Comparisons of Chemical Mechanisms



Climate-Chemistry
Working Group Meeting
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Goals and Questions

HUMAN HEALTH AND AIR QUALITY SCIENTIFIC QUESTIONS:

What is the impact of the choice of <u>resolution</u> on the determination of human health impacts?

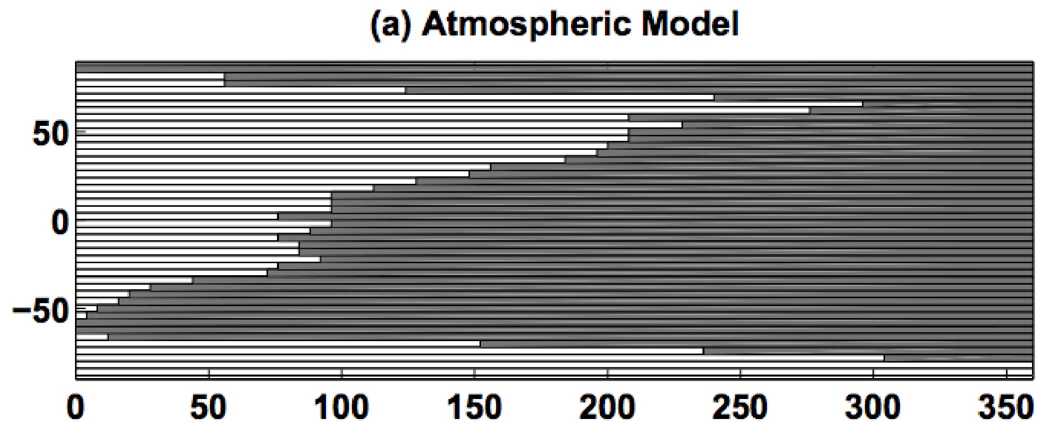
What is the impact of the choice of <u>chemical mechanism</u> on the determination of human health impacts?

MODEL UNCERTAINTIES

What is the impact of:
spatial and temporal resolution,
meteorology,
chemical mechanism, and model
on the quality of the simulated atmosphere and chemistry?

What leads to a sufficient climate-chemistry simulation (including uncertainties)?

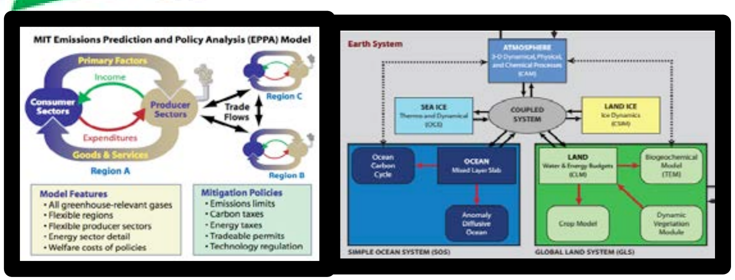
Efficiency vs. Sufficiency



Wang et al. (1998)

Table 1. Gaseous Phase Chemical Reactions Includ

Number	Reaction
(R1)	$O_3 + h\nu \rightarrow O(^1D) + O_2$
(R2)	$O(^1D) + H_2O \rightarrow 2OH$
(R3)	$O(^1D) + N_2 \rightarrow O + N_2$
(R4)	$O(^1D) + O_2 \rightarrow O + O_2$
(R5)	$CO + OH \rightarrow H + CO_2$
(R6)	$H + O_2 + M \rightarrow HO_2 + M$
(R7)	$HO_2 + NO \rightarrow OH + NO_2$
(R8)	$NO_2 + h\nu \rightarrow NO + O$
(R9)	$O + O_2 + M \rightarrow O_3 + M$
(R10)	$HO_2 + O_3 \rightarrow OH + 2O_2$
(R11)	$OH + O_3 \rightarrow HO_2 + O_2$
(R12)	$NO + O_3 \rightarrow NO_2 + O_2$
(R13)	$NO_2 + OH + M \rightarrow HNO_3 + M$
(R14)	$NO_2 + O_3 \rightarrow NO_3 + O_2$
(R15)	$NO_3 + NO_2 + M \rightarrow N_2O_5 + M$
(R16)	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$
(R17)	$H_2O_2 + h\nu \rightarrow 2OH$
(R18)	$H_2O_2 + OH \rightarrow HO_2 + H_2O$
(R19)	$HO + HO_2 \rightarrow H_2O + O_2$
(R20)	$HO + HO \rightarrow H_2O + O$
(R21)	$HO + HO + M \rightarrow H_2O_2 + M$
(R22)	$CH_4 + OH \rightarrow CH_3 + H_2O$
(R23)	$CH_3 + O_2 + M \rightarrow CH_3O_2 + M$
(R24)	$CH_3O_2 + NO \rightarrow CH_3O + NO_2$
(R25)	$CH_3O + O_2 \rightarrow CH_2O + HO_2$
(R26)	$CH_3O_2 + HO_2 \rightarrow CH_3O_2H + O_2$
(R27)	$CH_3O_2H + h\nu \rightarrow CH_3O + OH$
(R28)	$CH_3O_2H + OH \rightarrow CH_3O_2 + H_2O$
(R29)	$CH_2O + h\nu \rightarrow CHO + H$
(R30)	$CH_2O + OH \rightarrow CHO + H_2O$
(R31)	$CHO + O_2 \rightarrow CO + HO_2$
(R32)	$SO_2 + OH + M \rightarrow HOSO_2 + M$
(R33)	$HOSO_2 + O_2 \rightarrow HO_2 + SO_3$
(R34)	$SO_3 + H_2O \rightarrow H_2SO_4$
(R35)	$CFCl_3 + O(^1D) \rightarrow$ products
(R36)	$CFCl_3 + h\nu \rightarrow$ products
(R37)	$CF_2Cl_2 + O(^1D) \rightarrow$ products
(R38)	$CF_2Cl_2 + h\nu \rightarrow$ products
(R39)	$N_2O + h\nu \rightarrow N_2 + O(^1D)$
(R40)	$N_2O + O(^1D) \rightarrow 2NO$
(R41)	$N_2O + O(^1D) \rightarrow N_2 + O_2$

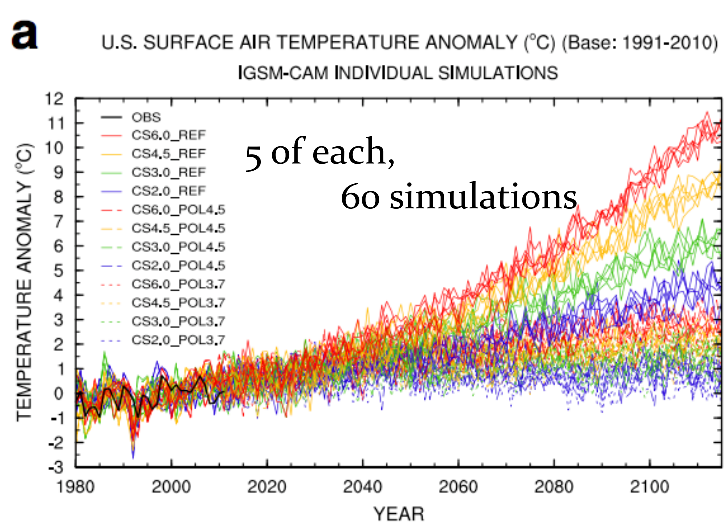


IGSM-CAM

Emissions
Meteorology

Aerosol Forcing
Ocean Heat Diffusion
Climate Sensitivities

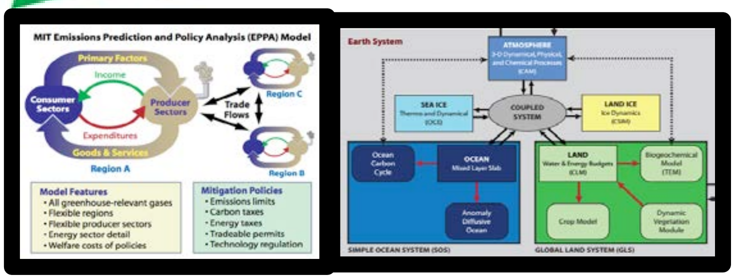
Initial Conditions

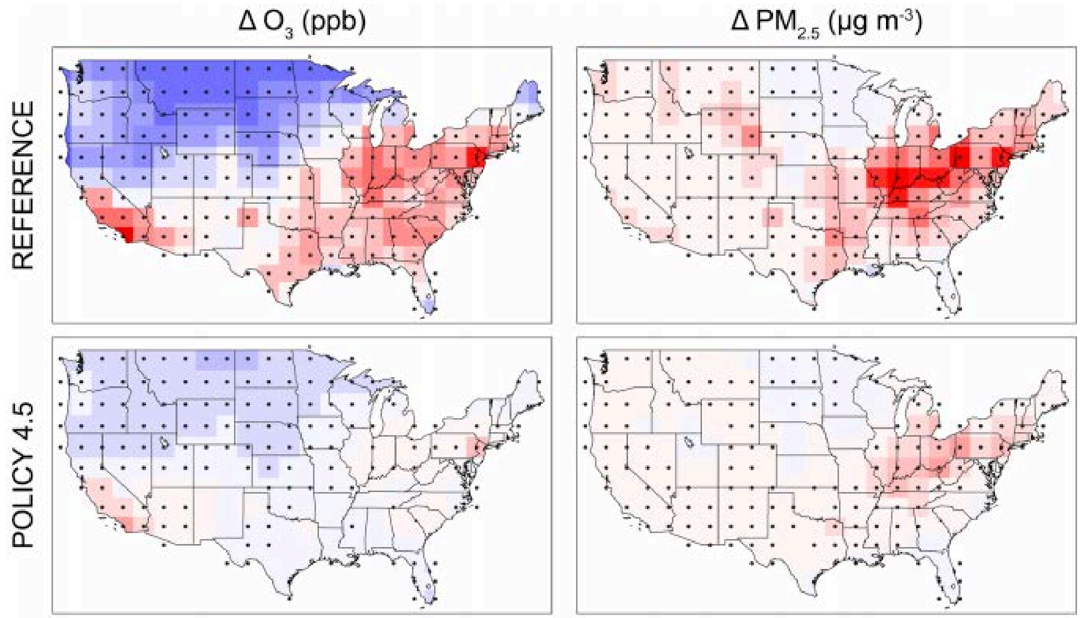


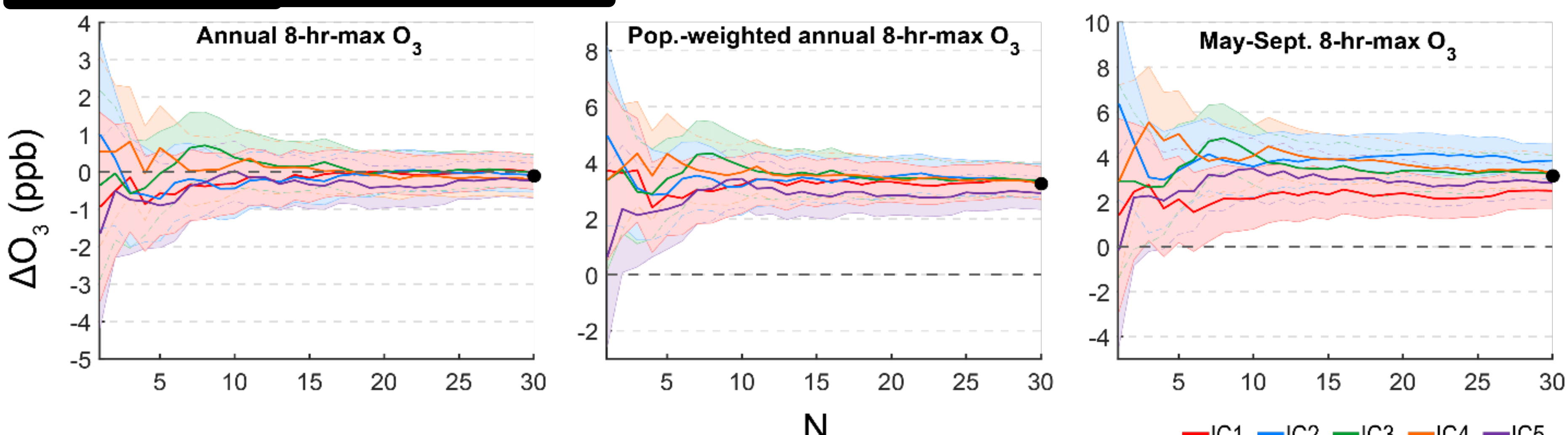
Monier et al. (2015)

Efficiency vs. Sufficiency Considering Uncertainty

Garcia-Mendendez et al. (2015)







Fernando Garcia-Menendez, Manuscript in Preparation, Do Not Cite

My work:
Climate-Chemistry Uncertainties

How do we add {some amount of} chemical complexity to the IGSM-CAM framework to address human health and air quality questions without compromising {too much} efficiency?

$$ccamchem\_off\_pd\_\begin{Bmatrix} T31 \\ 4x5 \\ 1.9x2.5 \end{Bmatrix}\_\begin{Bmatrix} GEOS5 \\ IGSM-CAM \end{Bmatrix}\_\begin{Bmatrix} trop\_mozart \\ trop\_moz\_MAM3 \\ trop\_BAM \\ \text{sup}er\_fast\_MAM3 \\ \text{sup}er\_fast\_BAM \end{Bmatrix}$$

$$geoschem\_off\_pd\_\begin{Bmatrix} 4x5 \\ 2x2.5 \\ 4x5_{(0.5x0.67)} \\ 4x5_{(0.25x0.31)} \end{Bmatrix}\_\begin{Bmatrix} GEOS5 \\ IGSM-CAM \end{Bmatrix}\_tropchem$$

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Also fast mechanism from Houweling et al. (1998)

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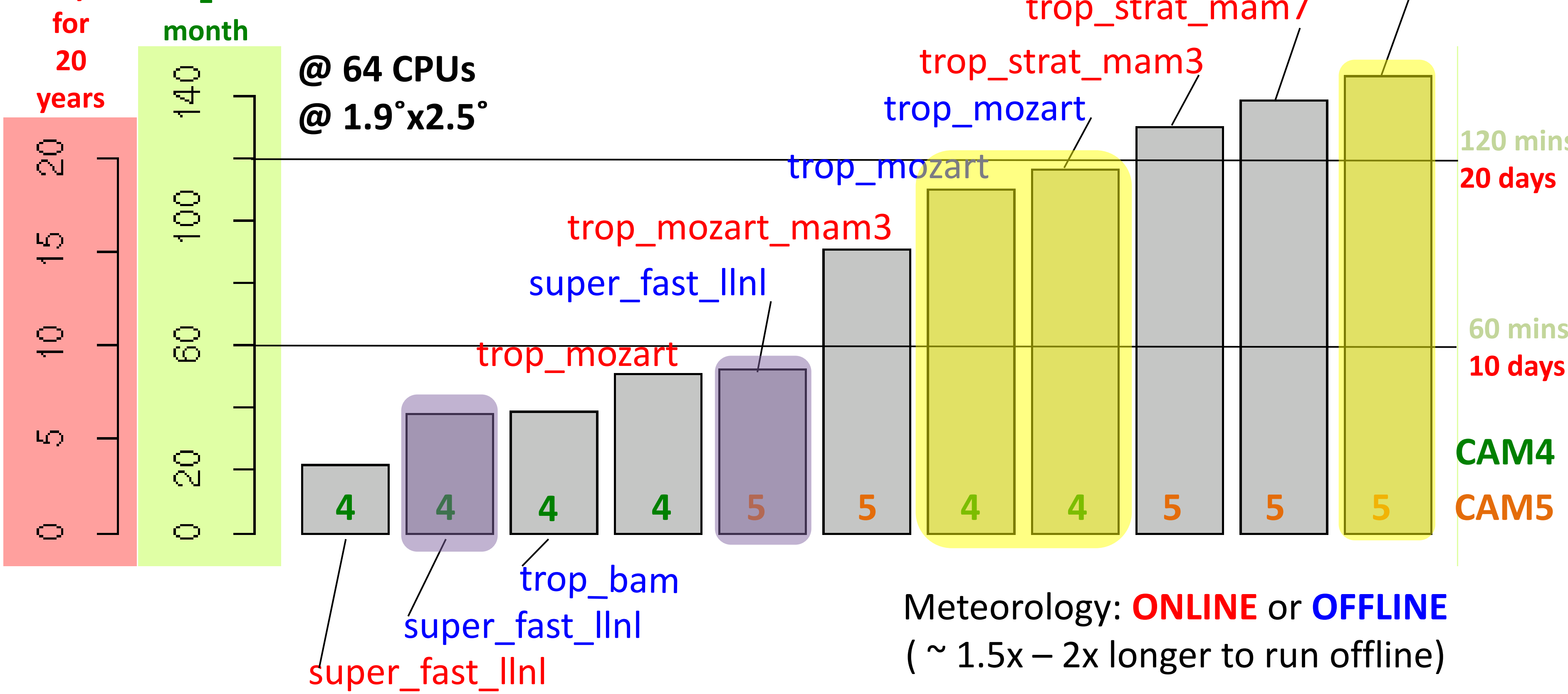
Benchmarking

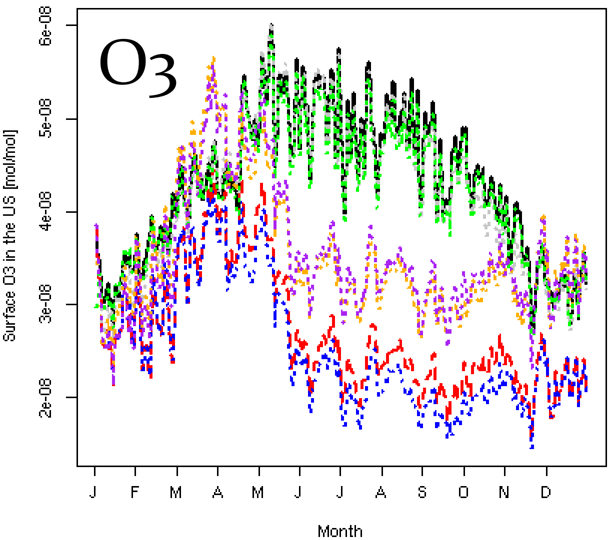


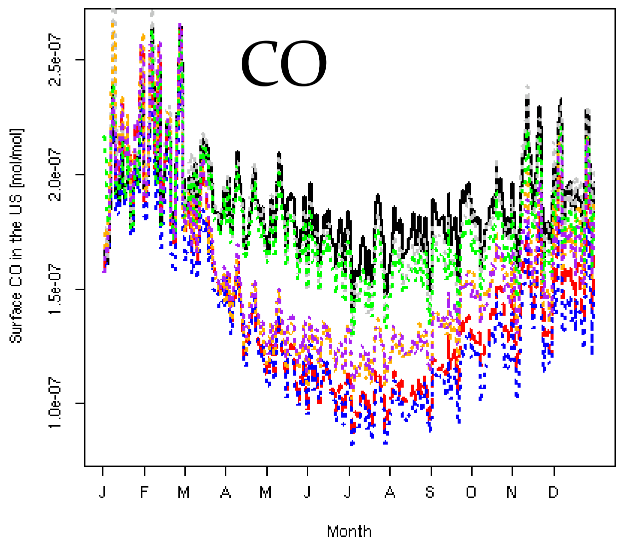
BIG DISCLAIMER: I haven't checked or optimized these simulations at all
I'm trying to get a feel for them, and a feel for the simulation length

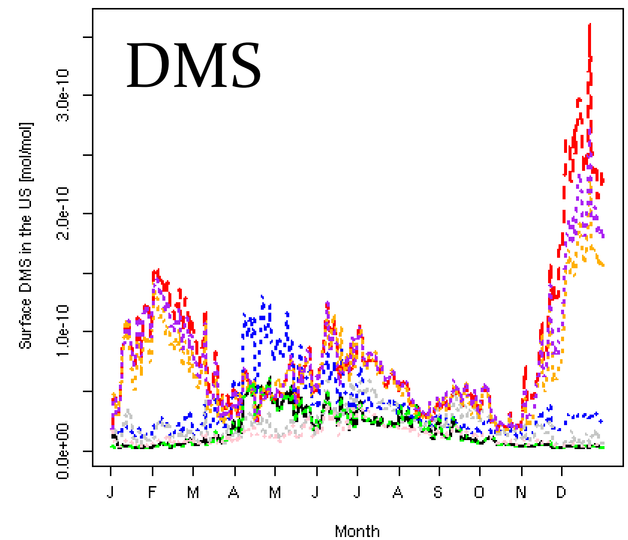
Comparison to GEOS-Chem: offline IGSM-CAM meteorology with trop_chem

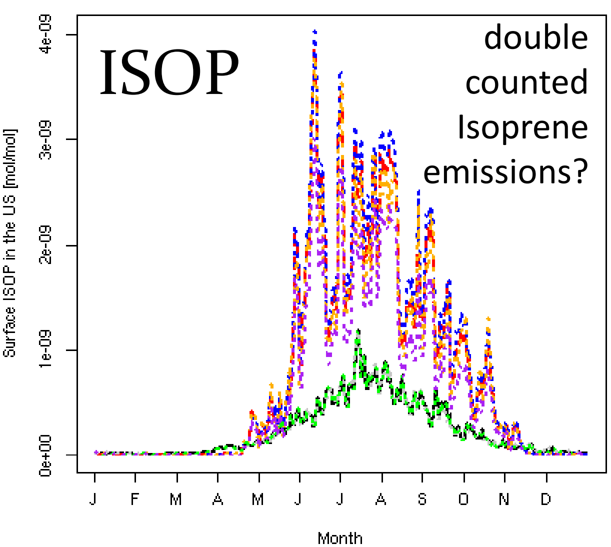
Ideal for IGSM Framework → Ensembles of Simulations, Offline Meteorology

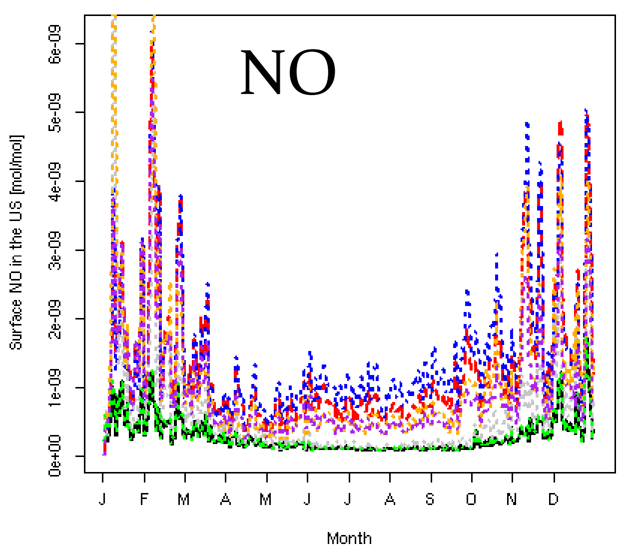
Chemistry Comparisons (**Preliminary**)
Ultimate Focus: O3 and PM Air Quality

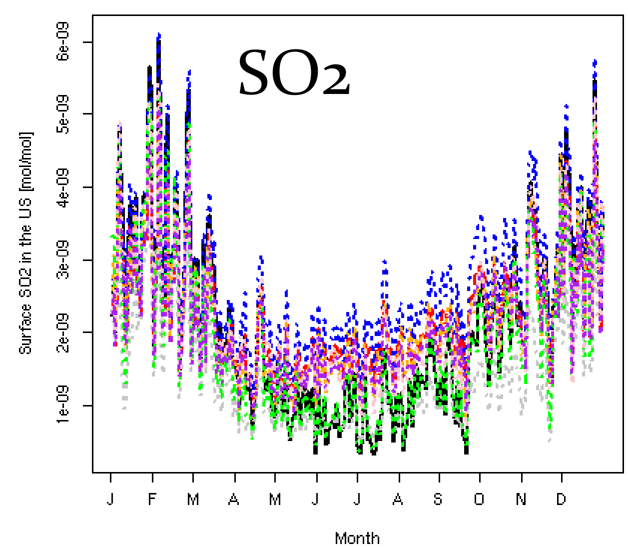








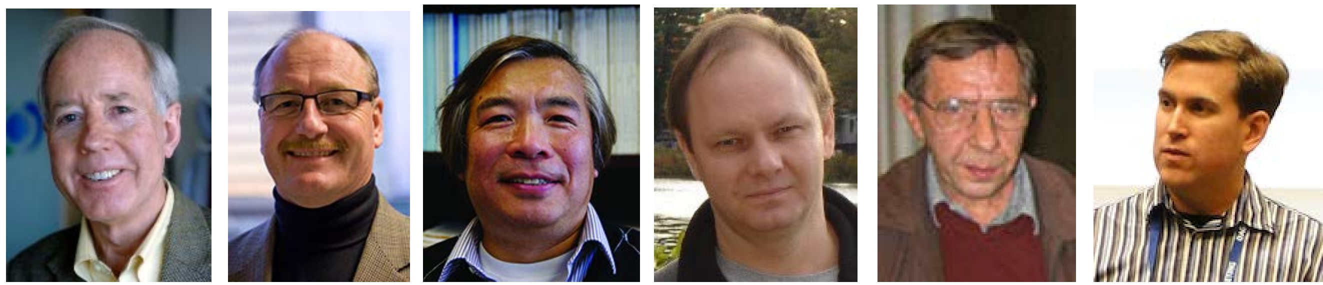




Next Steps

- This week: Perform Sanity Tests:
  - Using superfast chemistry for regional air quality?
  - Using full chemistry in an ensemble framework?
- This month: ensure and document consistency between configurations, try to isolate the parts we're interested in
- And beyond: Test runs to slim down the set of simulations to something more reasonable
- Run simulations, get results

Thanks!



IGSM

Wang, C., R.G. Prinn and A.P. Sokolov. A global interactive chemistry and climate model: Formulation and testing. Journal of Geophysical Research, 103(D3): 3399-3417, 1998.

Prinn, R.G., H.D. Jacoby, A.P. Sokolov, C. Wang, X. Xiao, Z. Yang, R.S. Eckaus, P.H. Stone, A.D.Ellerman, J.M. Melillo, J. Fitzmaurice, D. Kicklighter, G. Holian and Y. Liu. Integrated global system model (IGSM) for climate policy assessment: Feedbacks and sensitivity studies. Climatic Change, 41(3): 469-549, 1999.

Reilly, J., S. Paltsev, K. Strzepek, N. Selin, Y. Cai, K.-M. Nam, E. Monier, S. Dutkiewicz, J. Scott, M. Webster and A. Sokolov. Valuing Climate Impacts in Integrated Assessment Models: The MIT IGSM. Climatic Change, 2012.

IGSM-CAM

Monier, E., J.R. Scott, A.P. Sokolov, C.E. Forest and C.A. Schlosser. An integrated assessment modeling framework for uncertainty studies in global and regional climate change: the MIT IGSM-CAM (version 1.0). Geoscientific Model Development, 6: 2063–2085, 2013

Garcia-Menendez, F., R.K. Saari, E. Monier, and N.E. Selin. U.S. Air Quality and Health Benefits from Avoided Climate Change under Greenhouse Gas Mitigation. Environmental Science & Technology, 49(13): 7580–7588, 2015

Garcia-Menendez, F. et al. (in preparation)