

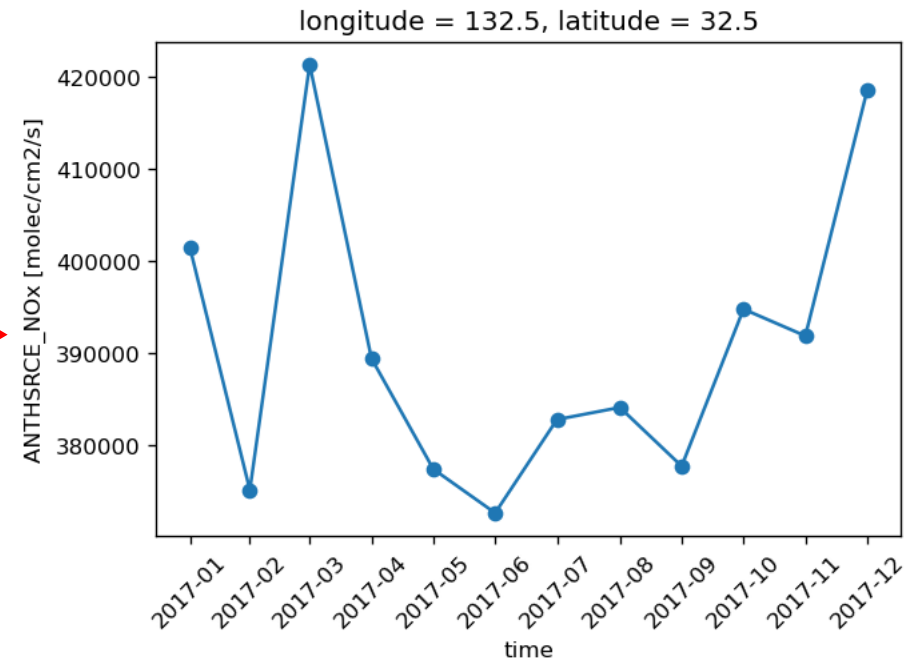
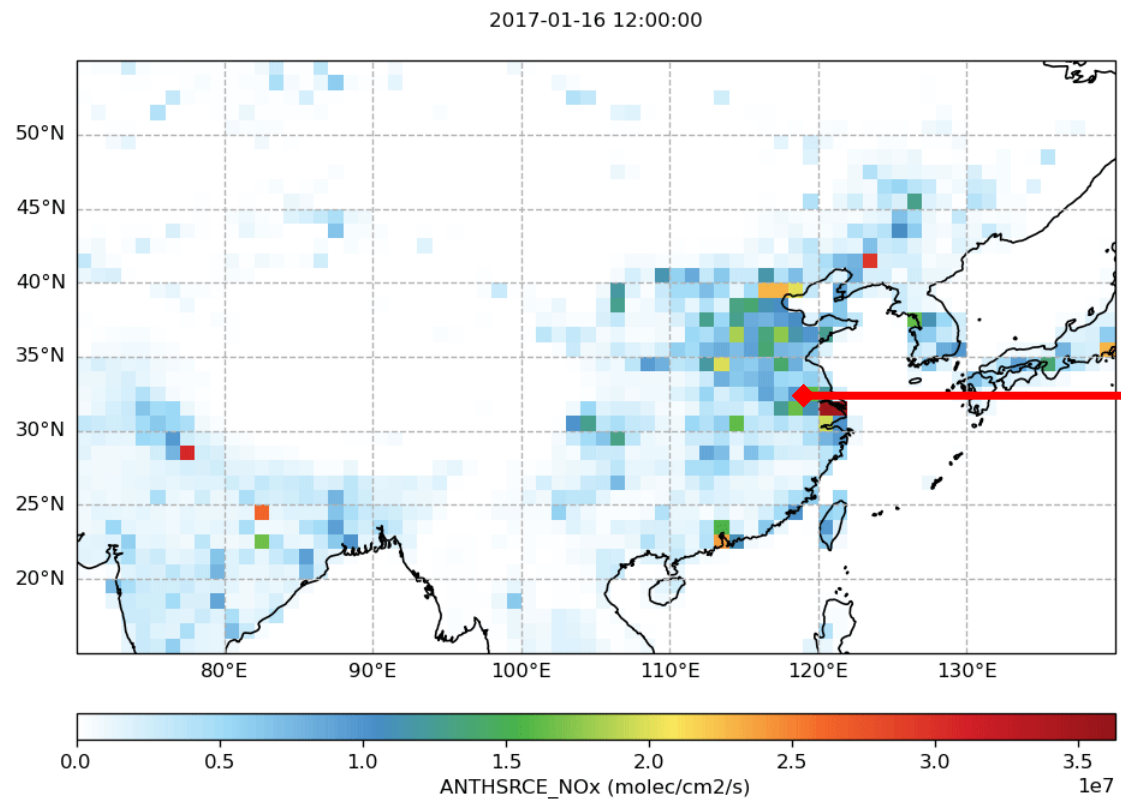


# Inferring NO<sub>x</sub> emissions from GEMS data

Fei Yao, Paul I. Palmer, Xiaolin Wang, Daven K. Henze, Liang Feng, Gitaek T. Lee, Rokjin J. Park

# Conventional bottom-up emission inventories for atmospheric pollutants suffer from infrequent updates

For instance, a harmonised, publicly available emission inventory for the whole of Asia is current only up to 2017 and provides data only at a monthly scale.

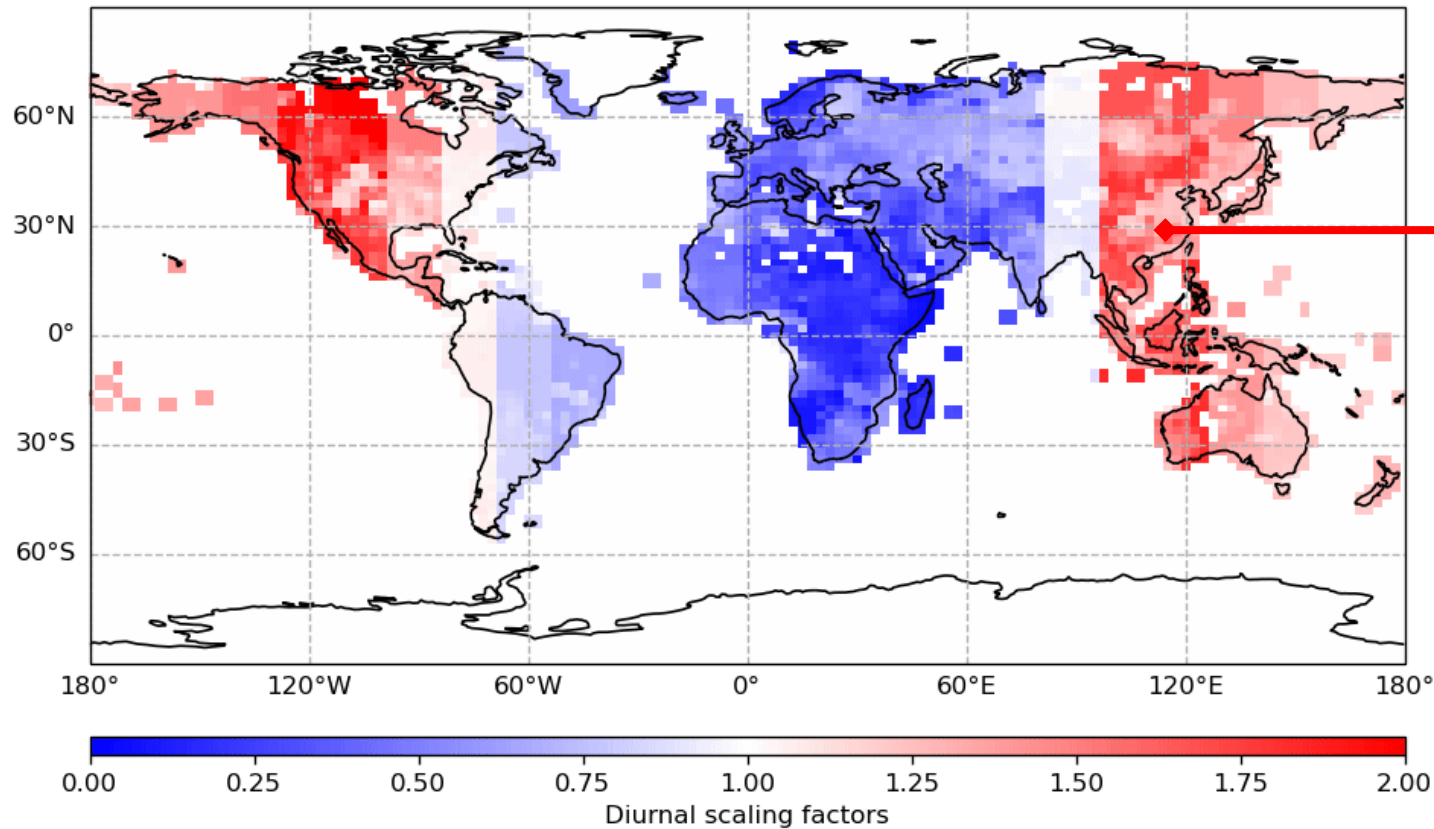




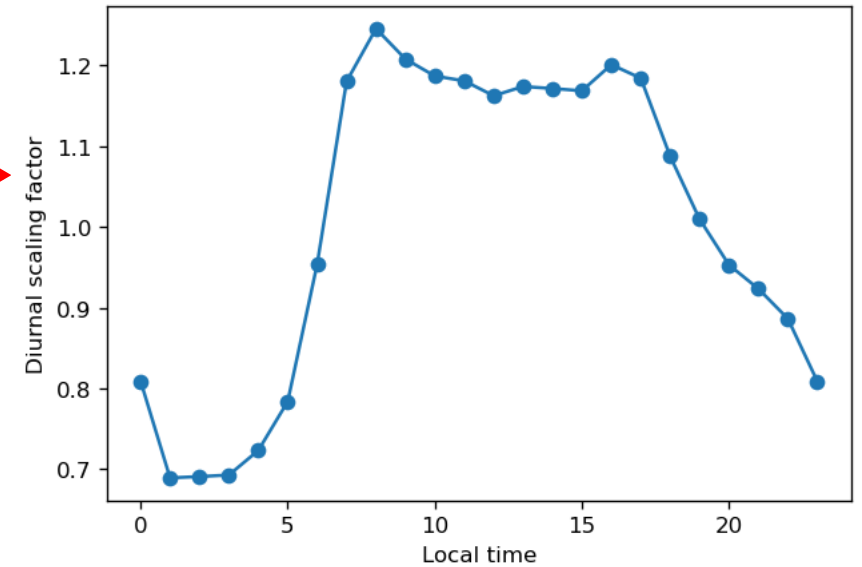
# Conventional bottom-up emission inventories for atmospheric pollutants suffer from large uncertainties

Monthly emissions are converted to hourly emissions in the model only by applying some prescribed diurnal scaling factors.

time: 00

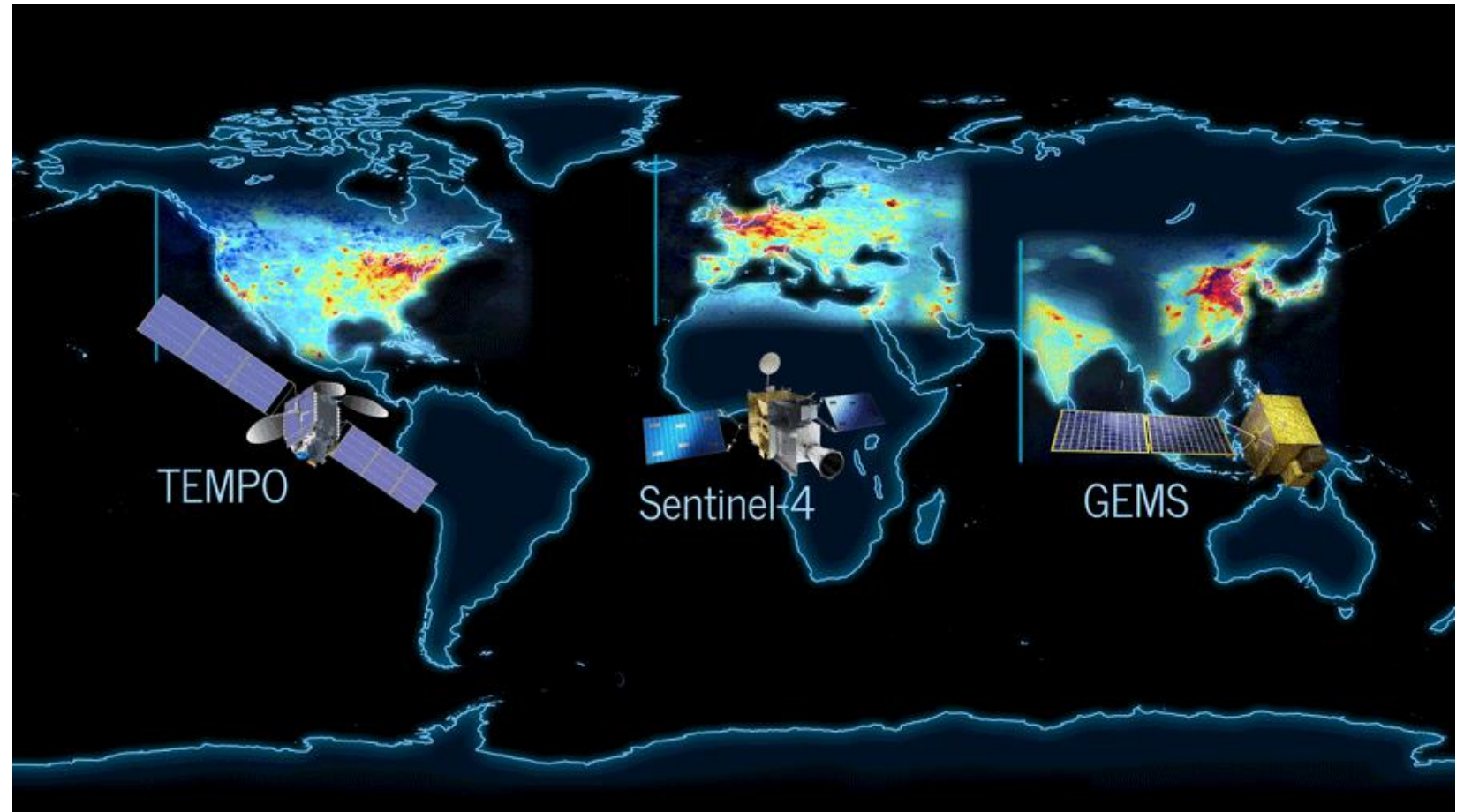


lon = 115.000, lat = 32.000



# Geostationary satellite data can complement bottom-up emission inventories by providing top-down estimates of air pollutant emissions

Pollution-monitoring instruments from NASA, the European Space Agency (ESA), and the Korea Aerospace Research Institute (KARI) will together form a geostationary air quality constellation.

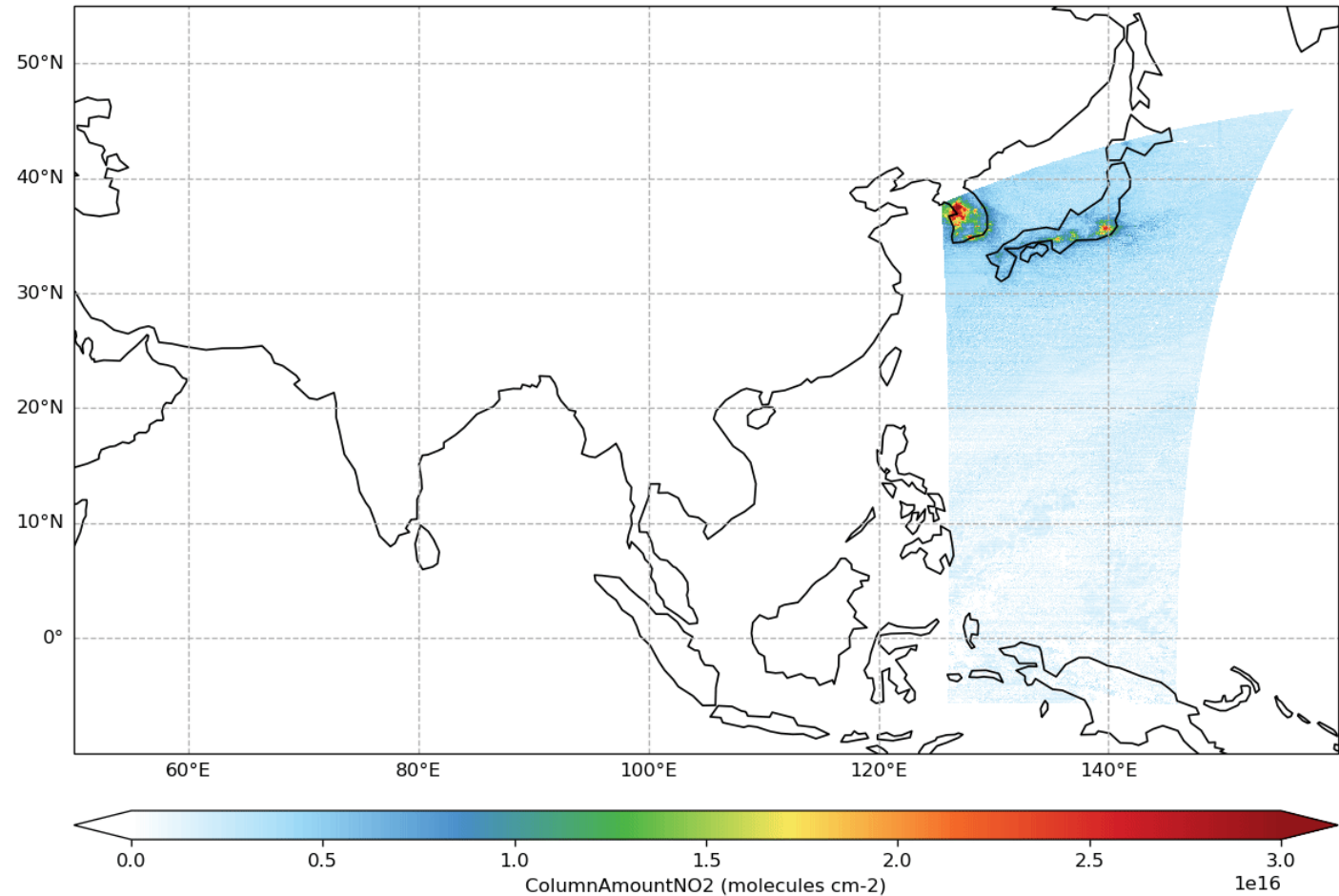


c/o Tim Marvel

# GEMS is the first environmental monitoring satellite in geostationary Earth orbit (GEO)

The Geostationary Environmental Monitoring Spectrometer (GEMS) now provides **columnar** measurements for key atmospheric pollutants, including tropospheric ozone ( $O_3$ ), aerosols, and their precursors ( $NO_2$ ,  $SO_2$ , HCHO, and glyoxal), on an hourly basis throughout the sunlit day.

GK2\_GEMS\_L2\_20210101\_0045\_NO2\_HE-ETC\_DPRO\_ORI.nc





# An efficient inverse modelling approach is essential to analyse these large volumes of geostationary data

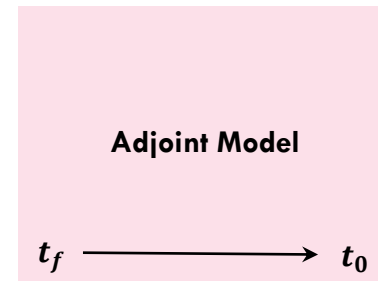
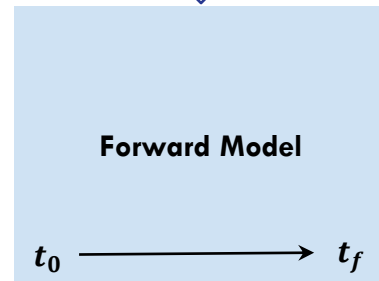
The GEOS-Chem Adjoint model is a strong candidate for such a task. The adjoint model only requires an additional 2x CPU time. The optimisation will generally form within 40 iterations of forward and backward runs.

**However**, each application requires extra code development, some of which involves code validation, e.g., new emission inventories, chemistry, etc.

## Optimization flowchart

Scaling the parameters

$$\mathbf{p} = \boldsymbol{\sigma} \mathbf{p}_a$$



Obtaining new scaling factors



$\boldsymbol{\sigma}'$

Optimization

$$\nabla_{\boldsymbol{\sigma}} J$$

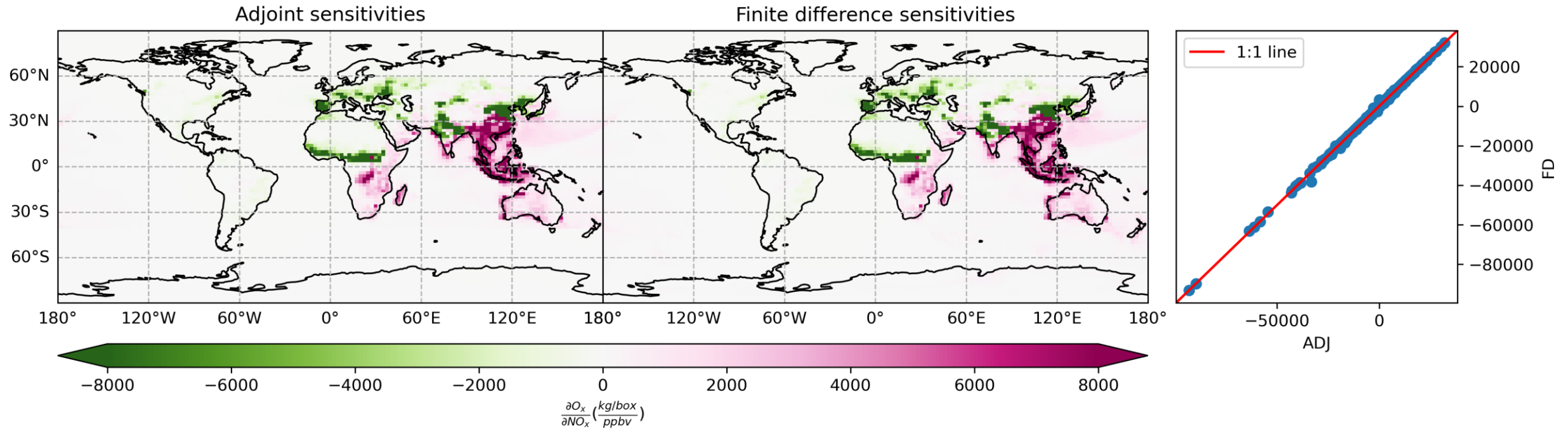
Cost function

$$J = \frac{1}{2} \sum_{\mathbf{c} \in \Omega} (\mathbf{H}\mathbf{c} - \mathbf{c}_{obs})^T \mathbf{S}_{obs}^{-1} (\mathbf{H}\mathbf{c} - \mathbf{c}_{obs}) + \frac{1}{2} \gamma_r (\boldsymbol{\sigma} - \boldsymbol{\sigma}_a)^T \mathbf{S}_{\boldsymbol{\sigma}}^{-1} (\boldsymbol{\sigma} - \boldsymbol{\sigma}_a)$$

$$\mathbf{c} \longrightarrow \frac{\partial J}{\partial \mathbf{c}}$$

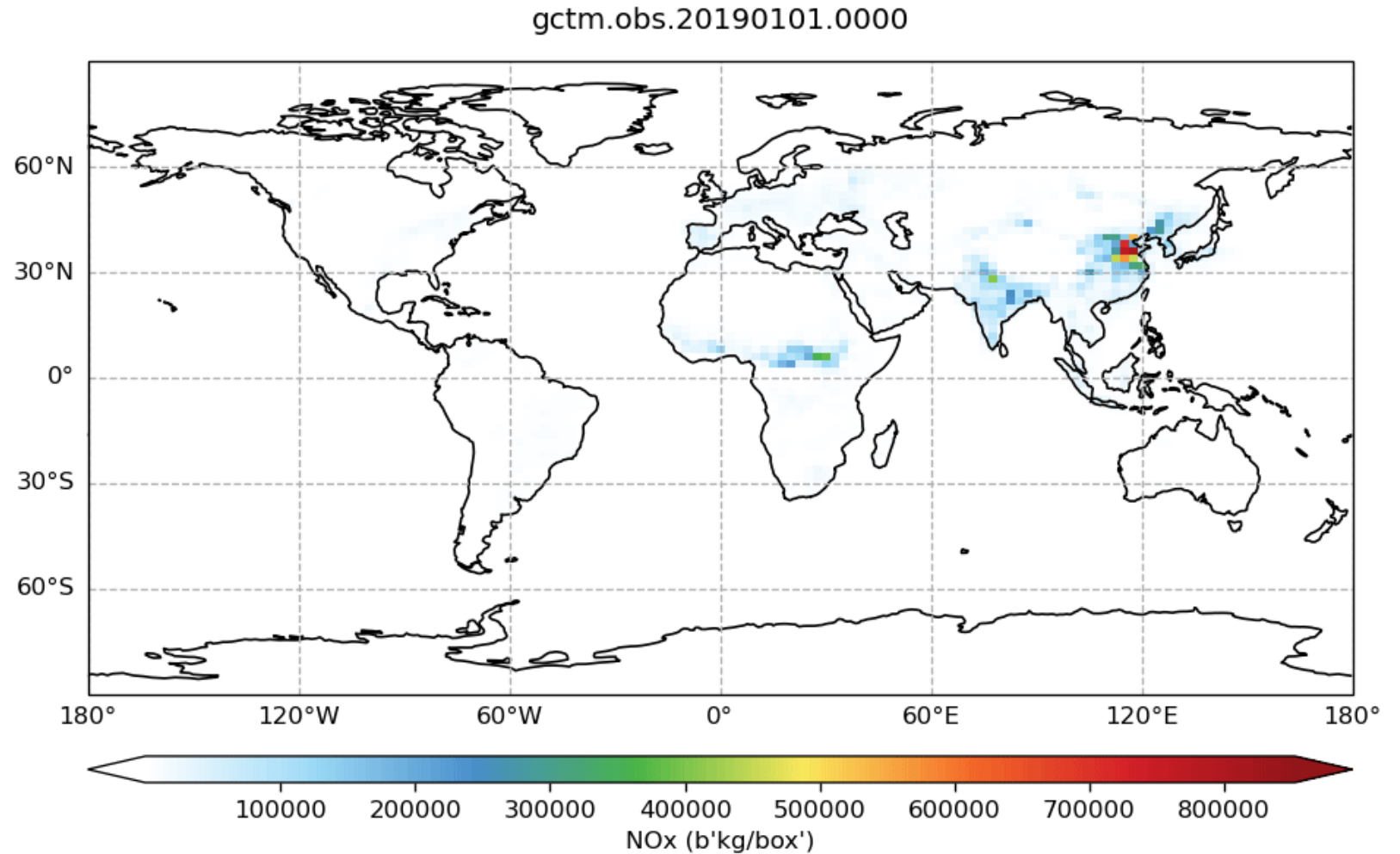
# Global tests of a subset of the adjoint model

The adjoint sensitivities from the updated code are strictly comparable to those from finite differences.



# Observing system simulation experiments (OSSEs) for evaluating the model performance in 4D variational (4D-Var) assimilations

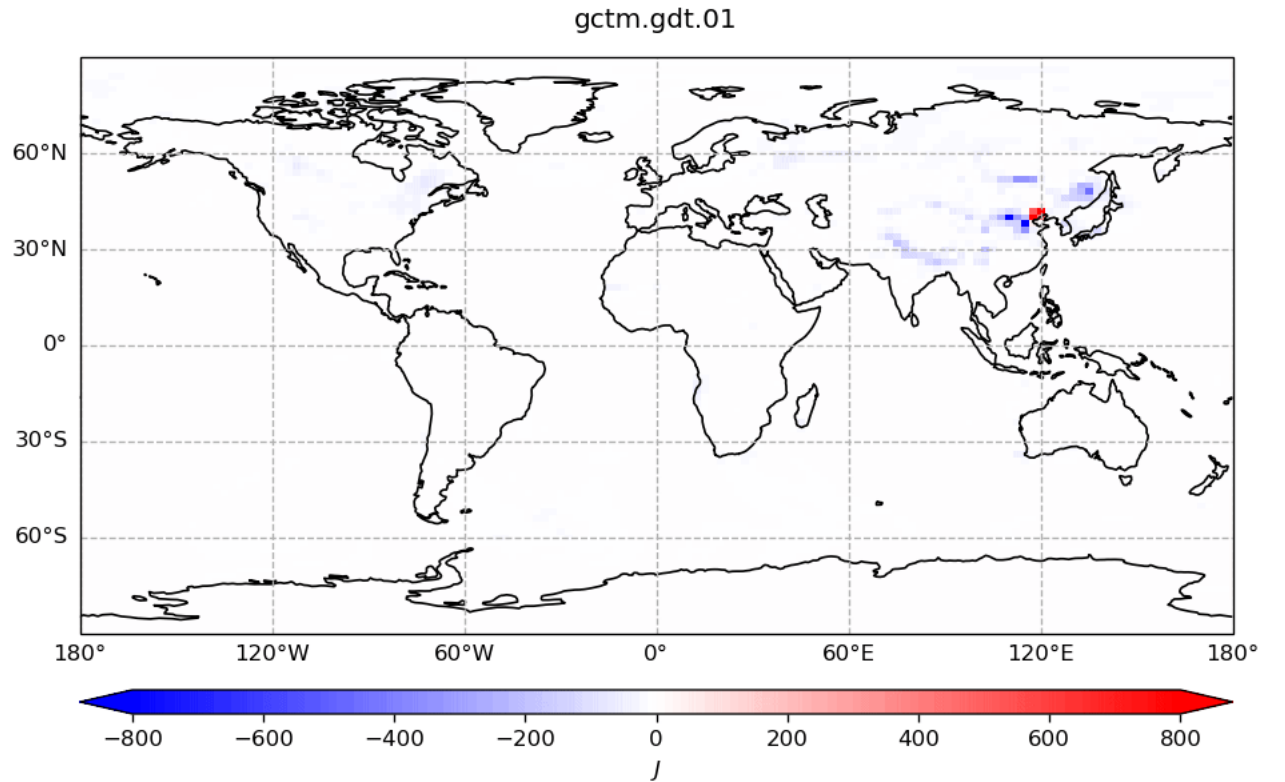
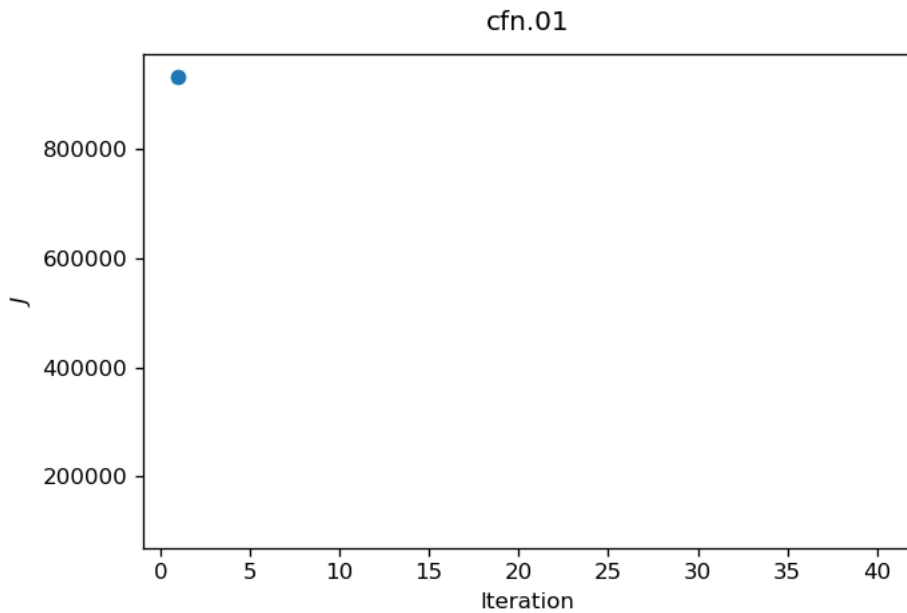
Pseudo-observations of NO<sub>x</sub>, which will ultimately be replaced by GEMS NO<sub>2</sub> data in 4D-Var, are generated from the forward GEOS-Chem model with controlled initial conditions and emissions.





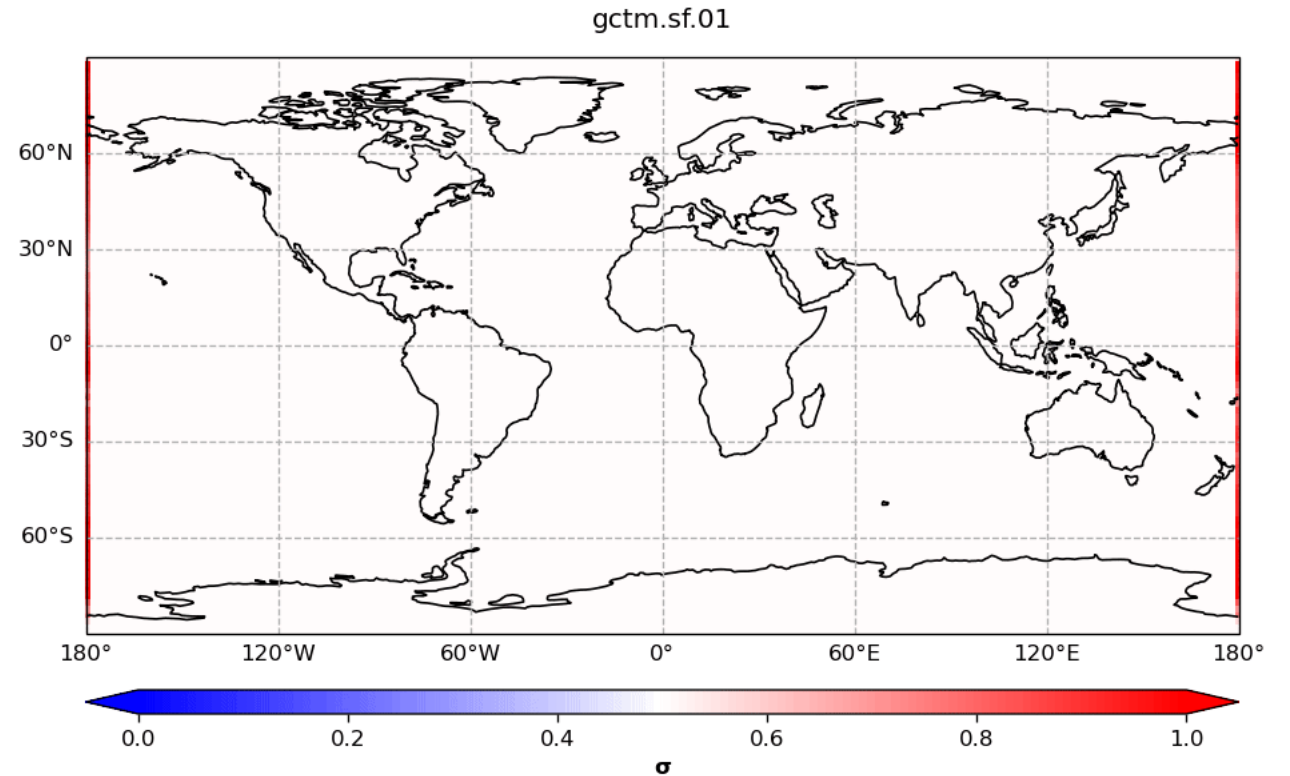
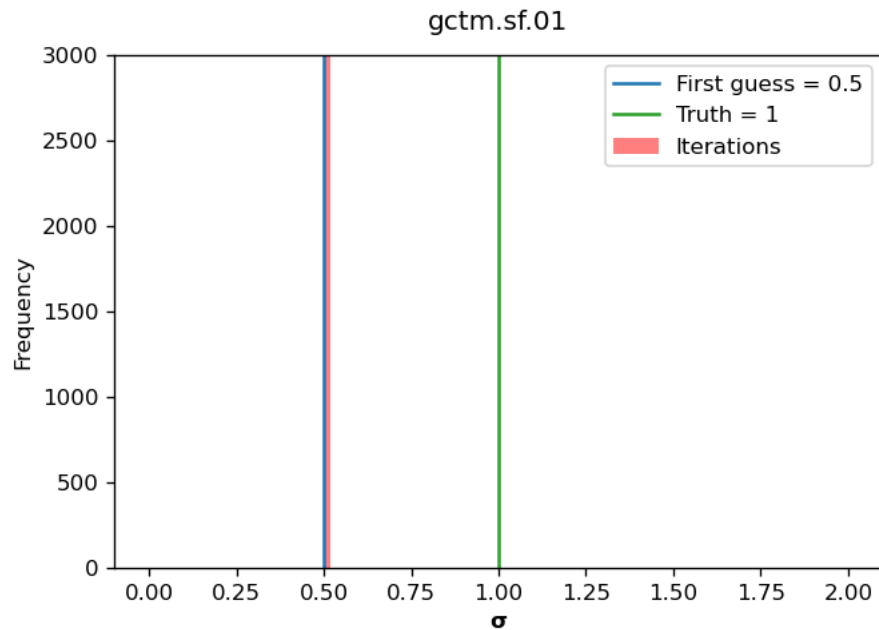
# Observing system simulation experiments (OSSEs) for evaluating the model performance in 4D variational (4D-Var) assimilations

Intentionally set the “initial guess” of scaling factors to be some value other than one and then try to converge to values of one, guided by the gradients of the cost function with respect to model parameters.



# Observing system simulation experiments (OSSEs) for evaluating the model performance in 4D variational (4D-Var) assimilations

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$$\gamma_r = 1$$

- ❑ The GEOS-Chem Adjoint full chemistry code has been updated to support recent emission inventories (including MEIC+MIX and GFED4) and chemistry (e.g., aromatics). These updates have been strictly verified to ensure that the model remains as good as the original code in computing sensitivities/gradients as well as in OSSEs.
- ❑ New code to interface GEMS data (*V2.0* → *V3.0*) is in progress.
- ❑ The work can be easily expanded to interpret data from TEMPO and Sentinel-4 once these data are available.



- What is an adjoint model and why you should care about it?
- Comparative results from the original GEOS-Chem Adjoint model
- Tropospheric  $NO_x$  chemistry

# What is an adjoint model and why you should care about it?

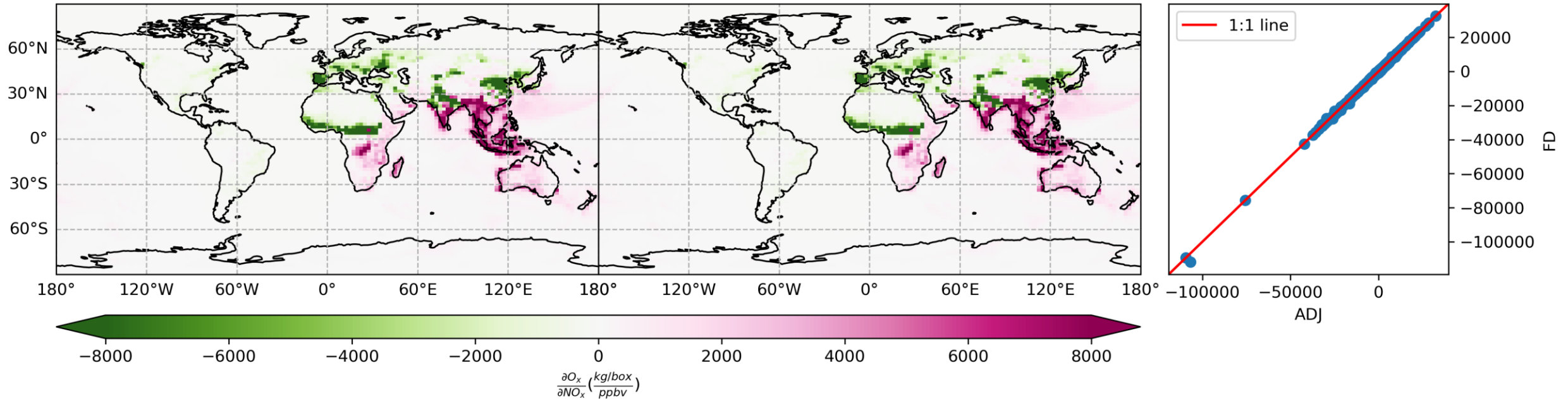
Refer to the separate [slides](#)

# Comparative results from the original GEOS-Chem Adjoint model

Global tests of a subset of the adjoint model

Adjoint sensitivities

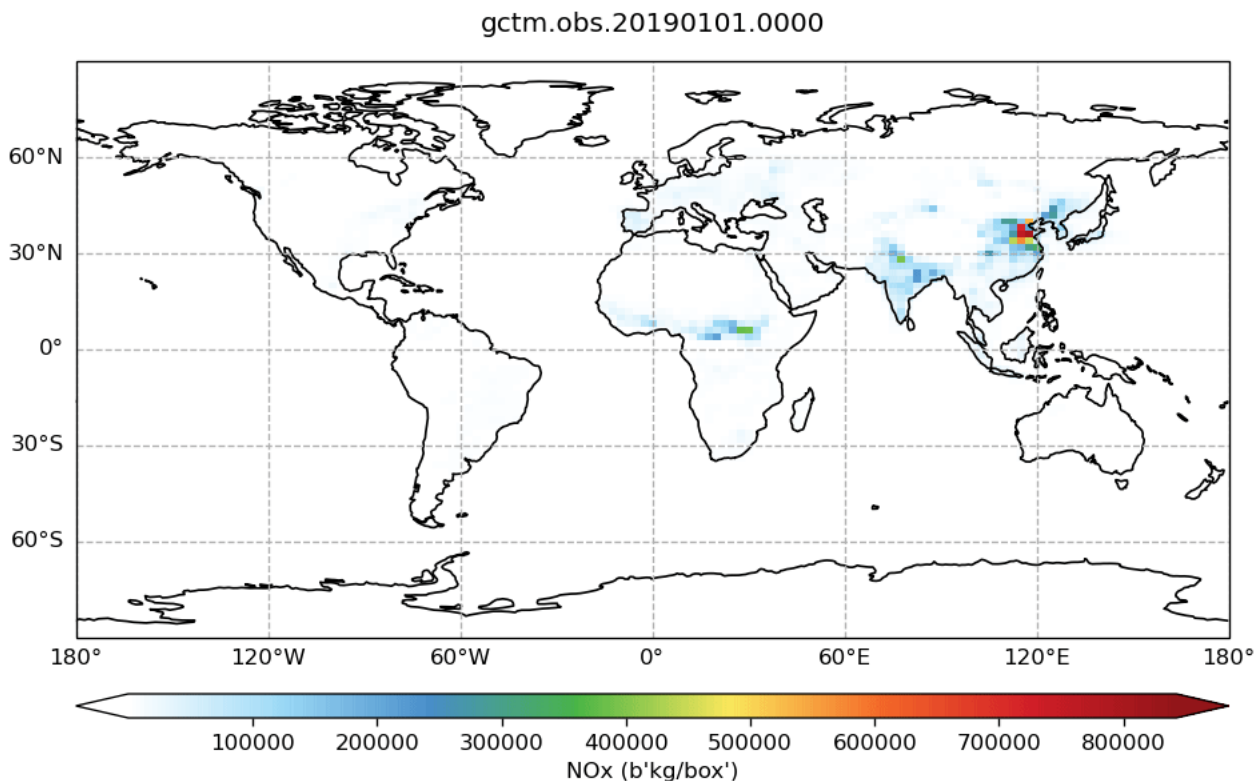
Finite difference sensitivities





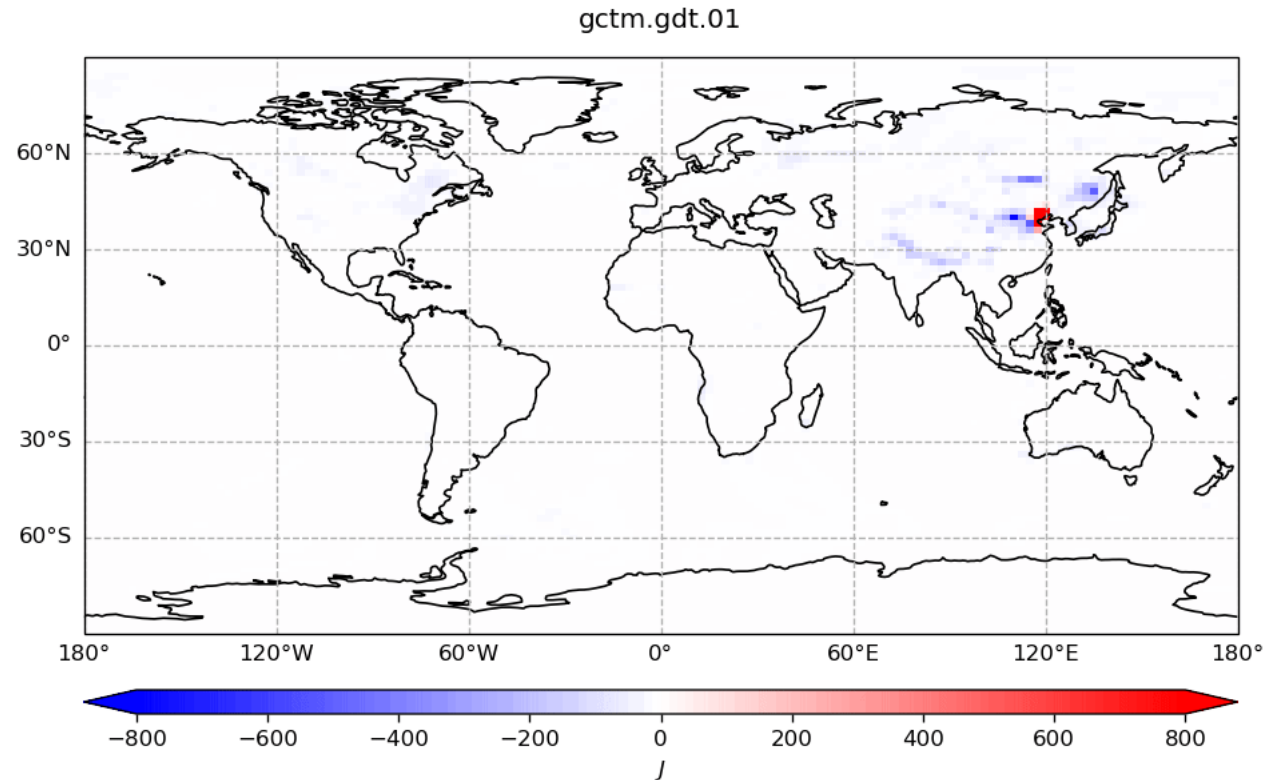
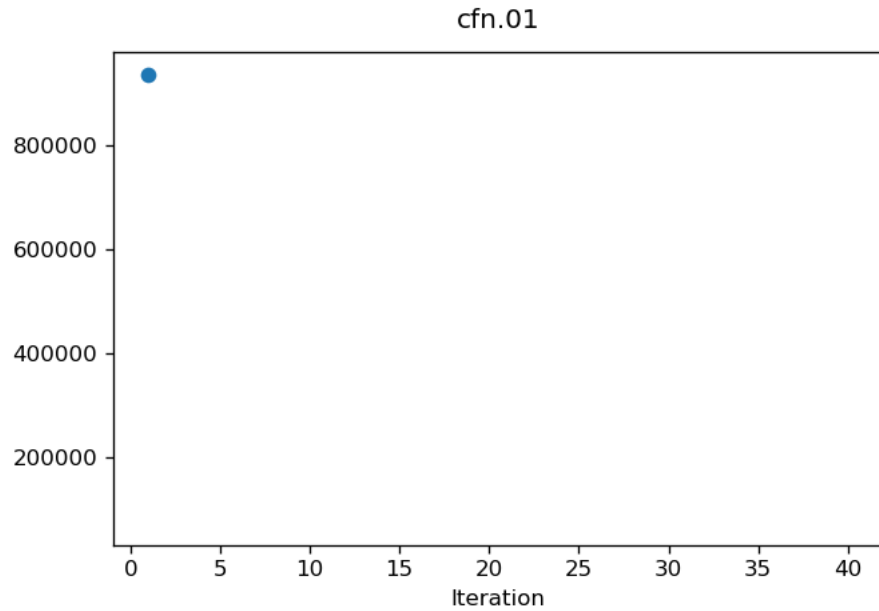
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Observing system simulation experiments (OSSEs) for evaluating the model performance in 4D variational (4D-Var) assimilations



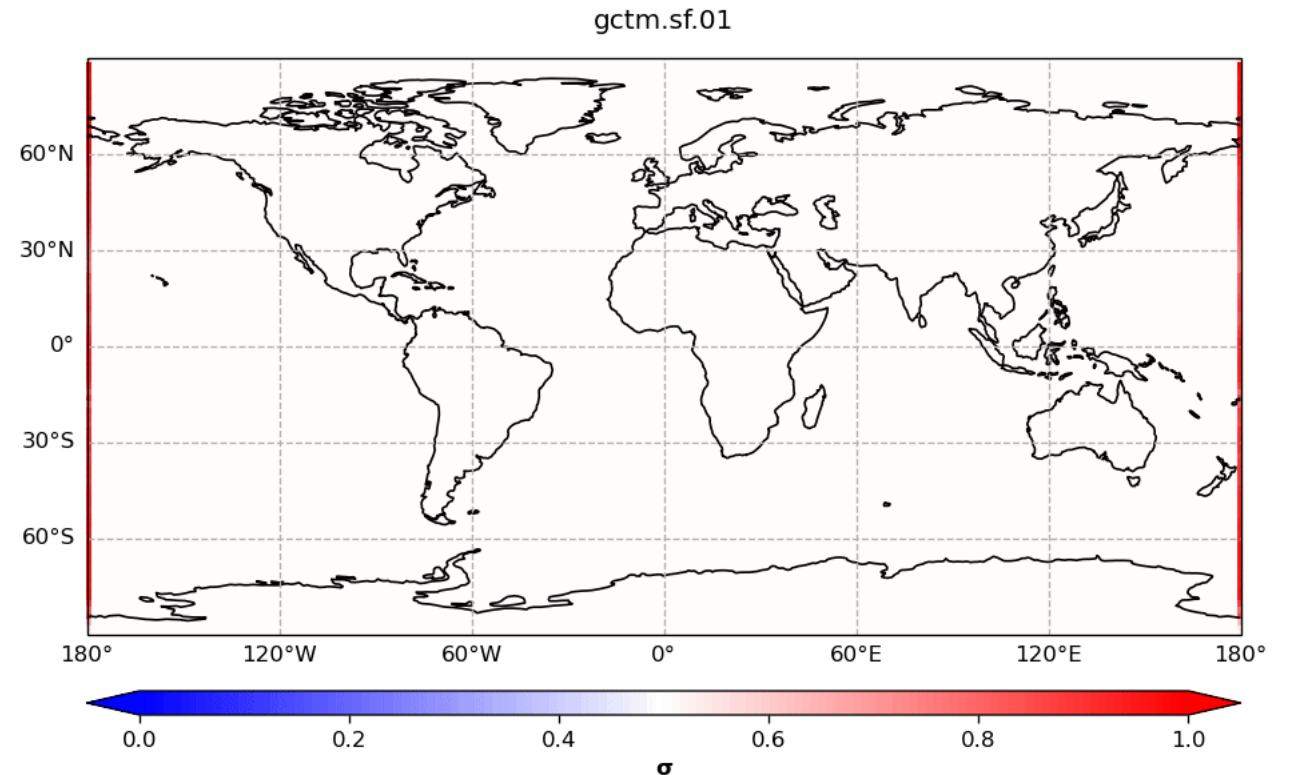
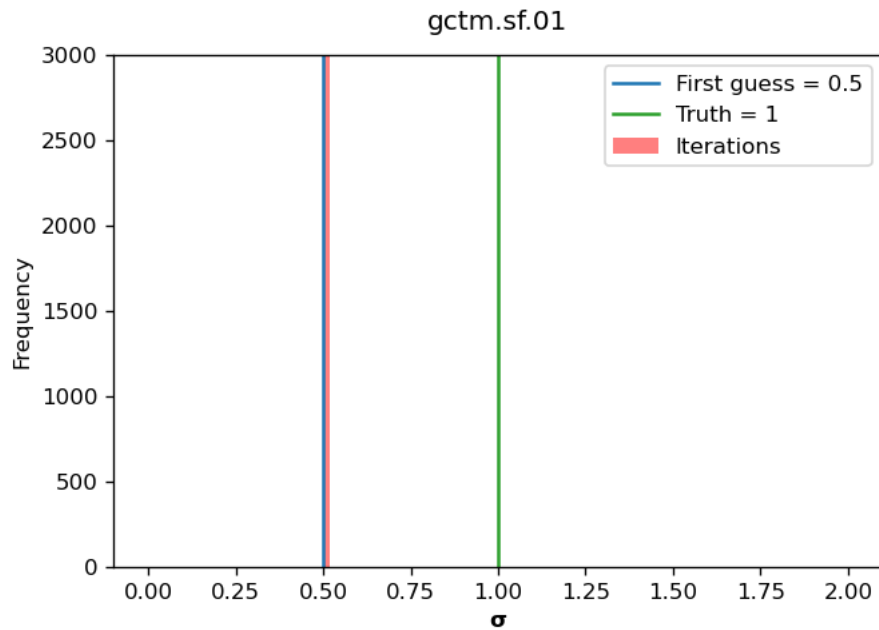
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# Why do we care about NO<sub>x</sub>?

NO<sub>x</sub> ≡ NO+NO<sub>2</sub> are important precursors of ozone (O<sub>3</sub>) and particulate matter pollution, and NO<sub>2</sub> itself is harmful to public health.

