Refining nested GEOS-Chem emissions during the CalNex campaign by assimilation of TES ammonia observations

Shannon Capps[1,2], Daven Henze[3], Zhe Jiang[4], Karen Cady-Pereira[5], Armistead Russell[1], Athanasios Nenes[1]

[1]Georgia Institute of Technology
[2]US Environmental Protection Agency
[3]University of Colorado, Boulder
[4]University of Toronto
[5]AER, Inc.

NASA Earth Systems Science Fellowship
Phillips66 Model Development Support
ORISE Postdoctoral Fellowship with US EPA

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This presentation may not reflect the official policies or views of the US EPA.

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Motivation

Human health degradation through $PM_{2.5}$ exposure

Pope & Dockery, 2006

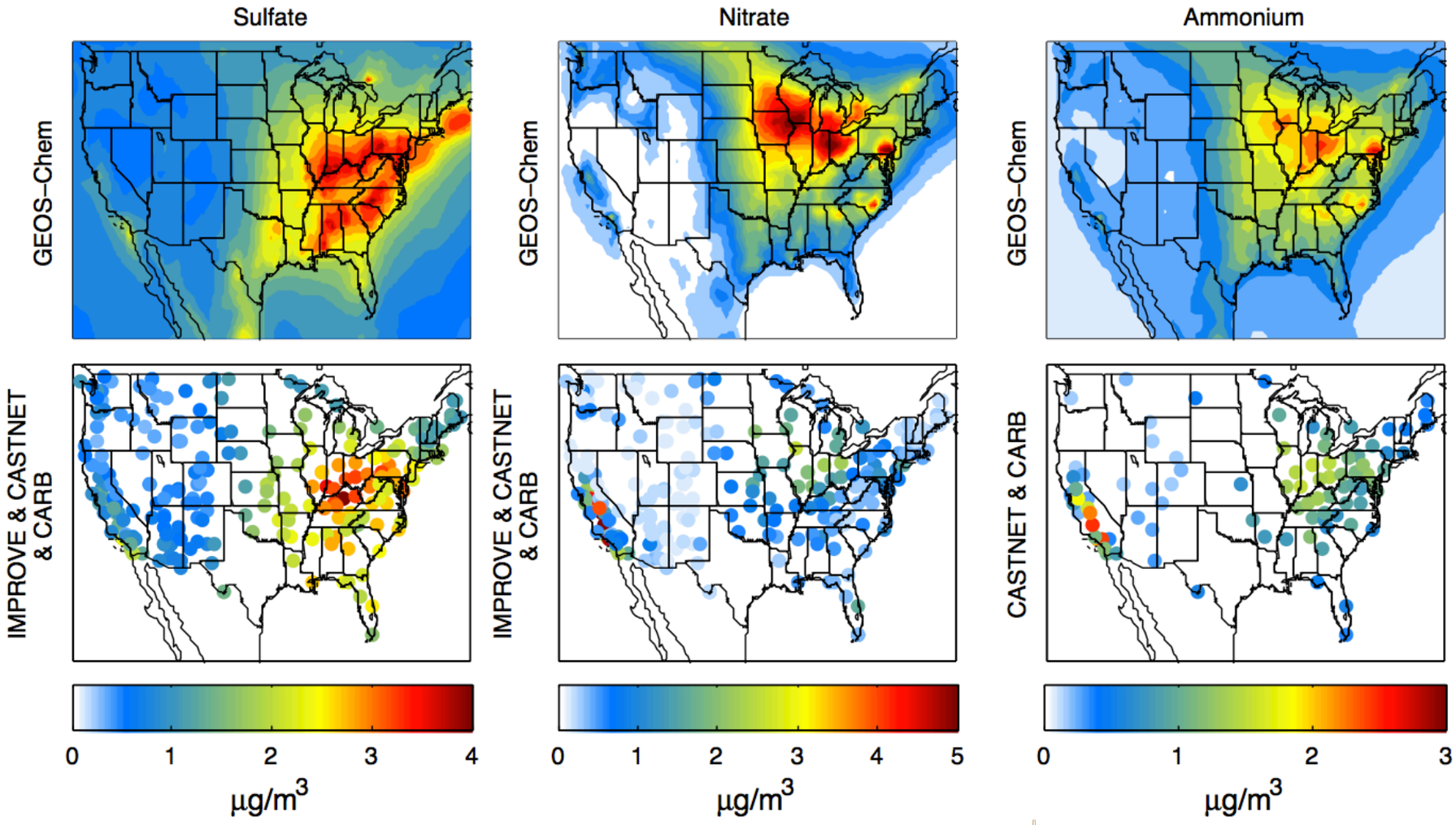
Radiative forcing directly and by altering cloud albedo

Haywood & Boucher, 2000

Ecosystem perturbations by reactive nitrogen deposition

Galloway et al., 2003

Discrepancies in modeled and observed inorganic $PM_{2.5}$ mass and, specifically, ***ammonium nitrate*** have been consistently demonstrated.



2009 annual mean - Walker et al., 2012
(similar to Heald et al., 2012 findings)

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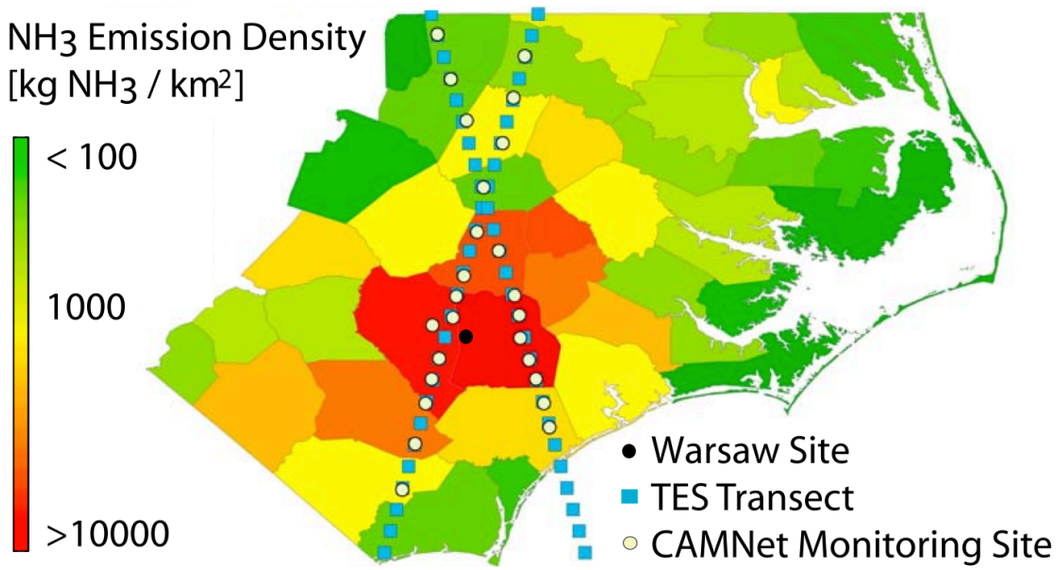
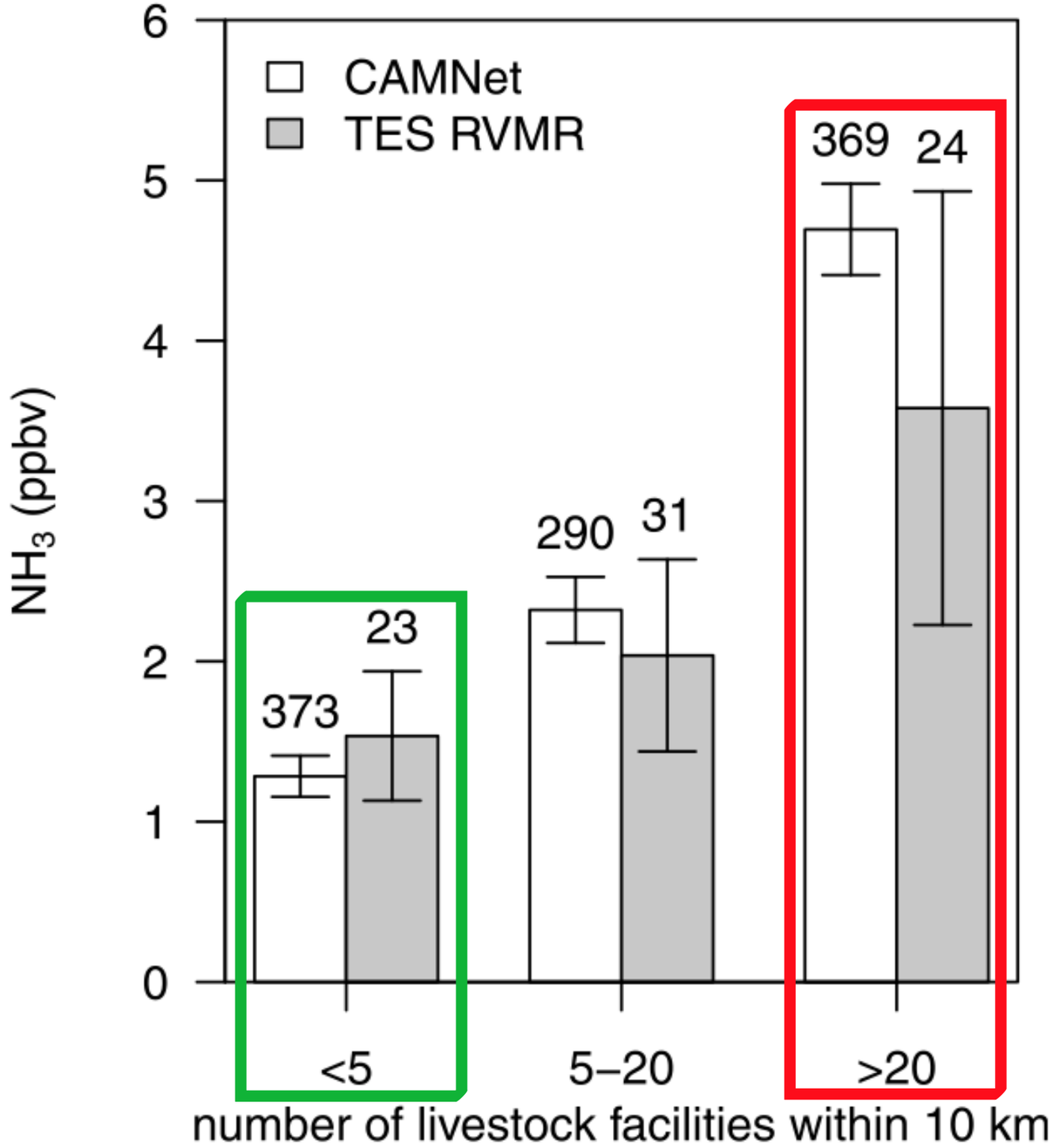
Motivation

Ammonia emissions sources from agricultural or livestock operations are hard to constrain from bottom-up inventories.





Satellite-based TES and in situ (CAMNet) observations of 2009 daytime NH_3 in North Carolina - Pinder et al., 2011

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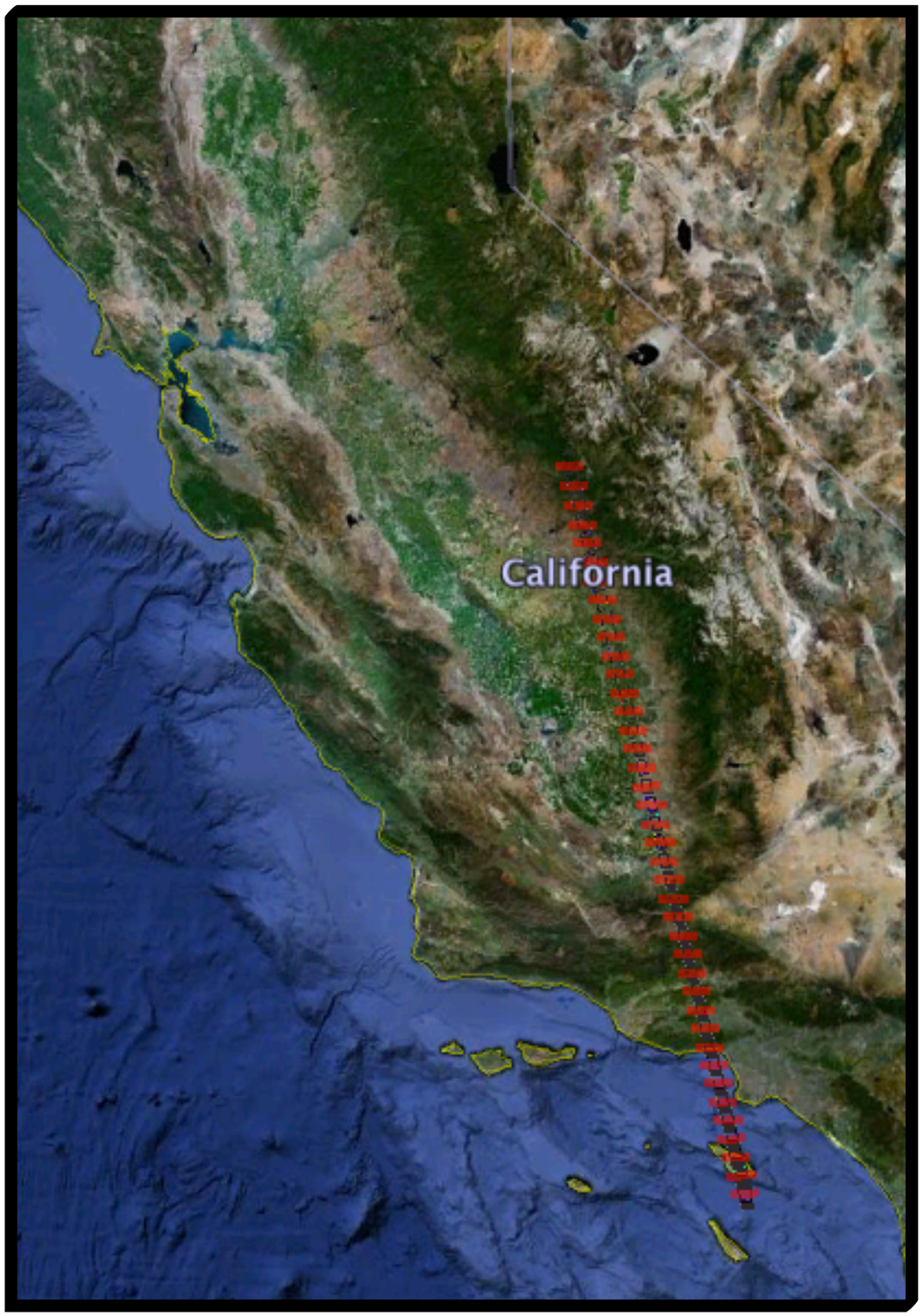
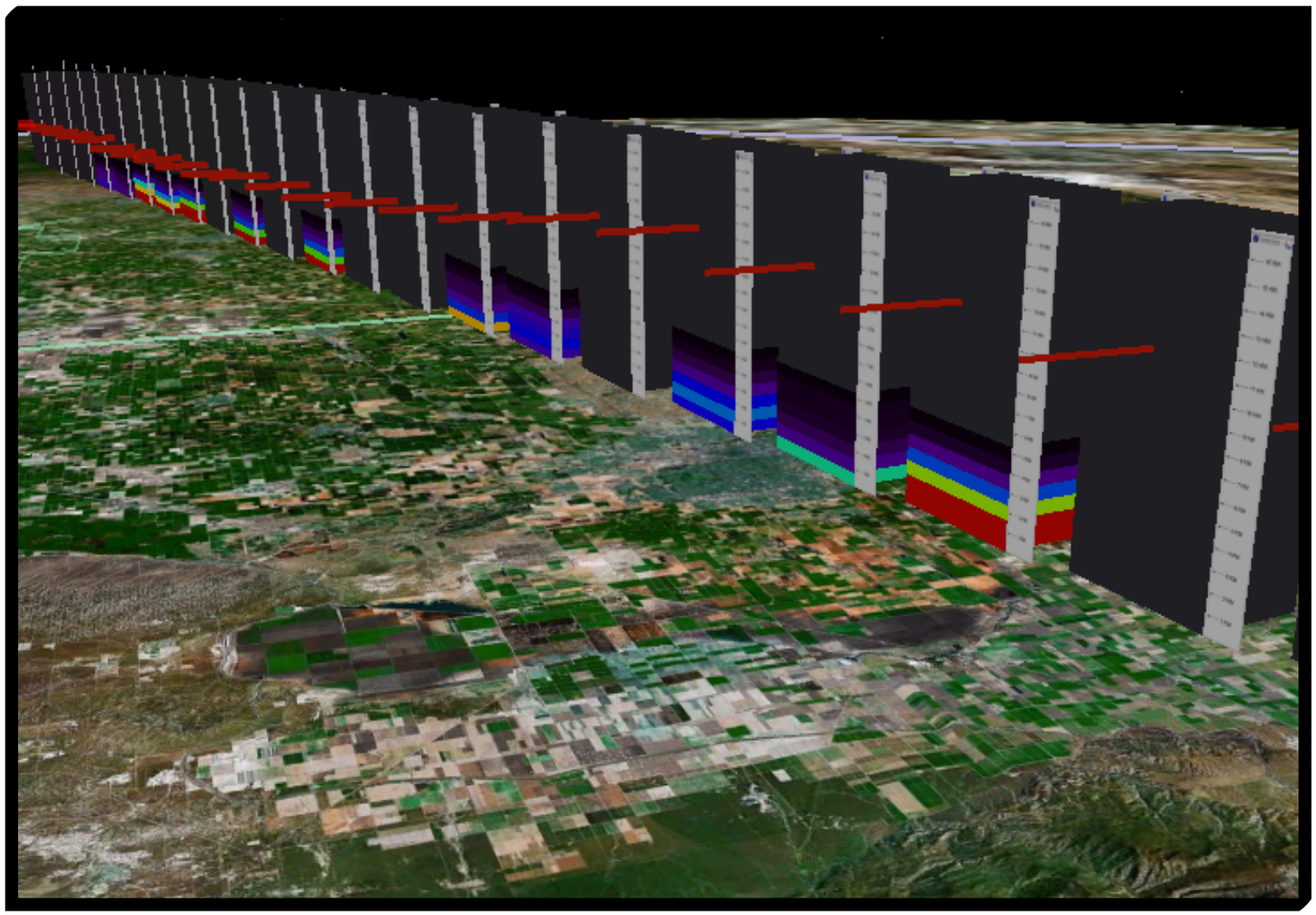
Bakersfield Transects



10 April 2010



indicates tropopause

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TES NH3 Retrieval
Shephard et al., 2011

Google Earth projection of TES NH3 Retrieval
tes.jpl.nasa.gov/visualization/

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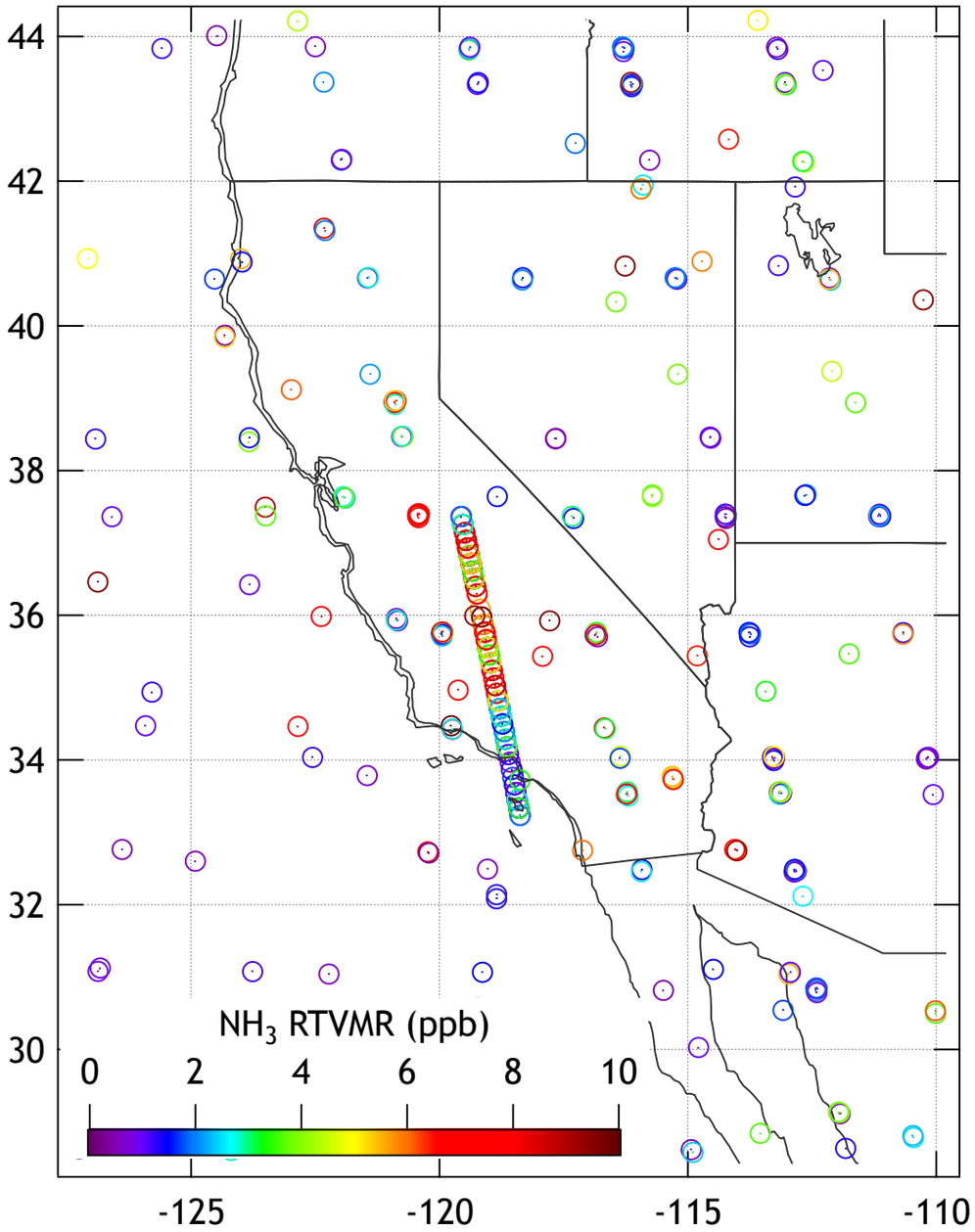
Bakersfield Transects

April - July 2010



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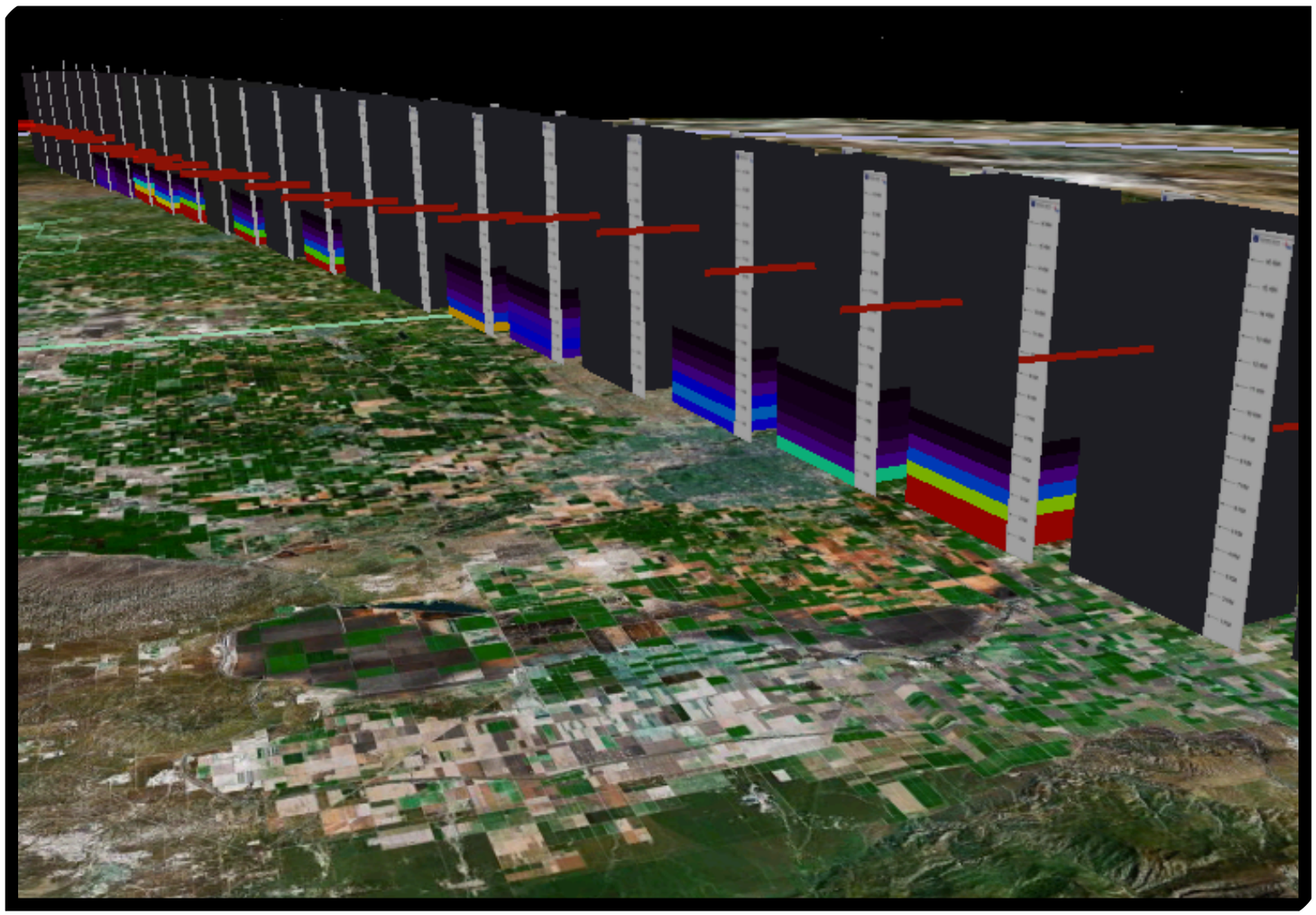

indicates tropopause

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Lite files
tes.jpl.nasa.gov/data/

Google Earth projection of TES NH3 Retrieval
tes.jpl.nasa.gov/visualization/

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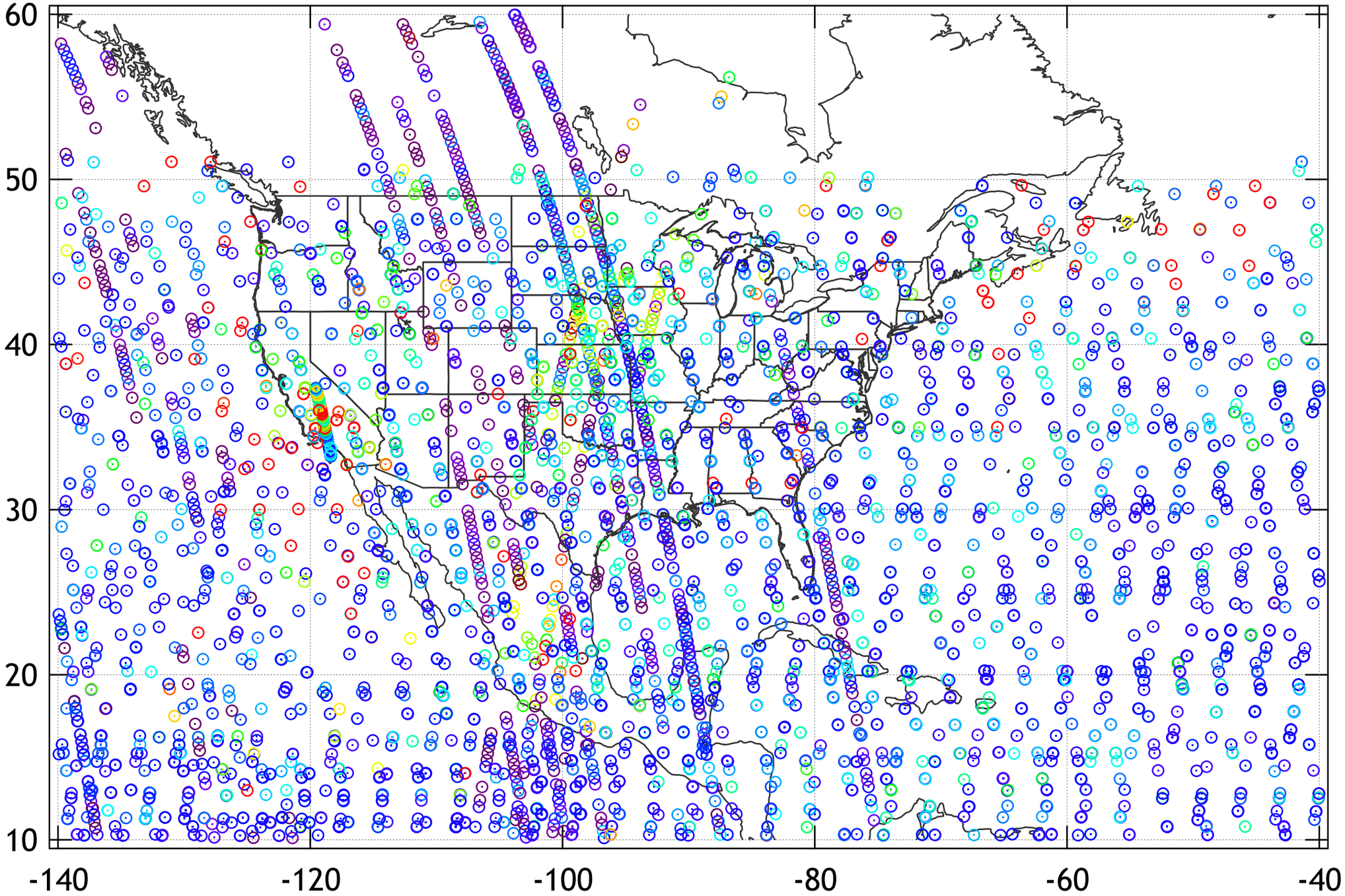
TES NH_3 Observations

April - July 2010



NH_3 Representative Tropospheric Volume Mixing Ratio (ppb)

0 2 4 6 8 10

tes.jpl.nasa.gov/data/

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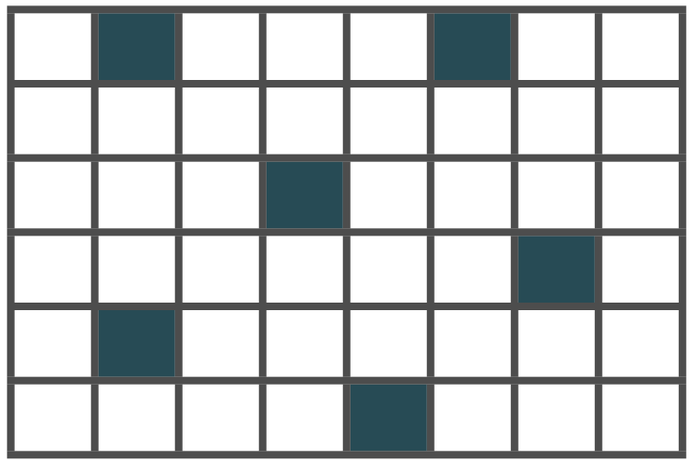
Assimilation Approach

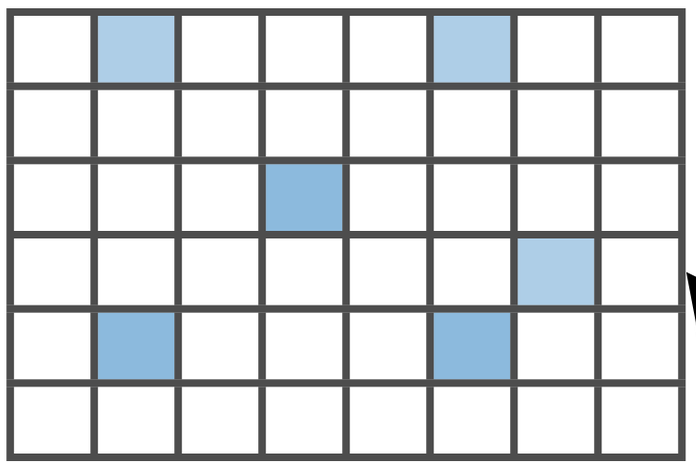
Iteratively minimize *J*

$$J = \sum_{c \in \Omega} (\mathbf{Hc} - (\mathbf{c}_{obs} - \mathbf{b}))^T S_{obs}^{-1} (\mathbf{Hc} - (\mathbf{c}_{obs} - \mathbf{b}))$$

NH_3 from TES, $\mathbf{c}_{obs}$ - **b**

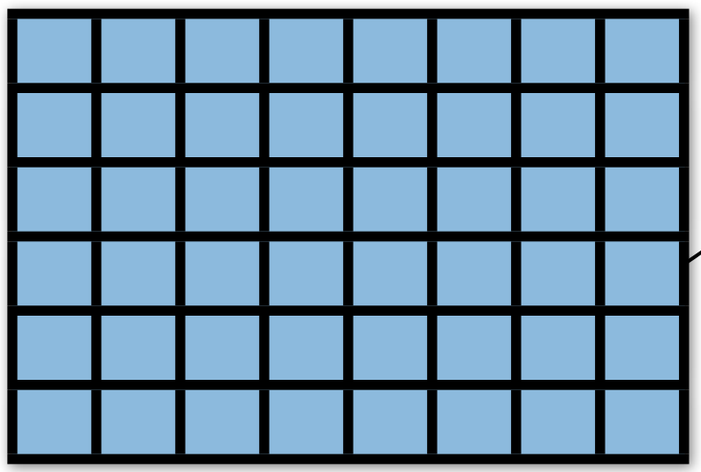


NH_3 from GEOS-Chem, ***H*c**



Observation operator, H

Modeled concentrations, **c**



Zhu et al., 2013

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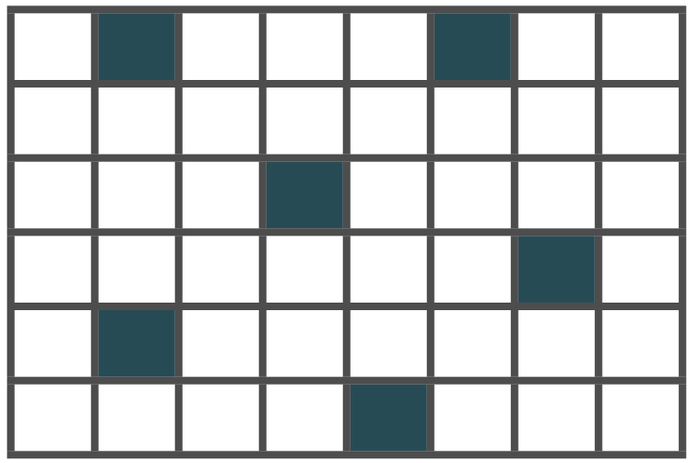
Assimilation Approach

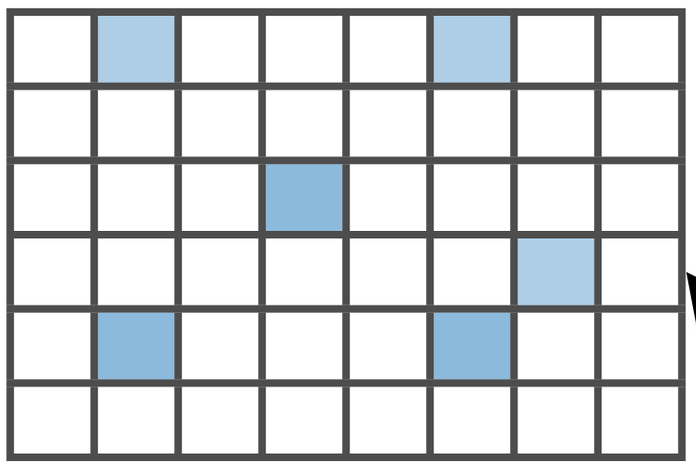
Iteratively minimize *J*

$$J = \sum_{c \in \Omega} (Hc - (c_{obs} - b))^T S_{obs}^{-1} (Hc - (c_{obs} - b))$$

NH_3 from TES, c_{obs} - **b**

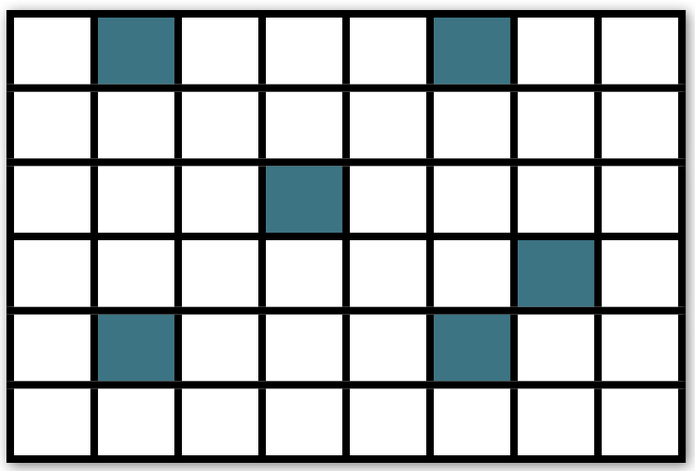


NH_3 from GEOS-Chem, *Hc*

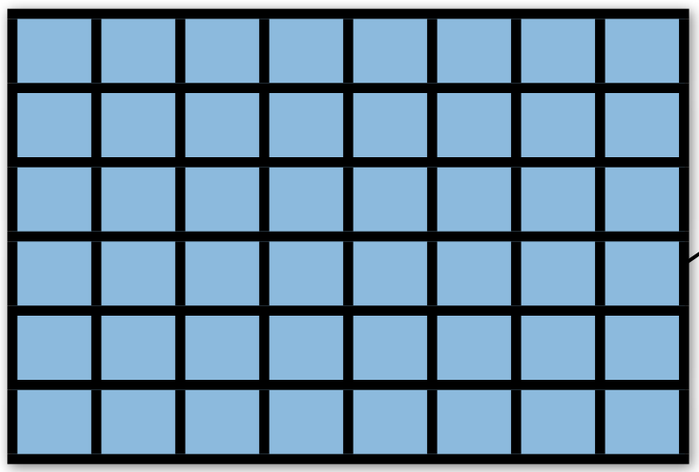


Observation operator, H

Observation error weighted difference, *J*



Modeled concentrations, **c**



Zhu et al., 2013

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Assimilation Approach

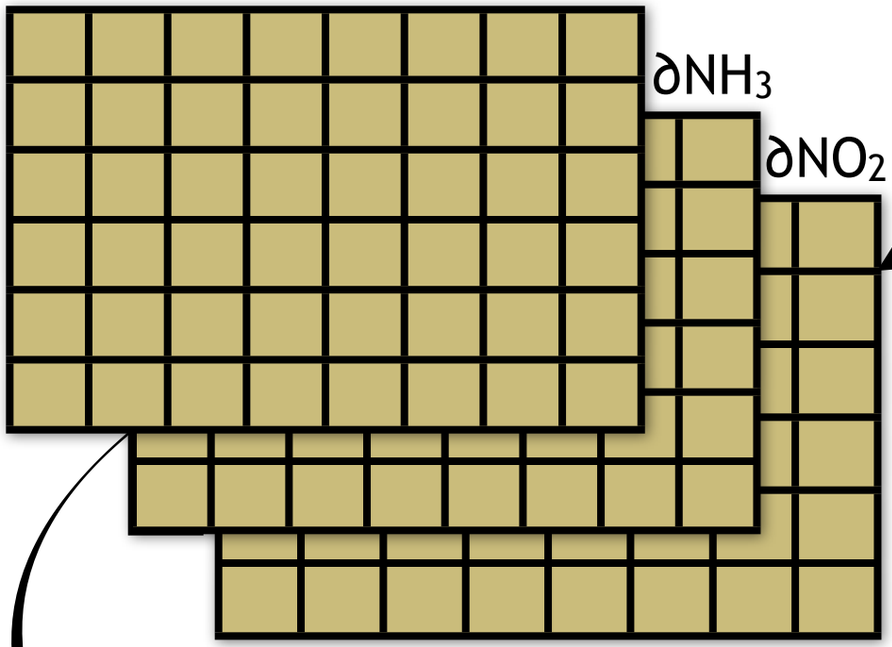
Iteratively minimize *J*

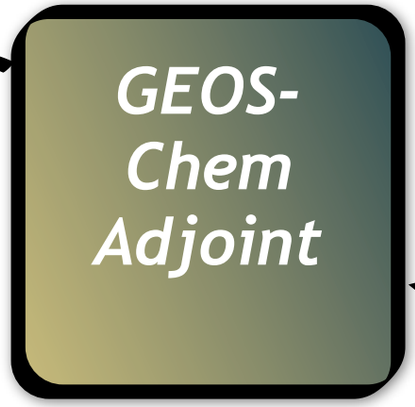
Emissions Scaling Factors

∂SO_2

∂NH_3

∂NO_2

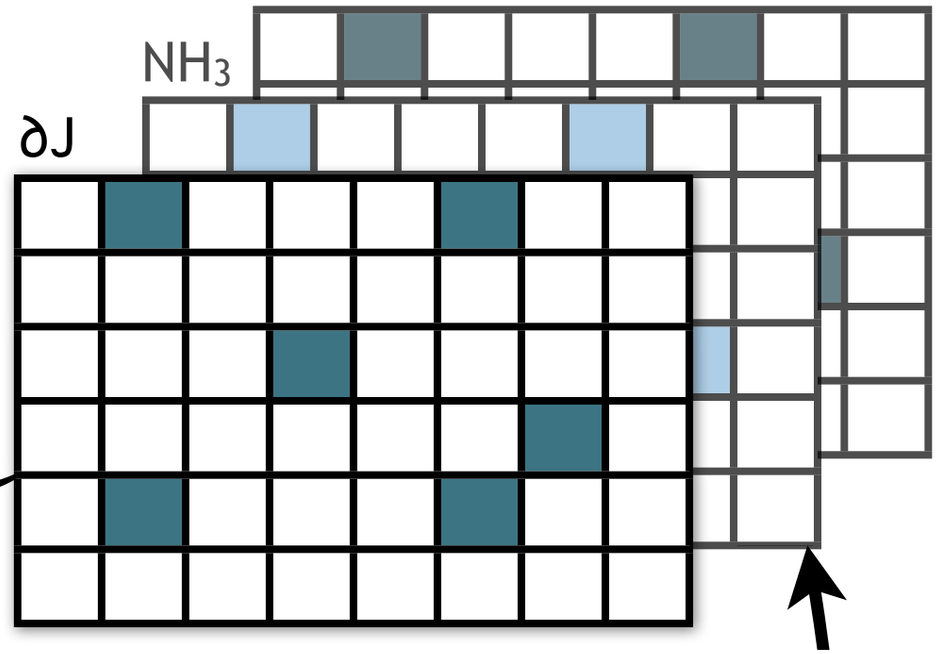




NH_3 from TES

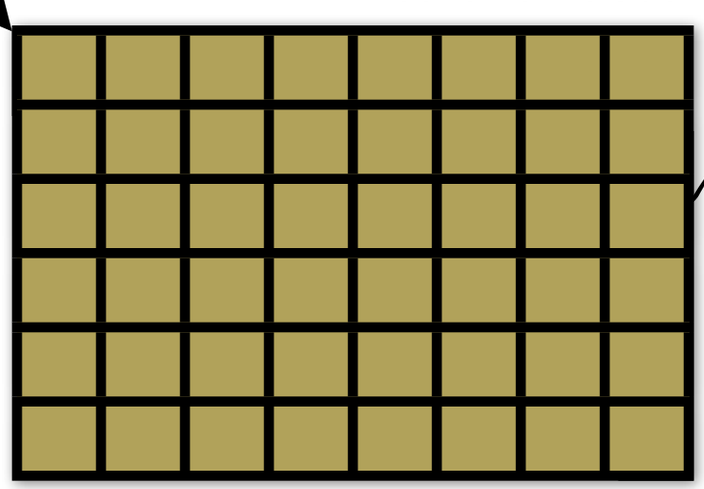
NH_3

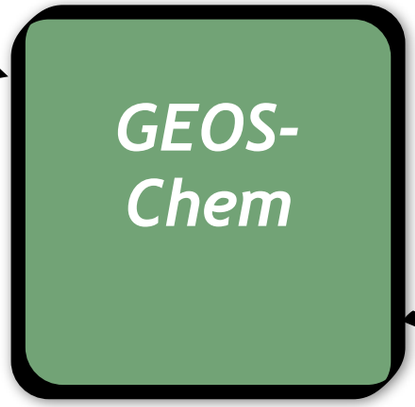
∂J



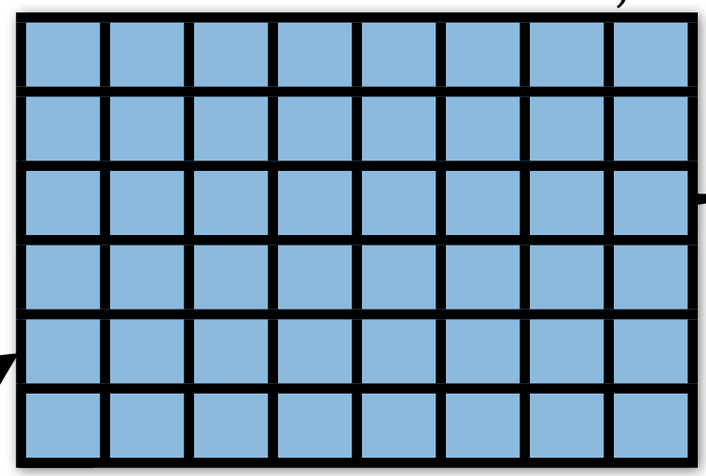
Observation operator, H

Emissions rates





Modeled concentrations, **c**



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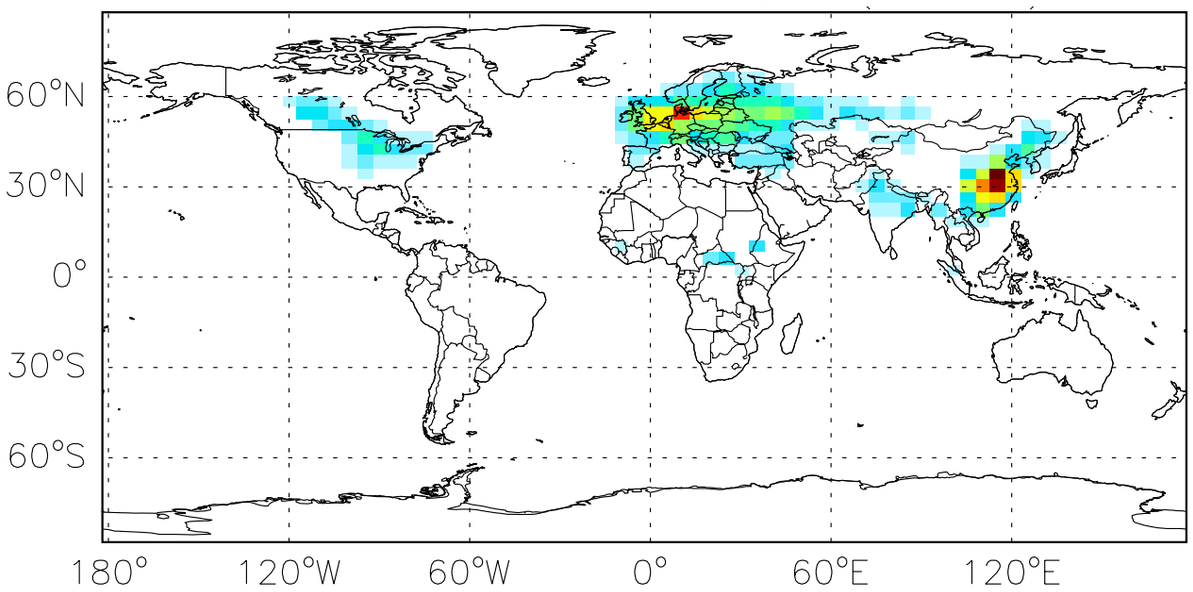
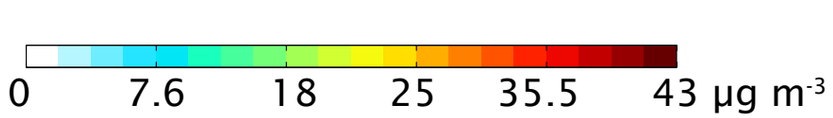
Aerosol Thermodynamics

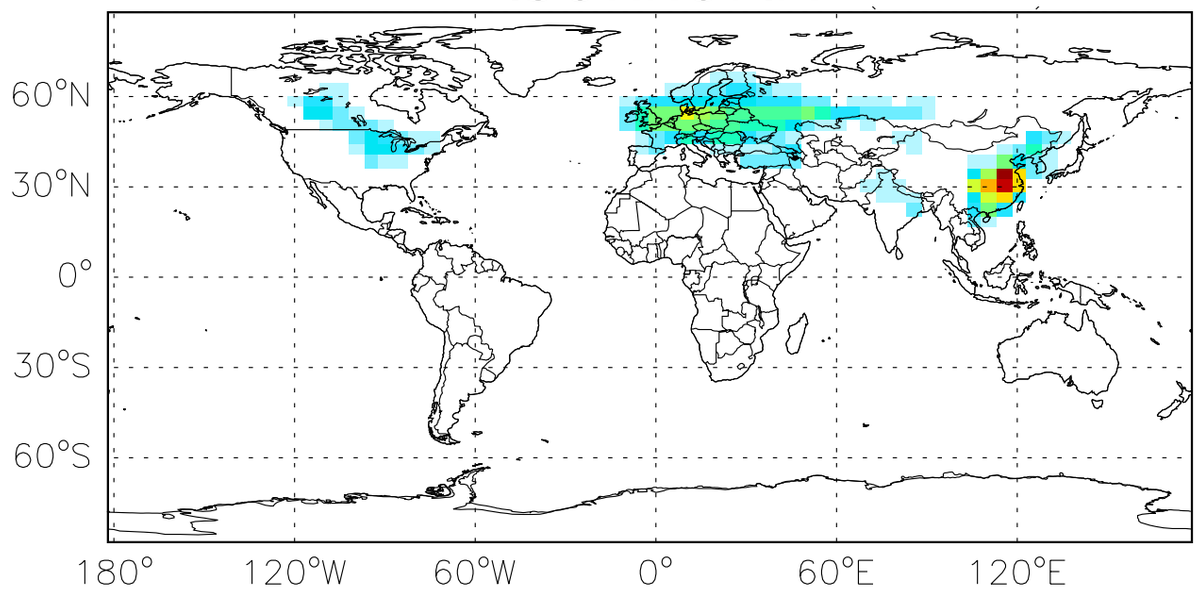
Mean $NO_{3,(p)}^-$ February 2008

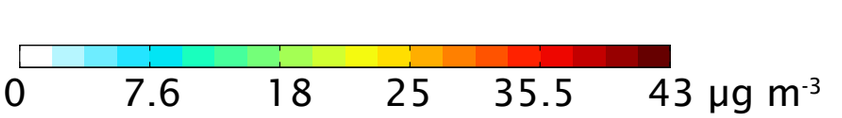
RPMARES



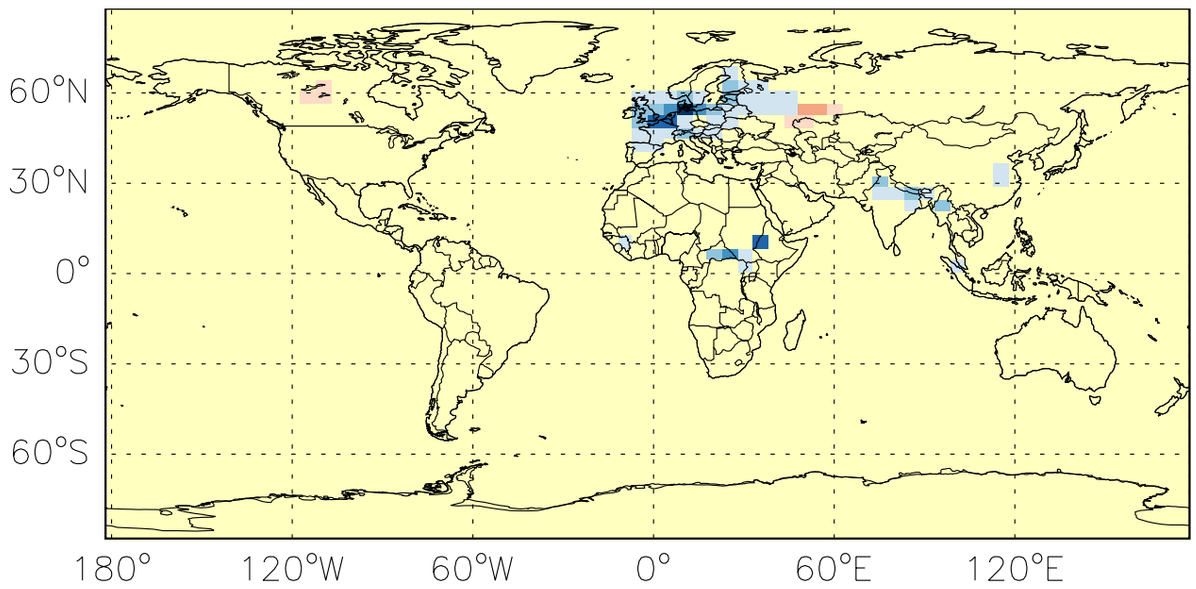


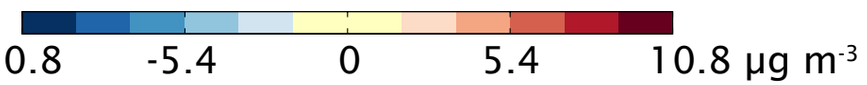
ISORROPIA





RPMARES - ISORROPIA





Capps et al., 2012

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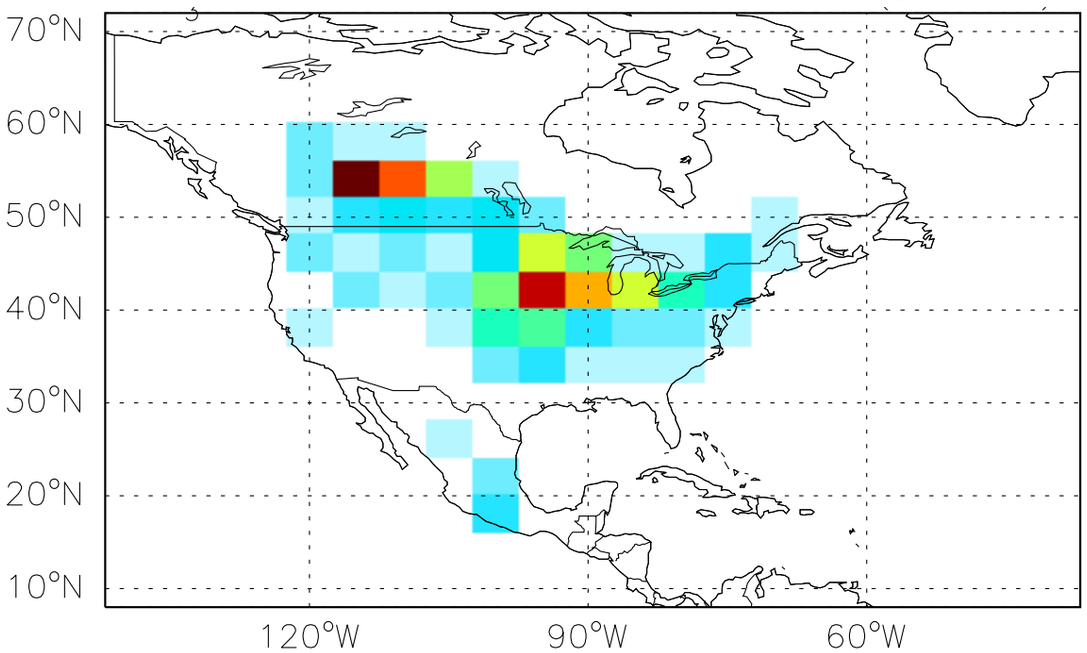
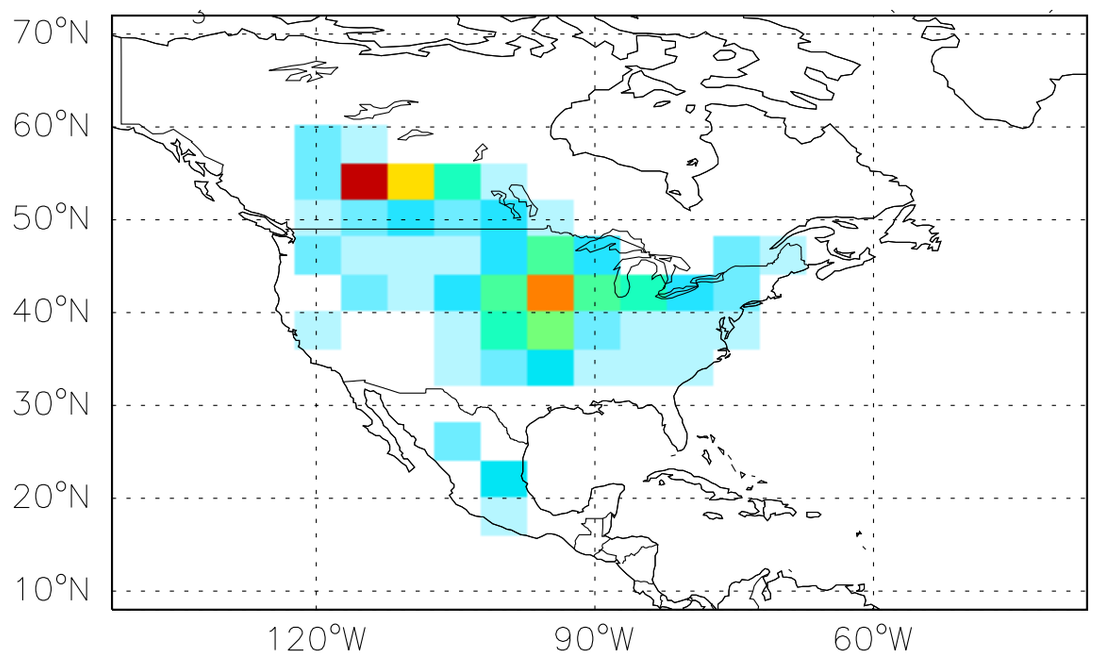
Aerosol Thermodynamics

February 2008

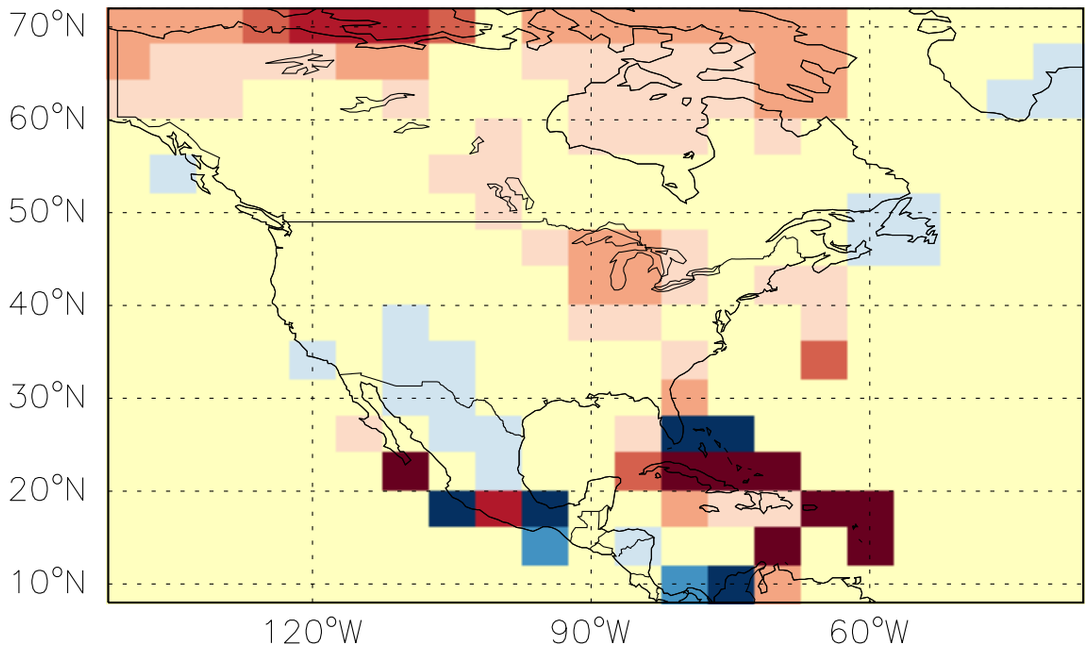
$\frac{\partial[\text{fine mode aerosol}]}{\partial(\sigma_{NH3,an})}$ | RPMARES

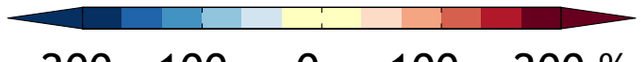


$\frac{\partial[\text{fine mode aerosol}]}{\partial(\sigma_{NH3,an})}$ | ANISORROPIA



ANISORROPIA - RPMARES





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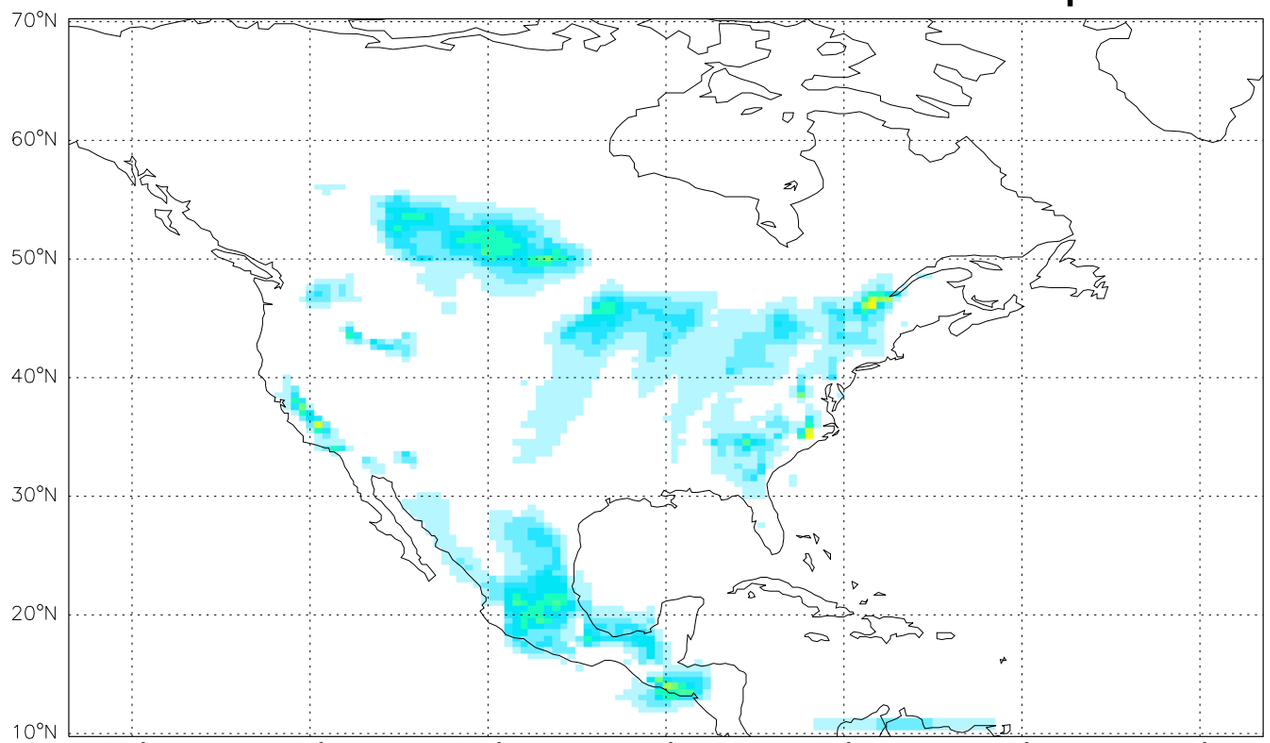
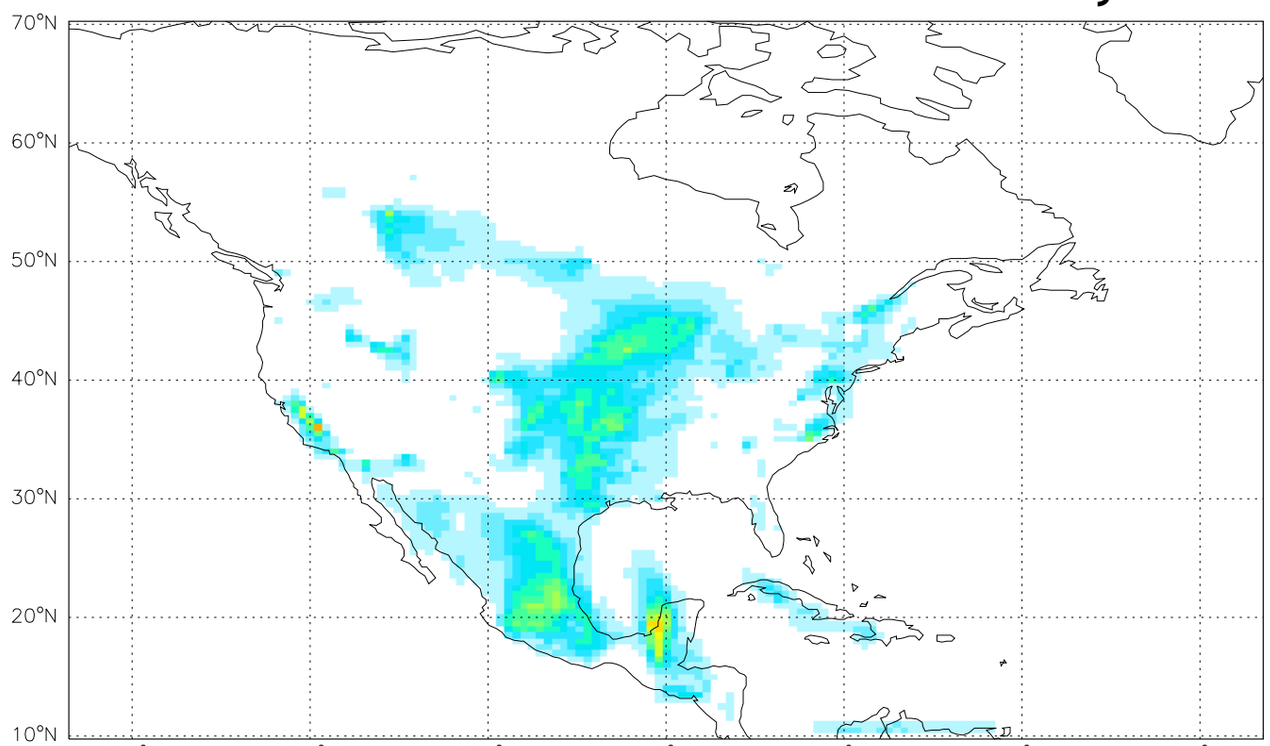
Preliminary Results

Average surface NH_3

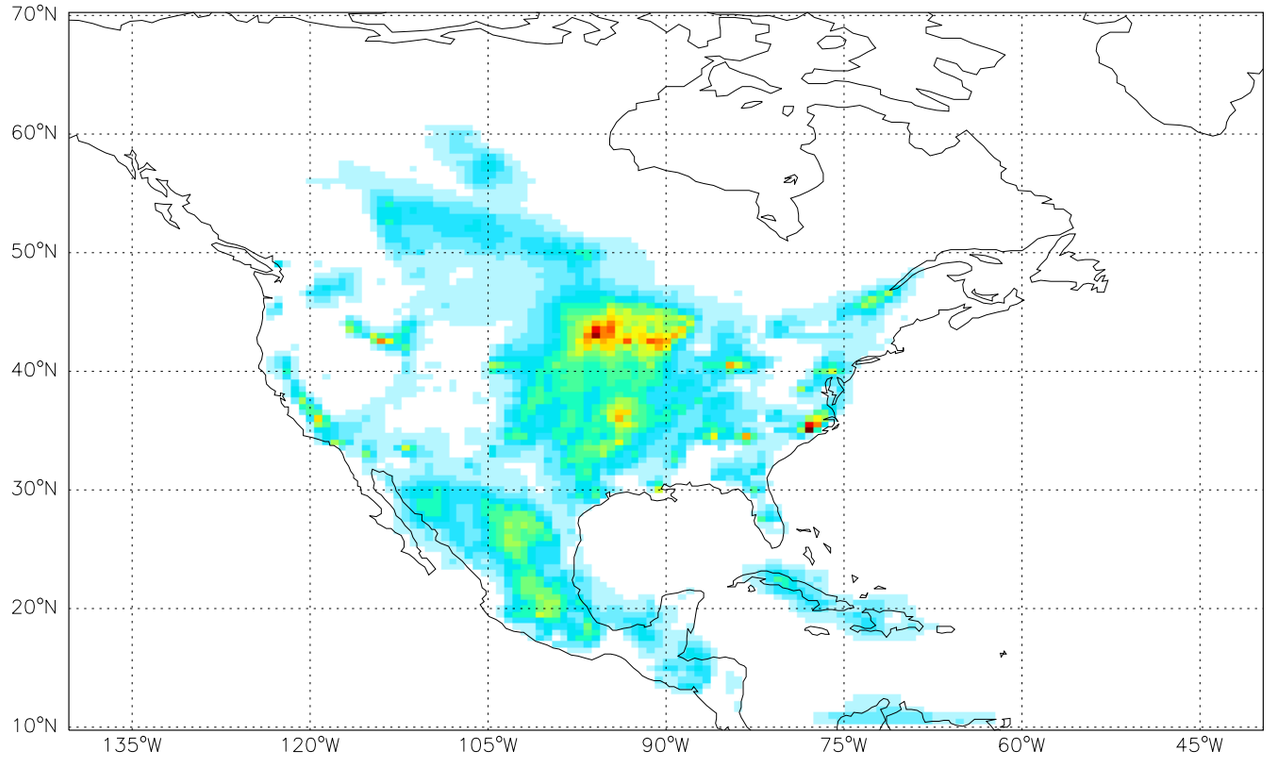
2 Apr 2010



1-3 May 2010



1-3 Jun 2010



GEOS-Chem adjoint v33
(adjoint wiki)

North American nested
grid 0.5° x 0.66° adjoint
(Zhe Jiang et al.)

ANISORROPIA
(Capps et al., 2012)

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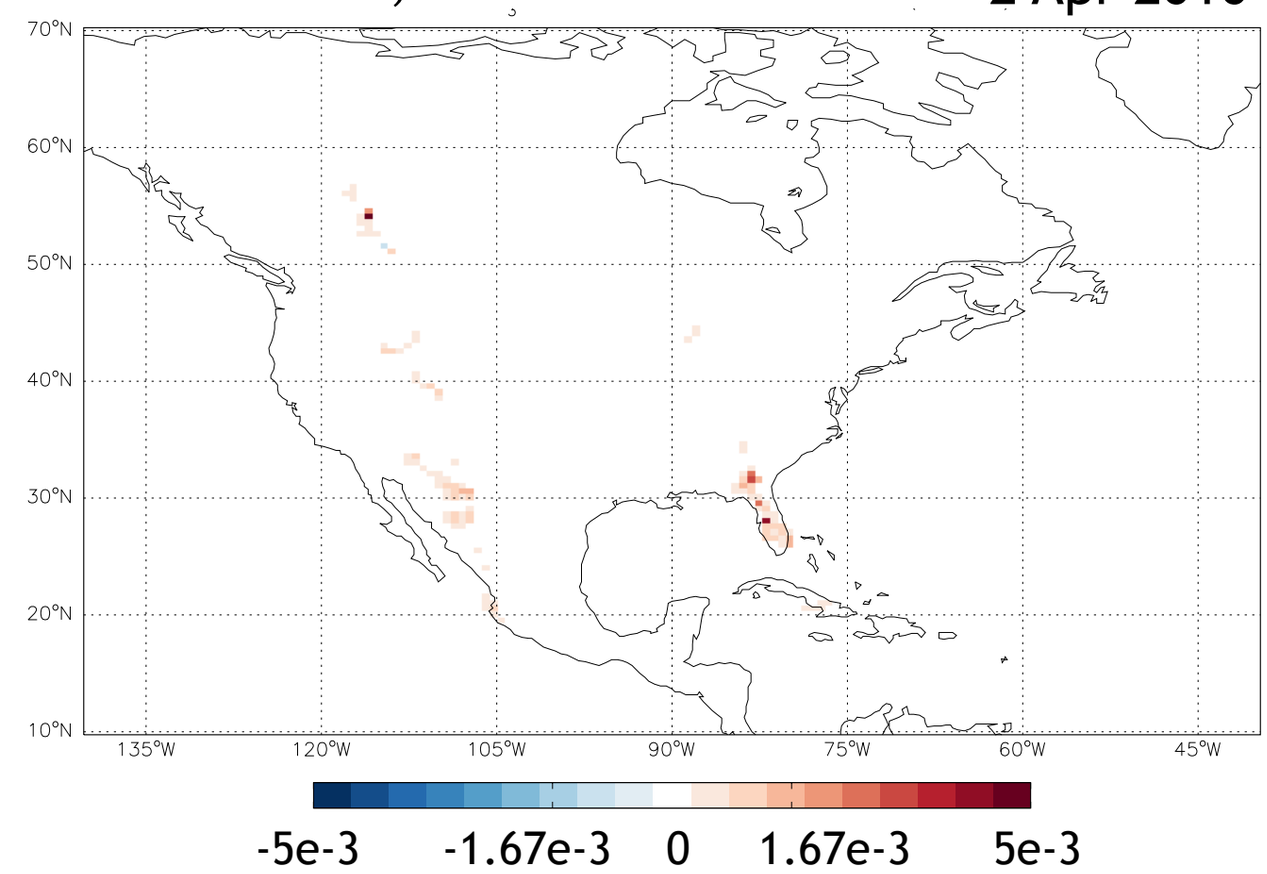
Preliminary Results

$\partial J/\partial NH_{3,an}$

2 Apr 2010



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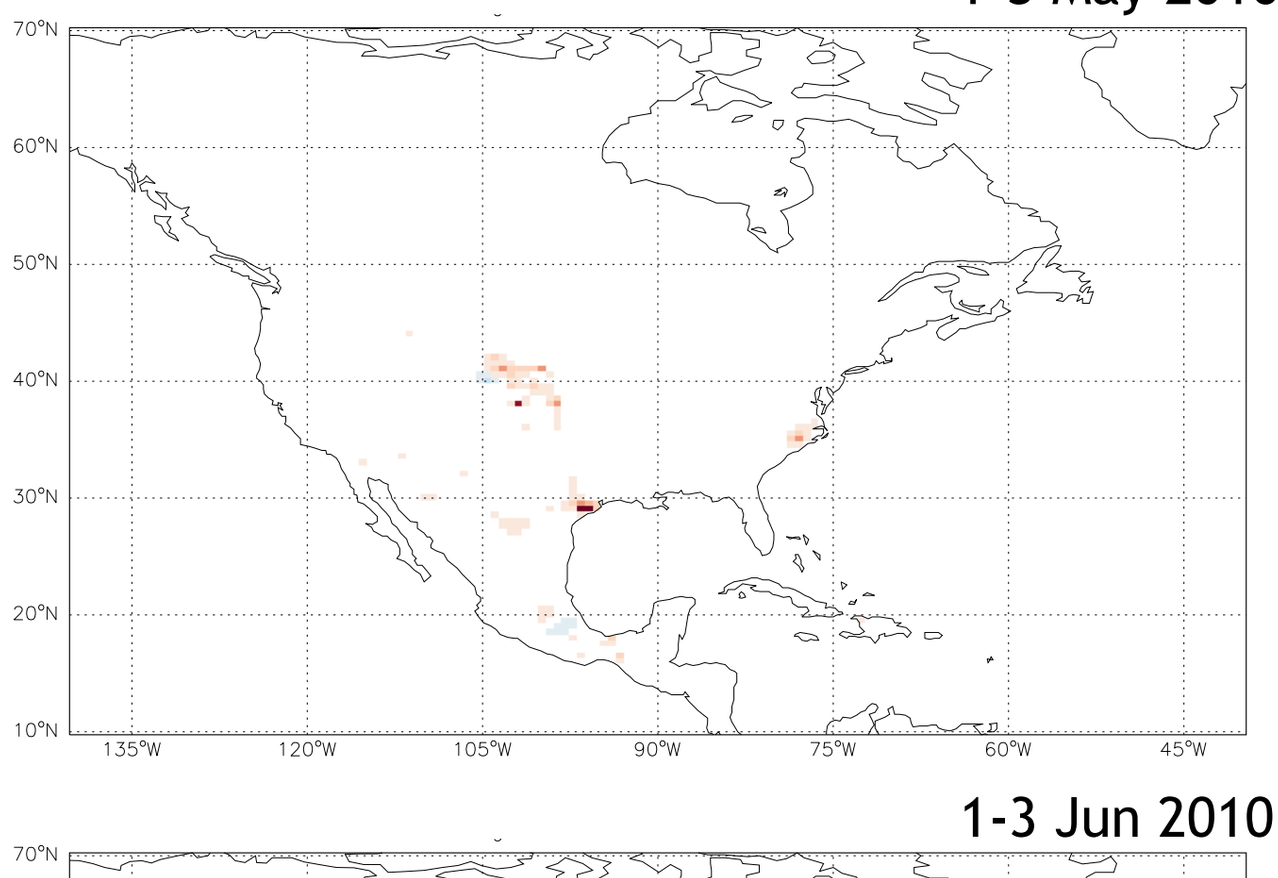

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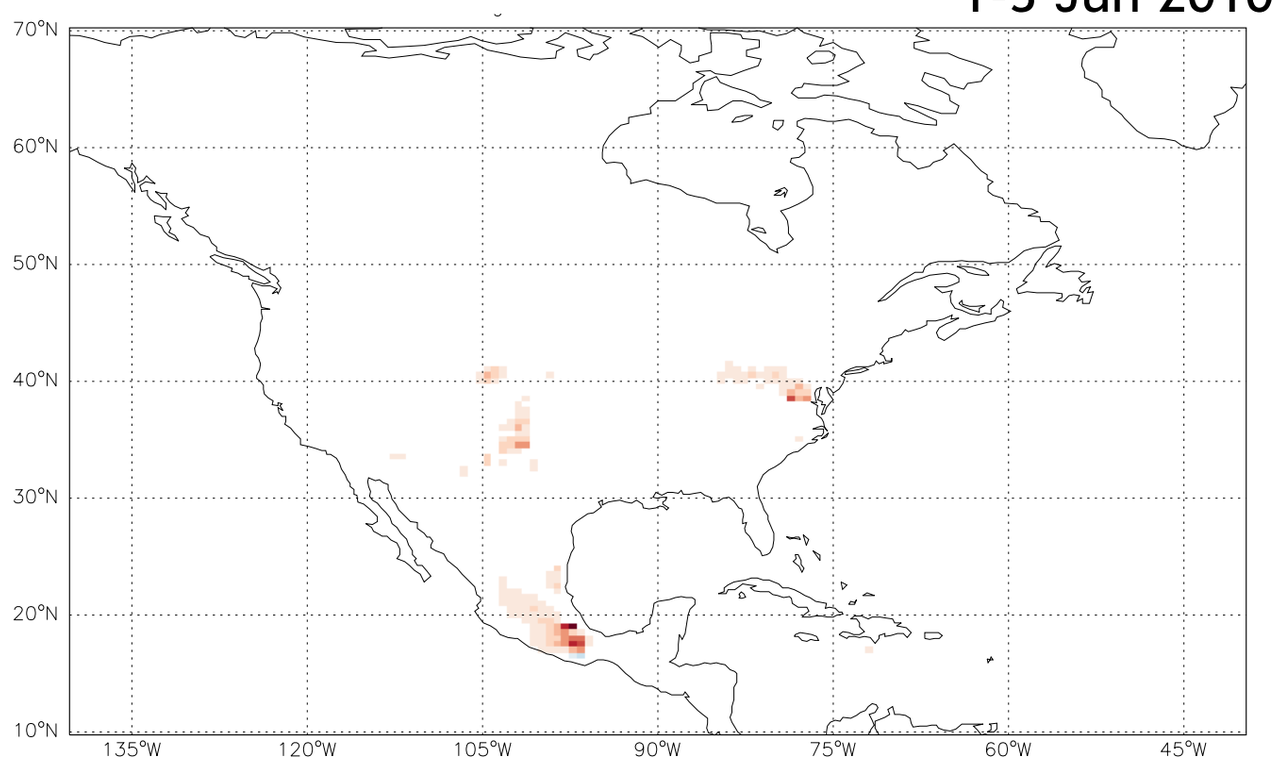

Sensitivity of cost function with respect to anthropogenic NH_3 emissions

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Highlights & Ongoing Work

- Demonstrated functionality of GEOS-Chem Adjoint with ANISORROPIA
- Running data assimilation with 0.5˚ x 0.66˚ nest over North America
- Including global swath & special observations from April - July 2010
- As we complete the inversion, a host of in situ measurements to which we can compare revised emissions independently exists

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