Assimilating Tropospheric Emission Spectrometer profiles in GEOS-Chem

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Motivation

Adjoint models are powerful tools widely used in meteorology and oceanography for applications

- data assimilation
- model tuning
- sensitivity analysis
- determination of singular vectors

GEOS-Chem Adjoint (GCv7_ADJ)

- Created an adjoint model of geos-4 v7 of GEOS-Chem
  - Tested each science process adjoint separately
  - Consistency check after integrating all processes together
  - Completely parallelized adjoint code
- Added 4-D variational data assimilation and sensitivity analysis capabilities
- Provided with choices of operations to choose from as per the need, plug-n-play functions for cost function calculations
- Adjoint code quite similar to forward mode – same coding convention

Forward and Adjoint Code Flow

Forward Mode	Adjoint Mode
CONVERT_UNITS(kg->vv)	**CALL DO_WETDEP_ADJ**
CALL DO_UPBDFLX	Read_CHEM_CHK(Date,Time) **CALL DO_CHEMISTRY_ADJ** ▪ *Emission, dry deposition handled inside chemistry.*
CALL DO_TRANSPORT	CONVERT_UNITS(vv->kg)
CALL DO_PBL_MIX	Read_CONV_CHK(Date,Time) **CALL DO_CONVECTION_ADJ**
Make_CONV_CHK(Date,Time) **CALL DO_CONVECTION**	**CALL DO_PBL_MIX_ADJ**
CONVERT_UNITS(vv->kg)	**CALL DO_TRANSPORT_ADJ**
CALL DO_DRYDEP CALL DO_EMISSIONS ▪ *Updating emission and dry deposition rates.*	**CALL DO_UPBDFLX_ADJ**
Make_CHEM_CHK(Date,Time) **CALL DO_CHEMISTRY**	CONVERT_UNITS(kg->vv)
CALL DO_WETDEP	

Definitions

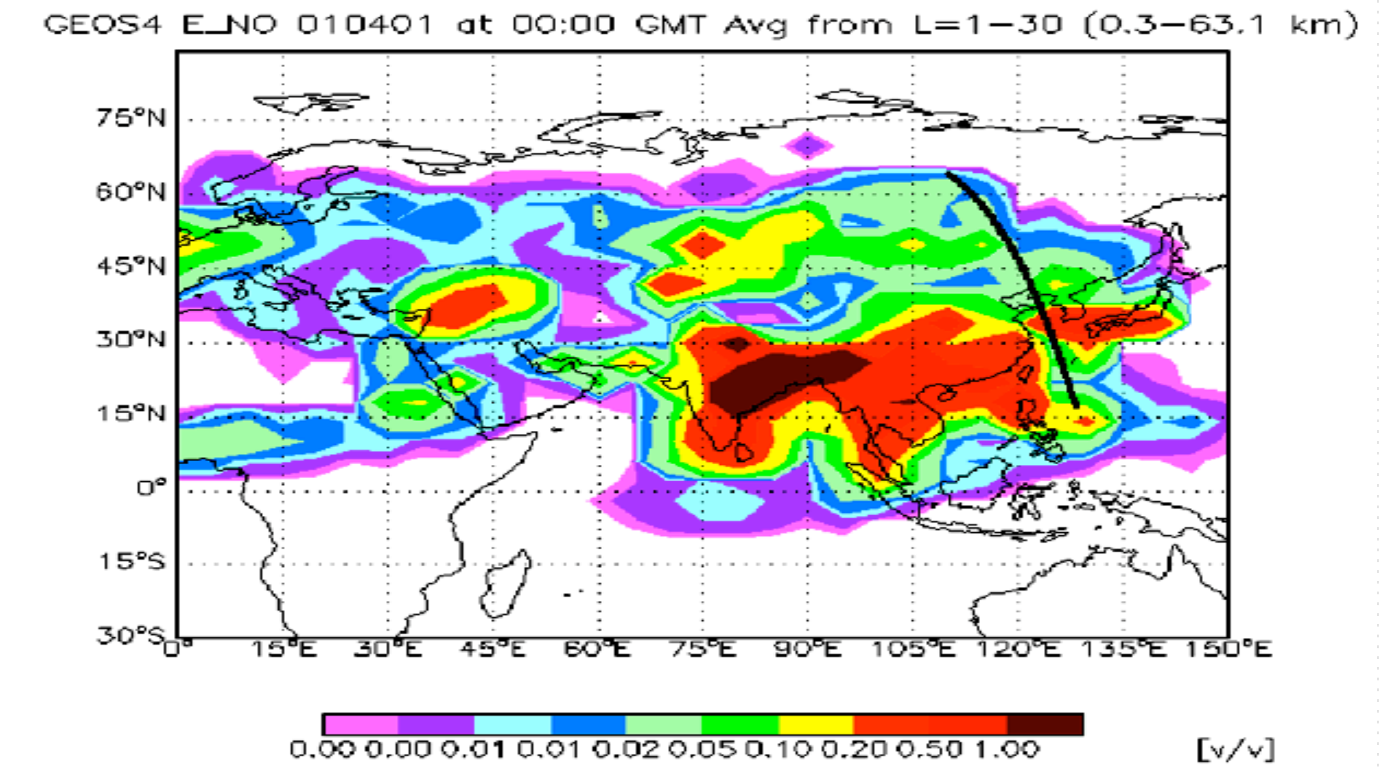
- Sensitivity Analysis

  Adjoint model is efficient in calculating sensitivities of a few output variable or metrics with respect to a large number of (input) parameters

- Data Assimilation

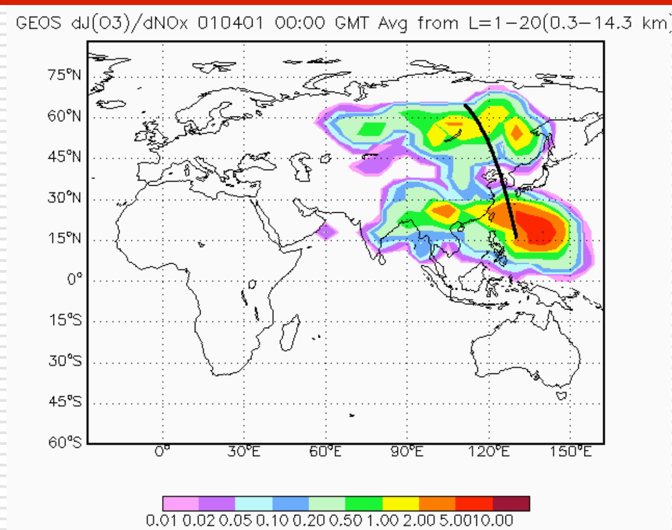
  Variational data assimilation allows the optimal combination of three sources of information: an a priori (background), estimate of the state of the atmosphere, knowledge about the physical and chemical processes

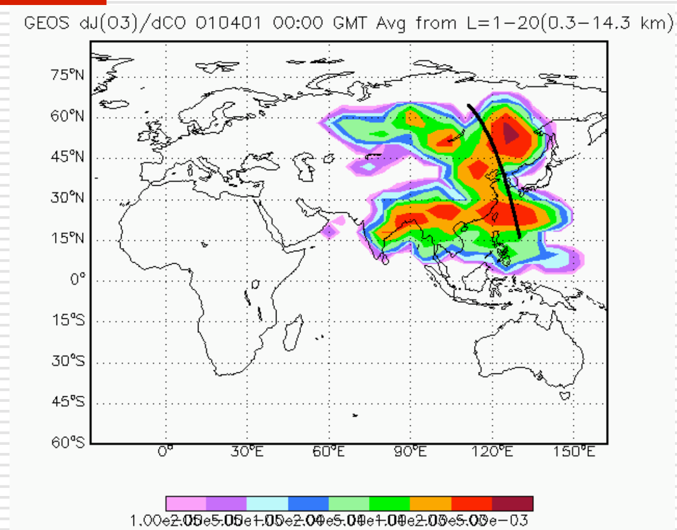
Sensitivity Analysis (emission species)

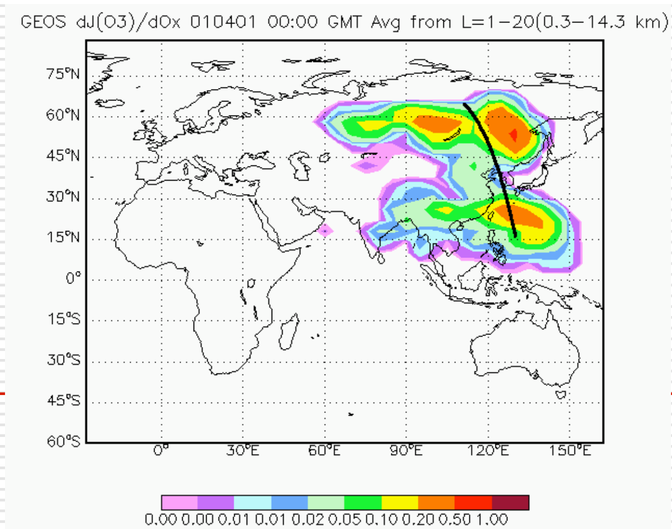


Sensitivity of the O3 column measured by TES with respect to total NOx emissions over Asia on April 1st, 2001

Sensitivity Analysis (tracer concentrations)







4-D Variational Data Assimilation Framework

- At iteration 0, $x_0 = c_p^{\,0}$
- At each subsequent iteration i (i≥1),

  $x_{i+1} \leftarrow$ L-BFGS (x_i, f, g)

  $c_{op}^{\,0} \leftarrow x_{i+1}$

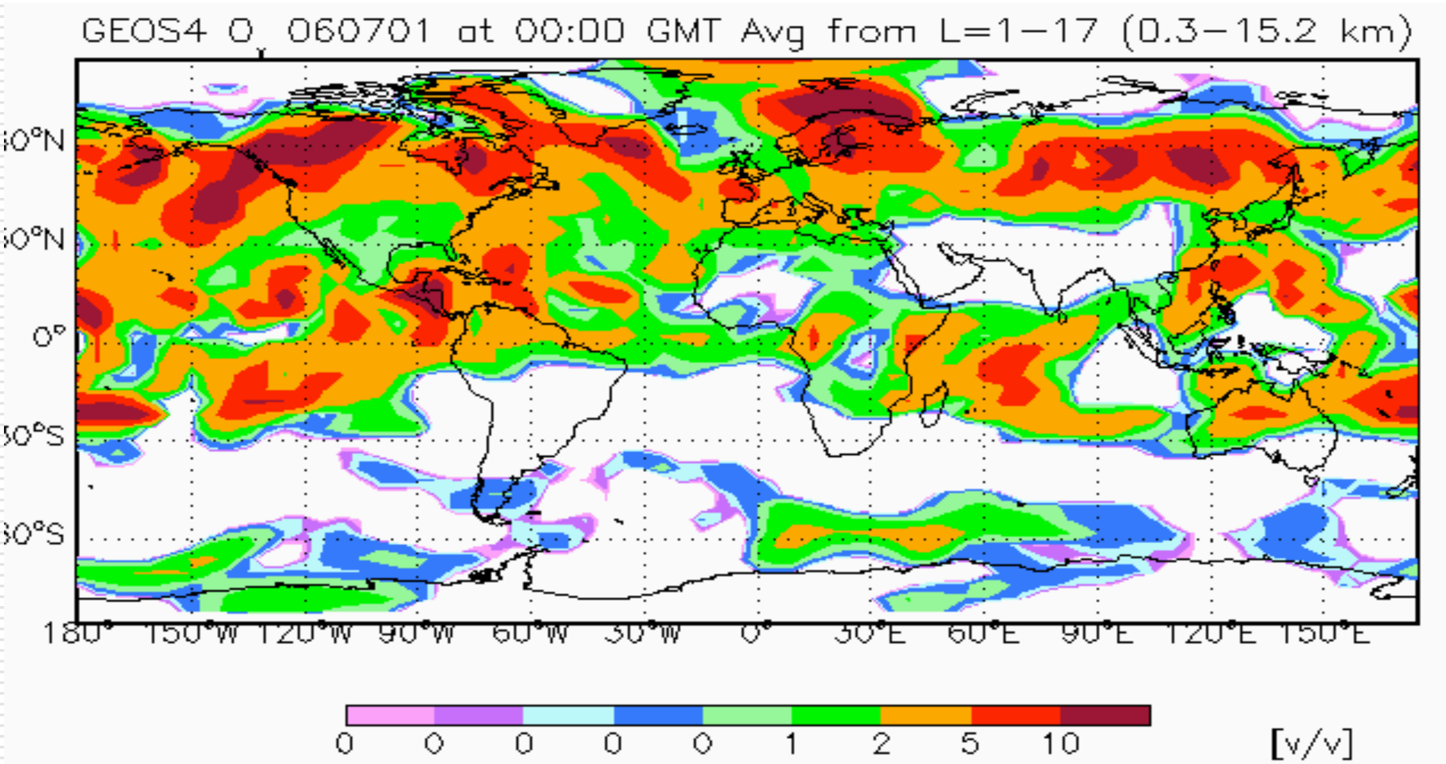
  (f, g) $\leftarrow$ Reverse Mode ($c_{op}^{\,0}$)

  where, f is the cost function and g is the gradient of the cost function.
- In our test case, the cost function and its gradient are defined as:

$$J(x_0) = \frac{1}{2}(x_0 - x_0^B)^T B^{-1}(x_0 - x_0^B) + \frac{1}{2}\sum_{k=1}^{N}(Hx_k - y_k)^T R_k^{-1}(Hx_k - y_k)$$

$$g(x_0) = B^{-1}(x_0 - x_0^B) + \sum_{k=1}^{N} R_k^{-1}(Hx_k - y_k)$$

4-D Variational Data Assimilation



A 4-day animation of plots from difference between background trajectory and analysis trajectory through TES profile retrievals for 2006 summertime GEOS-Chem data

3-D Variational Data Assimilation Framework

- At iteration 0, $x_0 = c_p^{\,0}$
- At each subsequent iteration i (i≥1),

  $x_{i+1} \leftarrow$ L-BFGS (x_i, f, g)

  $c_{op}^{\,0} \leftarrow x_{i+1}$

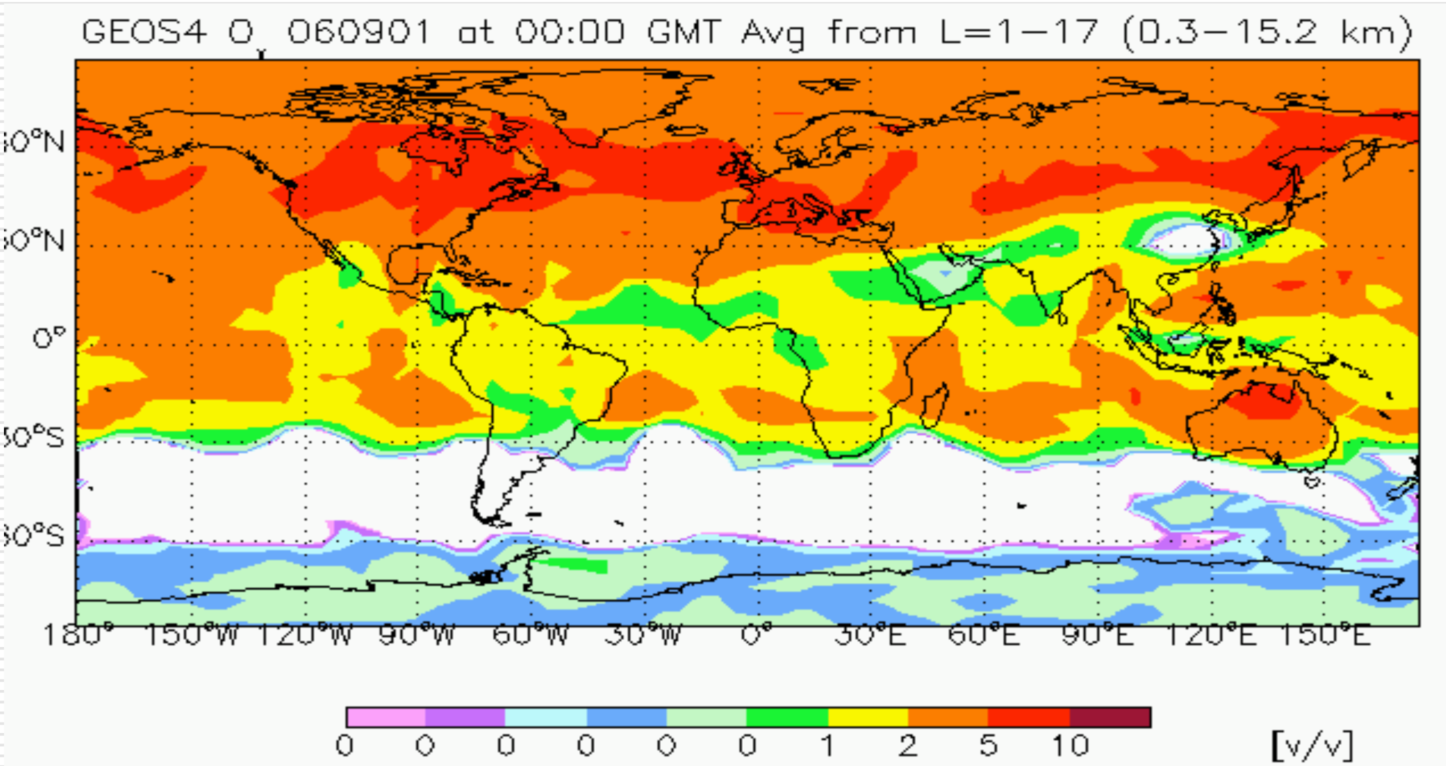
  (f, g) $\leftarrow$ Observation Operator and its adjoint ($c_{op}^{\,0}$)

  where, f is the cost function and g is the gradient of the cost function.
- In our test case, the cost function and its gradient are defined as:

$$J(x_0) = \frac{1}{2}\left(x_0 - x_0^B\right)^T B^{-1}\left(x_0 - x_0^B\right) + \frac{1}{2}\left(Hx_0 - y_0\right)^T R^{-1}\left(Hx_0 - y_0\right)$$

$$g(x_0) = B^{-1}\left(x_0 - x_0^B\right) + R^{-1}\left(Hx_0 - y_0\right)$$

3-D Variational Data Assimilation



A plot of difference between background trajectory and analysis trajectory through TES profile retrievals for 2006 summertime GEOS-Chem data through 3-D variational data assimilation for 2 months with diagonal background error covariance matrix.

Non-Diagonal Background Covariance Matrix

$$\mathbb{B}_0 = \mathbb{C}_{\text{lat}} \otimes \mathbb{C}_{\text{long}}$$

$$\mathbb{C}_{\text{lat}} = \text{correlation in the latitude direction} = \exp -(\tfrac{d_x}{l_x})^2$$

$$\mathbb{C}_{\text{long}} = \text{correlation in the longitude direction} = \exp -(\tfrac{d_y}{l_y})^2$$

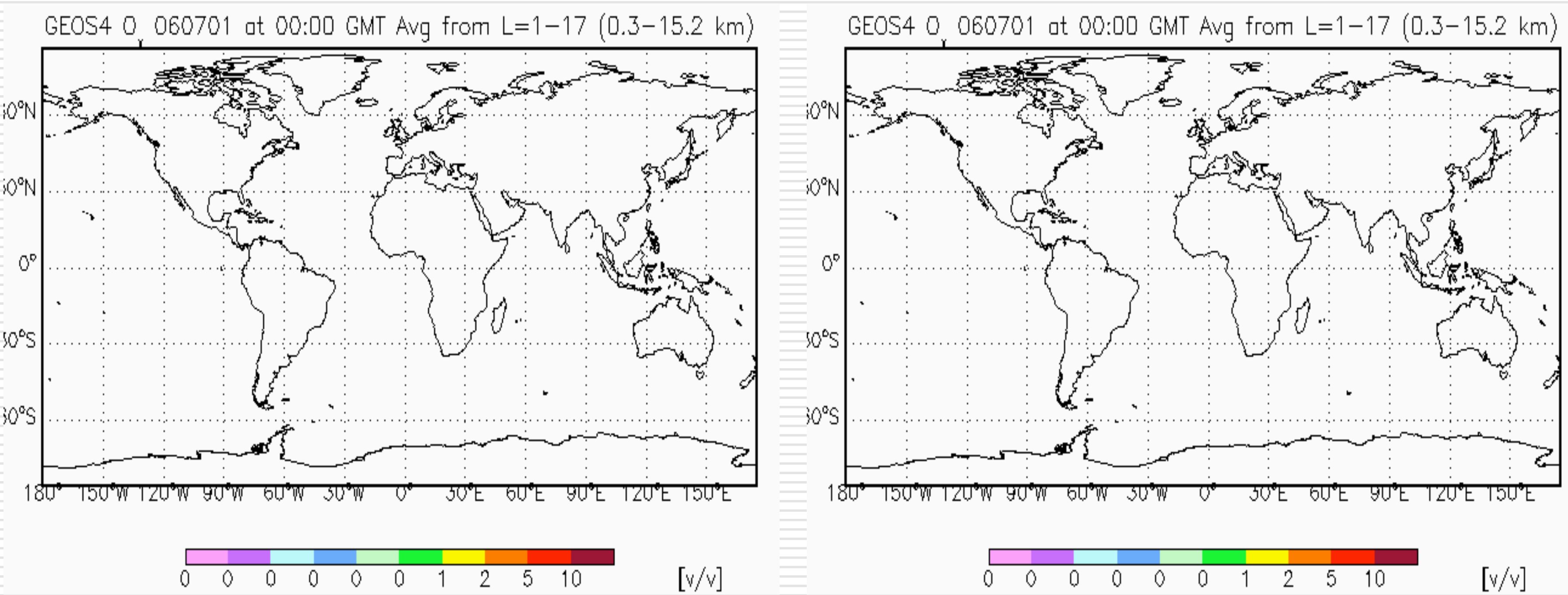
$\mathbb{C}_{\text{lat}} = U_{\text{lat}}\, \Sigma_{\text{lat}}\, U_{\text{lat}}$ SVD of the symmetric $\mathbb{C}_{\text{lat}}$

$\mathbb{C}_{\text{long}} = U_{\text{long}}\, \Sigma_{\text{long}}\, U_{\text{long}}$ SVD of the symmetric $\mathbb{C}_{\text{long}}$

$$\mathbb{B}_0^{-1} = \left[\mathbb{C}_{\text{lat}} \otimes \mathbb{C}_{\text{long}}\right]^{-1} = \left[\mathbb{C}_{\text{lat}}^{-1} \otimes \mathbb{C}_{\text{long}}^{-1}\right] =$$

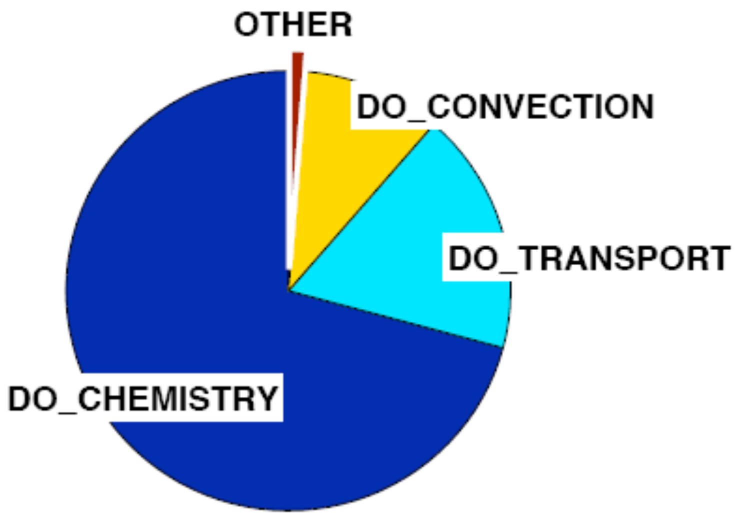
$$\left[U_{\text{lat}}\, \Sigma_{\text{lat}}^{-1}\, U_{\text{lat}}\right] \otimes \left[U_{\text{long}}\, \Sigma_{\text{long}}^{-1}\, U_{\text{long}}\right]$$

3-D Variational Data Assimilation

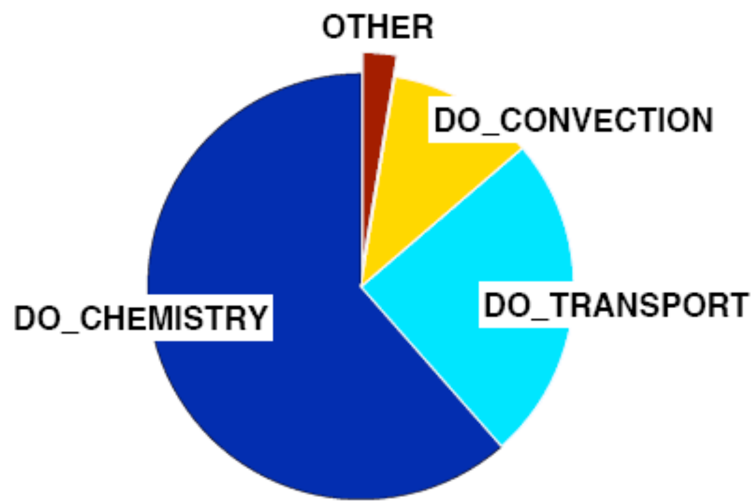


A 3-week animation of plots from difference between model predictions trajectory and assimilated trajectory through TES profile retrievals for 2006 summertime GEOS-Chem data for 3-D variational data assimilation with diagonal(*left*) and non-diagonal (*right*) background covariance.

Time Distribution of GC processes



(a) 1 cpu (12 min 46 sec)



(b) 8 cpus (2 min 7 sec)

GEOS-Chem simulation times on one and on eight cores. The majority of the computational time is spent in three processes: chemistry, transport, and convection.

KPP Chemistry using CUDA

Ironical - Working on improving air quality by running model codes on power hungry architectures

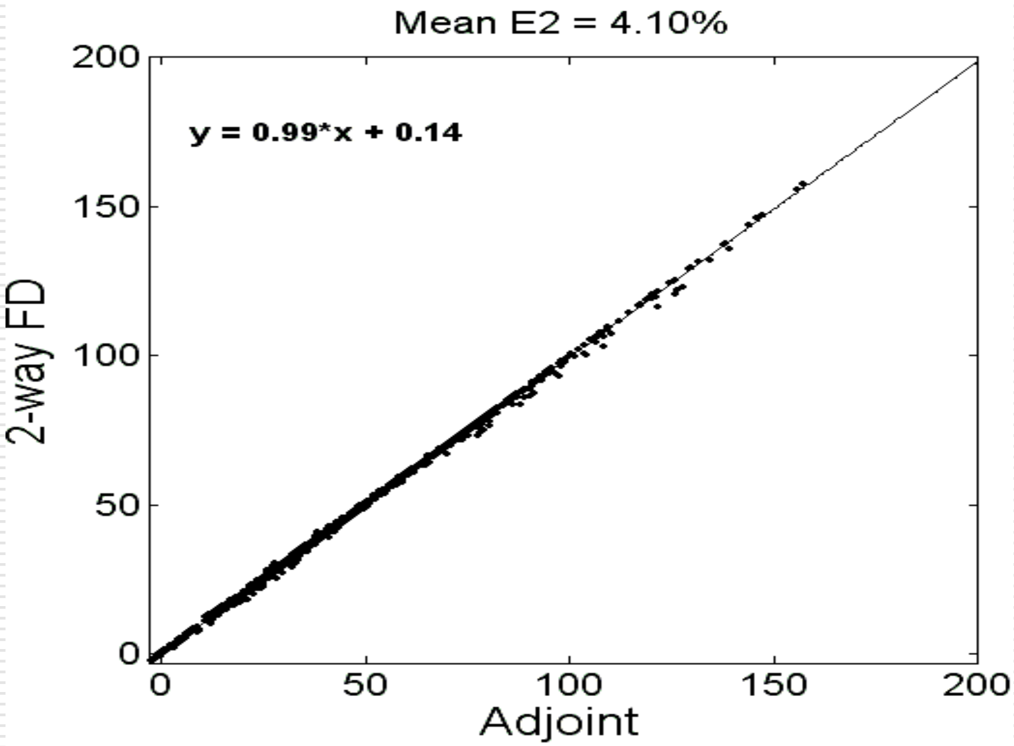
- Successful implementation of double precision CUDA chemistry code
- Achieved 2x speed up as compared to the serial CPU version

Conclusion

- Designed and developed parsers to automatically interface KPP with GEOS-Chem v7
- Developed an adjoint model of GEOS-Chem v7
- Parallelized adjoint code completely
- Added 3-D and 4-D Variational data assimilation, and sensitivity analysis capabilities
- Implemented non-diagonal background error covariance matrix
- Added TES satellite observation operator and its adjoint
- Developed CUDA KPP chemistry for GPGPUs

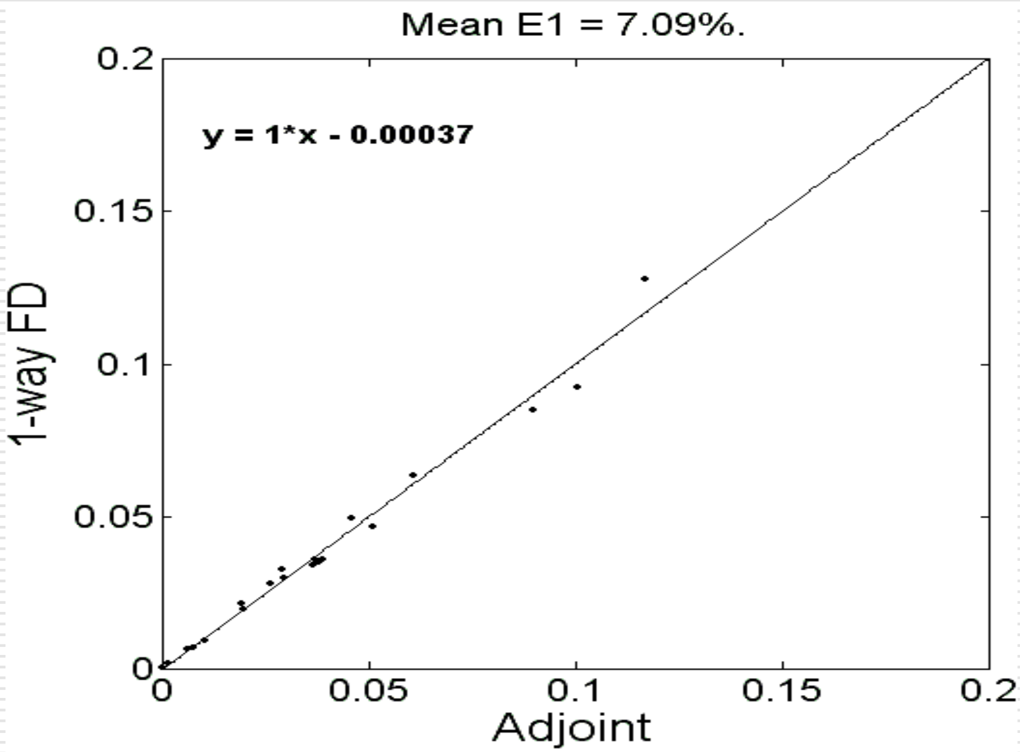
Questions

Validation results



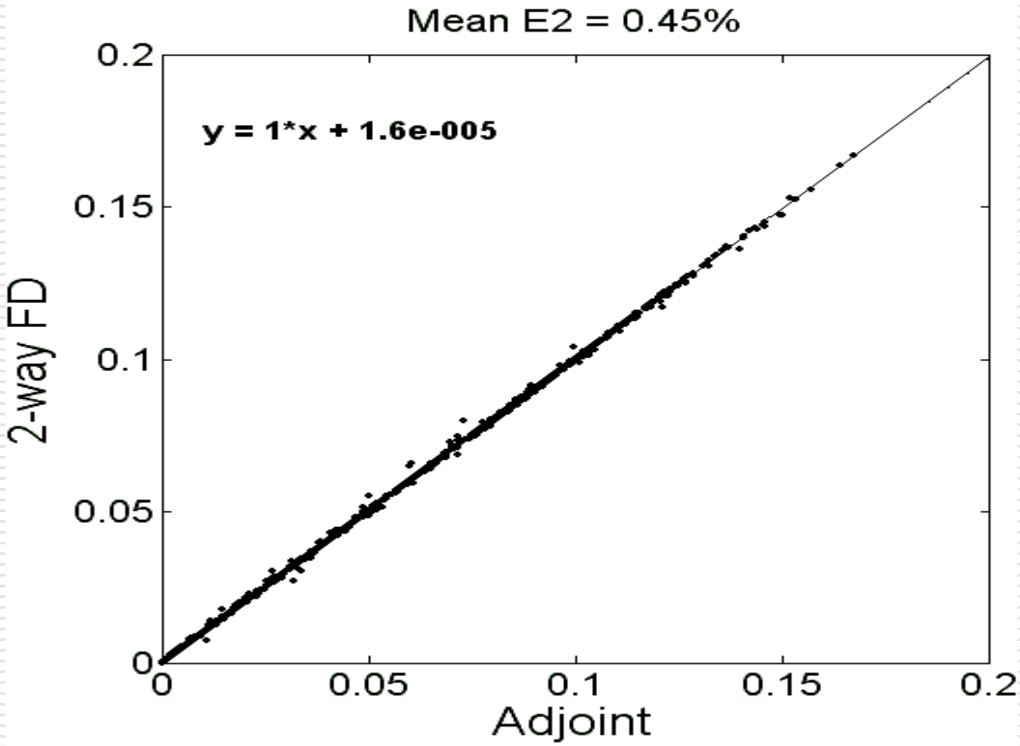
Scattered plot of adjoint vs. central finite difference values over all the grid points, generated by running GEOS-Chem v7 adjoint, **chemistry** only simulation for 6 days from 2001/04/01 to 2001/04/07, for SO4 with respect to NOx concentrations, layer 10

Validation results



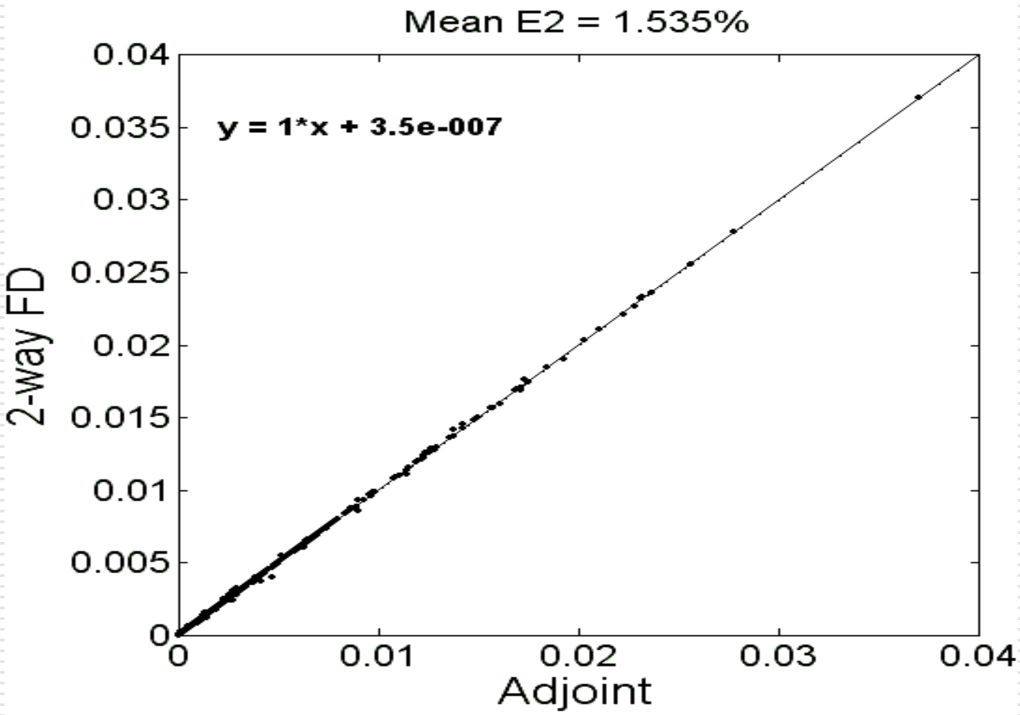
Scattered plot of 1-way finite difference vs. adjoint values generated by running GEOS-Chem v7 adjoint, **advection** only, for 2 days from 2001/07/01:00 to 2001/07/03:00, for NOx concentrations (continuous adjoint).

Validation results



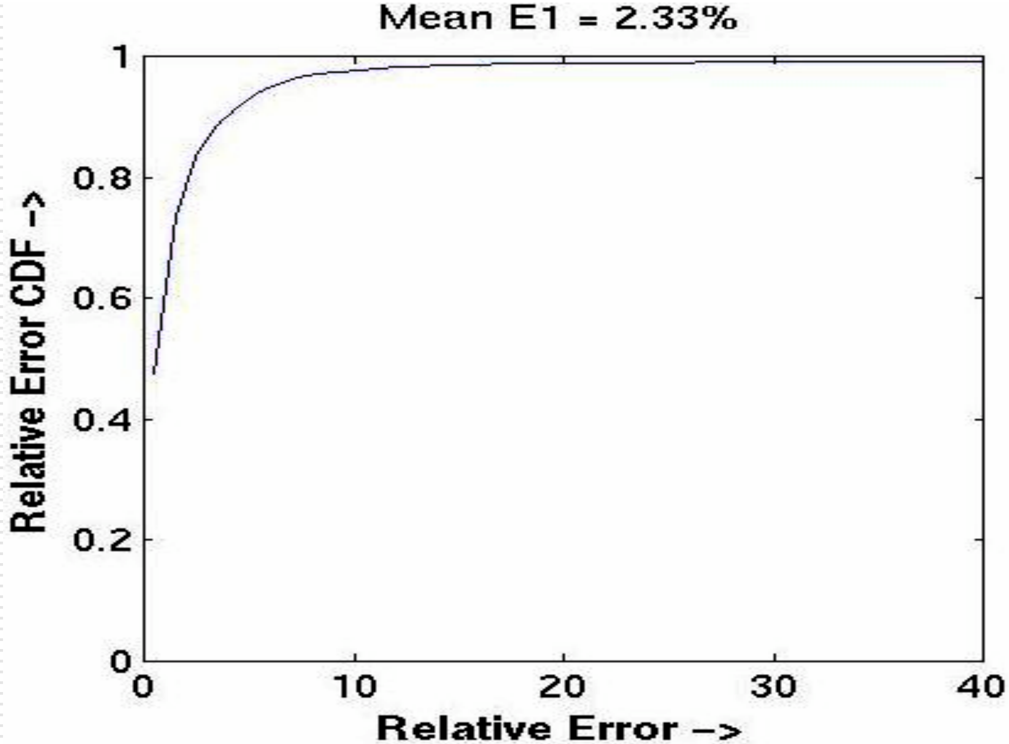
Scattered plot of 2-way finite difference vs. adjoint values generated by running GEOS-Chem v7 adjoint, **convection** only, for 6 days from 2001/07/01 to 2001/07/07, for NOx concentrations. A perturbation was introduced at layer 2 and was tracked at layer 9

Validation results



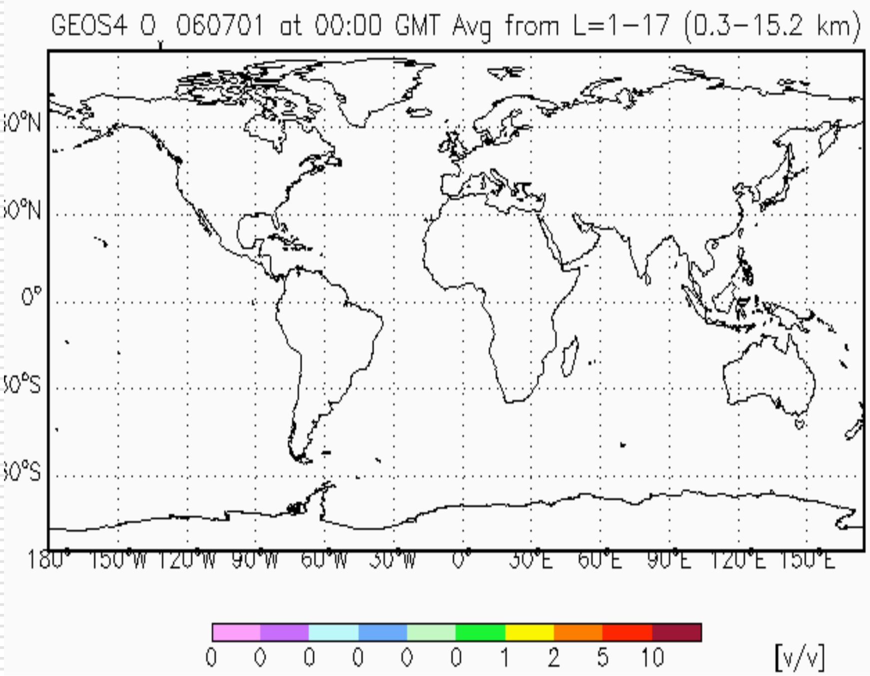
Scattered plot of central finite difference vs. adjoint values generated by running GEOS-Chem v7 adjoint, **wet deposition** only, for one week from 2001/07/01 to 2001/07/08. We consider the wet deposition process acting on H2O2 concentrations. The perturbation was introduced at layer H=9 and measured at layer L=5

Validation results

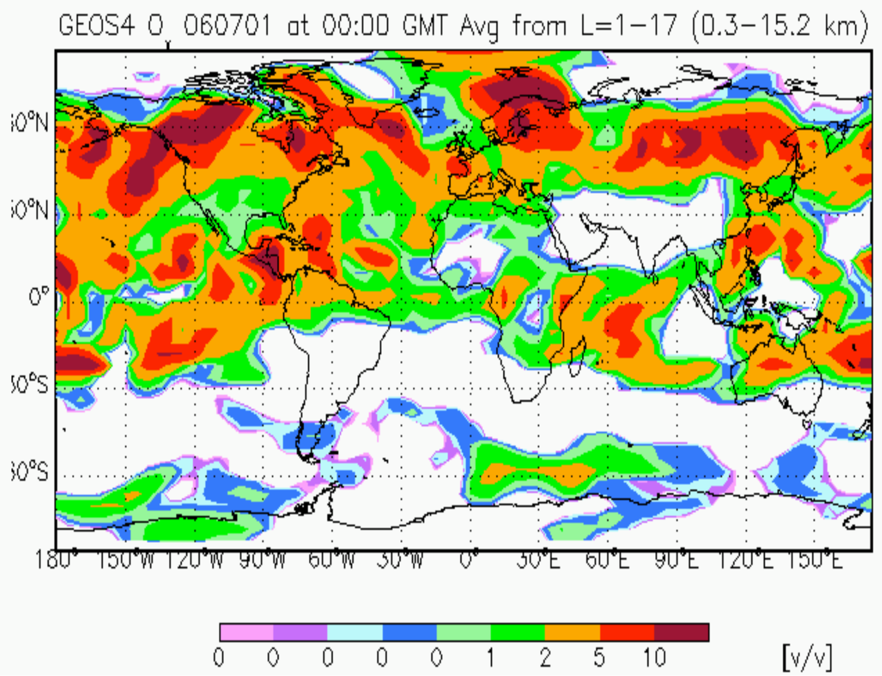


1-way finite difference vs. adjoint relative error cumulative distribution function plot generated by running GEOS-Chem v7 adjoint **emissions/dry-deposition** only, 2 days from 2001/07/01:000000 to 2001/07/03:000000, for changes in Ox concentrations with respect to NOx emissions

4-D Variational Data Assimilation

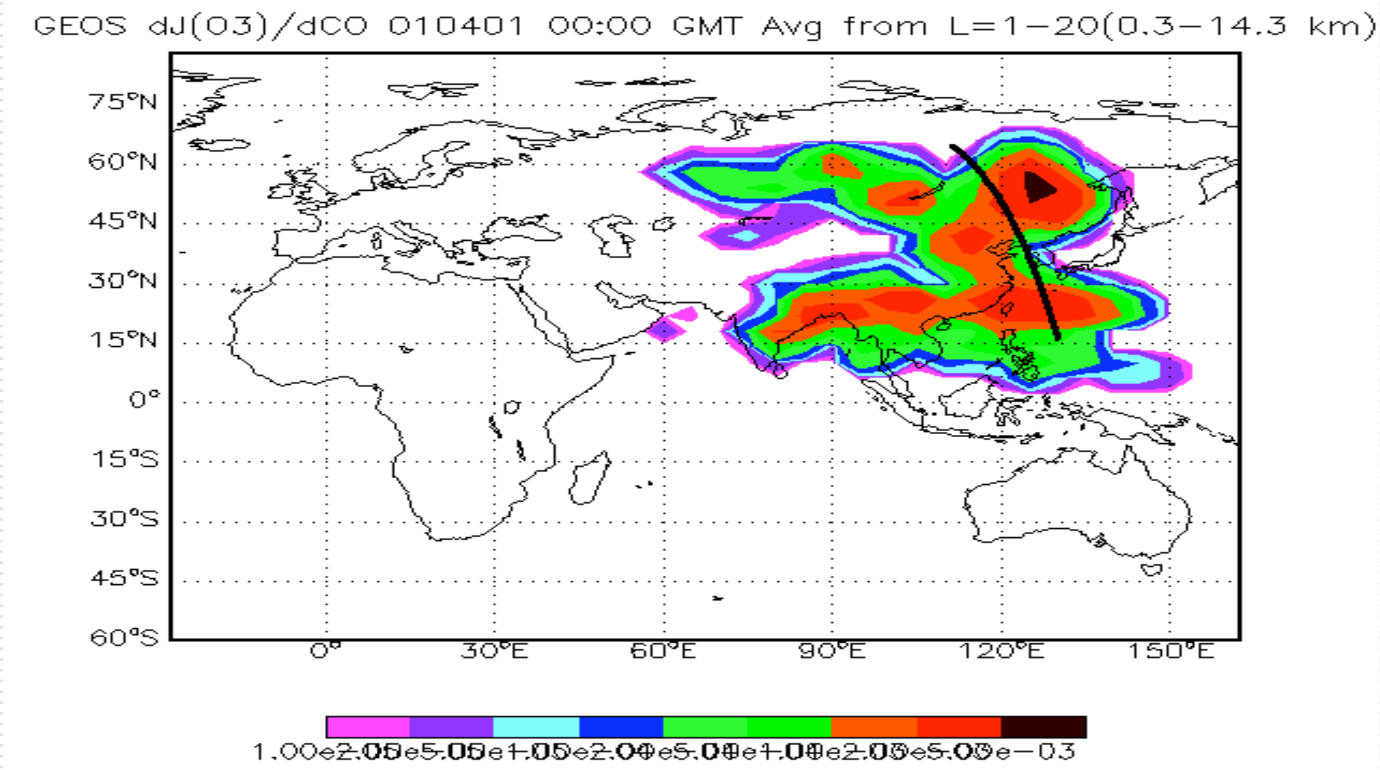


Difference between initial guess and background concentration ($c_p^0 - c_0^0$)



Difference between analysis and background concentration ($c_{op}^0 - c_0^0$)

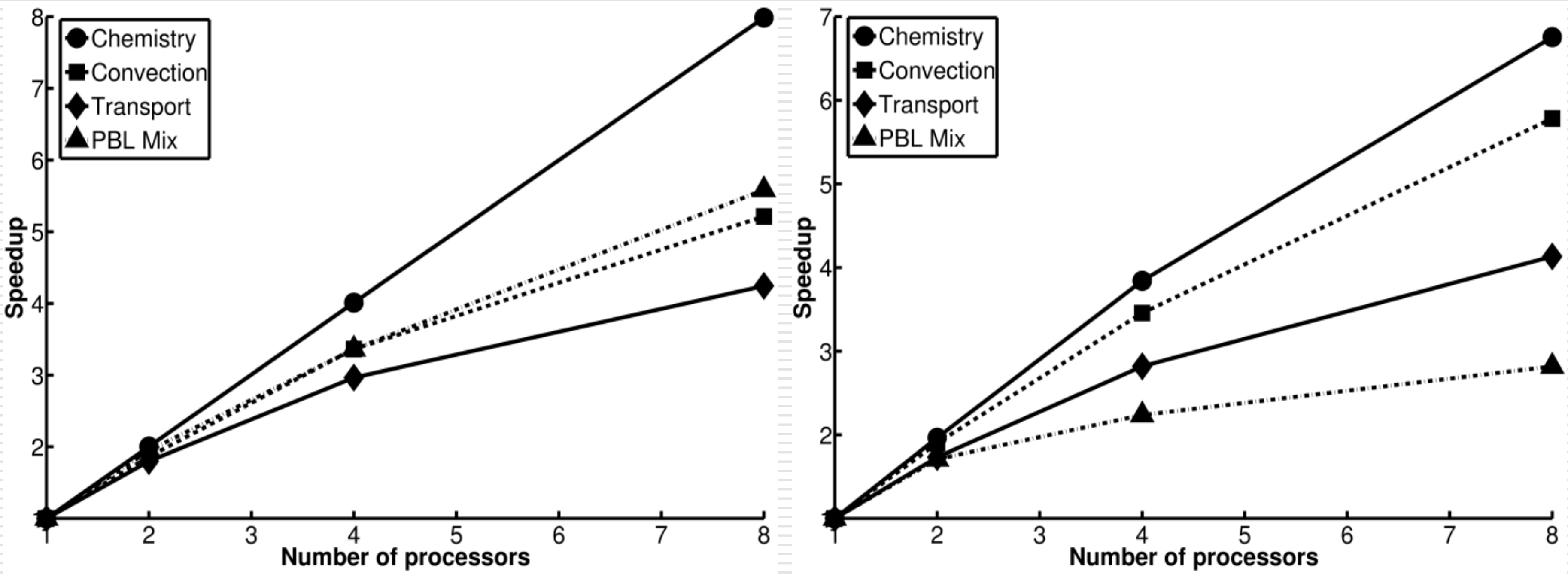
Sensitivity Analysis (emission species)



Sensitivity of the O3 column measured by TES with respect to the CO over Asia on April 1st, 2001

VirginiaTech Invent the Future

Adjoint Model Speed-up Graphs



Speedup graphs for chemistry, convection, advection and planetary boundary mixing subroutines in forward(*left*) and adjoint(*right*) mode on 1, 2, 4 and 8 processors. The simulation window for this analysis was 24 hours performed on July 2001 GEOS-Chem data