO, MW = 96.00 g mol ⁻¹) volume mixing ratio dry air	mol mol ⁻¹
FRSEAI E	tyx	ice covered fraction of tile	1
FRSNO	tyx	fractional area of land snowcover	1
GLYX	tzyx	Glyoxal (CHOCHO, MW = 58.00 g mol ⁻¹) volume mixing ratio dry air	mol mol ⁻¹
HCHO	tzyx	Formaldehyde (CH ₂ O, MW = 30.00 g mol ⁻¹) volume mixing ratio dry air	mol mol ⁻¹
HNO ₂	tzyx	Nitrous acid (HNO ₂ , MW = 47.00 g mol ⁻¹) volume mixing ratio dry air	mol mol ⁻¹
IO	tzyx	Iodine monoxide (IO, MW = 143.00 g mol ⁻¹) volume mixing ratio dry air	mol mol ⁻¹
NO ₂	tzyx	Nitrogen dioxide (NO ₂ , MW = 46.00 g mol ⁻¹) volume mixing ratio dry air	mol mol ⁻¹
O ₃	tzyx	Ozone (O ₃ , MW = 48.00 g mol ⁻¹) volume mixing ratio dry air	mol mol ⁻¹
OCIO	tzyx	Chlorine dioxide (OCIO, MW = 67.00 g mol ⁻¹) volume mixing ratio dry air	mol mol ⁻¹
PHIS	tyx	surface geopotential height	m+2 s-2
PS	tyx	surface pressure	Pa
Q	tzyx	specific humidity	kg kg ⁻¹
SNODP	tyx	snow depth	m
SNOMAS	tyx	Total snow storage land	kg m-2
SO ₂	tzyx	Sulfur dioxide (SO ₂ , MW = 64.00 g mol ⁻¹) volume mixing ratio dry air	mol mol ⁻¹
T	tzyx	air temperature	K
TROPPB	tyx	tropopause pressure based on blended estimate	Pa
U2M	tyx	2-meter eastward wind	m s-1
V2M	tyx	2-meter northward wind	m s-1
ZPBL	tyx	planetary boundary layer height	m

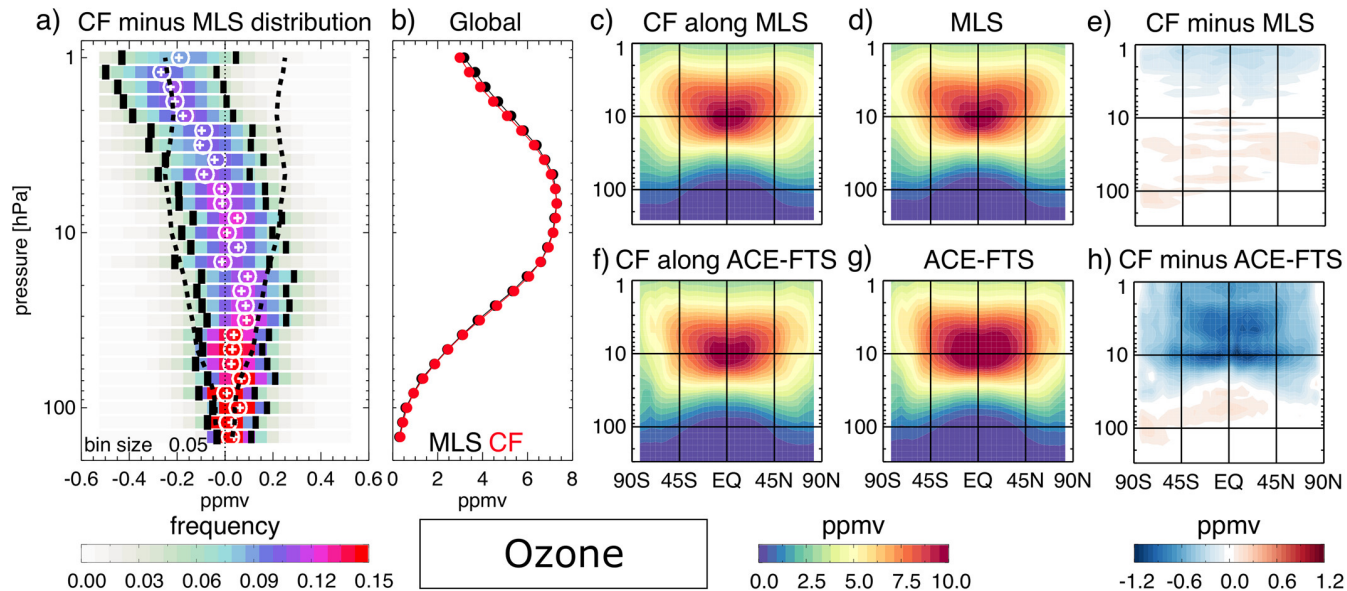


Knowland et al., 2022, JAMES

GEOS-CF vs SAGE III/ISS



Knowland et al., 2022, JAMES



Knowland et al., 2022, JAMES