Adjoint Clinic:
Introduction for new users.

International GEOS-Chem Meeting 9

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2. Resources

Adjoint WIKI

- http://wiki.seas.harvard.edu/geos-chem/index.php/GEOS-Chem_Adjoint

Code Management (aka GitLab)

- http://adjoint.colorado.edu:8080

Trello Board

- https://trello.com/board/geos-chem-adjoint/4fe505dd72fb60941e2f6c3c

Code flowchart

- http://adjoint.colorado.edu/~daven/gcadj_std/flowchart.pdf

Plotting tools

- http://adjoint.colorado.edu/~daven/gcadj_std/tools.tar.gz

Background papers and presentations

- http://adjoint.colorado.edu/~daven/gcadj_std/adj_articles.tar.gz

3. Obtaining the Code

a) Sign up for the geos-chem-adjoint mailing list to receive updates about code bugs and developments
b) Create an account on the GEOS-Chem wiki
c) Use your GEOS-Chem wiki account to add yourself to the list of users and projects at the GEOS-Chem adjoint wiki page
d) Review the policies on code use and distribution
e) Request a GIT account by sending an email to the mailing list
f) CHANGE YOUR PASSWORD by going to http://adjoint.colorado.edu:8080/profile/account
g) Generate your SSH Keys by going to http://adjoint.colorado.edu:8080/profile/keys
h) git clone git@adjoint.colorado.edu:yanko.davila/gcadj_std.git

4. Model structure and key files

```
code/
   define.h
   adjoint/
      define_adj.h
      inverse_driver.f
      geos_chem_adj_mod.f
   modified/
      geos_chem_mod.f

runs/
   v8-02-01/
      geos4/  - (default config for CO pseudo obs benchmark)
      geos5/  - (default config for fullchemistry global finite difference benchmark)
         OptData/
         diagadj/
         adjtmp/
         STR_ID
         RXN_ID
         input.gcadj
         input.geos
         run

.git/  - (Contain all the information about commits, history, log, etc.)
.gitignore
```

Key output files:

```
runs/
   v8-02-01/
      geos5/  - (default config for full chemistry benchmark)
        OptData/
          cfn.**              : cost function
          gctm.gdt.**         : gradients
          gctm.sf.**          : scaling factors
        diagadj/
          gctm.adj.**         : tracer adjoints
          gctm.fd.**          : finite difference results
          gctm.fdglob.**      : finite difference results
          ems.adj.**          : non-normalized emissions sensitivities
          gctm.iteration      : iteration vs function evaluation
         log                  : cost function from penalty term
```

The run script

```
#################################################################
# Set run parameters.
# - X
# - XSTOP
# - RNAME
#
# These need to be set and checked  before every run.
# X = 0 creates observations.  X_STOP < X only
# creates a backup of the program directory.
#################################################################
# Set the start (or current ) iteration number
X=1

# Set the stopping iteration number
XSTOP=3
# Give every run a unique name (default is $PBS_JOBID)
RNAME=gcadj_std

# Specify Type of Run "DEFAULT, HDF, SAT_NETCDF, LIDORT"
TYPE=DEFAULT

# Set Compiler Options. For a list of all compiler options
# type 'make help' on the code directory.
# example IFORT_OPT="DEBUG=yes TRACEBACK=yes"

IFORT_OPT=""

# Recompile geos on every iteration.
# NOTE: If you have IPO set to yes we recommend not to recompile.
# IPO optimization make linking process slow.

RECOMPILE=NO

# Save packages to temporary storage before and after execution
# Note: Need to set DSAVE below
SAVE=NO

# Archive packages to permanent storage after execution
# Note: Need to set DARCHIVE below
ARCHIVE=NO

# Set compiler, if necessary
#source /usr/projects/compilers/intel/9.1.043/bin/ifortvars.sh
```

Setting X and XSTOP

Sensitivity	Finite difference	Pseudo obs
X=1	X=1	X=0
XSTOP=1	XSTOP=3	XSTOP=10

Input.gcadj (default configuration for Finite Difference $\frac{\partial Ox}{\partial NOx}$)

```
GEOS-CHEM ADJOINT SIMULATION v35n
------------------------------+---------------------------------------------
%%% ADJOINT SIMULATION MENU %%%
Do adjoint run    LADJ         : T
Selecet one simulation type    :---
Inverse problem   L4DVAR       : F
Kalman filter     L3DVAR       : F
Sensitivity       LSENS        : T
 => spot finite diff  FD_SPOT  : F
 => global finite diff FD_GLOB : T
------------------------------+---------------------------------------------
%%% FORWARD MODEL OPTIONS %%%
adjoint chemistry LADJ_CHEM    : T
aerosol thermo    LAERO_THEM   : T
 => ISORROPIAII                : F
------------------------------+---------------------------------------------
%%% ADJOINT MODEL OPTIONS %%%
Include a priori term APSRC    : F
 => offdiagonal                : F
Compute DFP inverse Hessian    : F
Compute BFGS inverse Hessian   : F
Include rxn rate sensitivities : F
Delete chk files LDEL_CHKPT    : T
Scale up and FILL adj transport: F
------------------------------+---------------------------------------------
%%% DIRECTORIES %%%
Optimization output            : OptData/
Temporary adjoint dir adjtmp   : adjtmp/
Diagnostics ouptut             : diagadj/
-------------------------------------------------------------------------------
%%% CONTROL VARIABLE MENU %%%
Initial conditions LICS        : T
... OR emissions   LADJ_EMS    : F
 => strat prod/loss LADJ_STRAT : F
 => reaction rates LADJ_RRATE  : F
>------------------------------<
          FOR LICS             :
NSOPT: number of tracers opt   : 1
  => opt these tracers------>  : TRC# trc_name SF_DEFAULT REG_PARAM ERROR
Tracer  #1                     : 1    NOx      1          1         1
>------------------------------<
          FOR LADJ_EMS         :
NNEMS: ems groups implemented  : 33
Emission entries ------------> : EMS# ems_name       opt  SF_DEFAULT REG_PARAM ERROR CORR_LX CORR_LY
Emission #1                    : 1    IDADJ_ENH3_an  T    1          1         1       100     100
Emission #2                    : 2    IDADJ_ENH3_na  T    1          1         1       100     100
Emission #3                    : 3    IDADJ_ENH3_bb  T    1          1         1       100     100
Emission #4                    : 4    IDADJ_ENH3_bf  T    1          1         1       100     100
Emission #5                    : 5    IDADJ_ESO2_an1 T    1          1         1       100     100
Emission #6                    : 6    IDADJ_ESO2_an2 T    1          1         1       100     100
Emission #7                    : 7    IDADJ_ESO2_bf  T    1          1         1       100     100
Emission #8                    : 8    IDADJ_ESO2_bb  T    1          1         1       100     100
Emission #9                    : 9    IDADJ_ESO2_sh  T    1          1         1       100     100
Emission #10                   : 10   IDADJ_EBCPI_an T    1          1         1       100     100
Emission #11                   : 11   IDADJ_EBCPO_an T    1          1         1       100     100
Emission #12                   : 12   IDADJ_EOCPI_an T    1          1         1       100     100
Emission #13                   : 13   IDADJ_EOCPO_an T    1          1         1       100     100
Emission #14                   : 14   IDADJ_EBCPI_bf T    1          1         1       100     100
Emission #15                   : 15   IDADJ_EBCPO_bf T    1          1         1       100     100
Emission #16                   : 16   IDADJ_EOCPI_bf T    1          1         1       100     100
Emission #17                   : 17   IDADJ_EOCPO_bf T    1          1         1       100     100
Emission #18                   : 18   IDADJ_EBCPI_bb T    1          1         1       100     100
Emission #19                   : 19   IDADJ_EBCPO_bb T    1          1         1       100     100
Emission #20                   : 20   IDADJ_EOCPI_bb T    1          1         1       100     100
Emission #21                   : 21   IDADJ_EOCPO_bb T    1          1         1       100     100
Emission #22                   : 22   IDADJ_ENOX_so  T    1          1         1       100     100
Emission #23                   : 23   IDADJ_ENOX_li  T    1          1         1       100     100
```

```
Emission #24                  : 24   IDADJ_ENOX_ac  T    1          1         1       100     100
Emission #25                  : 25   IDADJ_ENOX_an  T    1          1         1       100     100
Emission #26                  : 26   IDADJ_ENOX_bf  T    1          1         1       100     100
Emission #27                  : 27   IDADJ_ENOX_bb  T    1          1         1       100     100
Emission #28                  : 28   IDADJ_ECO_an   T    1          1         1       100     100
Emission #29                  : 29   IDADJ_ECO_bf   T    1          1         1       100     100
Emission #30                  : 30   IDADJ_ECO_bb   T    1          1         1       100     100
Emission #31                  : 31   IDADJ_EISOP_an T    1          1         1       100     100
Emission #32                  : 32   IDADJ_EISOP_bf T    1          1         1       100     100
Emission #33                  : 33   IDADJ_EISOP_bb T    1          1         1       100     100
Number emis time group MMSCL  : 1
>------------------------------<
        FOR LADJ_STRAT        :
NSTPL: strat prod & loss trcs : 0
Read reactions from STR_ID file: T
Strat prod & loss trc entries : ID# trc_name    opt   SF_DEFALUT  REG_PARAM ERROR
>------------------------------<
         FOR LADJ_RRATE       :
NRRATES: num of rxn rates     : 0
Read reactions from RXN_ID file: T
 ...or use these Rxn rates    : ID#   rxn_name  opt SF_DEFAULT REG_PARAM ERROR
-------------------------------------------------------------------------------
%%% OBSERVATION MENU %%%
%%%  for PSUEDO_OBS  %%%
%%%   or LSENSE      %%%
Observation frequency OBS_FREQ : 60
Limit number of observations?  : F
  =>  Forcing time till        : 20050701 050000
COST FUNCTION options for LSENS:---
  =>  tracer kg/box            : T
  =>  tracer ug/m3             : F
  =>  tracer ppb               : F
  =>  tracer ppm free trop     : F
  =>  species ppb w/averaging  : F
  =>  tracer ug/m3 pop weight  : F
  =>  tracer ug/m2/hr          : F
  =>  deposition based?        : F
      =>  dry dep (not kpp)    : F
      =>  dry dep (kpp)        : F
      =>  tracer wet LS dep    : F
      =>  tracer wet CV dep    : F
      =>  molec/cm2/s          : F
      =>  kgN/ha/yr            : F
      =>  eq/ha/yr             : F
      =>  kg/s                 : F
  =>  Regional mask?           : F
      =>  binary punch file?   : F
         =>  bpch mask name    : usa_mask.geos.4x5
      OR  netcdf file      ?   : F
         =>  nc mask file name : /home/hyungmin/Class_1/Class1.nc
         =>  nc mask var  name : NPS_16
 >------------------------------<
NOBS: number of tracers to obs : 1
  => obs these tracers------>  : TRC# tracer_name
Tracer  #1                     : 2    Ox
>------------------------------<
NOBS_CSPEC: # of species to obs: 0
  => obs these species------>  : species_name
Species #1                     : O3
-------------------------------------------------------------------------------
%%% FINITE DIFFERENCE MENU %%%
fd perturbation        FD_DIFF : 0.1
Numerator of derivative to test:---
 => longitude degree   LONFD   : 32
 => latitude  degree   LATFD   : 21
 => OR pick box by grid index? : T
   => longidute index  IFD     : 41
   => latitude index   JFD     : 32
 => altidude index     LFD     : 1
 => tracer (STT #)     NFD     : 2
Denomenator of deriv.   to test:
```

```
 => w/LEMS: emis group MFD     : 1
 => w/LEMS: sector     EMSFD   : 1
 => w/LICS: tracer     ICSFD   : 1
 => w/LSTR: tracer     STRFD   : 1
 => w/LRRATE: rate     RATFD   : 1
------------------------------------------------------------------------------
%%% DIAGNOSTICS MENU %%%
General                         : T
 => print debug  LPRINTFD       : F
 => jsave, jsave2               : F
 => adjoint traj LADJ_TRAJ      : F
   => w.r.t. scale factors?     : T
 => save iteration diags LITR   : T
 => sense w.r.t absolute emis   : F
CO satellite diganostics        : F
 => H(model)                    : F
 => h(obs)                      : F
 => H(model)-h(obs)             : F
 => adjoint forcing             : F
 => model bias                  : F
 => observation count           : F
 => DOFs                        : F
TES NH3 diagnostics             :---
 => BLVMR                       : F
HDF diagnostics                 :---
 => Level 2                     : F
 => Level 3                     : F
 ------------------------------------------------------------------------------
%%% CRITICAL LOAD MENU %%%
Critical Load obs               : F
 => N deposition                : T
 => Acidity deposition          : F
Critical Load file              : Exceedence.nc
GEOS-Chem file                  : Annual_Deposition.nc
------------------------------------------------------------------------------
END OF FILE                     :
--------------------------------+---------------------------------------------
```

Stratospheric production and loss

```
Strat prod & loss trc entries  : ID# trc_name    opt   SF_DEFALUT  REG_PARAM ERROR
Tracer  #1                     : 1    NOx_p      T     1           1         1
Tracer  #2                     : 2    Ox_p       T     1           1         1
Tracer  #3                     : 3    PAN_p      T     1           1         1
. . .
```

Reaction Rates

```
Rxn rate entries               : ID#   rxn_name                      opt   SF_DEFAULT   REG_PARAM   ERROR
Rate #1                        : 1     NO+O3                         T     1            1           1
Rate #2                        : 2     OH+O3                         T     1            1           1
Rate #3                        : 3     HO2+O3                        T     1            1           1
Rate #4                        : 4     NO2+O3                        T     1            1           1
Rate #5                        : 5     O3+MO2                        T     1            1           1
Rate #6                        : 6     2OH->O3+H2O                   T     1            1           1

. . .
```

define_adj.h

```
!*****************************************************************************
!  Include file "define_adj.h" specifies C-preprocessor "switches" that are
!  used to include or exclude certain sections of ADJOINT code, mostly for
!  controlling observation datasets used. The reason they are pre-processor
!  switches instead of logical flags is so that we can omit the code which
!  requires installation of hdf libaries and such. All are independent of
!  each other, but not of simulation and tracer type
!  (adj_group, 6/08/09)
!
!  List of "Switches"
!  ========================================================================
!  (1 ) TES_NH3_OBS         : Use NH3 data from TES
!  (2 ) PM_ATTAINMENT       : Compute PM attainment
!  (3 ) SOMO35_ATTAINMENT   : Compute ozone attainment
!  (4 ) SCIA_KNMI_NO2_OBS   : Use NO2 obs from SCIA KNMI retrieval
!  (5 ) IMPROVE_SO4_NIT_OBS : Use sulfate-nitrate from IMPROVE network
!  (6 ) CASTNET_NH4_OBS     : Use amonia from CASTNET network
!  (7 ) TES_O3_OBS          : Use O3 obs from TES
!  (8 ) SCIA_DAL_NO2_OBS    : Use NO2 obs from SCIA Dalhousie retrieval
!  (9 ) SCIA_DAL_SO2_OBS    : Use SO2 obs from SCIA Dalhousie retrieval
!  (10) MOPITT_V3_CO_OBS    : Use v3 CO obs from MOPITT
!  (11) MOPITT_V4_CO_OBS    : Use v4 CO obs from MOPITT
!  (12) SCIA_BRE_CO_OBS     : Use CO obs from SCIA Bremen retrieval
!  (13) AIRS_CO_OBS         : Use CO obs from AIRS (UMBC) retrieval
!  (14) PSEUDO_OBS          : Generate pseudo obs if no data selected
!  (15) LOG_OPT             : Optimized log of scaling factors
!  (16) SOMO35_ATTAINMENT   : Ozone attainment
!  (17) PM_ATTAINMENT       : PM    attainment
!  (18) LIDORT              : Online radiative forcing calculations
!  (19) GOSAT_CO2_OBS       : Use CO2 obs from GOSAT retrieval
!  (20) MODIS_AOD_OBS       : Use AOD obs from MODIS
!  (21) IMPROVE_BC_OC_OBS   : Use BC and OC aerosol obs from IMPROVE
!  (22) MOPITT_V5_CO_OBS    : Use v5 CO obs form MOPITT
!  (23) MOPITT_V6_CO_OBS    : Use v6 CO obs form MOPITT
!  (24) TES_O3_IRK          : Use radiative kernels for TES O3
!  (25) OMI_SO2_OBS         : Use OMI L3 SO2
!
! NOTES:
! (1 )  Replace MOPITT_IR_CO_OBS with MOPITT_V3_CO_OBS and MOPITT_V4_CO_OBS
!       (zhe, dkh, 02/04/11)
! (2 ) Add MODIS_AOD_OBS (xxu, dkh, 01/09/12, adj32_011)
! (3 ) Addd IMPROVE_BC_OC_OBS (yhmao, dkh/ 01/16/12, adj32_013)
! (4 ) Add MOPITT_V5_CO_OBS (zhej, dkh, 01/16/12, adj32_016)
! (5 ) Add CH4 obs operators (kjw, dkh, 02/12/12, adj32_023)
! (6 ) Add MOPIT_V6_CO_OBS and drop support for MOPITT v3 and v4 (zhe, dkh
06/2015)
!*****************************************************************************
!
!=============================================================================
! Undefine all "switches" so that they cannot be accidentally reset
!=============================================================================

#undef TES_NH3_OBS
#undef PM_ATTAINMENT
#undef SOMO35_ATTAINMENT
#undef SCIA_KNMI_NO2_OBS
#undef IMPROVE_SO4_NIT_OBS
#undef CASTNET_NH4_OBS
#undef TES_O3_OBS
#undef TES_O3_IRK
#undef SCIA_DAL_NO2_OBS
#undef SCIA_DAL_SO2_OBS
#undef SCIA_BRE_CO_OBS
#undef AIRS_CO_OBS
#undef GOSAT_CO2_OBS
#undef PM_ATTAINMENT
#undef SOMO35_ATTAINMNET
#undef PSEUDO_OBS
#undef LOG_OPT
#undef LIDORT
#undef LBKCOV_ERR
! (xxu, dkh, 01/09/12, adj32_011)
#undef MODIS_AOD_OBS
! (yhmao, dkh, 01/13/12, adj32_013)
#undef IMPROVE_BC_OC_OBS
! (zhej, dkh, 01/16/12, adj32_016)
#undef MOPITT_V5_CO_OBS
#undef MOPITT_V6_CO_OBS
! (kjw, dkh, 02/12/12, adj32_023)
#undef TES_CH4_OBS
#undef SCIA_CH4_OBS
#undef MEM_CH4_OBS
#undef LEO_CH4_OBS
#undef GEOCAPE_CH4_OBS
!mkeller
#undef OMI_NO2_OBS
! ( ywang, 04/21/15)
#undef OMI_SO2_OBS

!----------CO observations------
! pick any combination
! => MOPITT CO
!    => MOPITT v5
!    => MOPITT v6
! => AIRS CO
! => SCIA Bremen CO
!#define  MOPITT_V5_CO_OBS 'MOPITT_V5_CO_OBS'
!#define  MOPITT_V6_CO_OBS 'MOPITT_V6_CO_OBS'
!#define  AIRS_CO_OBS     'AIRS_CO_OBS'
!#define  SCIA_BRE_CO_OBS   'SCIA_BRE_CO_OBS'

!---------aerosol-related----------
!NH3 observations
! = > TES_NH3_OBS
!SO2 observations
! => SCIA_DAL_SO2_OBS
!Aerosol observations
! => PM_ATTAINMENT
! => IMPROVE_SO4_NIT_OBS
! => IMPROVE_BC_OC_OBS
! => CASTNET_NH4_OBS
!#define TES_NH3_OBS         'TES_NH3_OBS'
!#define SCIA_DAL_SO2_OBS    'SCIA_DAL_SO2_OBS'
!#define PM_ATTAINMENT       'PM_ATTAINMENT'
!#define IMPROVE_SO4_NIT_OBS 'IMPROVE_SO4_NIT_OBS'
!#define IMPROVE_BC_OC_OBS   'IMPROVE_BC_OC_OBS'
!#define CASTNET_NH4_OBS     'CASTNET_NH4_OBS'
!#define MODIS_AOD_OBS       'MODIS_AOD_OBS'

!--------ozone-related-------------
! => SOMO35_ATTAINMENT
! => TES O3
! => TES O3 IRKs
!#define SOMO35_ATTAINMENT 'SOMO35_ATTAINMENT'
!#define TES_O3_OBS    'TES_O3_OBS'
!#define TES_O3_IRK    'TES_O3_IRK'

!--------CH4 Observations------------
! => TES CH4
! => SCIA CH4
! => MEM CH4
! => Generic LEO instrument CH4
! => GEOCAPE CH4
!#define TES_CH4_OBS         'TES_CH4_OBS'
!#define SCIA_CH4_OBS        'SCIA_CH4_OBS'
!#define MEM_CH4_OBS         'MEM_CH4_OBS'
!#define LEO_CH4_OBS         'LEO_CH4_OBS'
!#define GEOCAPE_CH4_OBS     'GEOCAPE_CH4_OBS'

!-------NO2 observations------------
! => SCIA_KNMI_NO2_OBS
! => SCIA_DAL_NO2_OBS
!#define SCIA_KNMI_NO2_OBS   'SCIA_KNMI_NO2_OBS'
!#define SCIA_DAL_NO2_OBS    'SCIA_DAL_NO2_OBS'

!-------OMI NO2 tropospheric columns
!#define OMI_NO2_OBS 'OMI_NO2_OBS'

!-------CO2 observations------------
! => GOSAT_CO2_OBS
!#define GOSAT_CO2_OBS

!-------SO2 observations------------
! => OMI_SO2_OBS
!#define OMI_SO2_OBS         'OMI_SO2_OBS'

!------other options-----------------
!#define PSEUDO_OBS    'PSEUDO_OBS'
!#define LOG_OPT       'LOG_OPT'
!#define LIDORT        'LIDORT'
!#define LBFGS_INV     'LBFGS_INV'
!#define LBKCOV_ERR    'LBKCOV_ERR'
```

5. Examples

a. Inverse Modeling

Test if we can correct an error in anthro NO_x emissions using "observations" of O_x

- First generate a set of "observations" of O_x using base case (scaling factors = 1) NO_x emissions.

- Inversion begins with initial guess of NO_x emission = 1.5 * base NO_x emissions

- All other emissions assumed to be correct (so only optimize anthro NO_x emissions)

- Inversion uses Ox observations in every grid cell, at every hour, over the course of 1 day (so it better work!).

- Use the adjoint model to complete 10 iterations -- check to see if NO_x emission scaling factors converge to 1.0

- Full chemistry, geos5, 4x5

b. Sensitivity Test

Sensitivity of Ox with respect to NOx using initial conditions. See how much Ox changes with changes in NOx emissions.

- Sensitivity of Ox in level 1 at hour 6 with respect to NOx initial conditions in level 1

- geos5, 4x5

- full chemistry

C. Finite Difference

Compare adjoint sensitivities to sensitivities calculated using finite differences in each column of the model (horizontal transport off)

- Sensitivity of Ox in level 1 at hour 6 with respect to NOx initial conditions in level 1

- geos5, 4x5

- full chemistry

This is a standard test we do for every model version to benchmark code, see the google spreadsheet
https://docs.google.com/spreadsheet/ccc?key=0As2MewHKyWpDdDlTeFdPanU2RzlWc0luaFpEQXlyclE#gid=0

6. Useful GIT commands:

Initial download:

```
git clone git@adjoint.colorado.edu:yanko.davila/gcadj_std.git
```

Status of project vs the current repository:

```
git status
```

Check difference of files (differences have colors for easy reading)

```
git diff --color <wildcard> [<wildcard>] <path>/foo_mod.f
```

Checkout specific version

```
git checkout <wildcard>
```

Replacing a file with the newest version from the repository:

```
git checkout origin/master -- <path>/foo_mod.f
```

Merging changes in a file:

```
git merge -m <wildcard>
```

Comitting

```
git commit -a
```

Tagging a version

```
git tag -a TAGNAME
```

Deleting a tag

```
git tag -d TAGNAME
git push origin :refs/tags/TAGNAME
```

List the history of a file:

```
git log -- <path>/foo_mod.f
```

Add a file to the repository

```
git add <file_name>
```

Delete a file from the repository

```
git rm <file_name>
```

There are several wildcards that you can use on git for example:
"origin/master" - Latest version on the repository
"HEAD" - Latest version as of your last download
"v33i" - Specific TAG, find all tag names on GitLab or by typing " git tag "
"32d5c926e" - Specific COMMIT, find all commit numbers on GitLab