GEOS-Chem as a community model for air quality on urban to global scales in the satellite era

Daniel Jacob (Harvard), GEOS-Chem model scientist

GEOS-Chem
Surface NO$_x$ at C720 resolution (12.5 km) from GEOS-Chem within NASA GEOS-5
(graphic from U. York)
What GEOS-Chem aims to be

1. A grass-roots, open-access atmospheric chemistry model for global to urban scales that is well-supported and easy to use and modify;
2. An atmospheric chemistry module for weather/climate models.
GEOS-Chem is more than a model, it is a community

Model Support Team
Harvard, WashU, CU

contribute developments, report bugs

set development priorities through Working Groups:
support
implement priorities
review benchmarks

Model version updates

GEOS-Chem Steering Committee
Model scientist: Jacob (Harvard)
Model co-scientist: Martin (Washington U.)
Adjoint model scientist: Henze (U. Colorado)
Nested model scientists: Y. Wang (U.Houston), L. Zhang (PKU)
WRF-GC scientist: Fu (SUSTech)
Engineer: Yantosca (Harvard)
Aerosols WG: Heald (MIT), Alexander (UW), Pierce (CSU), Yu (SUNYA)
Chemistry WG: Henderson (EPA), Evans (York), Mao (U. Alaska), Hu (U. Montana)
Emissions and Deposition WG: Lin (PKU), Fischer (CSU), Millet (U. Minnesota),Marais (UCL)
Chemistry-Ecosystem-Climate WG: Liao (NUIST), Tai (CUHK), Murray (U. Rochester), Geddes (Boston U)
Carbon WG: Jones (U. Toronto), Bowman (JPL)
Adjoint and Data Assimilation WG:
J. Wang (U. Iowa), Henze (U. Colorado)
Transport WG: Liu (NIA), Molod (NASA)
Hg and POPs WG: Holmes (FSU), Fisher (U. Wollongong), Y. Zhang (Nanjing U.)
GCHP WG: Martin (WashU), Eastham (MIT)
Stratospheric WG: Jones (U. Toronto),
Strahan (NASA), Eastham (MIT)
Software Engineering WG: Lundgren (Harvard), Sulprizio (Harvard)
GMAO rep: Keller (NASA)
At large: Kasibhatla (Duke).

Emphasize user support, community spirit, nimble innovation, strong version control, documentation, traceability
Tutorial videos on GEOS-Chem YouTube
GEOS-Chem “Classic” off-line atmospheric chemistry model

Detailed chemical simulation of troposphere and stratosphere

Input meteorological data from NASA GEOS-5 system:
MERRA-2, 1980-present (0.5°x0.625°)
GEOS-FP, 2012-present (0.25°x0.3125°)

Model solves 3-D chemical continuity equations on global or nested domains, at native or coarser resolution

**Modules**
- transport (TPCORE)
- emissions (HEMCO)
- chemistry (KPP with FlexChem)
- photolysis (Fast-JX)
- aerosol microphysics (APM, TOMAS)
- deposition

Model adjoint
Under the hood, the core of GEOS-Chem is actually a column model…

\[ \frac{dC}{dt} = P - L + E - D \]

- chemistry
- emissions
- deposition

This enables:
- use of any meteorological fields
- massively parallel simulations with distributed memory (MPI)
- GEOS-Chem as on-line chemical module in weather/climate models
High-performance GEOS-Chem (GCHP)

- Massively parallel off-line GEOS-Chem with FV3 cubed-sphere advection using GEOS fields
- Efficient scaling on over 1,000 cores including on AWS cloud

Eastham et al., GMD 2018
Zhuang et al., JAMES 2020

Full chemistry at C360 (~25km) resolution: Junwei Xu and Aaron van Donkelaar
Stretched-grid capability for targeted high-resolution simulations using GCHP

C24
SF:  1.0 x
TLat:  0.0 ° N
TLon:  100.0° W

Liam Bindle and Randall Martin, Wash. U.
Stretched-grid capability for targeted high-resolution simulations using GCHP

- Transformation to the cube-sphere’s grid-boxes
- Grid-boxes shrink over target region
- Grid-boxes expand on the opposite face
- No added computational effort

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Liam Bindle and Randall Martin, Wash. U.
Stretched-grid simulation with C720 (12 km) resolution

Full chemistry simulation over California (surface ozone)

Liam Bindle, WashU

Complex topography and source structure better represented at fine resolution

Implicit 2-way ‘nesting’

At expense of global C48 (~2° x 2.5°)
GEOS-Chem as chemical module for weather/climate models

any 3-D grid specified at run time

Advection

Mixing Convection

Chemistry (FlexChem): \( \frac{dC}{dt} = P - L - D \)

Emissions (HEMCO): \( \frac{dC}{dt} = E \)

off-line GEOS-Chem model with input met. data

GEOS-Chem chemical module
GEOS-Chem as chemical module for weather/climate models

any 3-D grid specified at run time

GEOS-Chem chemical module

coupler

Chemistry (FlexChem):
\[ \frac{dC}{dt} = P - L - D \]

coupler

Emissions (HEMCO):
\[ \frac{dC}{dt} = E \]

coupler

Dynamics, chemical transport

weather/climate model with on-line GEOS-Chem
GEOS-Chem as chemical module for weather/climate models

any 3-D grid specified at run time

Off-line and on-line GEOS-Chem chemical modules use exactly the same code

Off-line GEOS-Chem users contribute model advances

Advances are incorporated into standard GEOS-Chem

...and are seamlessly passed to weather/climate model

Off-line GEOS-Chem model with input met. data

Advection

Mixing

Convection

GEOS-Chem chemical module

Chemistry (FlexChem):
\[ \frac{dC}{dt} = P - L - D \]

Emissions (HEMCO):
\[ \frac{dC}{dt} = E \]

Dynamics, chemical transport

weather/climate model with on-line GEOS-Chem
Global composition analyses and forecasts at NASA GMAO (GEOS-CF)

GEOS-Chem as on-line chemical module in GEOS system

Christoph Keller, GMAO
Coupling of GEOS-Chem with WRF (WRF-GC)

- Both WRF and GEOS-Chem are off-the-shelf; 1-way and 2-way couplings are mature
- Enables GEOS-Chem simulations at any resolution and with different WRF options

Simulation over Korea during KORUS-AQ aircraft campaign: three 2-way nested grids
Coupling of GEOS-Chem with NCAR CESM (CESM-GC)

OBJECTIVE 1

1. Implement GEOS-Chem as alternative to CAM-Chem in CESM2
2. Implement HEMCO as an independent emission tool for use, e.g., by CAM-Chem

Lizzie Lundgren, Haipeng Lin, Daniel Jacob (Harvard)
Seb Eastham, Thibaud Fritz (MIT)
Louisa Emmons, Forrest Lacey (NCAR)
HEMCO emissions tool

- Reads, combines, masks, modifies, regrids emission data from library of inventories on any grid with no change to GEOS-Chem source code.
- Can be used to serve emissions to other atmospheric chemistry models

On-disk emissions, masks, scaling factors

Keller et al., GMD 2014; Lin et al., in prep.
GEOS-Chem on the AWS cloud

- Mature single-node and multi-node capabilities, supported with detailed tutorials
- Scales efficiently to > 1000 cores

Current standard version of GEOS-Chem, properly configured and ready to execute

Configure/execute your run, analyze output

GEOS and HEMCO input data

GEOS data hosted free on AWS through agreement with Harvard

Zhuang et al., BAMS 2019, JAMES 2020
Future vision for GEOS-Chem:
one scientific base, three implementations

GEOS-Chem chemical module
- a single code for all implementations
- state-of-science, benchmarked, traceable

GEOS-Chem Classic
- easy to install and use, simple to modify
- adjoint and cloud capabilities available

GEOS-Chem high performance (GCHP)
- high-resolution simulations with MPI
- FV3 advection on cubed-sphere grid
- cloud capability available, adjoint soon

GEOS-Chem in weather/climate models
- chemistry-ecosystem-climate coupling
- access to any meteorology, resolution
- chemical data assimilation and forecasts