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Space Administration

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California Institute of Technology
Pasadena, California

GEOS-Chem Adjoint:
Status from the Adjoint Working Group

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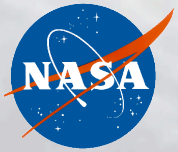
Jet Propulsion Laboratory

California Institute of Technology

Joint Institute for Regional Earth System Science and Engineering

University California, Los Angeles



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GEOS-Chem Adjoint Working Group

- **The adjoint working group started in 2007 to coordinate adjoint development activities between several groups**
  - ***Caltech***
  - ***Harvard***
  - ***Virginia Tech***
  - ***Jet Propulsion Laboratory***
- **The number of active participants has increased**
  - ***Caltech/ Columbia / NASA GISS / CU Boulder : Daven Henze***
  - ***Dalhousie: Randall Martin, Chulkyu Lee***
  - ***Harvard: Monika Kopacz, Lin Zhang, Peter Zoogman, Daniel Jacob***
  - ***JPL: Kevin Bowman, Changsub Shim, Paul Hamer, Sunita Verma***
  - ***UCLA: Qinbin Li***
  - ***U. of Toronto: Dylan Jones, Mark Parrington, Michael Seymour, Thomas Walker***
  - ***Virginia Tech: Adrian Sandu, Kumaresh Singh, Paul Eller, Mohammed Jardak***

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What Is an Adjoint Model?

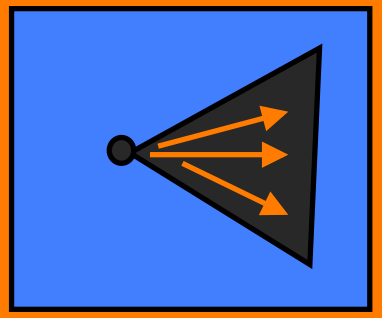
Ronald M. Errico
National Center for Atmospheric Research,* Boulder, Colorado

BAMS, 1997

Let *A* be a bounded operator on a Hilbert Space, *H*.
The adjoint operator is defined by:

$$A^* : H \to H \quad \langle Ax, y \rangle = \langle x, A^* y \rangle \quad \forall x, y \in E$$

$$\left(\frac{\partial \mathbf{x}^i}{\partial \mathbf{x}^0}\right)^\top = \left(\frac{\partial \mathbf{M}_{i-1}}{\partial \mathbf{x}_{i-1}} \cdots \frac{\partial \mathbf{M}_0}{\partial \mathbf{x}_0}\right)^\top$$



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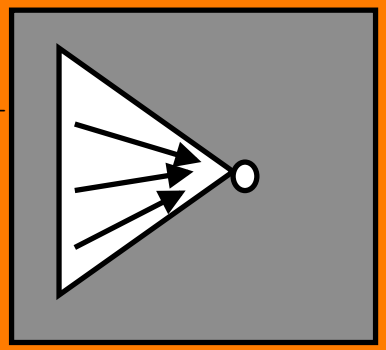

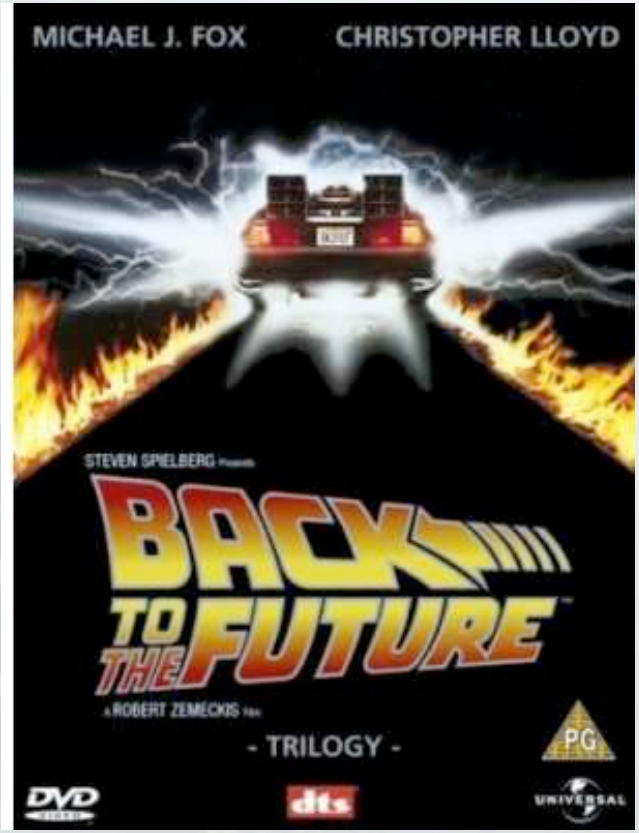

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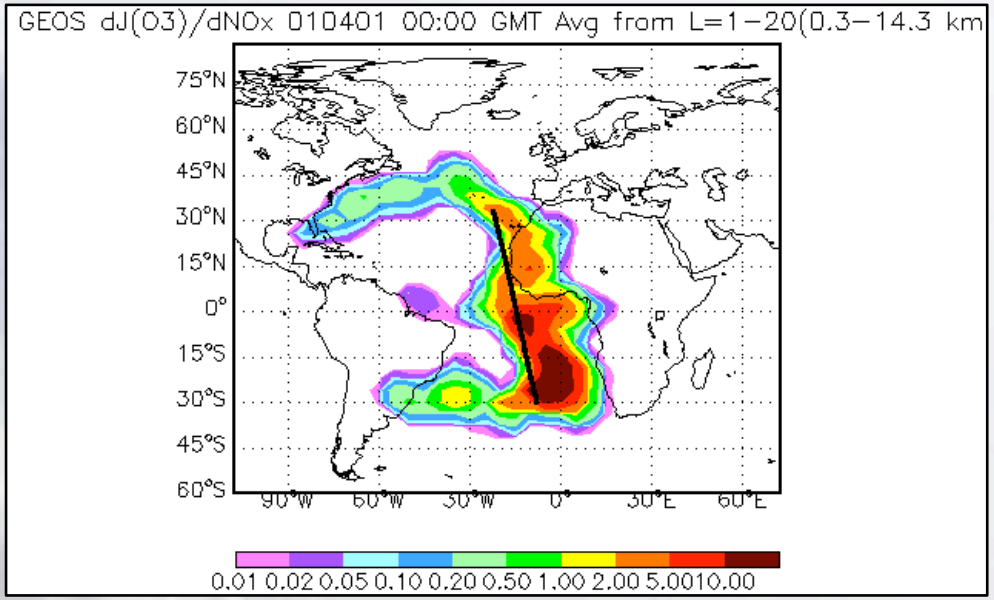
Sensitivity Analysis

- Sensitivity of O_3 along satellite track to global NO_x 2 days prior
- Receptor-based approach, so time marches backwards
- Adjoints are at the heart of
  - 4D-variational source and state estimation
  - Sensitivity analysis
  - Stability/perturbation analysis



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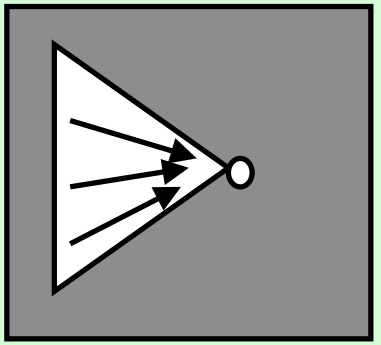

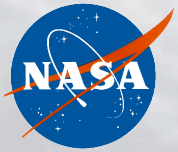

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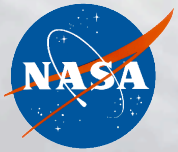
Adjoint Model Status

- **GEOS-Chem adjoint model versions:**
  - ***GEOS-Chem v6-02-05, full chemistry with online aerosols (Henze-CU Boulder)***
  - ***GEOS-Chem v6, tagged CO and Ox (Kopacz-Harvard)***
  - ***GEOS-Chem v7, full chemistry (Singh-Virginia Tech)***
- **Versions described at**
  - ***http://wiki.seas.harvard.edu/geos-chem/index.php/GEOS-Chem_Adjoint***
  - ***http://filebox.vt.edu/~kumaresh/***
  - ***http://spot.colorado.edu/~henzed/gc_adj.html/***



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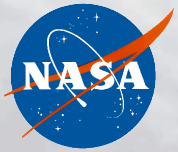
GEOS-Chem v6-02-05, full chemistry with online aerosols

- **GEOS-3 and GEOS-4 met fields**
- **2x2.5, 4x5 model resolution**
- **OpenMP parallelized**
- **Observational Operators**
  - ***IMPROVE PM2.5 (NO3, SO4, OC, BC)***
  - ***CASTNet (NH4+)***
  - ***GOME / SCIAMACHY NO2 column (KNMI and Dalhousie retrievals)***
  - ***TES NH3***
- **Control parameters**
  - ***Emissions scaling parameters (linear or log)***
    - SOx, NH3, primary BC/OC: anthro, natural, bioburn, biofuel, volcanoes
    - NOx: anthro, soil, lightning
  - ***Initial concentration scaling factors (all, linear)***
- **Adjoint sensitivities**
  - ***w.r.t control parameters***
  - ***of AQ attainment metrics***
  - ***of spatiotemporally averaged pollutant levels (e.g., arctic O3)***



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GEOS-Chem v6-02-05 (builds on dkh version), tagged CO and Ox

- **GEOS-3, GEOS-4 met fields**
- **4x5, 2x2.5 model resolution**
- **OpenMP parallelized**
- **Observational Operators**
  - ***MOPITT CO column***
  - ***SCIAMACHY CO column using Bremen retrieval***
  - ***AIRS CO column***
- **Control parameters**
  - ***Emissions (CO)***
  - ***Initial Conditions***
  - ***Ox production***
- **Adjoint sensitivity analysis**
  - ***w.r.t control parameters***

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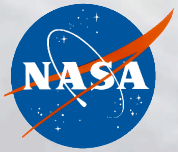
GEOS-Chem v7 with full chemistry

- **GEOS-4 met fields**
- **4x5 model, 2x2.5 resolution**
- **OpenMP parallelized**
- **Observational Operators**
  - ***TES O3***
- **Control Parameters**
  - ***Emissions scaling factors***
  - ***Initial Conditions***
- **Adjoint sensitivity analysis w.r.t control parameters**



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Adjoint Workshop goals

- **Adjoint model clinic (chairs: Kopacz, Singh, Henze)**
  - ***Thurs. 11-12:30pm***
  - ***Provide tutorials on adjoint usage with different model branches***
  - ***Please sign-up at registration desk for interested participants***
- **Adjoint model development planning group (chairs: Bowman, Henze)**
  - ***Thurs. 3:45- 5:15pm***
  - ***Assess how/whether adjoint branches should be merged***
  - ***Adjoint version releases relative to standard version releases***
  - ***Migration to GEOS-5 v8***
  - ***Next development milestones***
  - ***Funding opportunities***
  - ***Adjoint WG please sign up at registration desk***

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- **BACKUP**

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Adjoint operator

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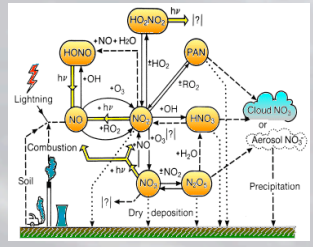
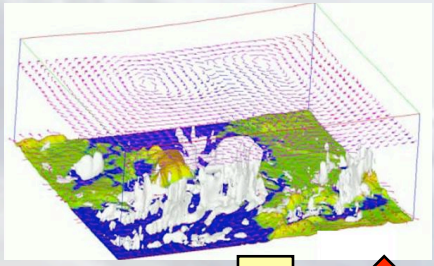
Advancement in atmospheric chemistry through modeling, observations and assimilation

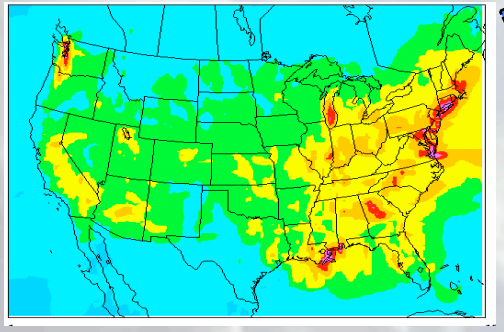
Transport
Meteorology

Chemical kinetics

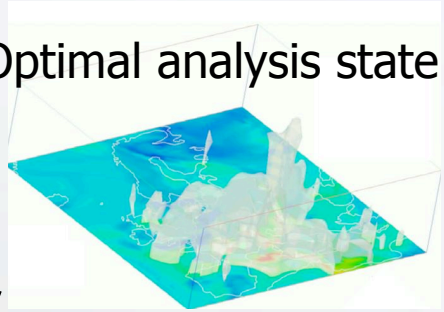




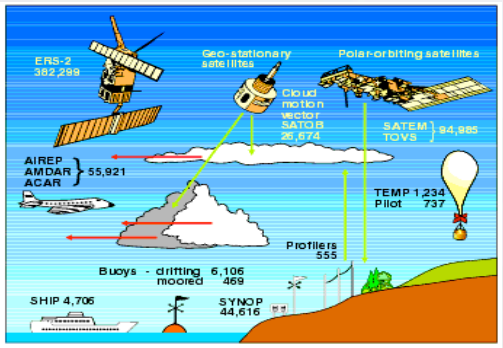
CTM



Optimal analysis state

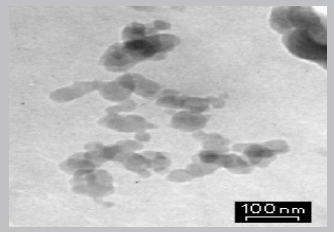


Observations



State/parameter estimation

Aerosols



Emissions

$$\min_{\mathbf{x}_0} C(\mathbf{x}) = \left\{ \sum_i (\mathbf{y}_i - \mathbf{F}_i(\mathbf{x}))^\top (\mathbf{S}_n^i)^{-1} (\mathbf{y}_i - \mathbf{F}_i(\mathbf{x})) + (\mathbf{x}_0 - \mathbf{x}_a)^\top \mathbf{S}_a^{-1} (\mathbf{x}_0 - \mathbf{x}_a) \right\}$$

- We want to understand the sensitivity of ozone to processes
- We can observationally constrain parameters defined within those processes

Courtesy, Adrian Sandu, VT