TEMPO Science Team Meeting:
Satellite evaluation and Assimilation in Hemispheric CMAQ

Presenter: Barron H. Henderson
US EPA Office of Air Quality Planning and Standards

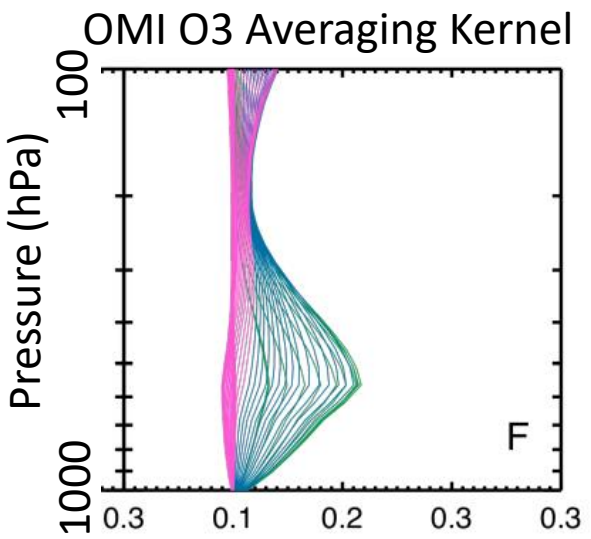
Co-Authors: James East, Shannon N. Koplitz, Sergey Napelenok, OAQPS Satellite Forum

Disclaimer: Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

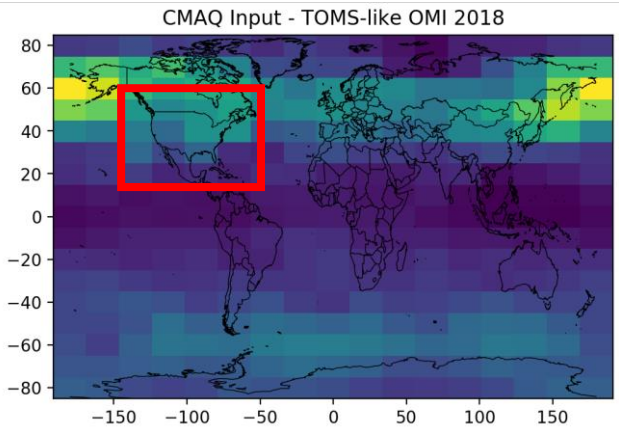
Where can TEMPO add value for the EPA model applications?

- How does EPA currently use satellite data in model applications?
  - Satellite screening of model inputs
  - Satellite model evaluation
- Progress on data assimilation
  - Assimilation webinar overview
  - Assimilation and inverse emissions methodology
  - Preliminary research results
- Considerations for TEMPO

How does EPA use satellite data regularly?



Fu et al. 10.5194/acp-13-3445-2013



CMAQ Model Input

Often not directly interpretable as surface

- Most often total column measurement with low sensitivity to the surface for some species.
- Requires model “priors” and “kernels” or “assimilation” for interpretation to ground level.

Meteorological Model Inputs

- Land use/Land Cover, Digital Elevation Maps
- GHR Sea Surface Temperatures
- Data assimilation (e.g, GEOS, CAMS, GDAS, WRF)

Emissions Model Inputs

- e.g., MEGAN, FINN, GFED, BlueSky
- Fire detection, land area burned

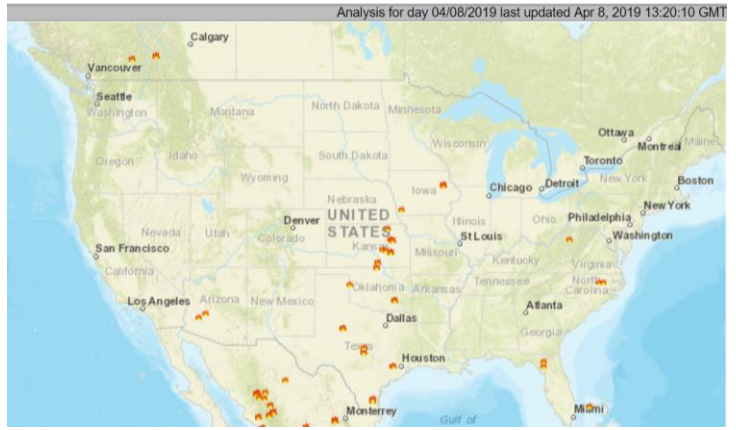
Air Quality Model Inputs

- Land use/Land Cover, Digital Elevation Maps
- ***Daily coarse*** TOMS/OMI Ozone to adjust j-values
- Other existing products, new products?

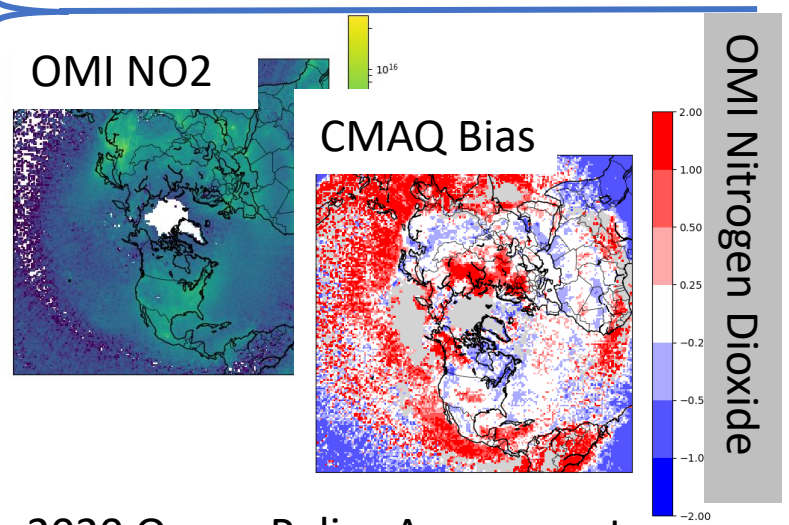
Air Quality Model or Emissions Evaluation*

- OMI Nitrogen Dioxide Tropospheric Columns
- OMI Ozone Tropospheric Columns
- OMI Formaldehyde Columns
- MODIS Aerosol Optical Depth
- CRIS Ammonia

Moving towards assimilation!*



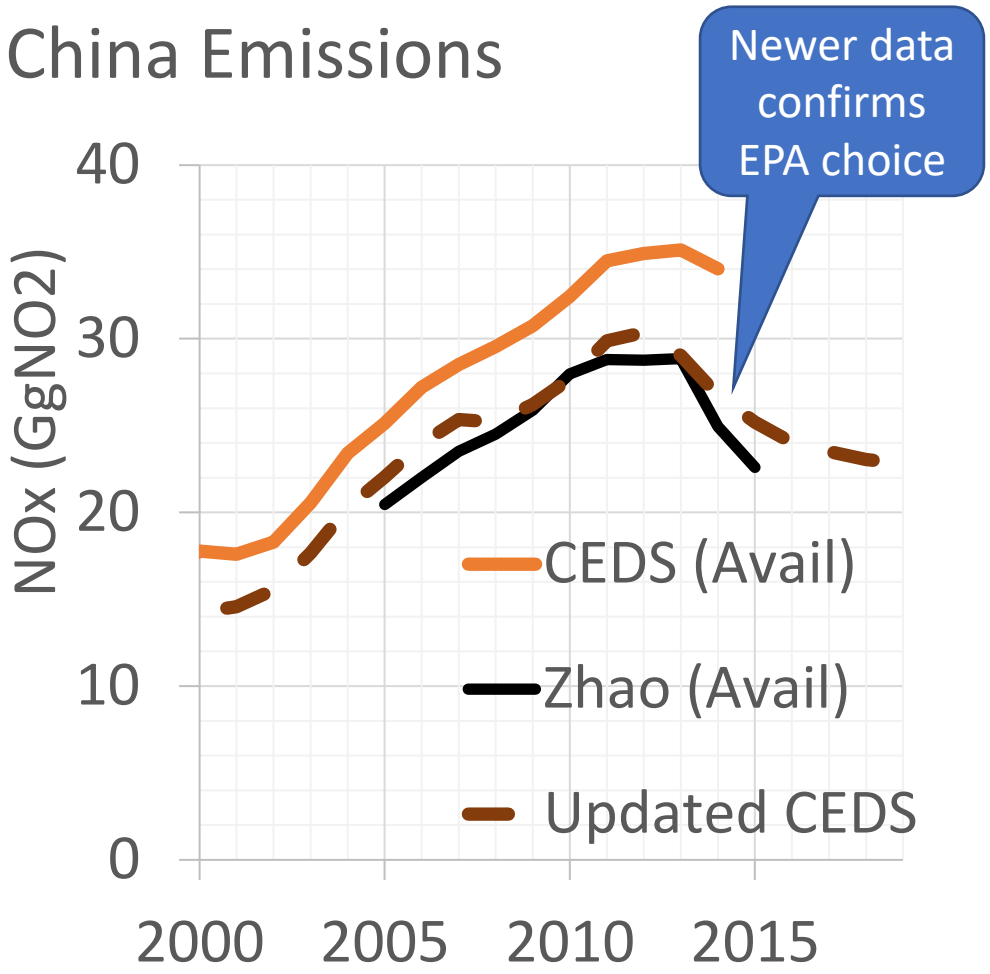
Fires from NOAA’s Hazard Mapping System



2020 Ozone Policy Assessment

Qualitative emission input screening

- 2016 hemispheric model emissions options
  - Hemispheric Transport of Air Pollutants v2 mosaic inventory was the base
  - CEDS CMIP6 inventory was released in time for us to incorporate updated trends out to 2014.
  - CEDS showed increase NOx/SOx;
  - Zhao et al [2015] showed decreases in recent years and lower magnitudes.
- Satellite showed decreases
  - van der A et al. 2017 doi:10.5194/acp-17-1775-2017; Krotkov, et al. 2016. doi: 10.5194/acp-16-4605-2016
  - Likely related to recent controls.
  - Updates to CEDS confirm decrease



Evaluation for surface concentration estimates

Model evaluation*

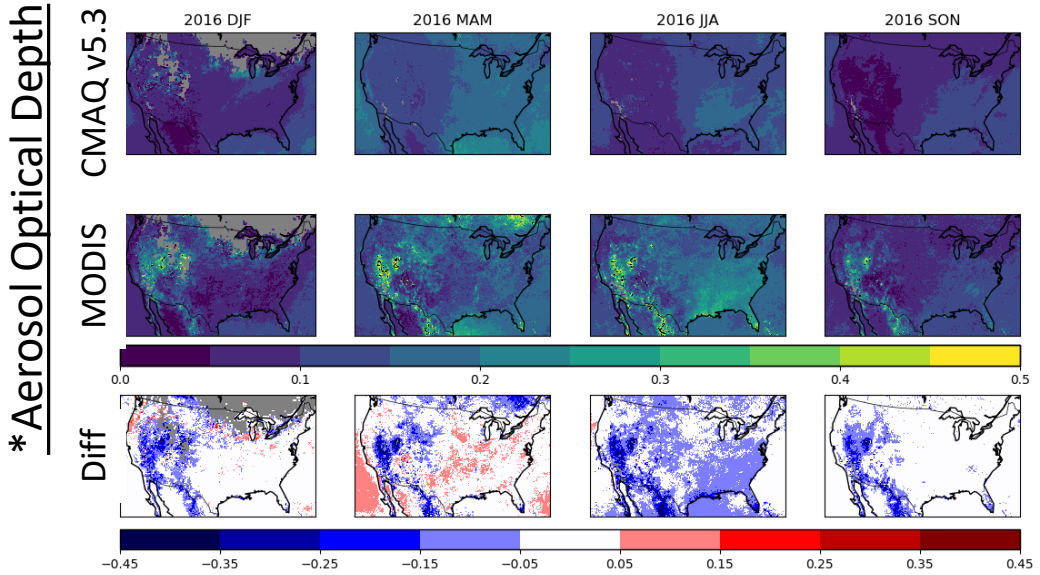
- 2020 Ozone Policy Assessment included evaluation against nitrogen dioxide, ozone, and formaldehyde
- Evaluation is performed quantitatively, but also considers uncertainties (e.g., AMF) qualitatively

Emissions Quality Assurance

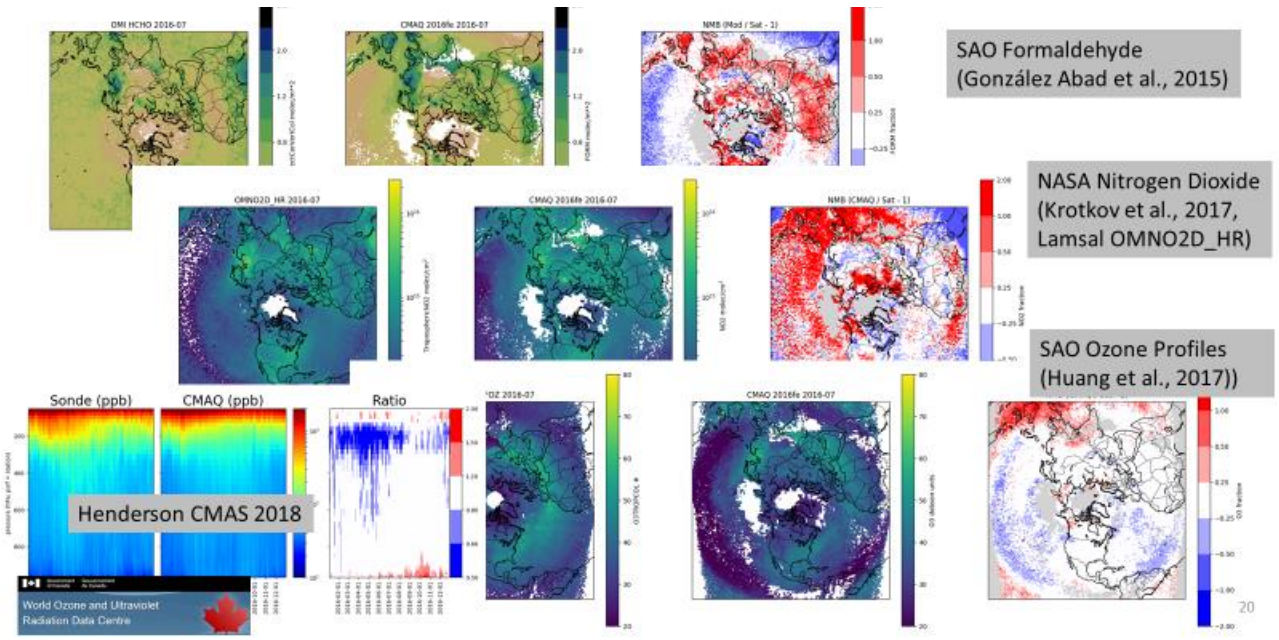
- NO2 and SO2 comparisons informed global emission inventory
- Useful for evaluating current inventories even if not directly applied

What about direct feedback?

Model processes and performance varies by time of day and at fine spatial scales that benefit from geostationary.



*Gases: NO2, O3, HCHO



JGR Atmospheres

Research Article | Full Access

Satellite Formaldehyde to Support Model Evaluation

Monica Harkey, Tracey Holloway, Eliot J. Kim, Kirk R. Baker, Barron Henderson

First published: 24 December 2020 | https://doi.org/10.1029/2020JD032881

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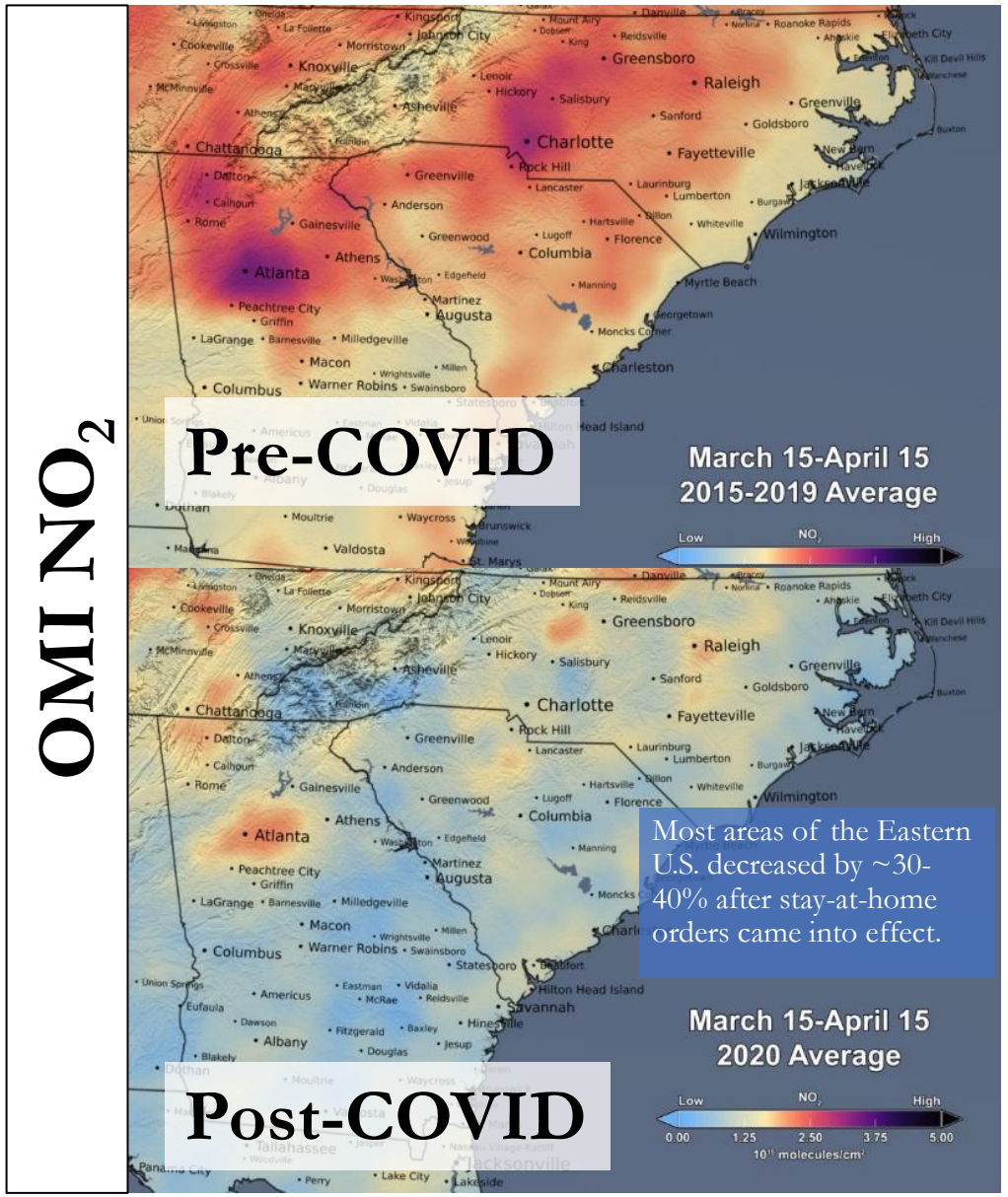
e2020JD032881

Policy-relevant modeling opportunities for satellite assimilation

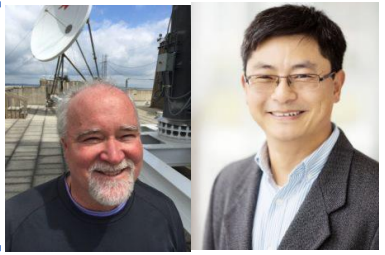
- Direct application of assimilation is not right for every application because it removes deterministic relationship between emissions and concentration.
- Regional modeling is dependent on global “boundary conditions”
  - Inter-continental anthropogenic transport and natural emissions largely contribute to what enters our model and is not the focus of controls.
  - International inventories are often updated less frequently or are a challenge to integrate into our platform
- Emission Inventory Development
  - Quality assurance by evaluation and comparison
    - Temporal and spatial variation
    - Existence or absence of “hotspots” or Regional outliers
  - Constraints on uncertain sources (NOx/VOC, but aerosol precursors)
    - Wildland fires, Soil NOx
    - International Emissions, Area sources
- Several reasons for interest in assimilation.

NASA OMI Team



Recent Webinar on Chemical Assimilation helping EPA toward routine application

- Motivated by Health and Air Quality Applied Science Team (HAQAST) project with Brad Pierce and Daniel Tong
  - Tiger Team projected included technology transfer.
  - Research fellow James East implementing at EPA
- Assimilation experts from NASA and Academia advised on:
  - Numerical assimilation frameworks that can improve air quality predictions
  - Practical applications relevant to criteria pollutants and associated uncertainties
  - Ongoing research needs for satellite validation and retrieval improvements
- Huge success! Great panelists! Great attendance!



Chairs:
Barron H. Henderson
Bryan N. Duncan

Panelists:
Ron C. Cohen
R. Bradley Pierce
Kazuyuki Miyazaki
Zhen Qu

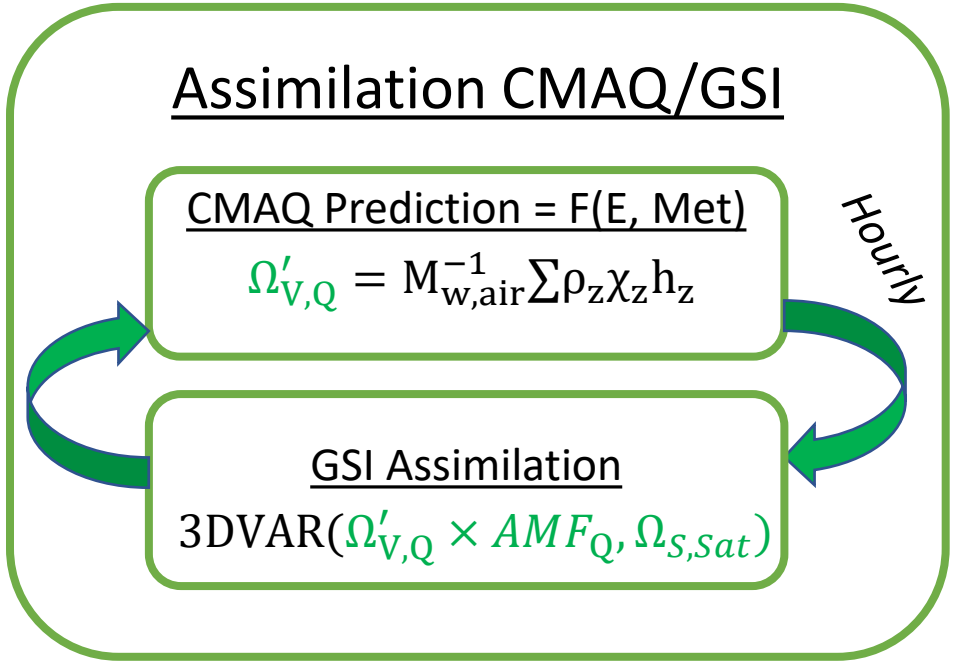
Attendees:
112 around the world

https://haqast.org/tiger-teams/#2017-tiger-teams

Assimilation overview

James East
ORISE Research Fellow

- HAQAST Collaboration:
  - R.B. Pierce, D. Tong, A. Lenzen
  - Provided framework applied to regional model and supported updates
- Hemispheric CMAQ Platform (2018)
  - Global emissions: HTAPv2 + China
  - Regional: EPA 2016 platform (expect some decrease to 2018)
  - Year-specific meteorology, biogenics, and fires
- Gridpoint Statistical Interpolation (GSI)
  - 3d-variational assimilation
  - Using **OMI** and **TropOMI** observation operators for comparison
- Assimilation
  - Improves fidelity w/r/t satellite = Good for improving lateral boundary conditions.
  - Removes deterministic relationship and mass conservation = Not as good for attribution.
- Also serves as a basis for updating global emissions.



Legend
Vertical Column: Ω_v
Slant Column: Ω_s

J. East

Iterative Inverse Emissions Estimation

A Priori Emissions
Global: HTAPv2 or
Regional: EPA platform

Initial E

Convergence Check
E' - E < tolerance

Yes

Posterior Emissions

E=E'

E' is new E

85 %

100 %

Sensitivity

$$\beta = \frac{\Delta E}{E} \frac{\Omega_{V,Q}}{\Omega_{V,Q85} - \Omega_{V,Q}}$$

Monthly

Finite Difference Mass Balance

$$E' = E\left(\beta \frac{\Omega'_{V,Q} - \Omega_{V,Q}}{\Omega_{V,Q}} + 1\right)$$

Monthly

Assimilation CMAQ/GSI

CMAQ Prediction = F(E, Met)

$$\Omega'_{V,Q} = M^{-1}_{w,air} \sum \rho_z \chi_z h_z$$

GSI Assimilation

$3DVAR(\Omega'_{V,Q} \times AMF_Q, \Omega_{S,Sat})$

Hourly

RAW CMAQ Prediction

$\Omega_{V,Q}$

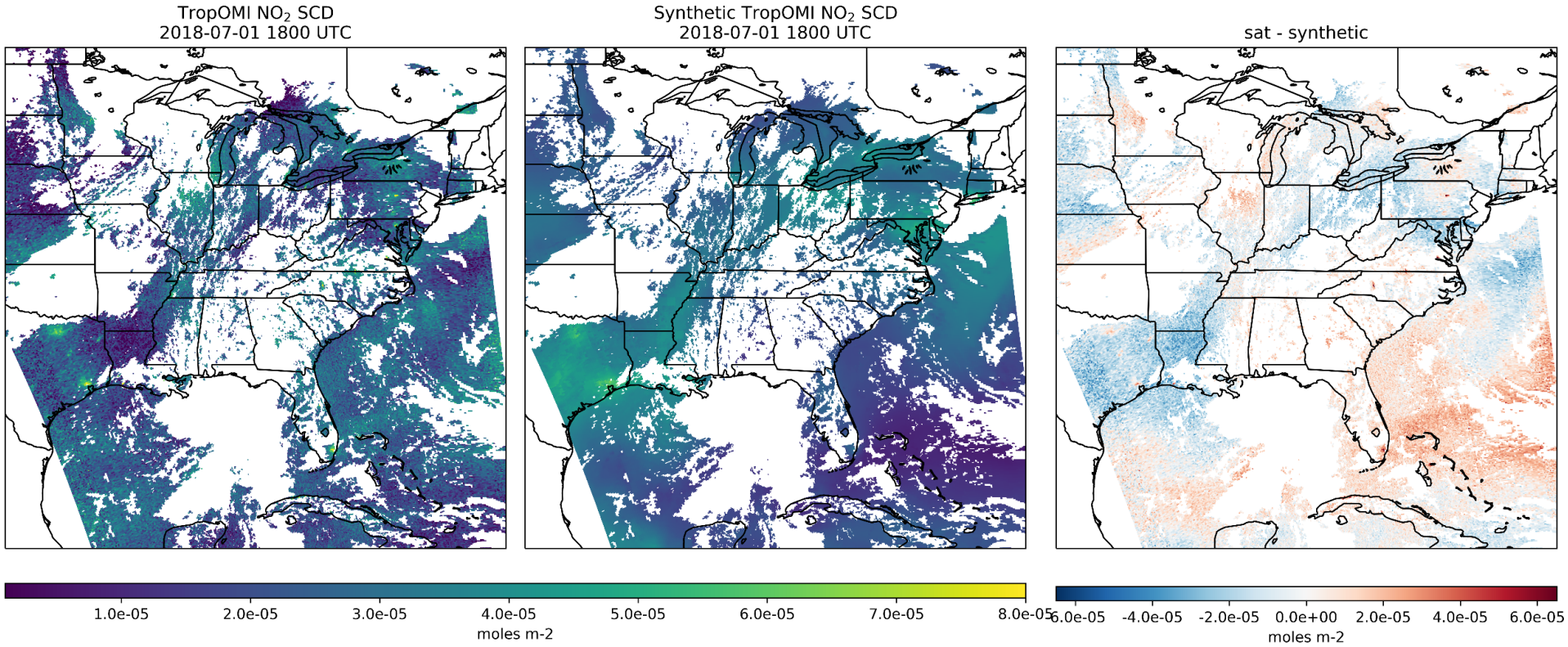
Legend
Vertical Column: Ω_v
Slant Column: Ω_s

*Only grid cells with substantial anthropogenic emissions are adjusted

TropOMI Slant Column Comparison

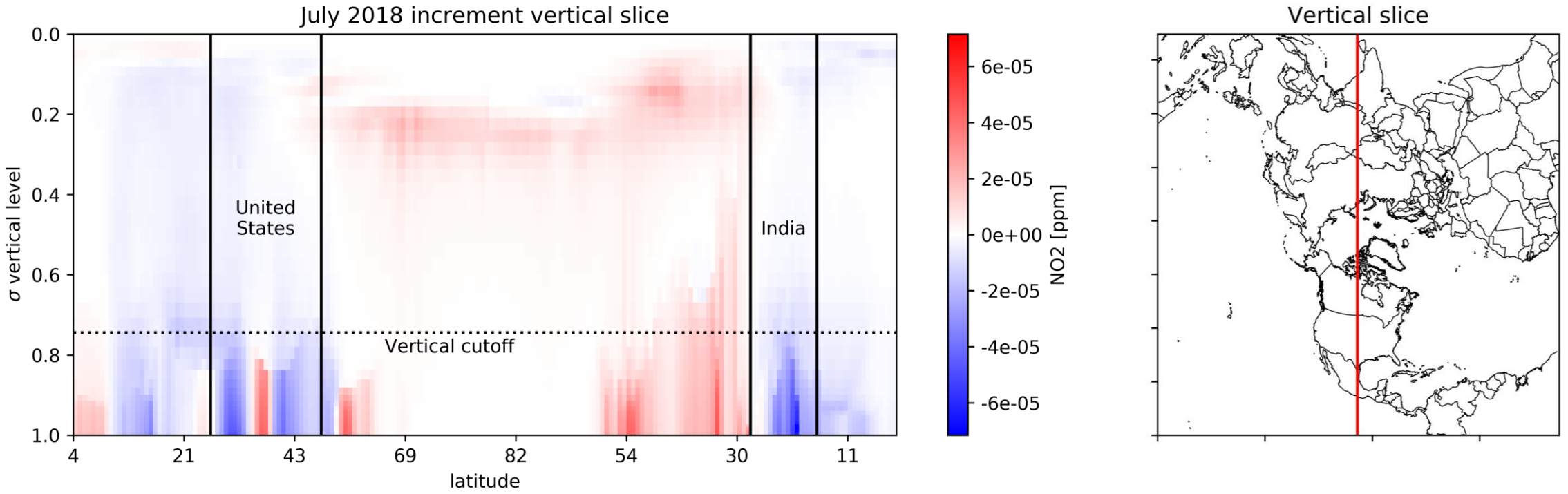
James East
ORISE Research Fellow

- Slant column comparison is the basis of assimilation.
- This prevents AMF uncertainty from direct influence
- GSI operator:
  - Interpolates to TropOMI
  - Applies scattering weight
  - Applies tropopause



2-dimensional picture

Challenges – vertical distribution of increment



- Cooper et al. (2017) showed spatial “smearing” by finite difference.
  - Conceptual disconnect between increment and assumptions in beta.
  - Adjoint accounts for this implicitly
- Step in the right direction: finite difference is to limit the vertical influence.

Iterative mass balance analysis

- Cooper et al. (2017) showed that basic mass balance converged toward the “truth” with an asymptote 4 or 5 iterations.

Cooper et al. (2017)

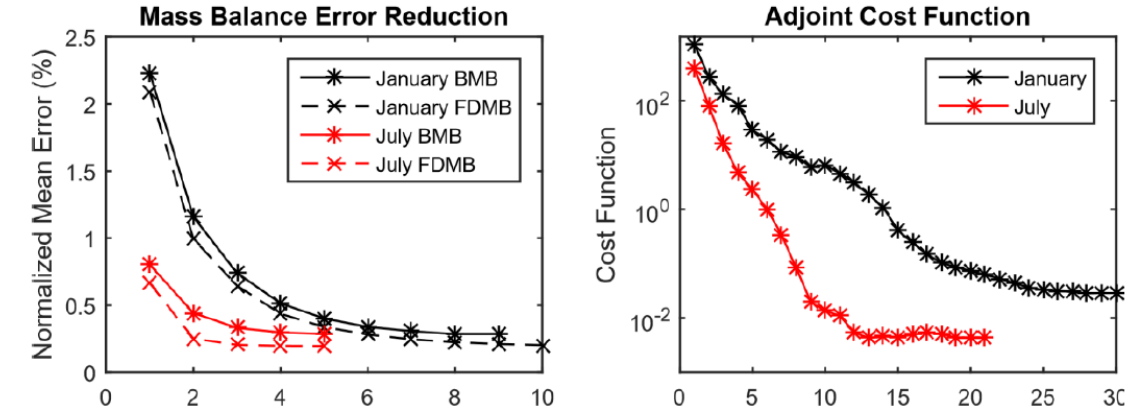
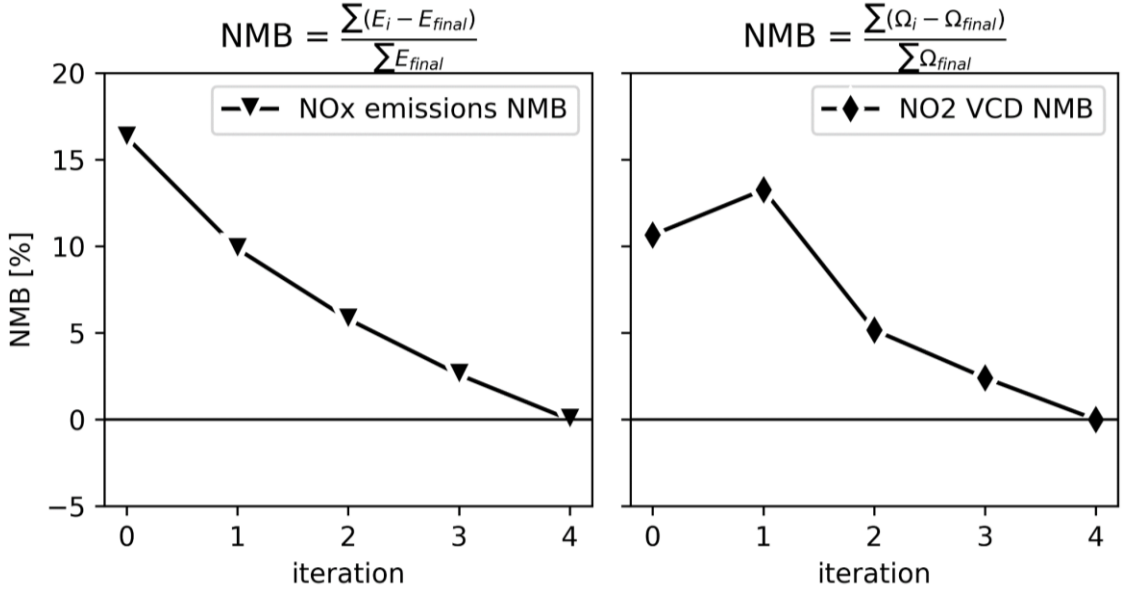


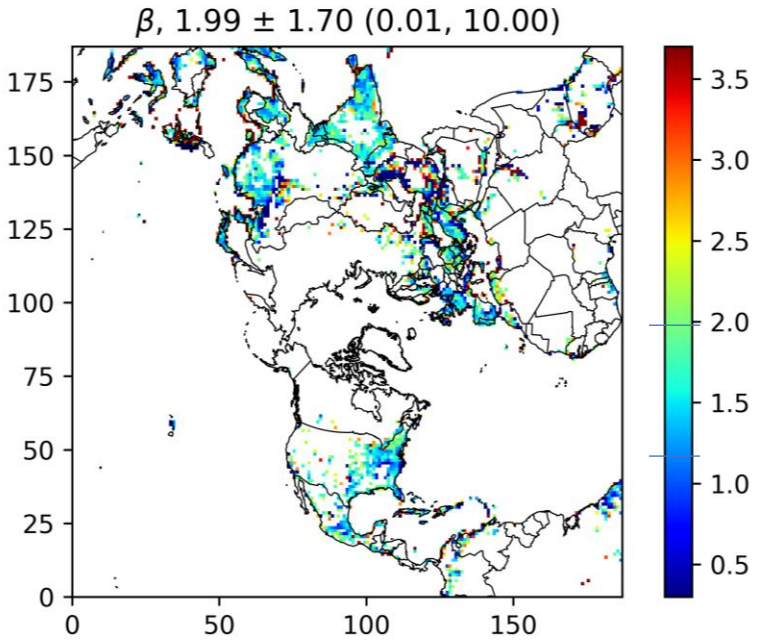
Figure S1. (Left) Normalized mean error reduction gained through an iterative method during the testing of horizontal smearing effects at 4°x5° resolution. Results using the basic mass balance (BMB) and finite difference mass balance (FDMB) methods are shown. (Right) Reduction in the adjoint cost function.

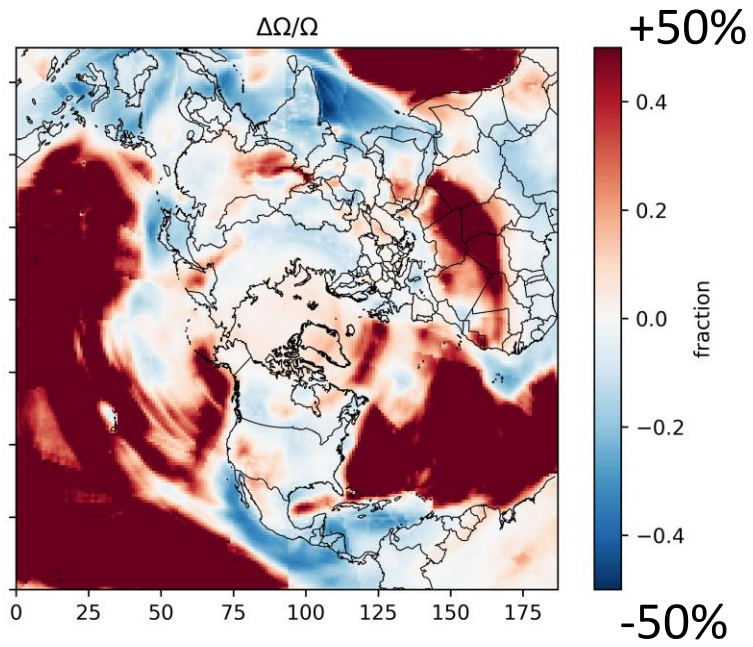
- Work in progress:
  - synthetic “truth” experiment not complete
  - iterative results show nominal convergence
  - More iterations in progress

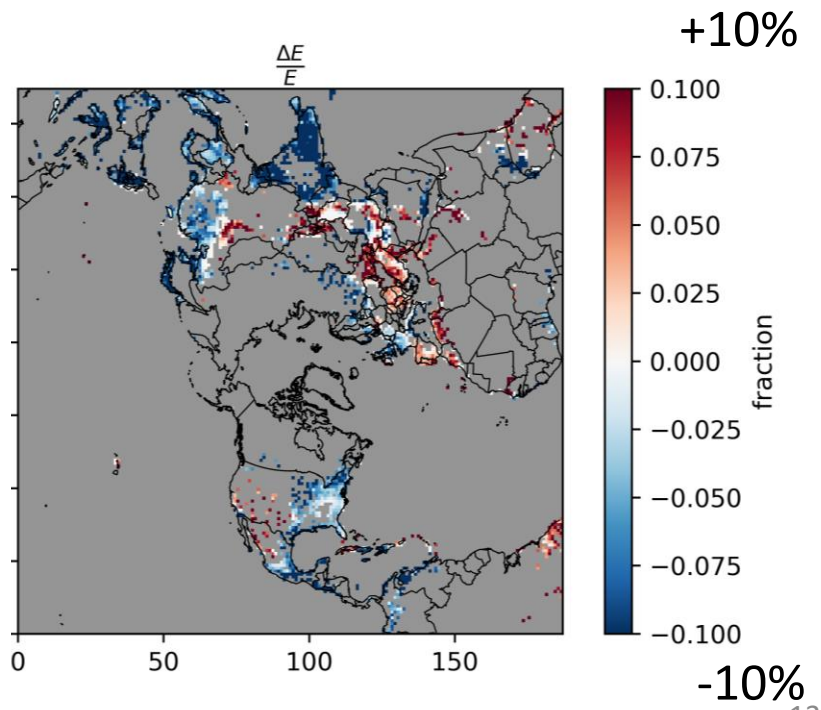


Preliminary Assimilation and inversion results

- Sensitivity parameter higher than previous literature (e.g., Lamsal 2011 = 1.16), partially due to outliers
- Large changes are seen over areas with little emissions and low vertical columns (lifetime or emissions?)
- Preliminary emission inversion (July 2018): heterogenous changes with some patterns

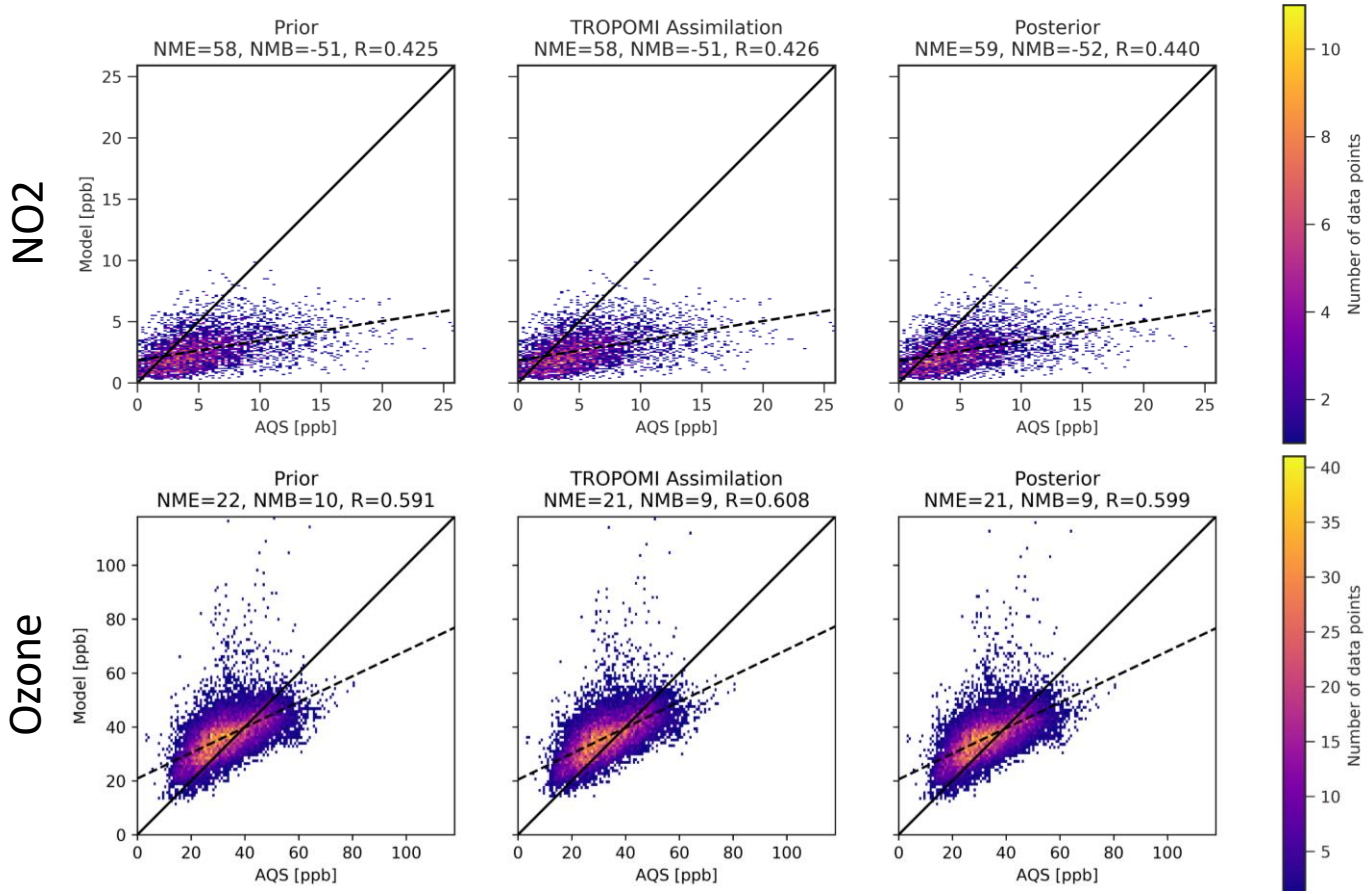






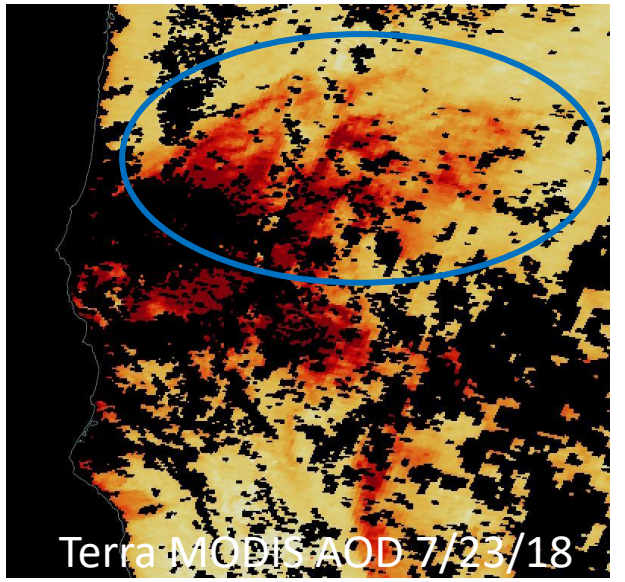
Impacts of preliminary assimilation and emissions update on model performance

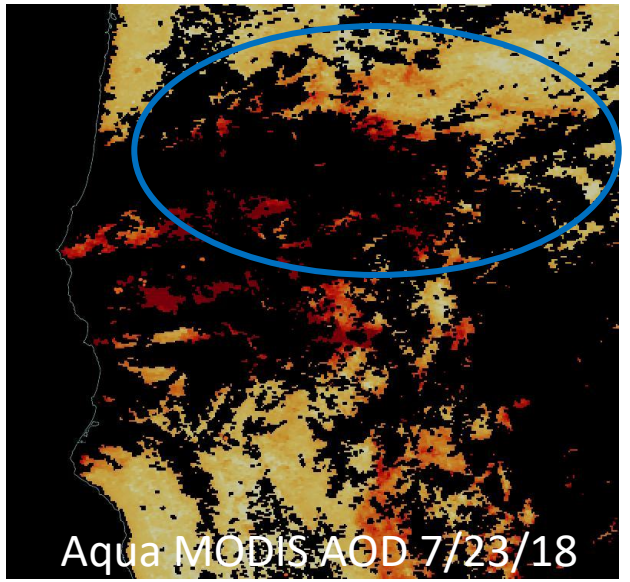
- Satellite performance improves, but what about surface?
- Small improvements in the right direction
- Correlation improved in both NO2 and ozone at the surface
  - NO2 correlation better in posterior than assimilation (better localization?)
  - Ozone correlation better in assimilation than posterior (more impact in the free trop?)
- No measurements from biggest changed areas (India and China)
  - Need surface measurements
  - OpenAQ processing



Possibilities with geostationary satellite information

- Imagine if we weren't looking once a day, but all day!
  - e.g., commuter traffic is at a minimum at mid-day
  - e.g., does the polar orbit cover peak electrical load times?
  - More complete coverage of episodic events – e.g. wildfire plumes
  - Better characterization of diurnal dynamics and interactions with emissions – e.g. land-sea breeze changes near coastal monitors
- Imagine if we had finer spatial resolution
  - More refined differentiation of proximal emission sources and chemical processes
  - Increased confidence in relationships between satellite data and surface concentrations
- The data management challenge will not be trivial.
  - Larger granules and more of them.
  - We need to start working with the data now to be ready when it arrives.



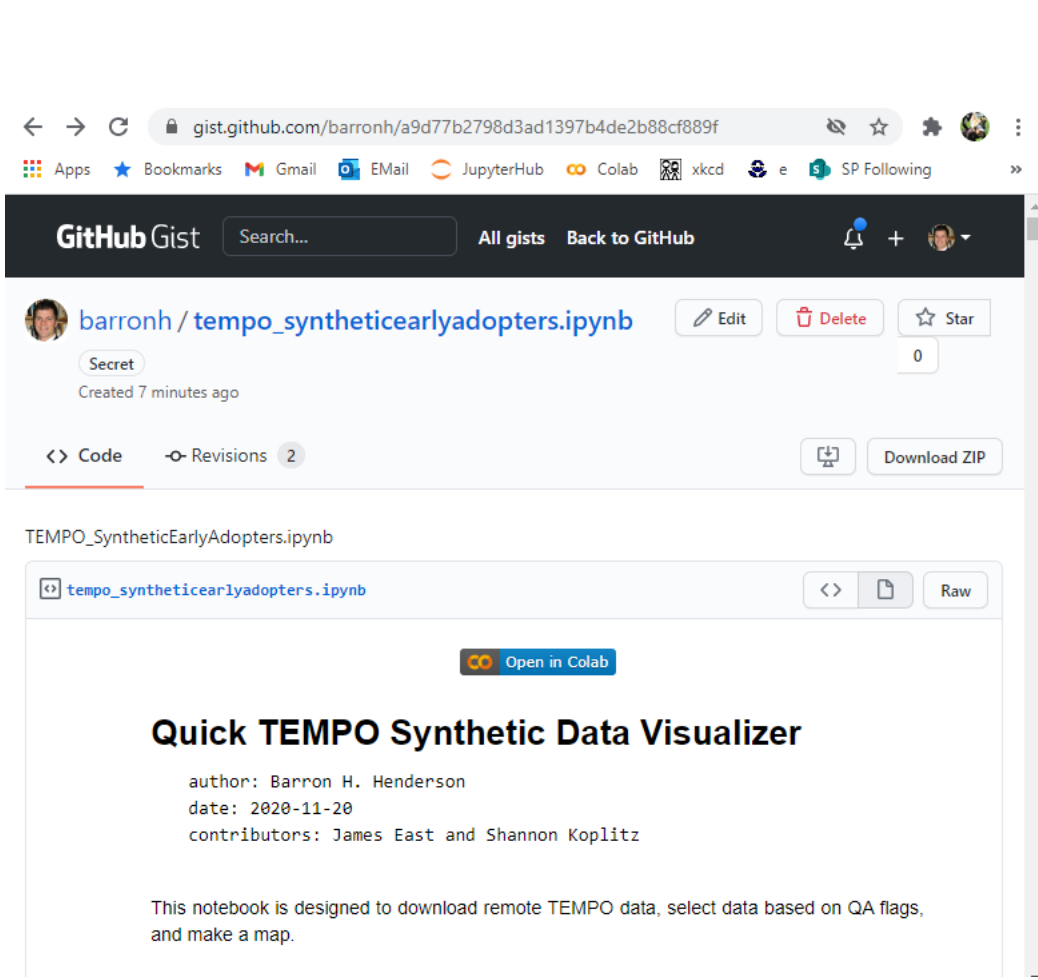


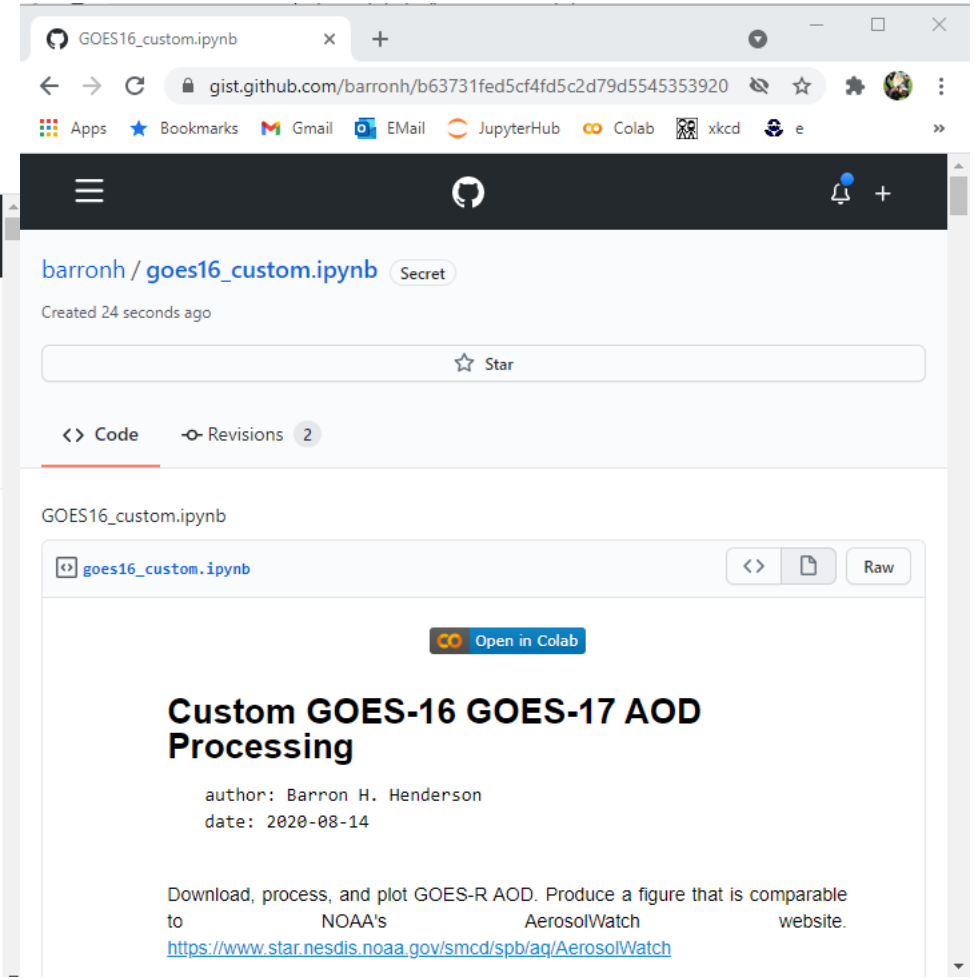
Images created with NASA Worldview

Processing for GOES and Synthetic TEMPO Data

If you want to get started with geostationary satellite data but aren't sure how, try plotting GOES-16 AOD or TEMPO Synthetic NO2 data.

These are primers, and not targeted toward specific applications.





https://gist.github.com/barronh/a9d77b2798d3ad1397b4de2b88cf889f

https://gist.github.com/barronh/b63731fed5cf4fd5c2d79d5545353920