UNIVERSITY of HOUSTON

IMAQS

Linking CMAQ with GEOS-CHEM

Daewon W. Byun, Nankyoung Moon

Institute for Multidimensional Air Quality Studies (IMAQS)

University of Houston

Daniel Jacob, Rokjin Park

Harvard University

Regional Air Quality Model requires prescription of IC/BCs

- Current usage; mostly rely on "climatological" fixed profiles

- Could be different at each sides of domain reflecting certain regional differences

- Works best when outside the boundaries of the domain does not have much direct emissions and no high concentration blobs already existing

- Need to study sensitivity of the model simulations to the different IC/BCs

- In reality fixed profiles are never accurate

Harvard/NASA GEOS-CHEM global model

(Goddard Earth Observing System-CHEMisrty)

This is a global 3-D model of atmospheric chemistry driven by assimilated meteorological observations from the Goddard Earth Observing System (GEOS) of the NASA Data Assimilation Office (DAO).

It is being developed by groups at Harvard, Duke, NASA/GSFC, U. Washington, Rutgers U., JPL, EPFL/Lausanne, CNRS/Toulouse, and the University of L'Aquila, Italy, as a versatile tool for application to a wide range of atmospheric chemistry problems.

NASA GEOS
DAO Products

First Look 4.0	Late Look 4.0
Conventional Final Dump - NCEP	Conventional CDAS Dump - NCEP
SSM/I (TPW only)	Wentz SSM/I (TPW only)
Operational Sea Ice	Operational Sea Ice
Interactive TOVS retrievals	Interactive TOVS retrievals
QuickSCAT	QuickSCAT
SBUV Ozone	SBUV Ozone
SST - Downstream Average	Reynolds SST - Centered Average
----	GADS (Passive)

Linkage between GEOS-CHEM and CMAQ

LAT-LON 2° X 2.5°
w/ GEOSCHEM
vertical coordinate

Chemistry Mapping
CB4 & SAPRC

GEOS2CMAQ INTERFACE

1. Read Input Data
2. Horizontal/Vertical Interpolation
3. Chemical Mapping (CB4/SAPRC99)

LAMBERT CONFORMAL
w/5D-3 hourly I/OAPI
on CMAQ/MM5
vertical coordinate

IC/BC Process

IC/BC for
CMAQ resolution

INPUT FILE - II

Vertical Height data

- GEOS-CHEM
  ; Monthly Mean Value
- CMAQ
  ; MCIP(GRIDCRO3D)

For Vertical Interpolation

INPUT FILE - III

Air Density Data

from GEOS-CHEM

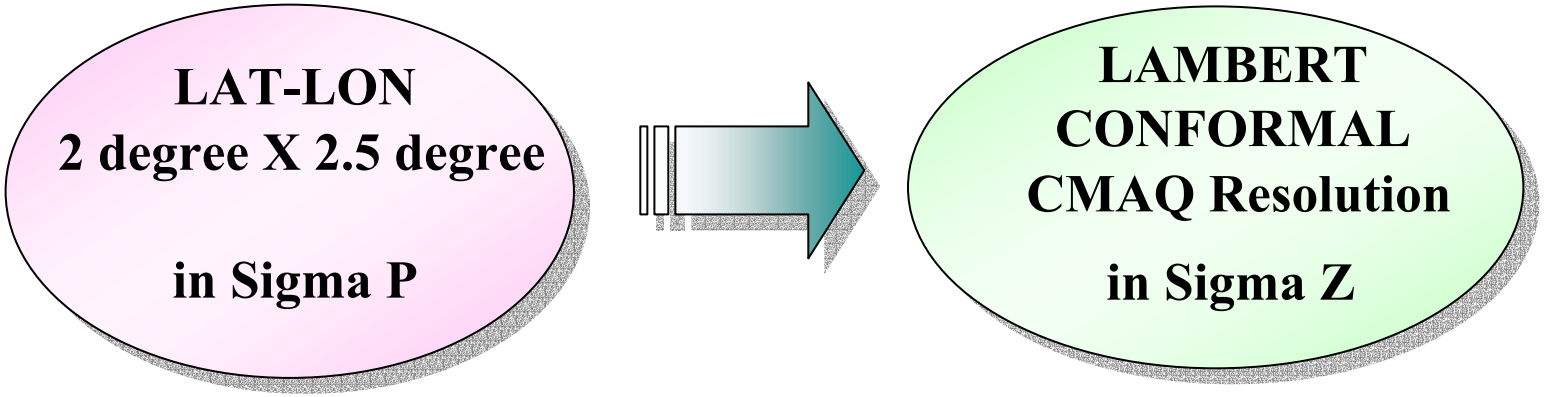
; Monthly Mean Value

For Unit Conversion

Horizontal & Vertical Interpolation

GEOS-CHEM Coordinate

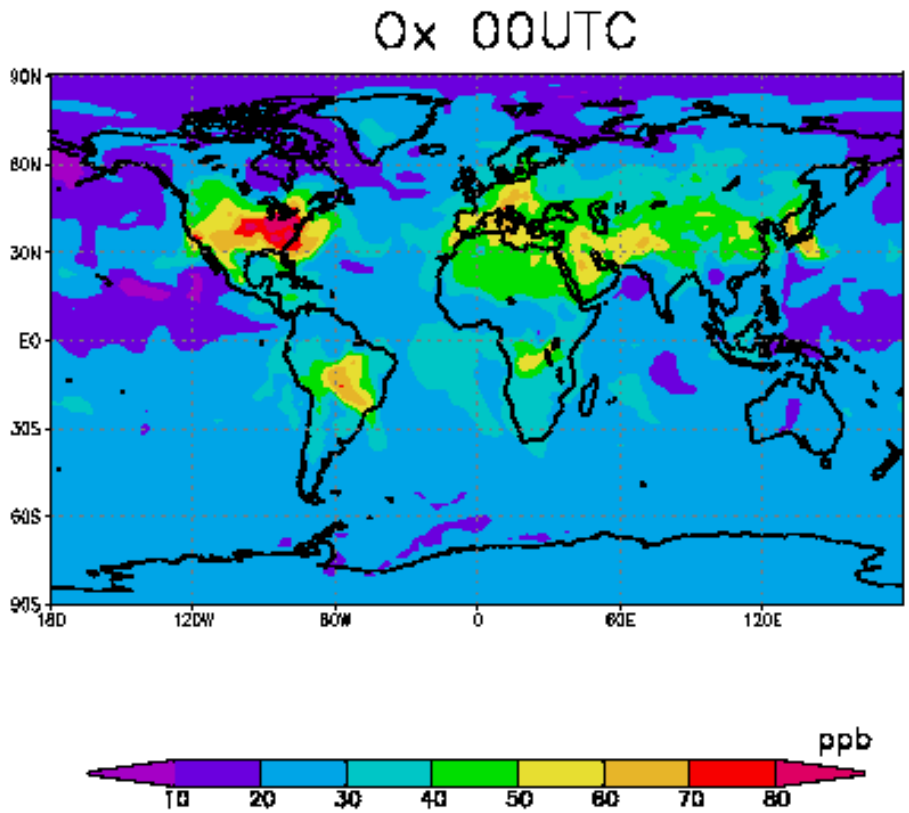
- Horizontal Coordinate
  - 4^o latitude x 5^o longitude (entire globe)
  - 2^o latitude x 2.5^o longitude (entire globe) → currently use
  - 1^o latitude x 1^o longitude (sub-region of globe)
- Vertical Coordinate
  σ_p Coordinate (SFC : 1000 hPa, TOP : 0.01 hPa)



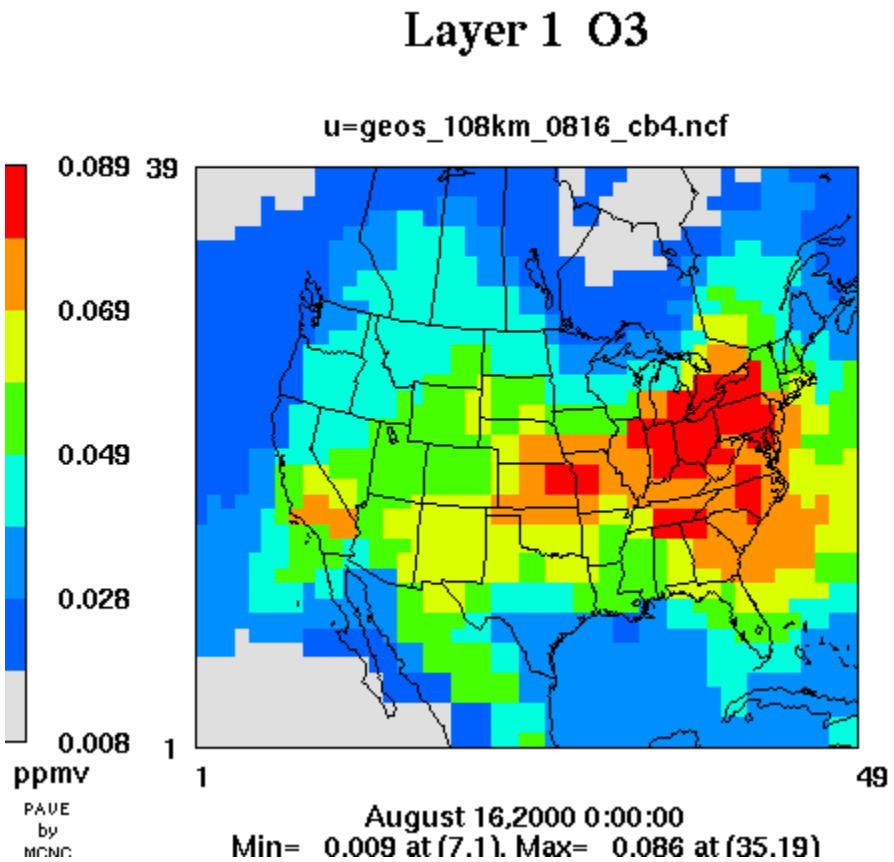
GEOS-CHEM
(Goddard Earth Observing System-CHEMisrty)

MODEL3 CMAQ
(Community Multiscale Air Quality Model)

Example result of initial condition for O_3 after GEOS2CMAQ Interface

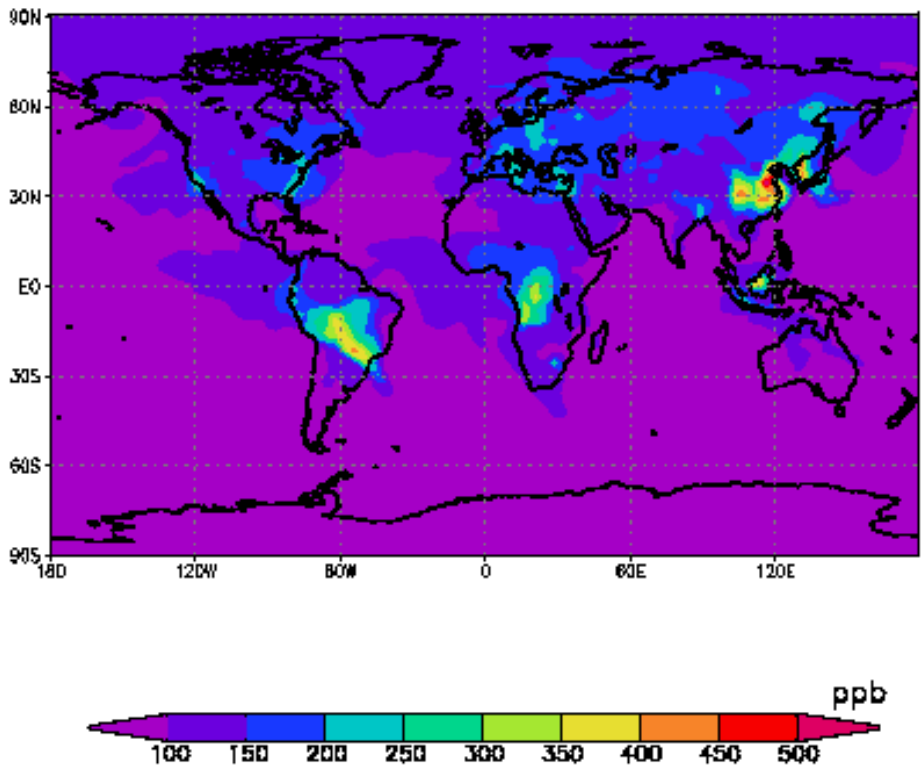


GEOS-CHEM
2° X 2.5° resolution



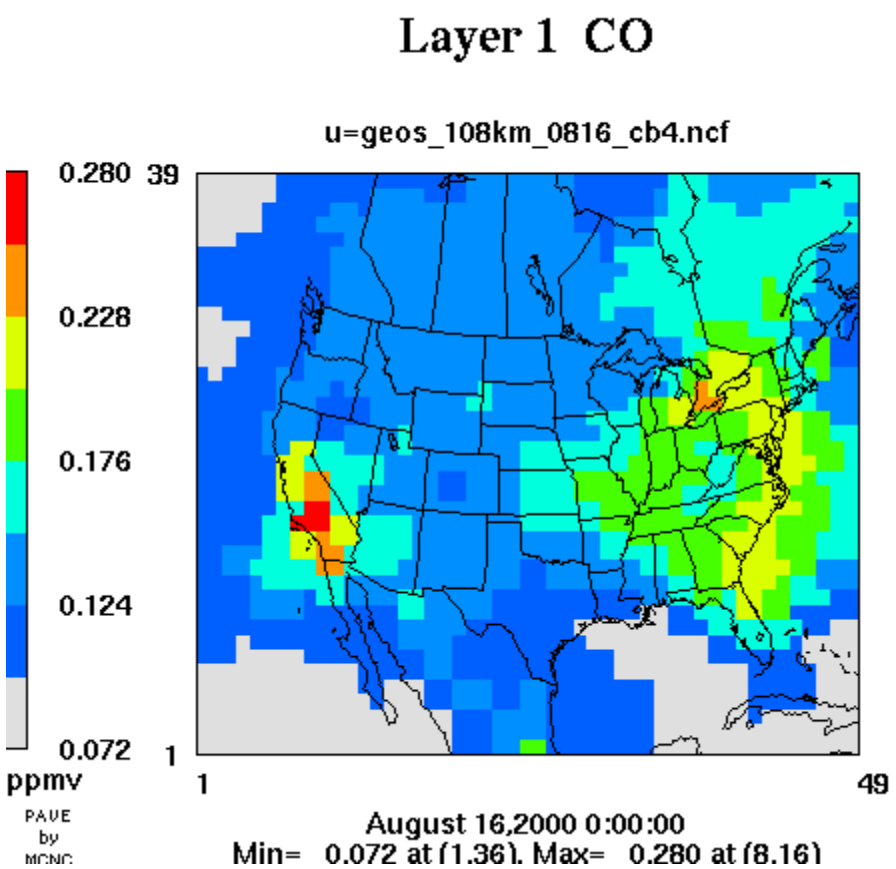
CMAQ-108km resolution

Example result of initial condition for CO after GEOS2CMAQ Interface



GEOS-CHEM

2° X 2.5° resolution



CMAQ-108km resolution

INPUT FILE - I

Standard GEOS-CHEM BINARY daily OUTPUT ; 31 species

Ox	Ox (O3+NO2)	MEK	Ketones(>C3)
NOx	NOx (NO+NO2)	ALD2	Acetaldehyde
HNO3	Nitric Acid	RCHO	Aldehyde(>C3)
N2O5	N2O5	ISOP	Isoprene
HNO4	Peroxynitric Acid	MVK	Methylvinylketone
CO	CO	MACR	Methacrolein
H2O2	Hydrogen Peroxide	MP	Methyl Hydroperoxide
CH2O	Formaldehyde	R4N2	Alkylnitrate(>C3)
SO2	SO2	NH3	Ammonia
PAN	PAN		
PMN	MPAN		
PPN	PPN		
C2H6	Ethane	**Aerosol Species**	
ALK4	Alkanes(>=C4)		
C3H8	Propane	SO4	Sulfate
PRPE	Propene	NH4	Ammonium
ACET	Acetone	NO3 (p)	Particulate Nitrate
		DMS	Dimethyl Sulfate
		MSA	Methyl Sulfionic Acid

Matching GEOS-CHEM and CMAQ chemistry mechanism

(EPA, 2001)

GEOS-CHEM		SAPRC-99	CB4
Ox	Ox (O3+NO2)	O3, NO2	O3, NO2
NOx	NOx (NO+NO2)	NO, NO2	NO, NO2
HNO3	Nitric Acid	HNO3	HNO3
N2O5	N2O5	N2O5	N2O5
HNO4	Peroxynitric Acid	HNO4	PNA
CO	CO	CO	CO
H2O2	Hydrogen Peroxide	H2O2	H2O2
CH2O	Formaldehyde	HCHO	FORM
SO2	SO2	SO2	SO2
PAN	PAN	PAN	PAN
PMN	MPAN	MA_PAN	PAN
PPN	PPN	PAN2	PAN
C2H6	Ethane	ALK1	0.4*PAR
ALK4	Alkanes(>=C4)	ALK3+ALK4+ALK5	4*PAR
C3H8	Propane	ALK2	3*PAR
PRPE	Propene	OLE1	(1*OLE)+ (1*PAR)
ACET	Acetone	ACET	3*PAR
MEK	Ketones(>C3)	MEK	4*PAR
ALD2	Acetaldehyde	CCHO	ALD2
RCHO	Aldehyde(>C3)	RCHO	ALD2
ISOP	Isoprene	ISOPRENE	ISOPRENE
MVK	Methylvinylketone	MVK	ISPD (products of isoprene rxns)
MACR	Methacrolein	METHACRO	ISPD (products of isoprene rxns)
MP	Methyl Hydroperoxide	COOH	UMHP
R4N2	Alkylnitrate(>C3)	RNO3	2*NTR
NH3	Ammonia	NH3	NH3
SO4	Sulfate	ASO4I+ASO4J	ASO4I+ASO4J
NH4	Ammonium	ANH4I+ANH4J	ANH4I+ANH4J
NO3 (p)	Particulate Nitrate	ANO3I+ANO3J	ANO3I+ANO3J
DMS	Dimethyl Sulfate		
MSA	Methyl Sulfionic Acid		