GEOS-Chem adjoint model: Recent developments and future directions

IGC5
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Daven K. Henze
University of Colorado Boulder

Kevin Bowman
NASA JPL, California Institute of Technology

with contributions from the entire adjoint group*

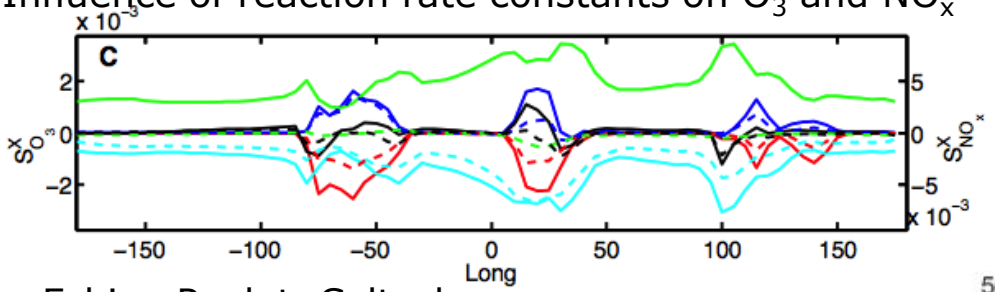
* 47 registered users at 20 institutions

An adjoint model...

...calculates gradients of a scalar model response with respect to all model parameters (emissions, initial conditions, rate constants, ...) at the native model resolution. Used for:

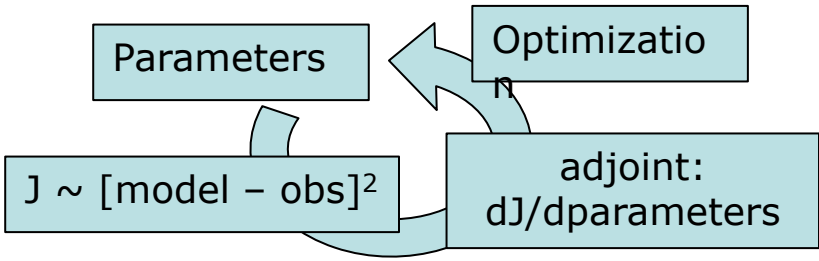
Sensitivity

Influence of reaction rate constants on O_3 and NO_x

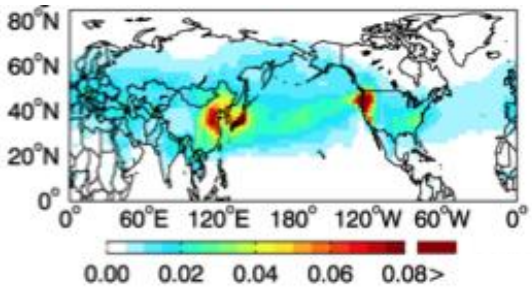


Fabien Paulot, Caltech

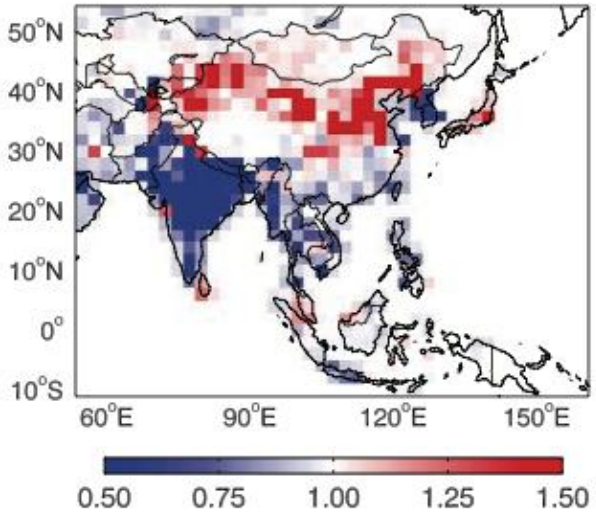
Inverse modeling / 4D-Var



Source attribution



sources of O_3 at Mt. Bachelor (Zhang et al., 2009)



top-down CO emission adjustments (Kopacz et al., 2009)

Adjoint model: current features

Standardized code: maintained / distributed via CVS
Code base: v8-02-01 with relevant fixes / updates up to v9-01-02

Meteorology: GEOS-3, GEOS-4, GEOS-5
Simulations: full chem; offline CO, O_x, CO_2
Resolution: 4x5, 2x2.5, Asia nested for offline CO
Observation operators: O_3, NO_2, CO, NH_3

Processes: all main forward model process *excluding:*
- non-local pbl mixing scheme
- aerosol microphysics, online het chem, ISORROPIA

Species: all forward model species *excluding:*
- dust, SOA, SO4s, NITs

see GC adj wiki page for details

Recent and current applications with mature capabilities

Aerosols:
- Source attribution of BC in Himalayas (Kopacz 2011)
- Assimilation of MODIS AOD (Xu, Wang, UNL)
- Top-down constraints on NH_3 (Zhu, Henze, CU Boulder)

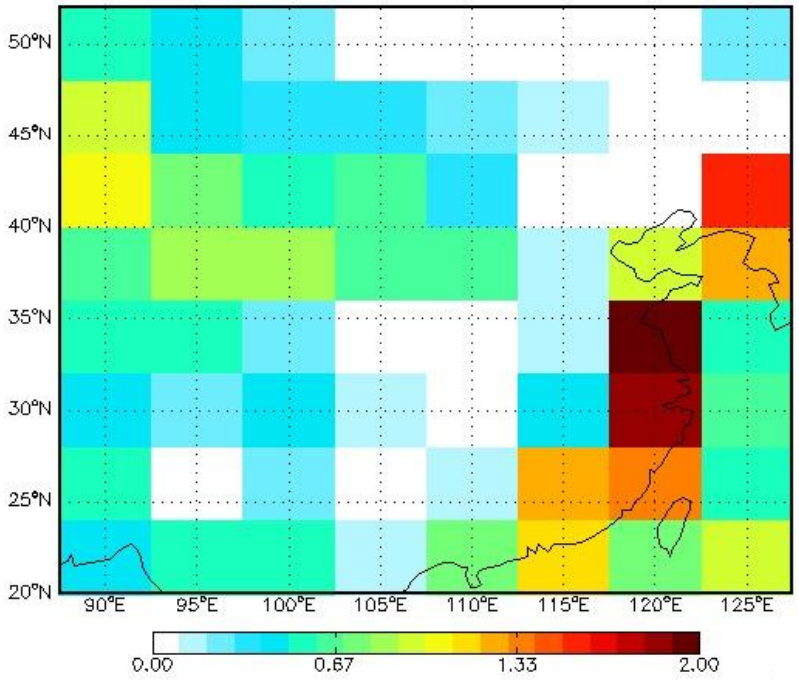
CO:
- CO constraints from AIRS, SCIA, TES, MOPITT (Kopacz 2010)
- Impact of model error on CO inversions (Jiang, submitted)

O_3 and NO_x:
- 3D-Var vs 4D-Var assimilation of TES O_3 (Singh 2011)
- TES and MLS O_3 assimilation (Bowman, Lee, NASA JPL)
- Arctic O_3 and NO_y (Walker, UT)
- Impacts of boreal biomass burning (Parrington, Edinburgh)
- Top-down constraints on NO_x (Bousserez, Padmanabhan, Dalhousie)

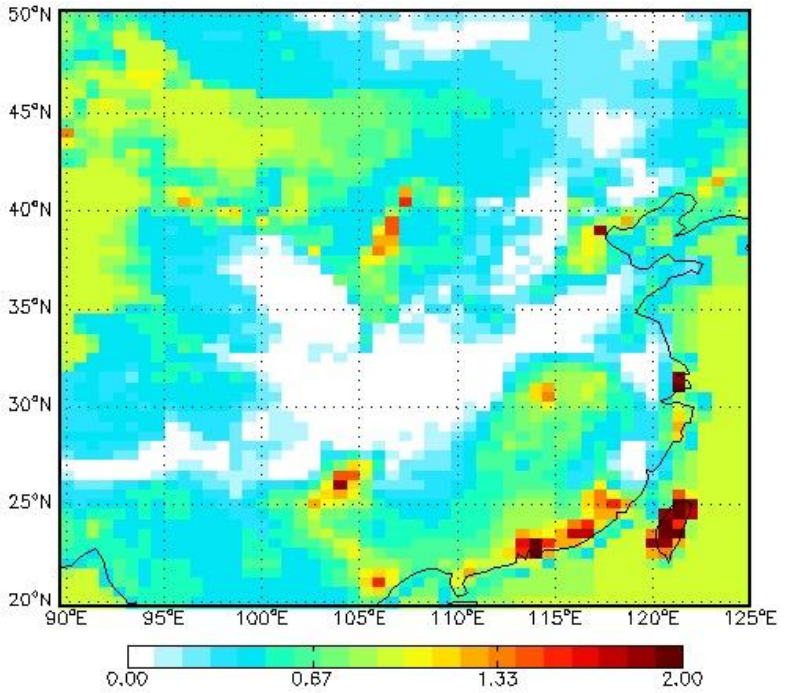
Recent developments: nested grid CO adjoint

in standard

CO inversion with MOPITT data: optimized emissions scaling factors



4° x 5°



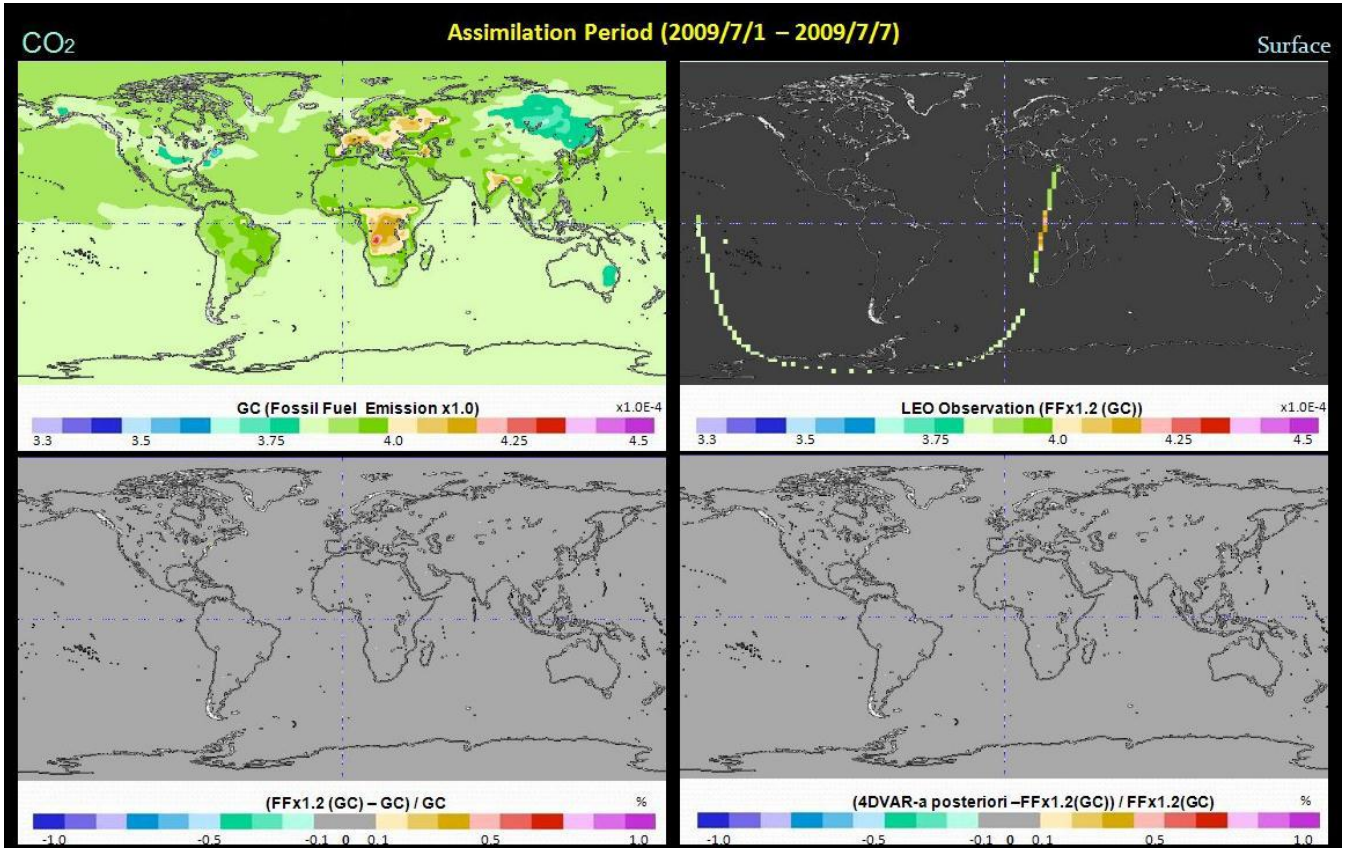
0.5° x 0.67°

Zhe Jiang, U Toronto

Recent developments: carbon dioxide adjoint

in standard

CO_2 OSSE studies, Meemong Lee:

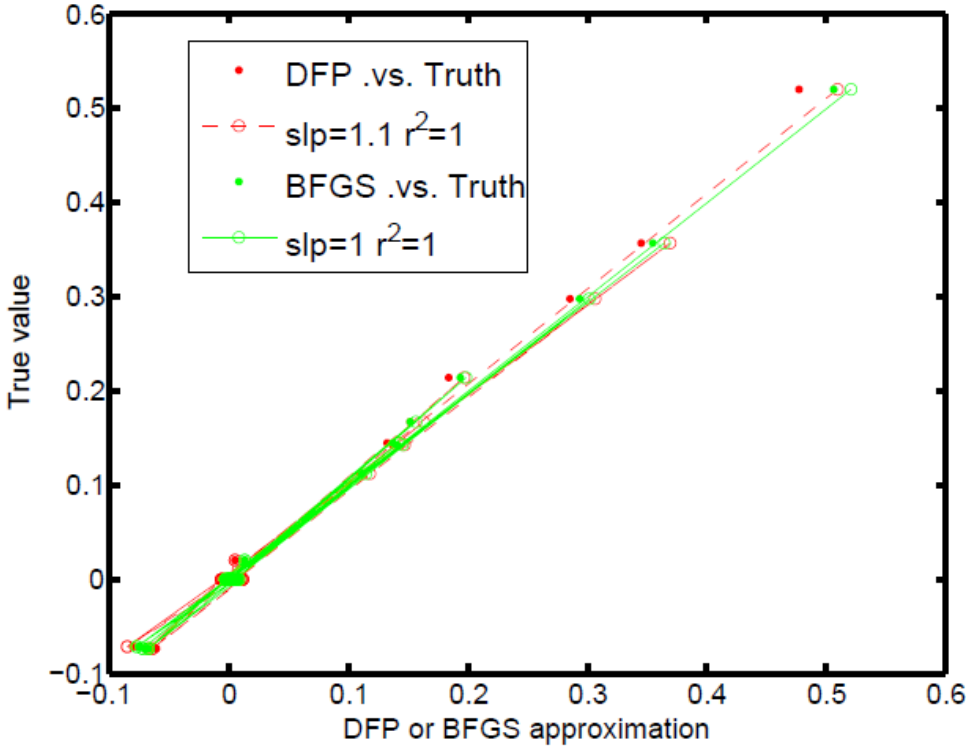


Many groups involved: U. Toronto, Env Canada, NASA JPL, Purdue, IAP.CAS, CU Boulder

Recent developments: Error analysis and constraints

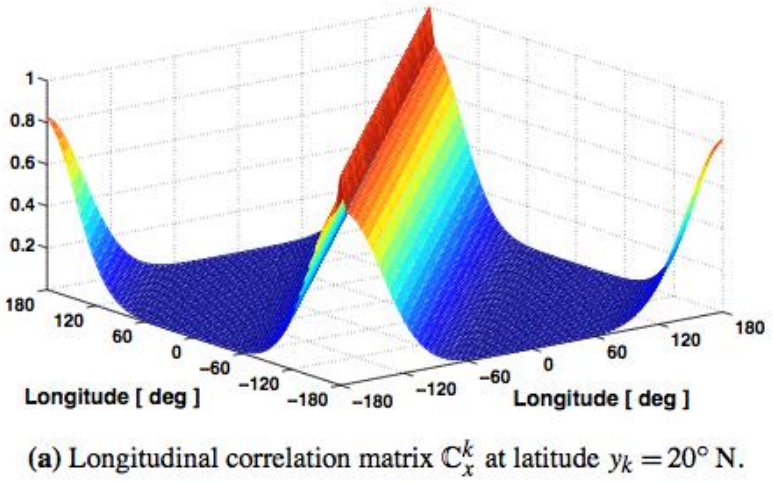
in pipeline

Posteriori error estimates
(i.e., inverse Hessian)



Jinyun Tang (Purdue)
updated from Henze et al.., 2009

Non-diagonal error
covariance matrices



(a) Longitudinal correlation matrix $\mathbb{C}_x^k$ at latitude $y_k = 20°$ N.

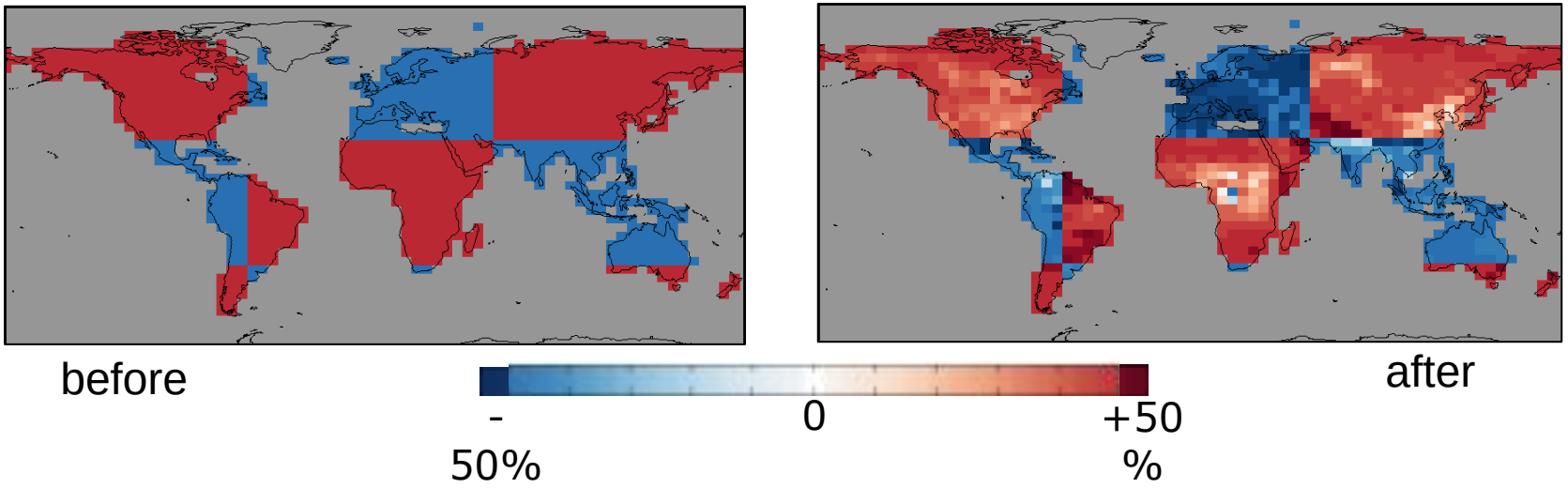
Singh et al., 2011

Recent developments: methane inversions

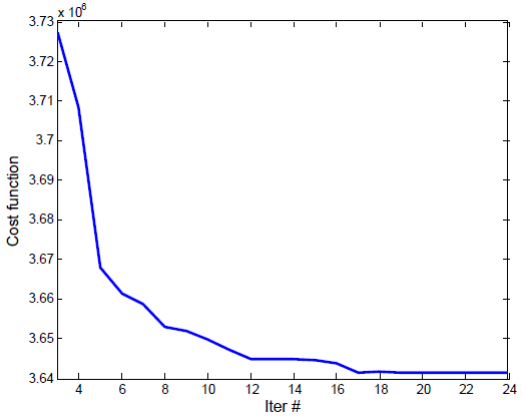
still testing

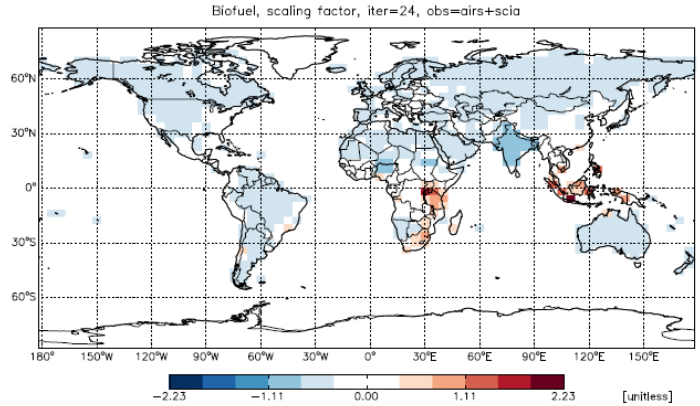
Kevin Wecht (Harvard): TES

Relative difference between optimized and "true" emissions



Jinyun Tang (Purdue): AIRS + SCIAMACHY



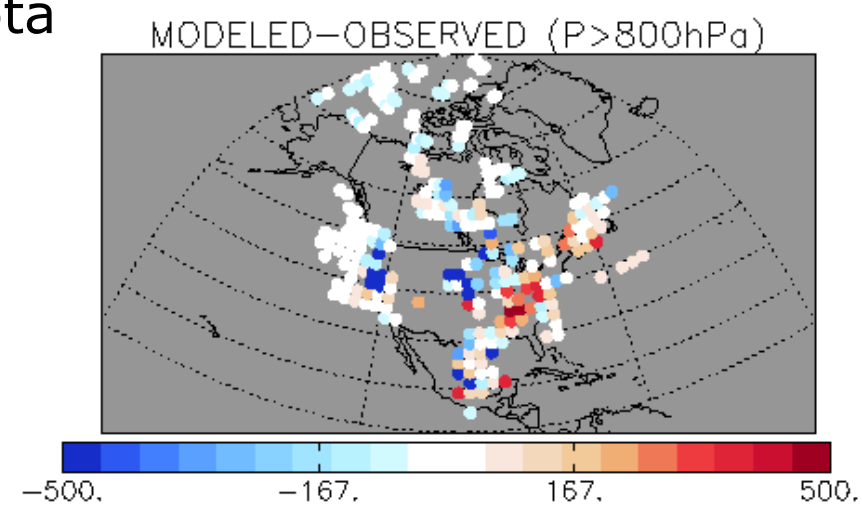


Posterior scaling factors

Recent developments: additional activities

still testing

- Ethanol: Dylan Millet, U. Minnesota



- Radiative forcing: Daven Henze, CU Boulder

- Sensitivity w.r.t. aviation emissions: Jamin Koo, MIT

- Sensitivity w.r.t. lighting NO_x injection height & yield: Nicolas Bousserez, Dalhousie

- others...

Future directions

My thoughts on the pipeline, ordered by perceived momentum:

- full chemistry nested
- more species (dust, ...)
- add ISORROPIA, update het chem adjoint
- more cost function options: deposition, ...
- more sensitivity output: convection, ...
- less hardcoding, more generalized inputs
- further consolidation of obs operators
- column model?
- additional meteorology? GCAP

use AD tools (better now!)

Address when warranted by science goals

- Develop better connections with other inverse approaches

- Quasi-adjoints: approximate or low res adjoint for inversions
  - that's how the meteorologists do it
  - Recently investigated for GC adjoint (Singh, VT)

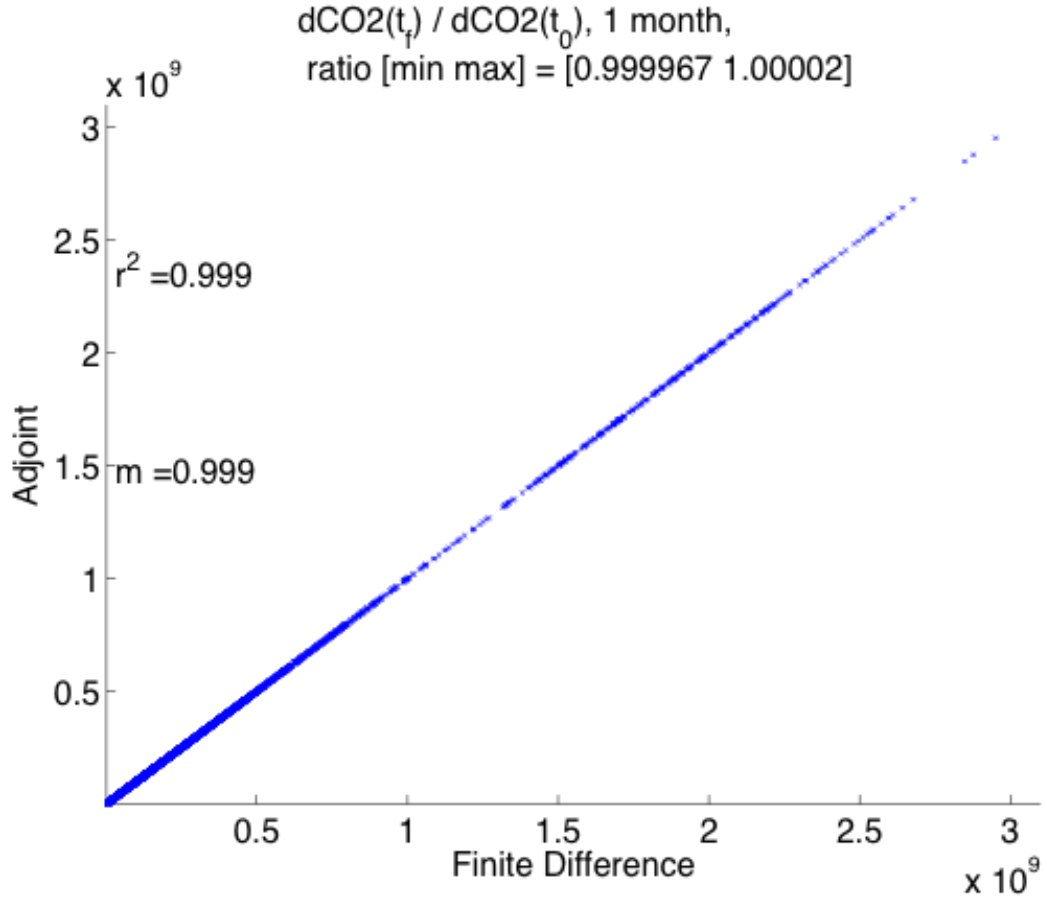
Stay tuned for the working group report...

the end

Recent developments: carbon dioxide adjoint

in standard

validation vs finite differences (Henze)



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Recent developments: carbon dioxide adjoint

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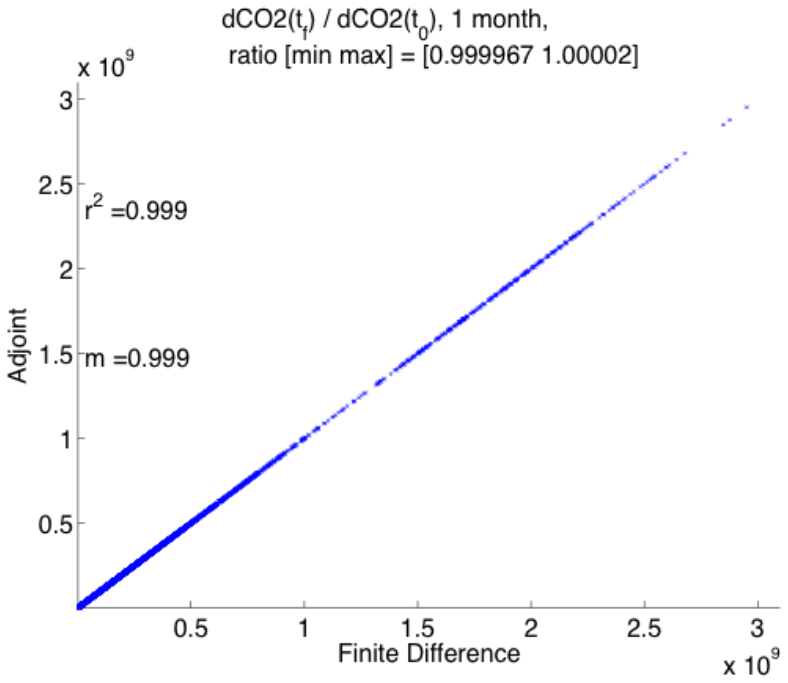
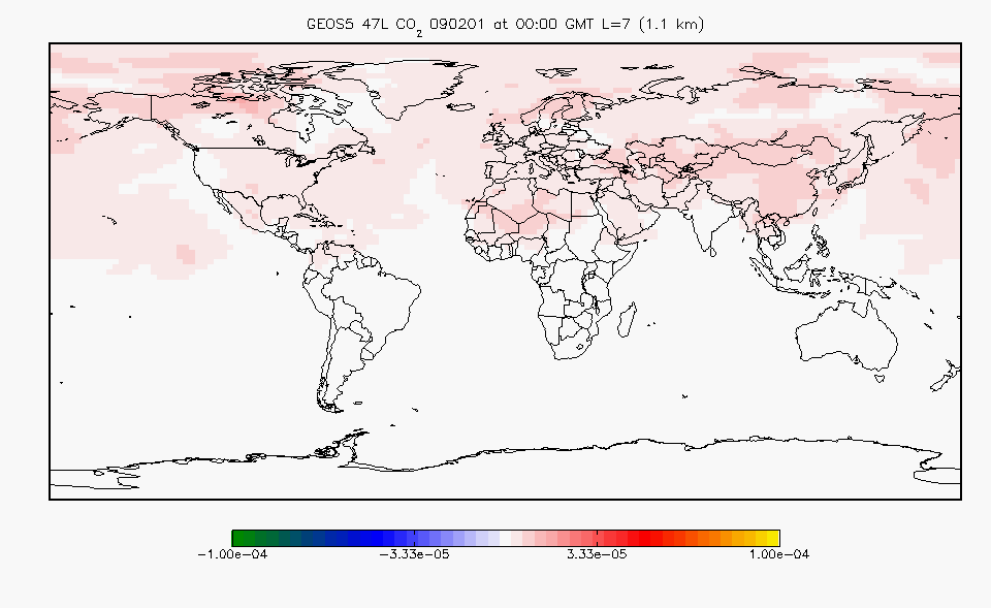
validation



sensitivity example



Henze

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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
- adjoint requires an additional x2 CPU time

Examples (on new dual hex-core Xeon 2.6 GHz):
- fwd+adj iteration of **full chem**, global 2x2.5, 1 month
    - 30 hours per iteration
    - 400 GB checkpoint files

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

GEOS-Chem adjoint history

Several different adjoint models attended the previous GC meeting:
- v6 adjoint (Henze et al., 2007; 2009)
- offline simulations (Kopacz et al., 2009; 2010; Zhang et al., 2010)
- v7 adjoint (Singh et al., 2011)

Following a merger held at VT in summer of 2009:
- consolidated most feature of previous versions
- updated the code to GEOS-Chem v8-02-01
- implemented support for GEOS-5

Since then:
- standardized adjoint code, maintained / distributed via CVS
- sync relevant bug fixes and updates up through v9-01-02
- model controlled via `define_adj.h` and `input.gcadj`
- user developed features rolled back into standard