

GEOS-Chem Adjoint Model and Data Assimilation Working Group

Daven K. Henze, CU Boulder, Adjoint Model Scientist

Jun Wang, U Iowa, Adjoint and Data Assimilation WG Co-Chair

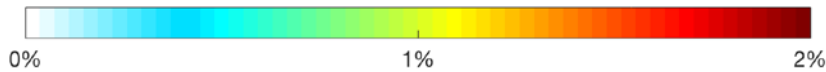
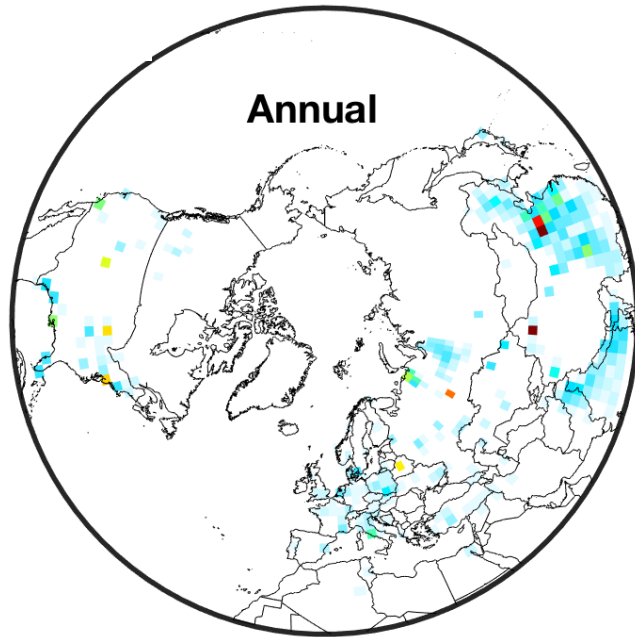
Yanko Davila, CU Boulder, Adjoint Model Code Support

...plus all of the GEOS-Chem adjoint modelers and data assimilators!

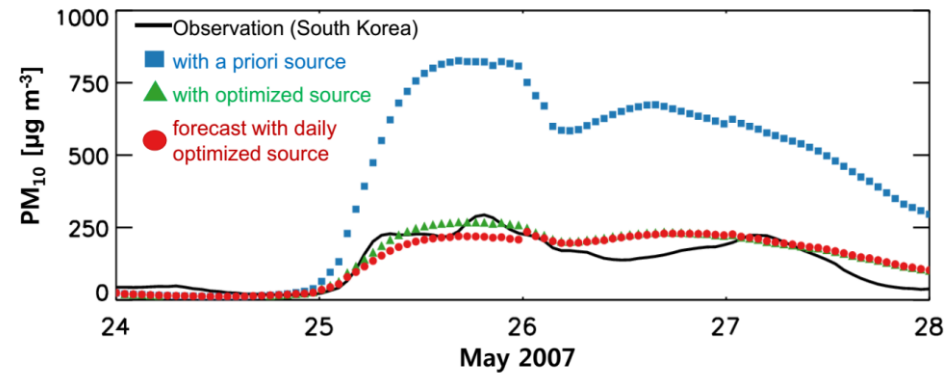
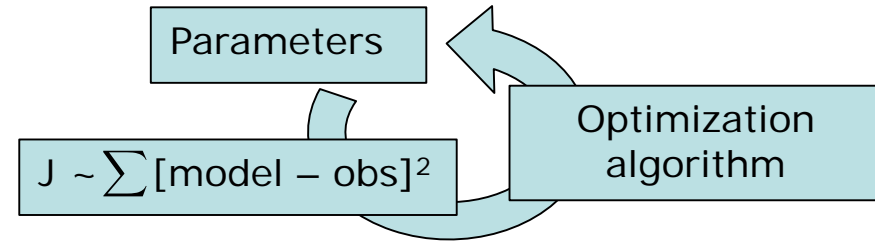
Adjoint Modeling and Data Assimilation

Adjoint sensitivity / source attribution

Inverse modeling / DA



Contributions to Arctic BC column concentrations from emissions in each grid cell computed very efficiently using the GEOS-Chem adjoint model (Junwei Xu et al., 2017)



Dust emissions optimized using GEOS-Chem 4D-Var and PM₁₀ measurements (Jaemin Jeong and Rokjin Park, 2018)

Adjoint sensitivity and source attribution: Recent and current applications

What is the impact of each of many (10^6) parameters on a single (or small number) of model response metrics?

→ computed efficiently with the adjoint model

Climate

- Aerosol Radiative forcing and Temperature (Lacey, CU Boulder)
- Ozone and CH_4 RF (Walker, JPL); Stratospheric O_3 (Dedoussi, MIT)
- CCN (Capps, Drexel)
- BC in the Arctic (Qi, UCLA; [Xu, Dalhousie](#))

Air quality

- $\text{PM}_{2.5}$ source attribution ([Zhang, Peking](#); [Lee, SNU](#))
- $\text{PM}_{2.5}$ health impacts (Dedoussi, Dasadhikari, MIT; Zhang, Tsinghua; Lee, Dalhousie; Lacey, CU Boulder; Koplitz, Harvard)
- O_3 health impacts ([Henze, CU Boulder](#))

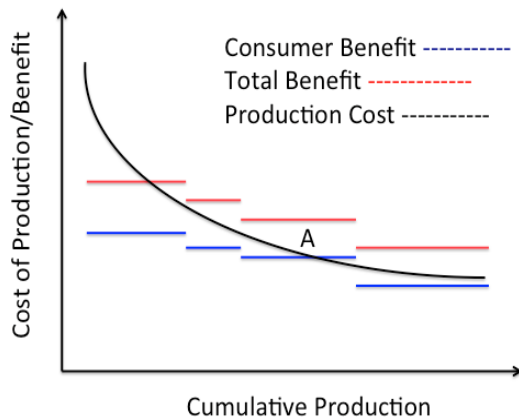
Ecosystem impacts

- O_3 vegetative exposure and crop loss (Lapina, CU Boulder)
- N deposition (Lee, CU Boulder; [Zhao, Zhang, Peking](#))

*Recent / active
projects
[GCA1 attendee](#)*

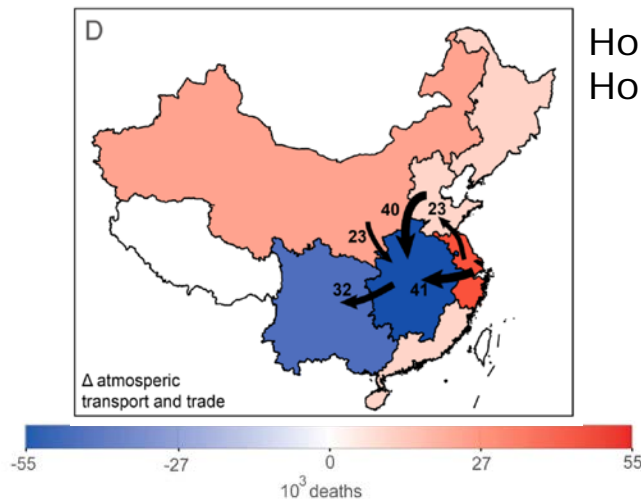
GEOS-Chem adjoint new directions: health impacts and integrated assessment

(e.g., Dedoussi, MIT; J. Lin and Q. Zhang, Peking/Tsinghua, Baublitz, Columbia; Henderson, EPA; Henze and Lacey, Keshavarzmohammadian, CUB)



Azi Keshavarzmohammadian et al. (submitted) use adjoint results (deaths per kg emission) from Dedoussi et al. (2014) to optimize electric vehicle market penetration

Impacts of atm transport vs trade on PM_{2.5} mortality in China



Hongyan Zhao et al., ACP, 2017
Hongyan Zhao et al., submitted

Inverse modeling and data assimilation: Recent and current projects

Aerosol and aerosol precursor emissions

- Aerosol with MODIS, CALIPSO ([Wang, UI](#); Lee, Dalhousie; Chen, Li, CNRS)
- Dust with surface PM₁₀ ([Jeong, SNU](#))
- NH₃ with TES and CrIS ([Zhang](#), Peking; Henze, CUB; Shim, KEI; Zhu, Sun Yat-Sen)
- SO₂ and NO₂ with OMI ([Wang, UI](#); [Qu](#), CU Boulder; Cooper, Dalhousie)

Greenhouse gases

- CH₄ (Turner, Harvard/UCB; Stanevich, UT;)
- CO₂ (Liu, Lee, Bowman, JPL; Deng, Jones, UT; Philips, NASA AMES)
- N₂O (Wells, U. Minnesota)



Reactive gas-phase species

- CO from MOPITT ([He, UT](#))
- Isoprene from OMI HCHO (Kaiser, Harvard)
- NMVOCs ([Cao](#), Peking)
- CO, NO₂ and O₃ ([Miyazaki](#), JAMSTEC/JPL; [Zhang](#), UT)
- Chem DA in GEOS (Keller, NASA GMAO)

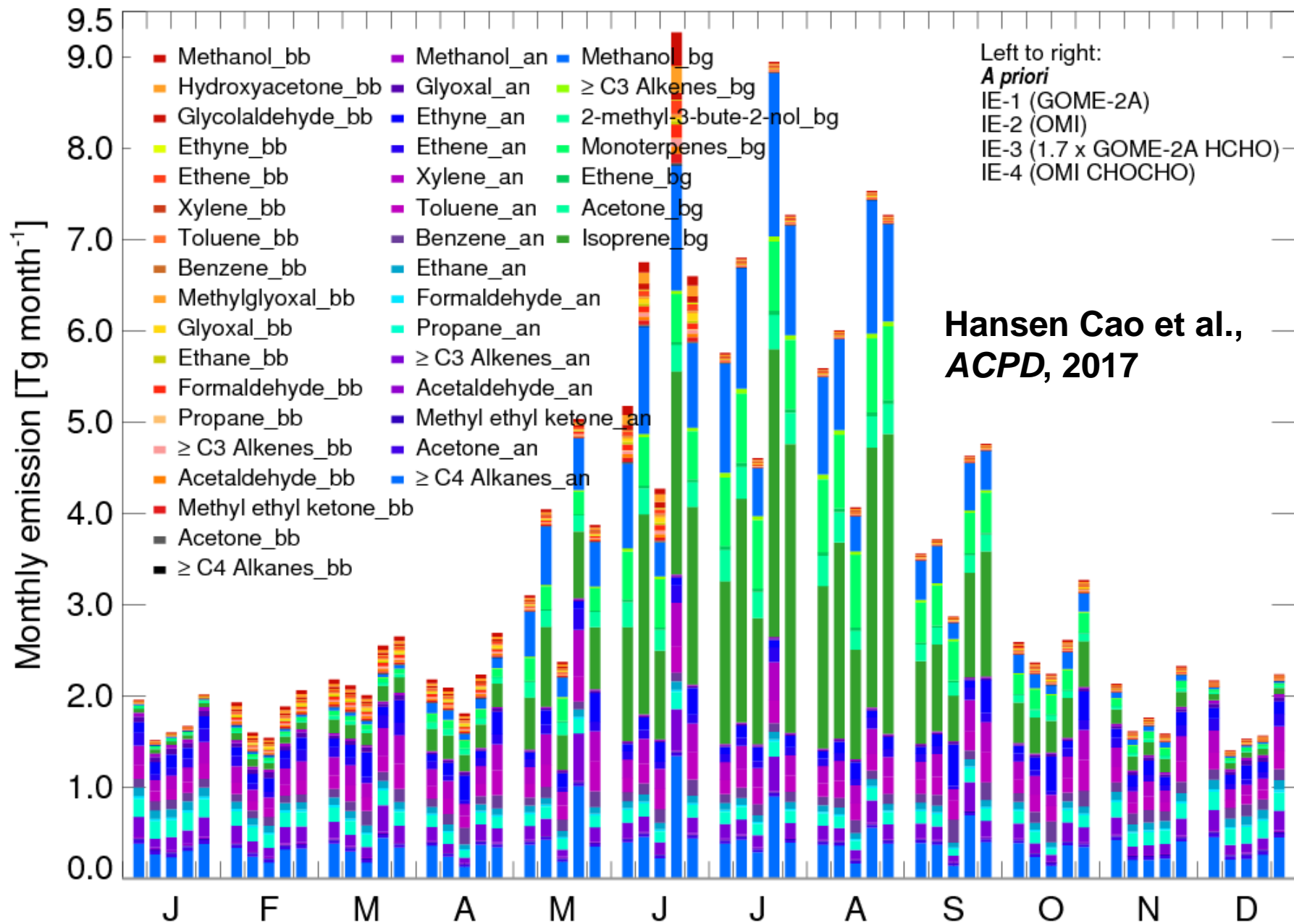
Satellite design

- GEO-CAPE (Bousserez; CU Boulder)
- CLARREO ([Wang, UI](#))

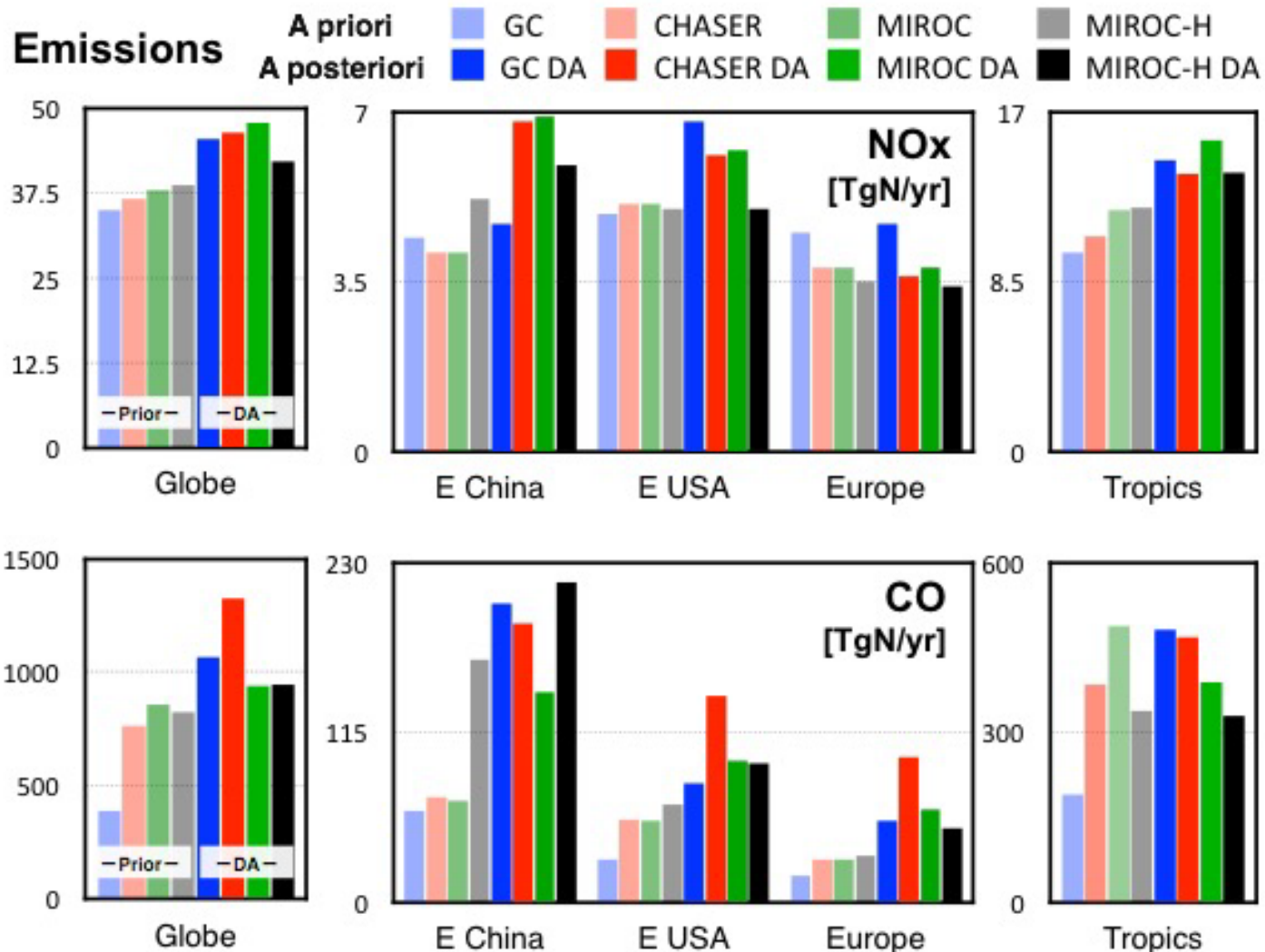
Method advancement and comparisons

- Weak constraint 4D-Var ([He](#), Stanevich, UT)
- Resolution errors (Stanevich, UT)
- UQ and model reduction (Bousserez, CU Boulder)
- 4D-Var and EnKF ([Miyazaki](#), JAMSTEC/JPL; Liu, JPL)
- Mass balance vs 4D-Var ([Qu](#), CU Boulder; Cooper, Dalhousie)

Adjoint inversion of Chinese NMVOC emissions using space-based observations of formaldehyde and glyoxal



Multi-species, multi-model EnKF Data Assimilation



Timely updates to SO₂ and NO₂ emissions with GEOS-Chem 4D-Var

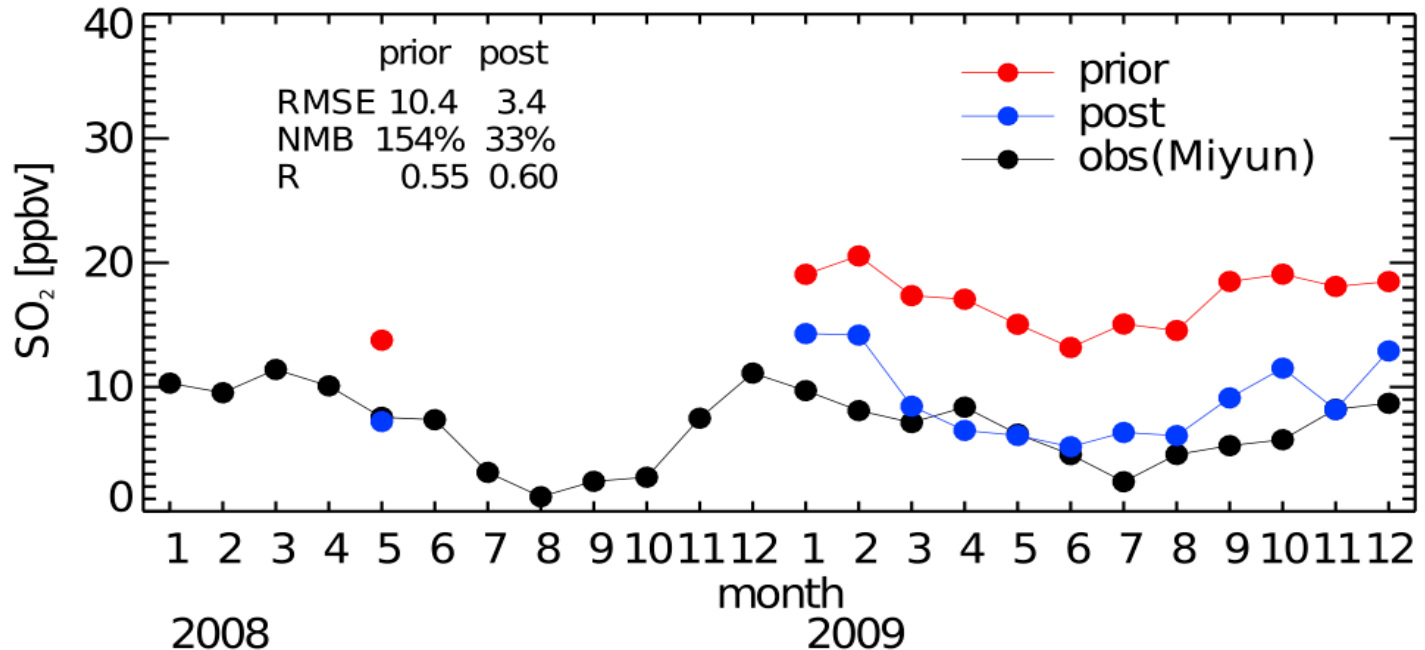
GEOPHYSICAL RESEARCH LETTER

Key Points:

- OMI and adjoint modeling can constrain monthly anthropogenic SO₂ emissions
- Twenty percent emission reduction during the Beijing Olympic Games made evident
- Posterior emissions improve model forecasts of surface and column

A new approach for monthly updates of anthropogenic sulfur dioxide emissions from space: Application to China and implications for air quality forecasts

Yi Wang^{1,2}, Jun Wang^{1,2}, Xiaoguang Xu^{1,2}, Daven K. Henze³, Yuxuan Wang^{4,5}, and Zhen Qu³



- GEOS-Chem adjoint operators for using OMI SO₂, NO₂, and MODIS radiances as constraint to optimize emissions have been developed.
- We're now actively looking for collaborators to test these satellite-added-value emissions in either research or operational model.

Adjoint model: current and **new** features

Standardized code: v**35m**, maintained / distributed via GIT

Code base : v8-02-01 with relevant fixes / updates **up to v10**

Meteorology: GEOS-4, GEOS-5, GEOS-FP, **MERRA2**

Simulations : full chem; **gly-chem**, offline CO, O_x, CO₂, CH₄, BC,
Dust, N₂O,

Resolution : 4x5, 2x2.5, 0.5 x 0.667, 0.25 x 0.3125

Processes: all main forward model process *excluding*:

- non-local pbl mixing scheme
- aerosol microphysics
- feedback of aerosols on photolysis or heterogeneous chemistry
- **UCX**, HEMCO
- **SOA**
- **diurnal variability of NH₃**

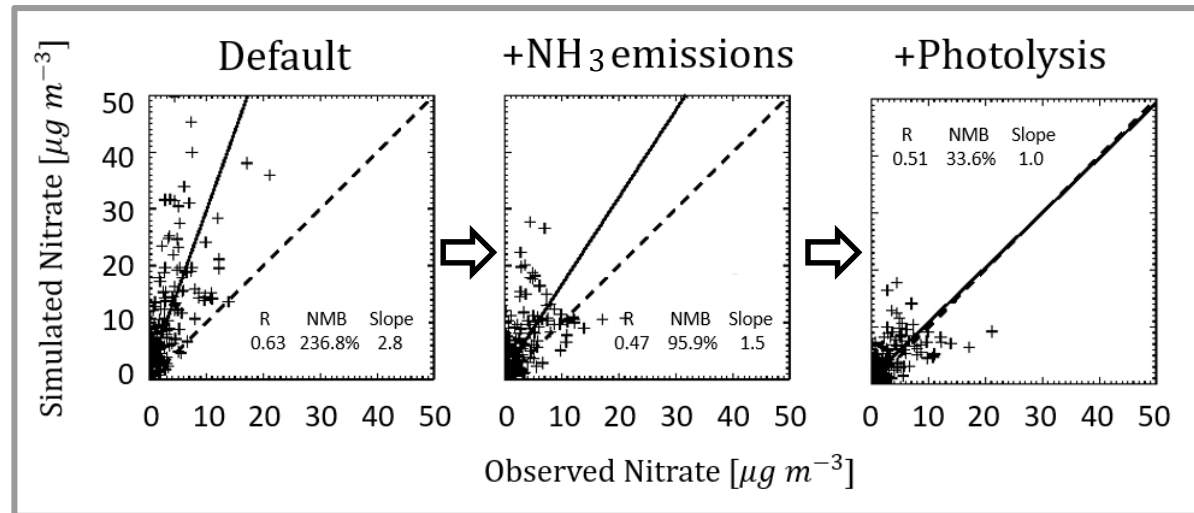
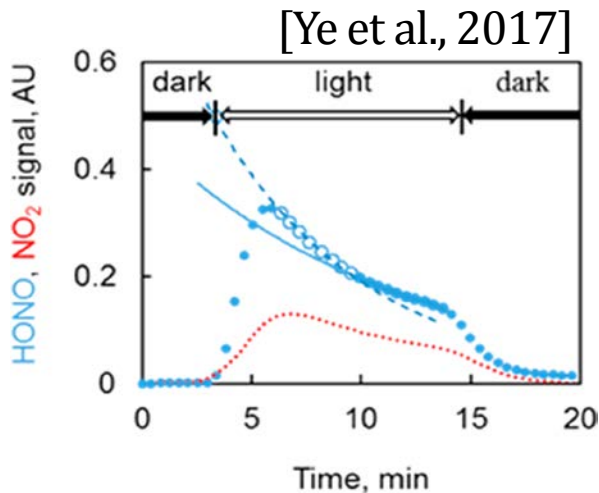
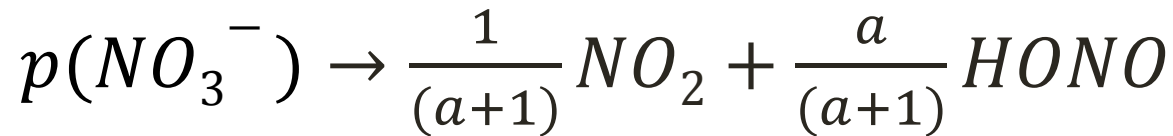
Species: forward full chemistry model species *excluding*:

- SO₄s, NITs, Br

Model update cycle slowed while waiting for GCHP / FlexChem...

Updates from SNU to Resolve the Nitrate Overestimation

1. Diurnal variation in NH_3 emission [Poullain et al., 2011; Zhu et al., 2015]
2. Additional Loss of NO_3^- by photolysis [Ye et al., 2017; Lee et al., in prep.]

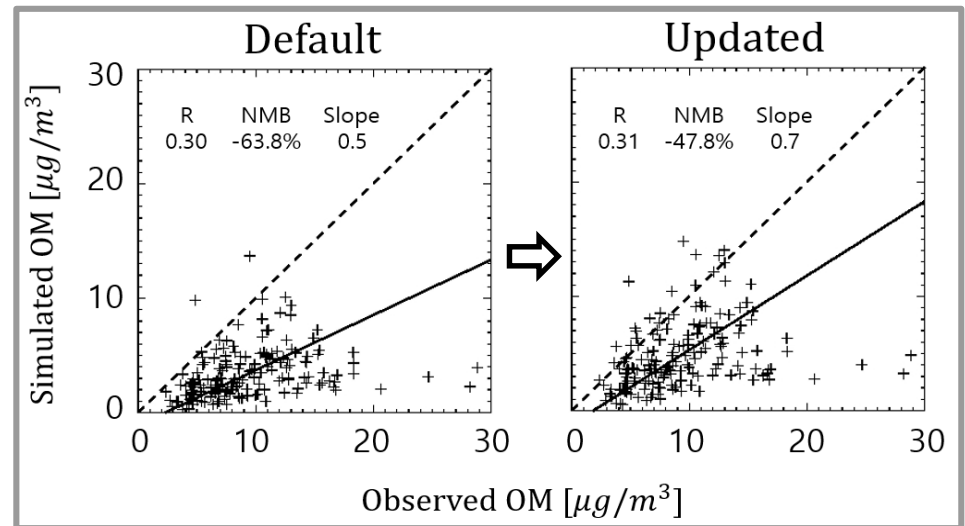


Updates from SNU to Resolve the OM Underestimation

1. SOA formation from anthropogenic aromatics oxidation (benzene, toluene, xylene) [Henze et al., 2008]
2. Yields(γ) are from simulation with VBS approach [Jo et al., 2013]

$$\gamma = \frac{SOA}{SOA + SOG}$$

γ : aerosol fraction of aromatic SOA from the GEOS-Chem simulation considering the VBS approach with chemical aging



Find out more...

Visit us at:

http://wiki.seas.harvard.edu/geos-chem/index.php/GEOS-Chem_Adjoint (wiki)

- manuals, instructions, publications
- code features
- current version overviews
- benchmarks

<http://adjoint.colorado.edu:8080> (code GitLab)

- code distribution

<https://trello.com/b/GTfHT38L/geos-chem-adjoint> (pipeline)

- code development cycle / pipeline

GEOS-Chem adjoint code support:

- yanko.davila@colorado.edu

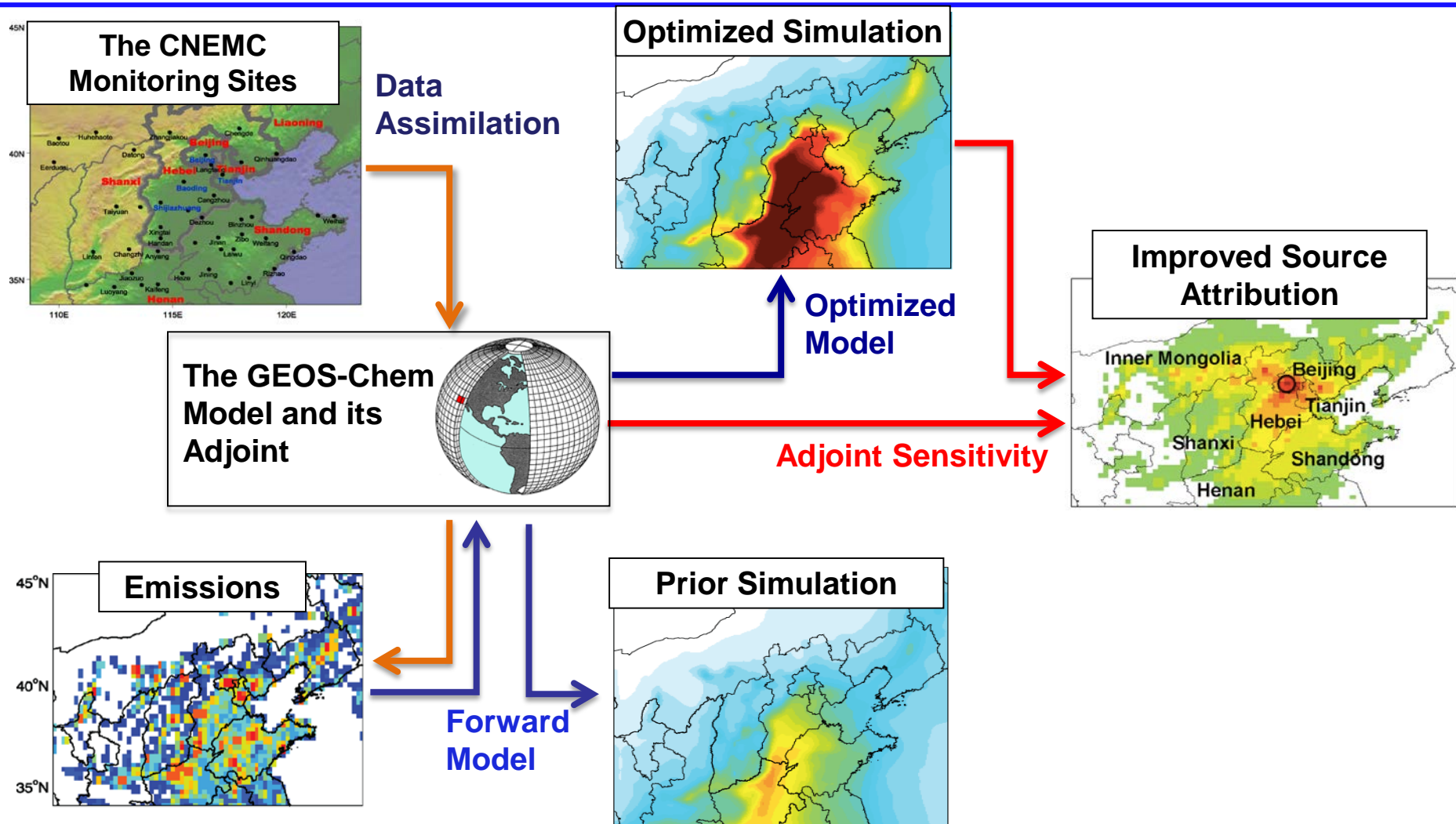
GEOS-Chem adjoint model clinic:

- **Wednesday 12:30 – 14:00**



bonus slides

Adjoint Application on PM_{2.5} pollution over China - Data Assimilation and Source Attribution

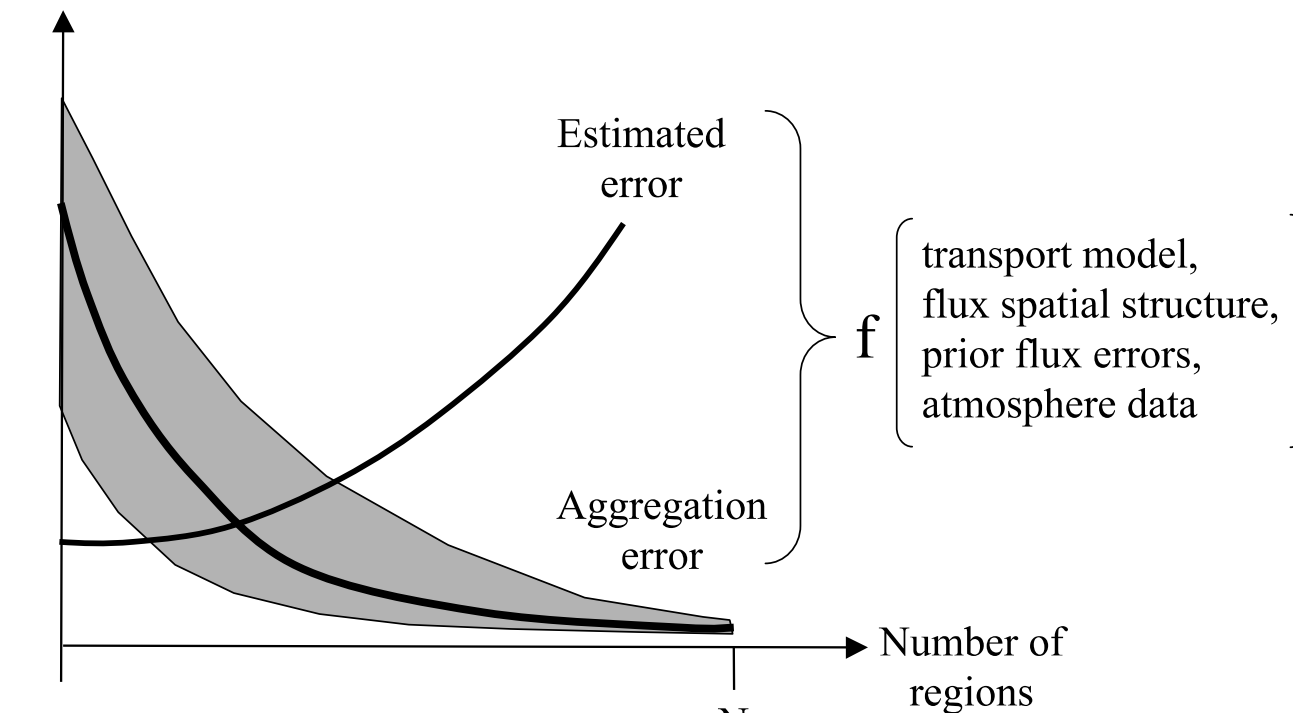


L. Zhang, et al., Sources and Processes Affecting Fine Particulate Matter Pollution over North China: An Adjoint Analysis of the Beijing APEC Period, ES&T, 2016.

GEOS-Chem adjoint major new directions

Overcoming outstanding challenges

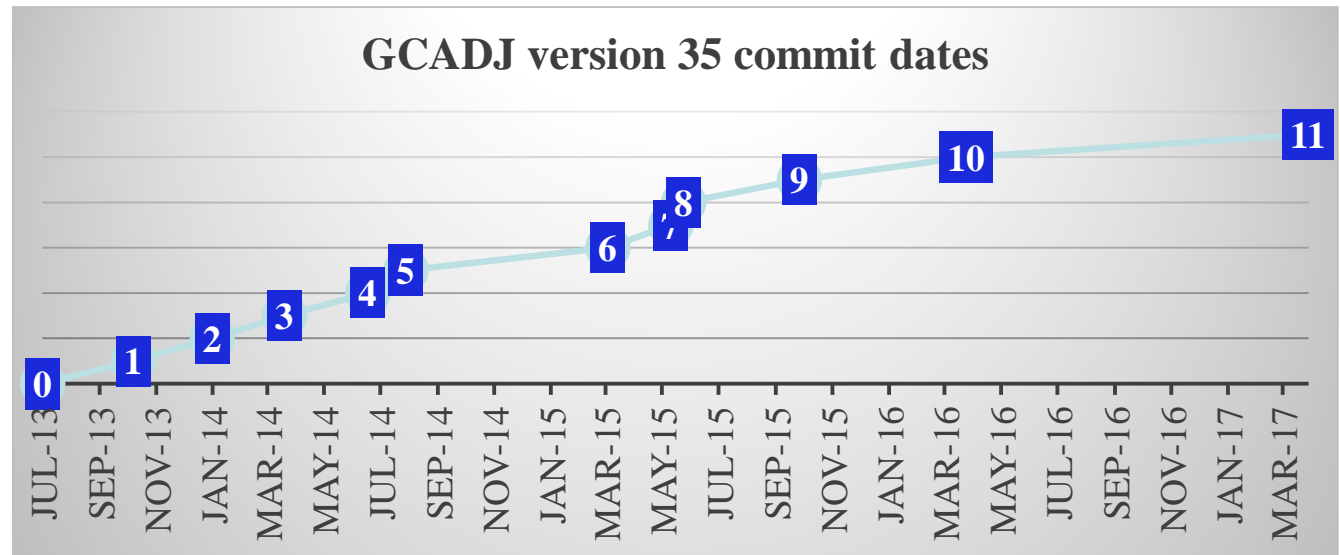
- assuming a perfect model (\Rightarrow weak constraint chem 4D-Var, UT)
- can't calculate posterior error (\Rightarrow MC and randomization, CU Boulder)
- aggregation vs inversion errors tradeoff in GHG flux constraints
(\Rightarrow Turner, Harvard, Boussez, CU Boulder)



Kaminski and Heimann (*Science*, 2001)

Adjoint code updates

Code update cycle



Significant forward model updates looming (GCHP, FlexChem)

Adjoint models often lag forward models – that's ok (for DA)
(e.g., ECMFW hasn't updated theirs in 4 yrs)

Adjoint model: tracking activities

See GC adjoint wiki page, GitLab and Trello for details:

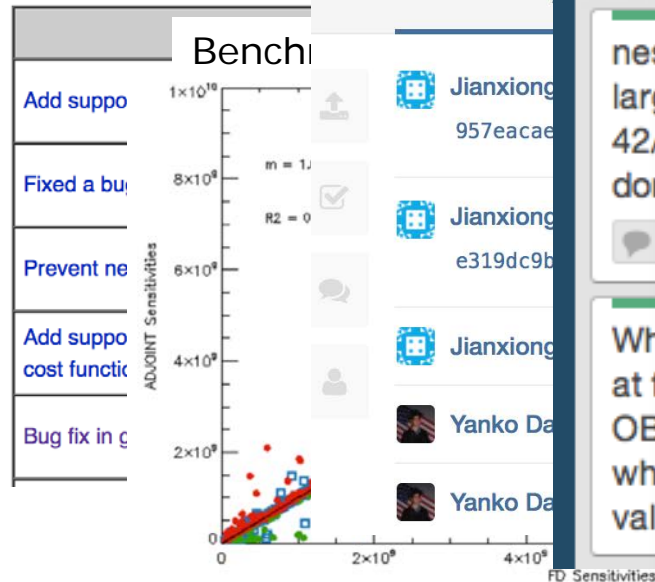
http://wiki.seas.harvard.edu/geos-chem/index.php/GEOS-Chem_Adjoint (wiki)

<http://adjoint.colorado.edu:8080> (code GitLab)

<https://trello.com/b/GTfHT38L/geos-chem-adjoint> (pipeline)

What's new in this version

GEOS-Chem Adjoint v35 contains



Bugs to fix

nested grid code crashes with

large

42/43

doma

2

Why

at first

OBS_

why a

value

Under development

Observation error variances for

In pipeline

Reaction rate sensitivities
(Paulot, Harvard; Walker, UT)

1

NAB HML

Cost function evaluated in unit of
flux ($\mu\text{g}/\text{m}^2/\text{hr}$)

HML

Recently Implemented

ANISO (Capps, Georgia Tech)

DKH fix for ITS_A_NEW_** to
account for simulations that
off month.

1

Add a card...

Adjoint model: requirements

Requirements:

- checkpointing: data written during fwd, read during adjoint
- forward model slower than standard owing to heavy i/o
- memory usage ~x4 of standard forward model
- adjoint requires x2-4 of standard forward CPU time

Examples (on dual hex-core Xeon 2.6 GHz):

- fwd+adj iteration of **full chem**, global 2x2.5, 1 month
 - 400 GB checkpoint files
 - 30 hours per iteration w/NFS scratch
 - 9 hrs per iteration w/local SS scratch

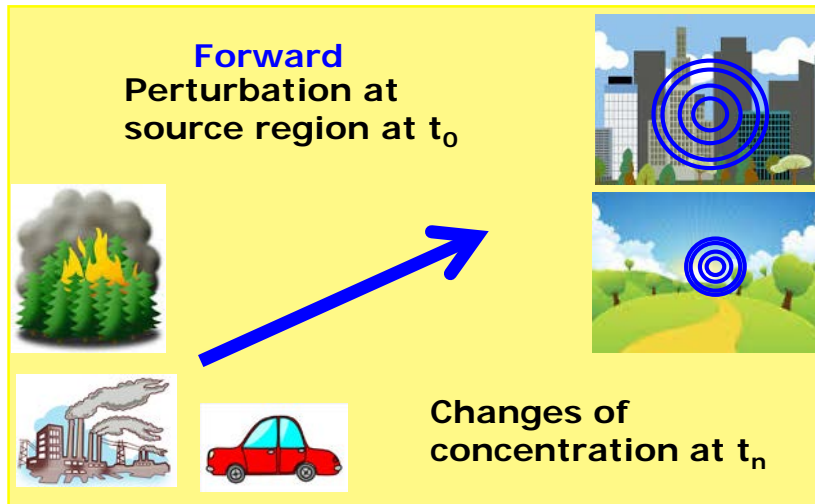
- fwd+adj iteration of **offline CO2**, global 2x2.5, 1 month
 - 2.5 GB checkpoint files
 - 2 hours per iteration

An adjoint model...

...efficiently calculates gradients of a scalar model response with respect to all model parameters (emissions, rate constants, ...) at the native model resolution.

Forward Model (source-oriented)

Sensitivity of all model concentrations to one model source

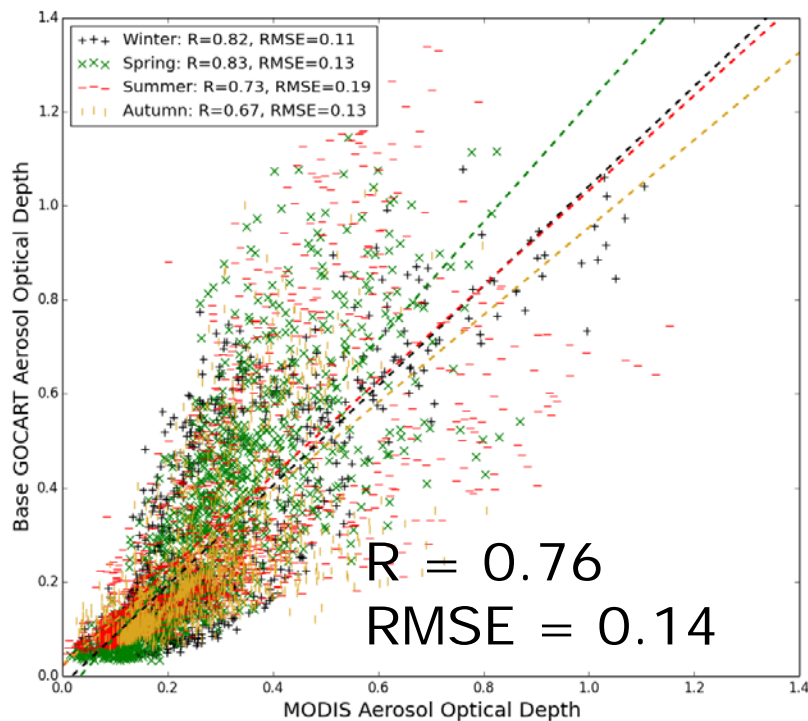


cost scales with # of sources

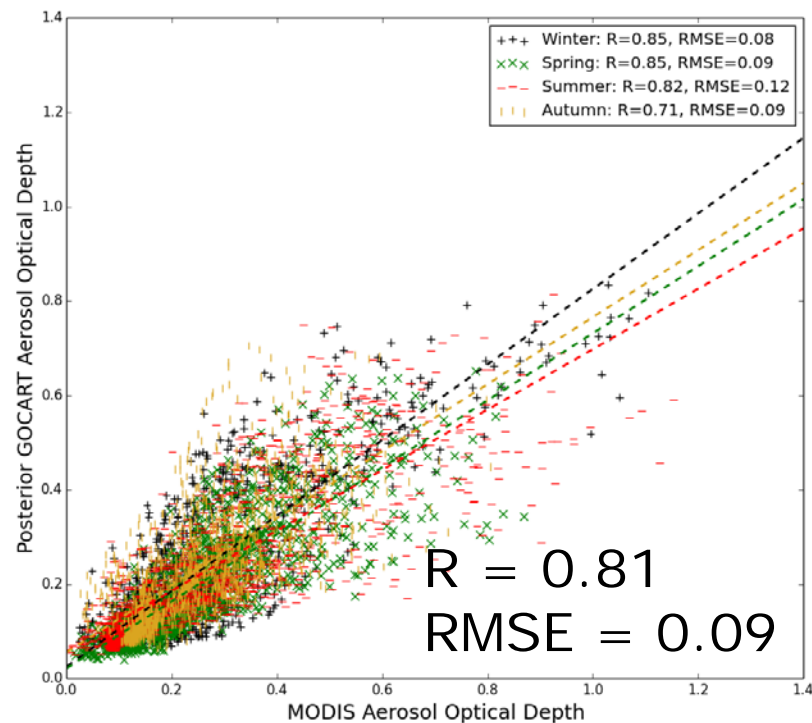
Inverse modeling evaluation: Try posterior emissions in different model

1. Inversion of speciated aerosol emissions in GEOS-Chem using new GRASP AOD retrieval from PARASOL
2. Evaluate posterior emissions in GOCART

Base GOCART

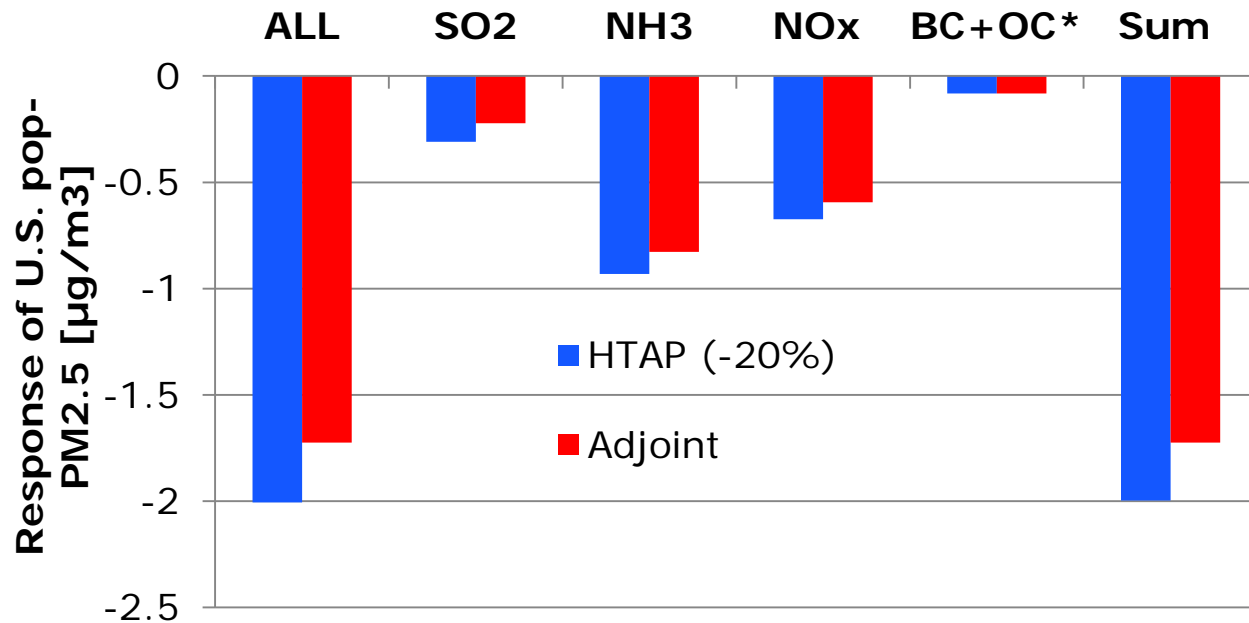


Posterior GOCART



Linearity as a function of species and region for PM_{2.5}

Experiment: Global SO₂, NH₃, NO_x and combined (ALL)

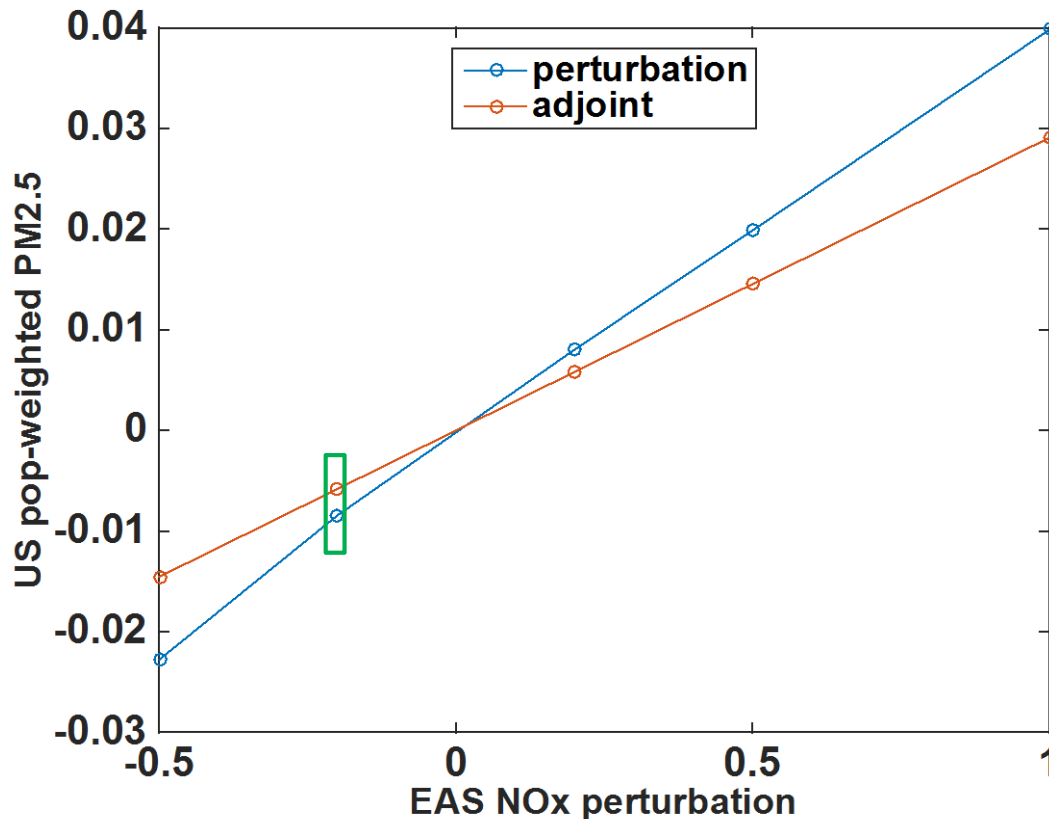


*BC+OC from HTAP not included, so used adjoint values (should match exactly for these linear species)

Results: Linearized estimates (adjoint) are fairly good representation of actual forward model responses, and results are additive.

Adjoint vs Perturbation: PM_{2.5}

Regional (EAS) NOx impact on US pop-weighted PM_{2.5}

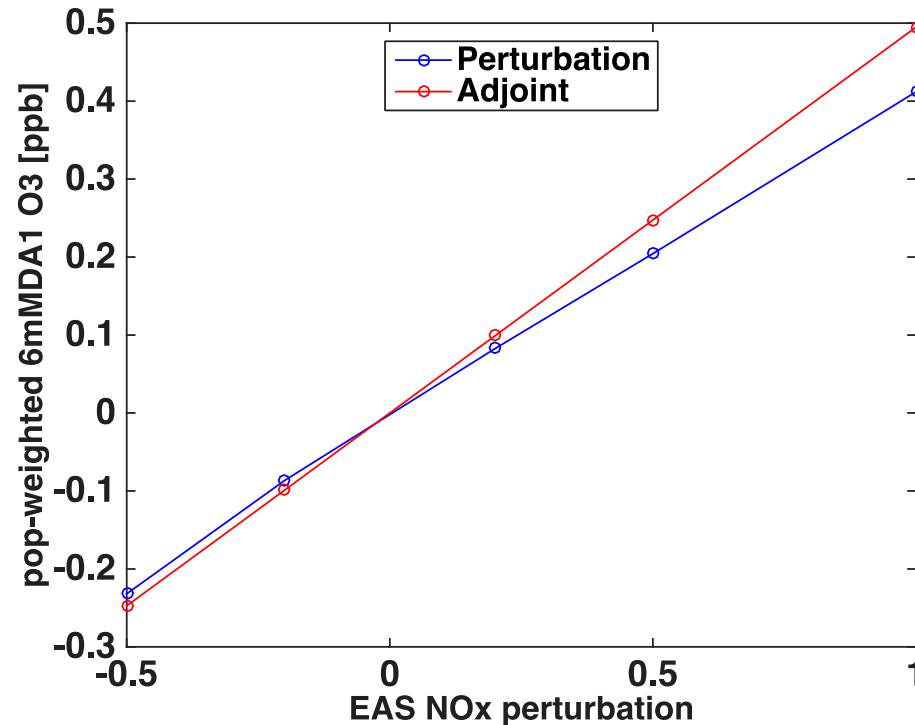


Results: Linearized (adjoint) agrees well with NOx emissions changes, with an underestimate in the response of 25%.

Range of 6 HTAP model estimates (green) is 44%.

Adjoint vs Perturbation: O_3

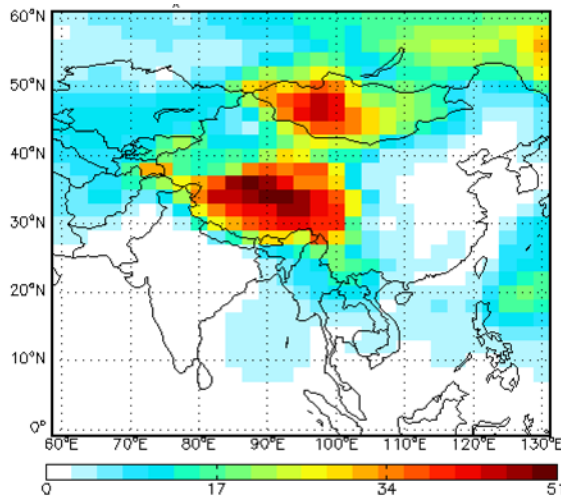
Regional (EAS) NOx impact on US pop weighted 6mMDA1 O_3



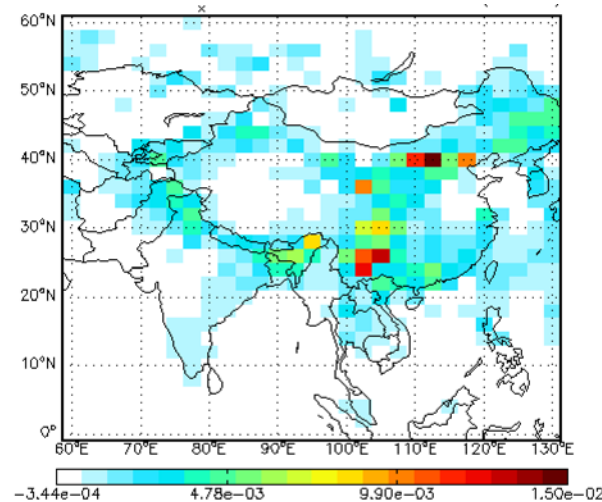
Results: Linearized (adjoint) agrees well with NOx emissions changes, with an overestimate in the response of 25%.

Sub-region variability in O₃ sensitivities

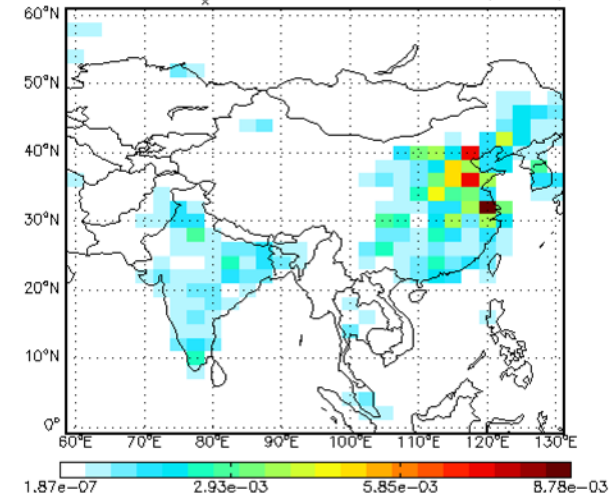
Experiment: EAS NO_x impact on US 6mMDA1 O₃



Sensitivities
(dO₃/dEN_{ox})



Contributions
(dO₃/dEN_{ox}) * EN_{ox}

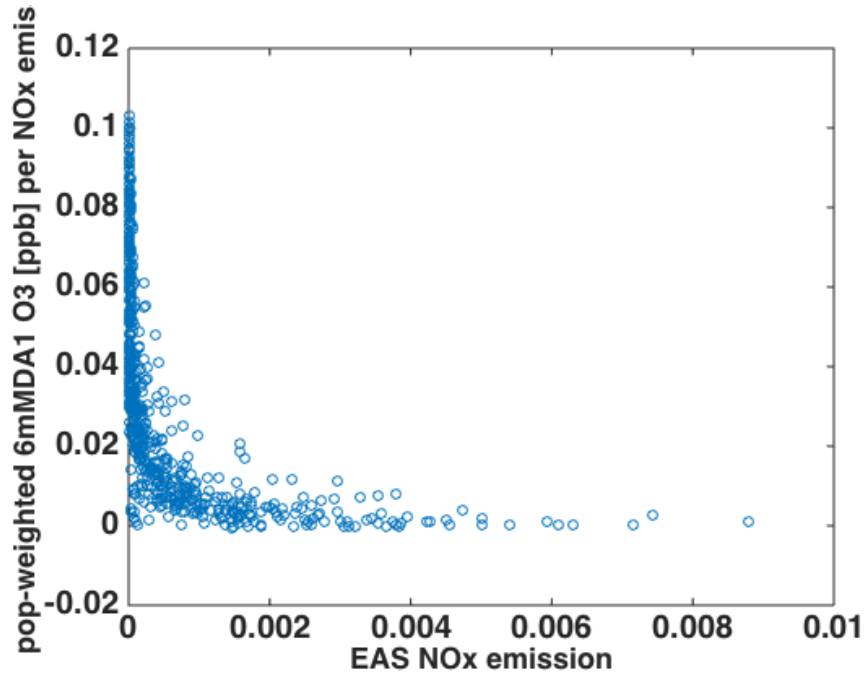


Emissions

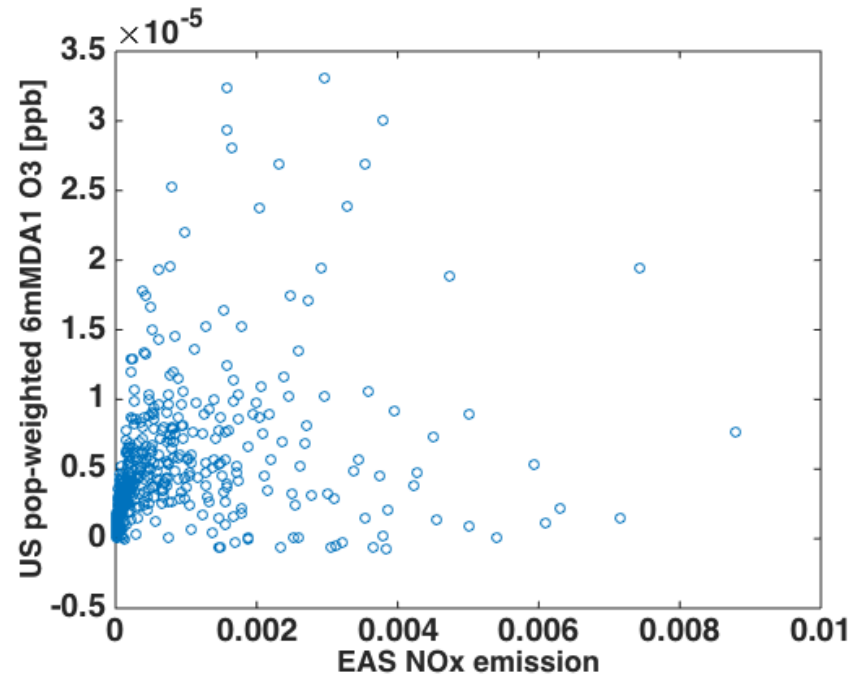
My sense here is that downscaling from HTAP-1 regions by emissions isn't going to work well, because Contributions \neq Emissions.

Sub-region variability in sensitivities

Experiment: EAS NO_x impact on US 6mMDA1 O₃



Sensitivities
(dO_3/dEN_{Ox})



Contributions
(dO_3/dEN_{Ox}) * EN_{Ox}

Sub-region variability in sensitivities

Experiment: EAS NO_x impact on US 6mMDA1 O₃ [ppb]

Region	HTAP	Adjoint
EAS	-0.087	-0.099
China	-0.081	-0.086
Japan	-0.004	-0.009

It would be nice to use SR tool to estimate impacts of emissions scenarios for regions other than ours (e.g., different provinces in China, or different countries in Easia), but this will be difficult w/o downscaling.