GEOS-Chem Adjoint and Data Assimilation Working Group

- Brief overview of current capabilities

- Review of current projects

- Update to policy / co-authoring

- Development tasks for adjoint model

- Incorporation of Data Assimilation into WG

- Personnel

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

Policy updates: code access and enforcing participation in WG wiki

Future policy: must follow these steps prior to getting an account to download the code:

1. Sign up for the geos-chem-adjoint mailing list to receive updates about code bugs and developments

2. Create an account on the GEOS-Chem wiki

3. Use your GEOS-Chem wiki account to add yourself to the list of users and projects at the GEOS-Chem adjoint wiki page

4. Review the policies on code use and distribution

5. Get an account on adjoint.colorado.edu by emailing daven.henze@colorado.edu

6. Follow the instructions in the user guide for using CVS to access the code.

Policy updates: co-authoring

Existing / previous: Kopacz, Shim, Singh and Henze on v8.
Apply to:
- Kopacz 2011 (almost)
- Jiang submitted
- Walker in prep
- Henze in prep

Then switch to feature specific co-author recommendations similar to forward model policy.

- (v31) Asian nested grid for tagged CO. Developer: Zhe Jiang, University of Toronto.
- (v31) MOPITT CO v3 and v4 observation operators. Developer: Zhe Jiang, University of Toronto.
- (v29) LIDORT. Developer: Daven Henze, University of Colorado Boulder. Collaborator: Rob Spurr.
- (v28) CO2 adjoint. Developer: Daven Henze, University of Colorado Boulder. Collaborators: Ray Nassar, Kevin Bowman, Dylan Jones.

Current (incomplete) projects

User Group	Description	Contact Person
CU Boulder	Aerosol precursors, CO2, O3; general adjoint code maintenance	Daven Henze
Harvard	Methane	Kevin Wecht
Purdue University	Methane (SICAMACHY, AIRS and IASI)	Jinyun Tang
MIT	Aircraft emissions	Jamin Koo
Princeton	BC sensitivities, general adjoint code development	Monika Kopacz, mkopacz [at] princeton.edu
Dalhousie University	Lightning NOx emissions and impact on tropical ozone using the adjoint	Nicolas Bousserez
JPL	Microwave Limb Sounder (MLS) Ozone assimilation	Meemong Lee
JPL	TES ozone assimilation/attribution of ozone radiative forcing	Kevin Bowman
University of Edinburgh	Quantifying the impact of boreal forest fires on tropospheric oxidants over the Atlantic	Mark Parrington
US EPA	Integration with economic models for future emission inventory scenario development	Farhan Akhtar
Peking University	Satellite constraints on VOC emissions	May Fu
CU Boulder	Aerosol precursor emissions	Alex Turner
IAP.CAS	CO2 assimilation	Chen
Purdue University	Feedback between terrestrial ecosystem processes and atmospheric co2 signals	Qing Zhu
University of Toronto	Sensitivity of ozone and reactive nitrogen to precursor emissions	Thomas Walker

Adjoint model development priorities

Model development	Development group	Priority level	Readiness	Difficulty
Off-diagonal error covariance matrix	JPL	high	med	low
Inverse Hessian	Tang (Purdue), JPL	high	med	low
Methane	Wecht (Harvard), Tang (Purdue)	high	high	low
CH4 obs operators: SCIA, AIRS, TES	Harvard / Purdue	med	med	low
generalized DOAS obs operator	Bousserez (Dal)	high	high	low
generalized TES obs operator	Lee (JPL)	med	med	med
full chemistry nested	Zhe Jiang (UT)	highest	low	med
CO/CO2	Jones (UT), Bowman (JPL)	high	low	med
BC offline adjoint	Yuhao Mao, Qinbin Li (UCLA)	high	low	low
heterogeneous chemistry (RDAER)	Henze (CU Boulder)	med	med	low
GISS tracer advection adjoint	Henze (CU Boulder)	low	low	low
GCAP convection	Henze (CU Boulder)	low	low	med
Column code adjoint		high, but wait	low	high
additional chemical mechanisms		med, but wait	low	med
Sensitivity of deposition	Yuanyuan Fang (Princeton), Henze (CU Boulder), Thomas Walker (UT)	high	low	low
Dust	Xu (UNL), Park (SNU), Li (UCLA)	high	med	low
Satellite obs operator sensitivity	Bowman, Lee (JPL)	med	med	low
Generic surface obs operator	Jones (UT)	med	med	low
Output rxn rate sensitivities	Paulot (Caltech/Harvard)	med	med	low
Joint initial condition & emissions opt	?	high	low	low
ISORROPIA adjoint	Shannon Capps (Georgia Tech)	med	med	med
Scaling factor "hooks" in forward model	work w/Bob and emissions group	high	low	low

Data Assimilation

Problem: our "Adjoint and Data Assimilation" WG doesn't incorporate much of the DA work.

Ongoing DA activities
- 3D-Var
- EnKF
- LTKF
- suboptimal KF

Need to represent on wiki

Standardize / distribute drivers

Specific overlaps with 4D-Var / adjoint
- covariance matrix
- assimilation window vs update cycle
- how implement scaling factors

Personnel

Adjoint scientific programmer support

Cultivation of future adjoint model gurus

Backup

Adjoint Working Group

Outstanding issues for development from IGC4

- GEOS-5
    - large bookkeeping task
    - minimal adjoint code dev task
- nested
- aerosol adjoints
    - size
    - optics
    - RT
- generic tagged adjoint? (PK)
- GEOS-Chem version 8?
- ESMF?

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

Developments: rank by priority (high, med, low) and assign point people or groups

Pipeline or recent features:

- off-diagonal covariance matrices for a priori error covariance

- inverse hessian approximation

- CH_4 simulation

- specific obs operators

Developments: rank by priority (high, med, low) and assign point people or groups

New adjoint features

- full chemistry nested

- dust (Park, Wang)

- joint CO/CO2 adjoint

- Hg? Fe?

- offline aerosol?

- add ISORROPIA (Capps)

- update het chem adjoint (Henze)

- additional meteorology?

    - for GCAP need the adjoint of GCAP convection

    - can run with GISS advection?

    - run in column model

- other chemical mechanisms (glyoxal chem or isoprene)

Developments: rank by priority (high, med, low) and assign point people or groups

New adjoint features:

- more cost function / sensitivity options:
    - deposition
    - sensitivities wrt to satelllites
    - sensitivity software configuration
    - general function/interface for surface obs
    - further consolidation of obs operators
    - MDA8
    - SOMO35 O3 (Henze)
- more/improved sensitivity output:
    - convection
    - rxn rate sensitivities (Paulot)
- joint optimization of initial conditions with emissions
- proper labeling of isoprene emissions