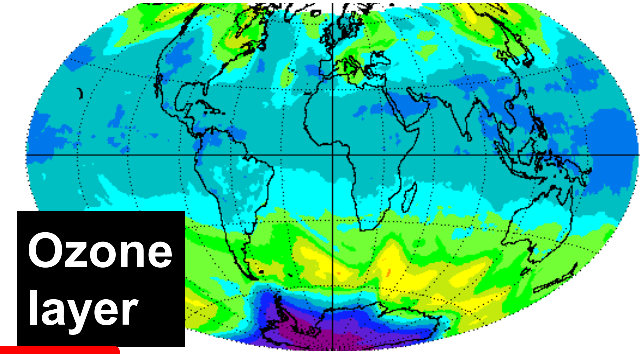
GEOS-Chem: building of a grass-roots community atmospheric chemistry model

Daniel Jacob, GEOS-Chem model scientist

GEOS-Chem

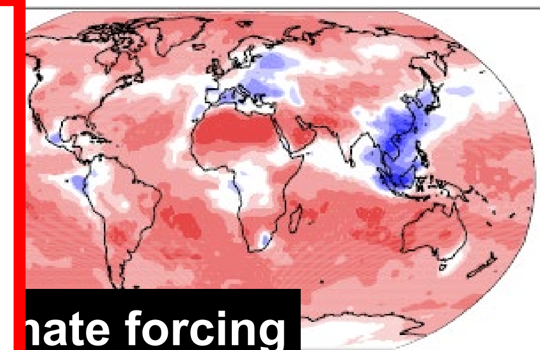
Surface NO_x at C720 resolution (12.5 km) from GEOS-Chem within NASA GEOS-5 *(graphic from U. York)*

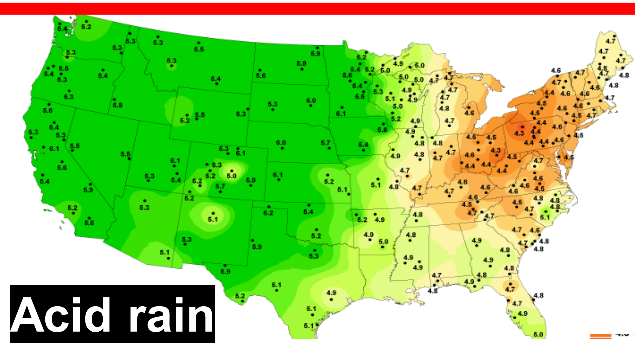
Atmospheric chemists are interested in a wide range of issues



We need models to:

- Understand processes
- Interpret observations
- Make forecasts and projections



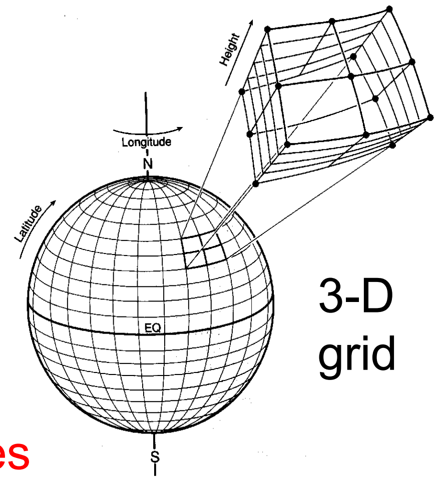


LOCAL
< 100 km

REGIONAL
100-1000 km

GLOBAL
> 1000 km

How to model atmospheric chemistry



3-D grid

transport
chemistry
aerosol microphysics

species **X** $\longrightarrow$ species **Y**

emission $\uparrow$ X

Y $\downarrow$ deposition

Solve continuity equations for concentrations $\mathbf{n} = (n_1, \ldots n_K)$ of K chemically coupled species in individual grid cells:

$$\frac{\partial n_i}{\partial t} = -\nabla \cdot (n_i \underbrace{\mathbf{U}}_{\text{wind}}) + \underbrace{P_i(\mathbf{n})}_{\text{production}} - \underbrace{L_i(\mathbf{n})}_{\text{loss}}$$

local change in concentration | transport (flux divergence) | emissions, deposition, chemical and aerosol processes

Challenges:

- Chemical coupling between large numbers of species
- Coupling between transport and chemistry on all scales

Break down dimensionality of continuity equation by operator splitting

Solve for transport and local terms separately over time steps Δt

$$\frac{\partial n_i}{\partial t} = -\nabla \cdot (n_i \mathbf{U}) + P_i(\mathbf{n}) - L_i(\mathbf{n})$$

Advection (and other transport):

$$\frac{\partial n_i}{\partial t} = -\nabla \cdot (n_i \mathbf{U})$$

Chemistry (and other local processes)

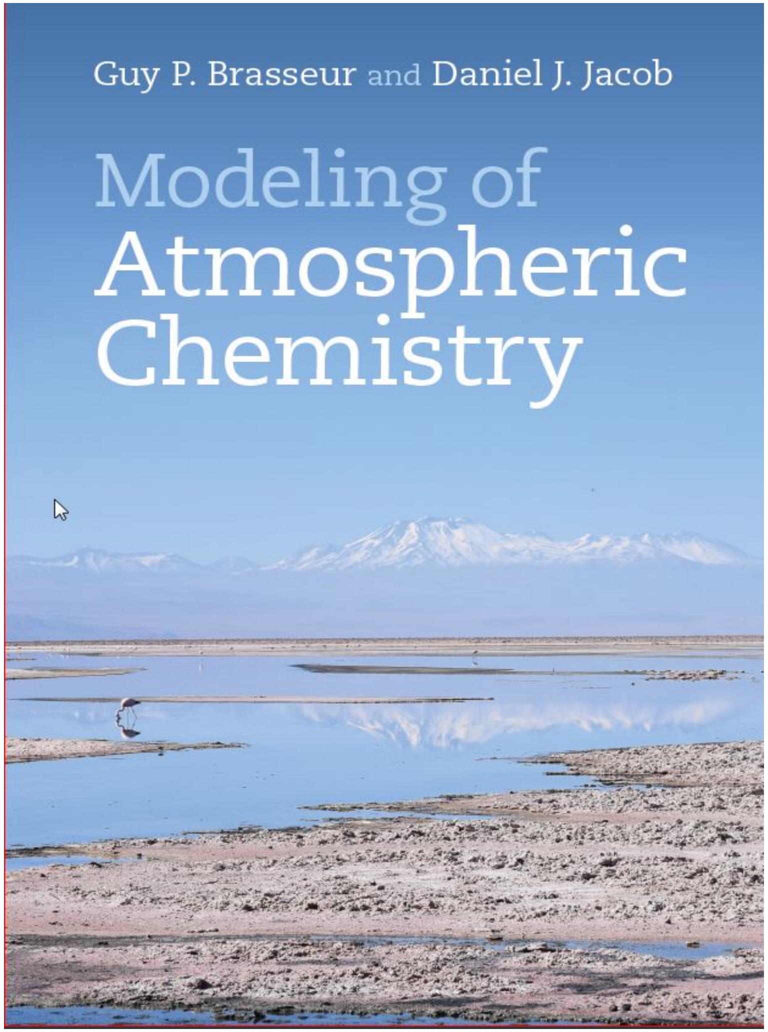
$$\frac{dn_i}{dt} = P_i(\mathbf{n}) - L_i(\mathbf{n})$$

$$\mathbf{n}(t) \xrightarrow{\Delta t} \mathbf{n}^* \xrightarrow{\Delta t} \mathbf{n}(t+\Delta t)$$

Advection equations:
PDEs with no coupling
between species

Chemical equations:
K-dimensional system of ODEs

An excellent book…



Cambridge University Press, 2017

Chapter 1: The concept of model

Chapter 2: Atmospheric structure and dynamics

Chapter 3: Chemical processes

Chapter 4: Model equations, numerical approaches

Chapter 5: Radiative, chemical, aerosol processes

Chapter 6: Numerical methods for chemical systems

Chapter 7: Numerical methods for advection

Chapter 8: Parameterization of small scales

Chapter 9: Surface fluxes

Chapter 10: Model evaluation

Chapter 11: Inverse modeling

also available electronically

On-line and off-line approaches to modeling atmospheric chemistry

On-line: coupled to dynamics

Meteorological model:
air mass: $\partial\rho_a/\partial t = \ldots$
momentum: $\partial\mathbf{U}/\partial t = \ldots$
heat: $\partial\theta/\partial t = \ldots$
water: $\partial q/\partial t = \ldots$
chemicals: $\partial\mathbf{n}/\partial t = \ldots$

Off-line: decoupled from dynamics

Meteorological model:
air mass: $\partial\rho_a/\partial t = \ldots$
momentum: $\partial\mathbf{U}/\partial t = \ldots$
heat: $\partial\theta/\partial t = \ldots$
water: $\partial q/\partial t = \ldots$

↓

3-D meteorological archive
(averaging time ~ hours)

↓

Chemical transport model:
$\partial\mathbf{n}/\partial t = \ldots$

PROs of off-line vs on-line approach:

- computational cost
- simplicity
- meteorological fidelity across scales
- compute sensitivities back in time

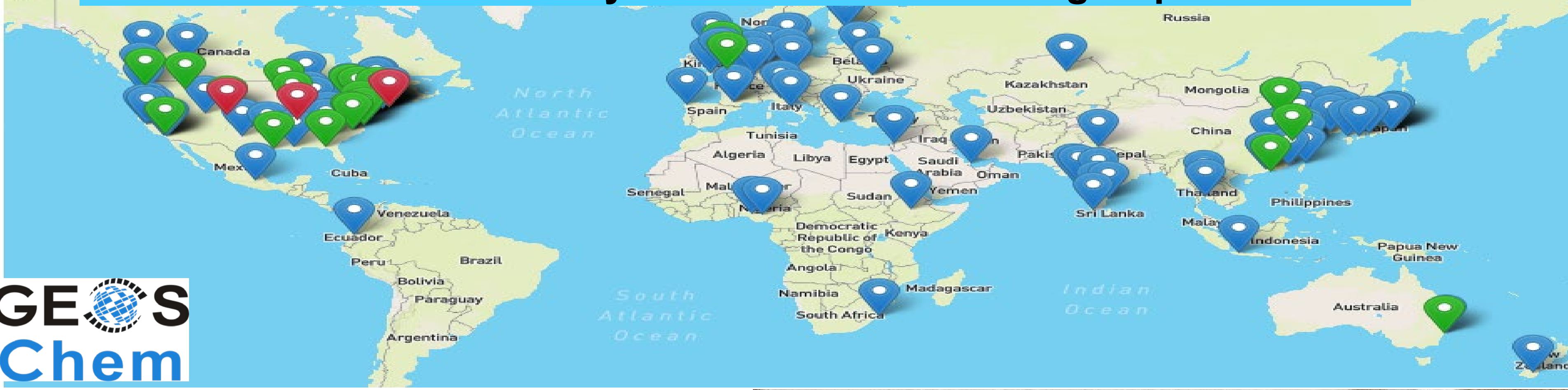
CONs:

- no fast chemical-dynamics coupling
- need for meteorological archive
- transport errors

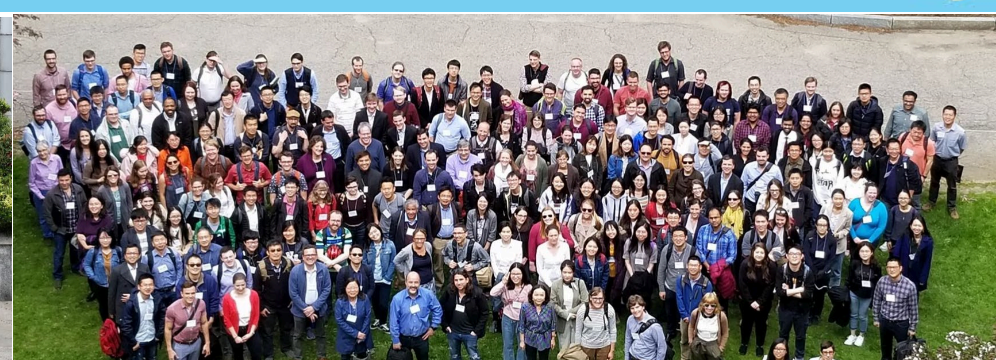
The GEOS-Chem atmospheric chemistry model

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.

The GEOS-Chem community: hundreds of research groups worldwide



1st GEOS-Chem Asia meeting (GCA1)
Nanjing, May 2018



9th International GEOS-Chem meeting (IGC9)
Harvard, May 2019

GEOS-Chem is more than a model, it is a community

contribute developments, report bugs

support

set development priorities through Working Groups:

implement priorities review benchmarks

Model Support Team
Harvard, WashU

Model version updates

Emphasize user support, community spirit, nimble innovation, strong version control, documentation, traceability
Tutorial videos on GEOS-Chem YouTube

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: Alexander (UW), Pierce (CSU), Yu (SUNYA)
Chemistry WG: Henderson (EPA), Evans (York), Mao (U. Alaska), Hu (U. Montana)
Emissions and Deposition WG: Lin (PKU), 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: Schuh (CSU), Orbe (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), Wales (NASA), Eastham (MIT)
Software Engineering WG: Lundgren (Harvard), Sulprizio (Harvard)
GMAO rep: Keller (NASA)
At large: Kasibhatla (Duke).

Model scientists

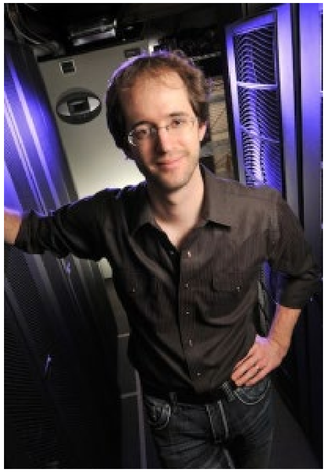
Model scientist

Daniel Jacob
Harvard

Model co-scientist

Randall Martin
WashU

Model adjoint scientist



Daven Henze
CU-Boulder

Nested model co-scientists

Yuxuan Wang
U. Houston

Lin Zhang
Peking U.

WRF-GC model scientist

Tzung-May Fu
SUSTC

GEOS-Chem Support Team

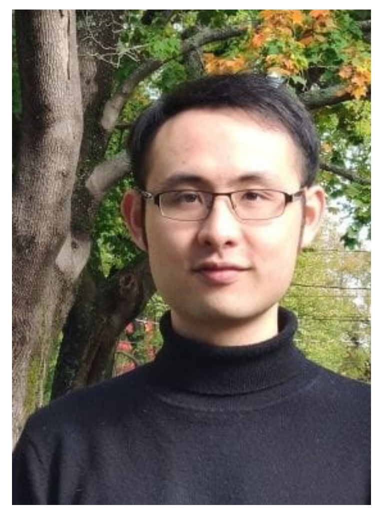
Lizzie Lundgren
Harvard

Melissa Sulprizio
Harvard

Bob Yantosca
Harvard

Lucas Estrada
Harvard

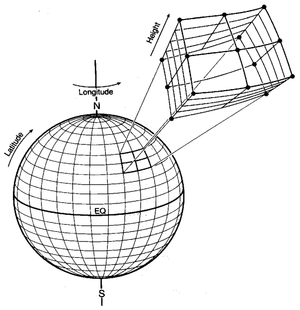
Liam Bindle
WashU



Yanshun Li
WashU

GEOS-Chem "Classic" off-line chemical transport model

Detailed chemical simulation of troposphere and stratosphere



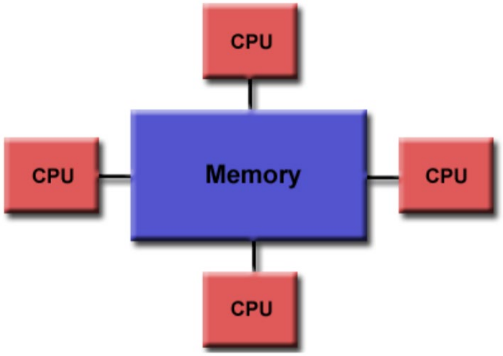
Input meteorological data from NASA GEOS system:
MERRA-2, 1980-present (0.5°x0.625°)
GEOS-FP, 2012-present (0.25°x0.3125°)

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

Shared-memory (Open-MP) architecture: run on single node,
scales well up to 30 cores



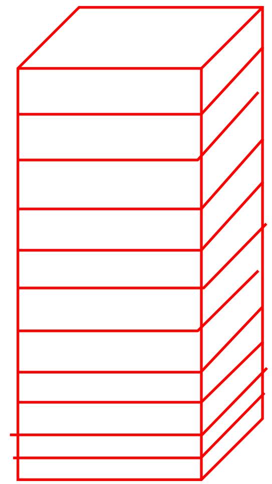
Under the hood, the core of GEOS-Chem is actually a column model…

Chemical module:

$dn_i /dt = P_i(\mathbf{n}) - L_i(\mathbf{n})$

- chemistry
- emissions
- deposition
- aerosol microphysics

$\mathbf{n}(\mathbf{x}, t) \xrightarrow{\text{transport}}$



$\longrightarrow \mathbf{n}(\mathbf{x}, t + \Delta t)$

(x, y)

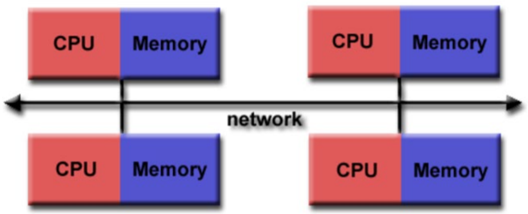
…updating concentration fields on any model grid specified at runtime

This enables:

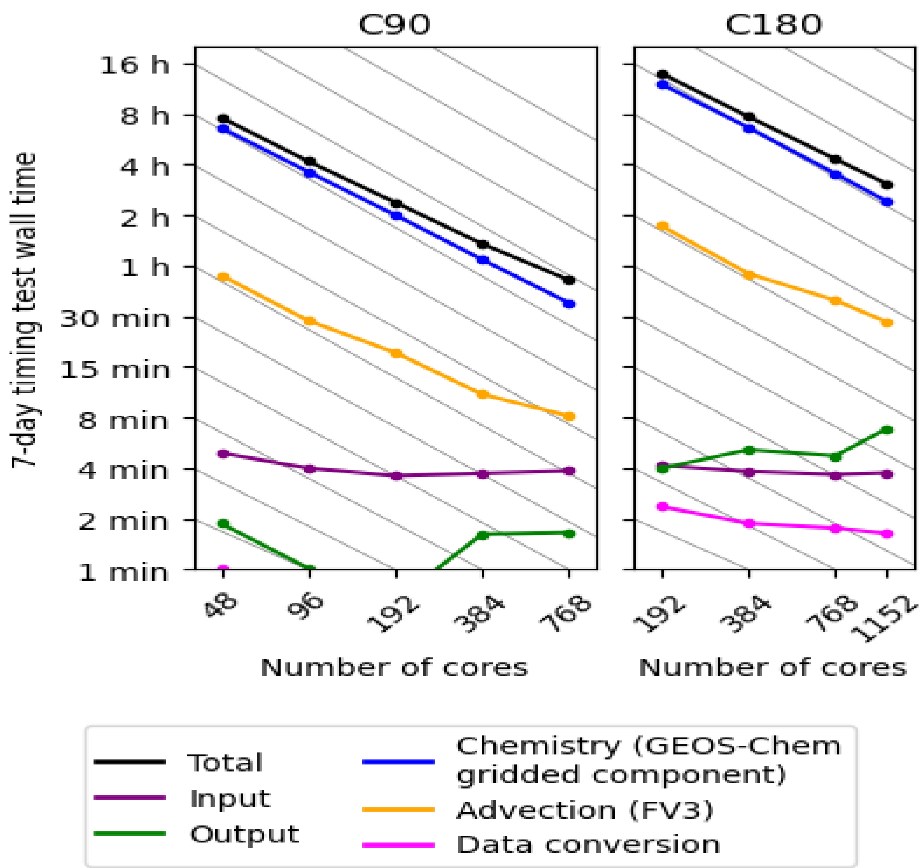
- use of any meteorological fields on any grid
- massively parallel simulations with distributed memory (MPI)
- GEOS-Chem as on-line chemical module in weather/climate models

High-performance GEOS-Chem (GCHP)

- Distributed-memory (MPI) architecture



- Massively parallel off-line capability on native NASA GEOS cubed-sphere grid
- Efficient scaling on over 1,000 cores including on AWS cloud
- Chemistry is expensive! But it parallelizes near perfectly

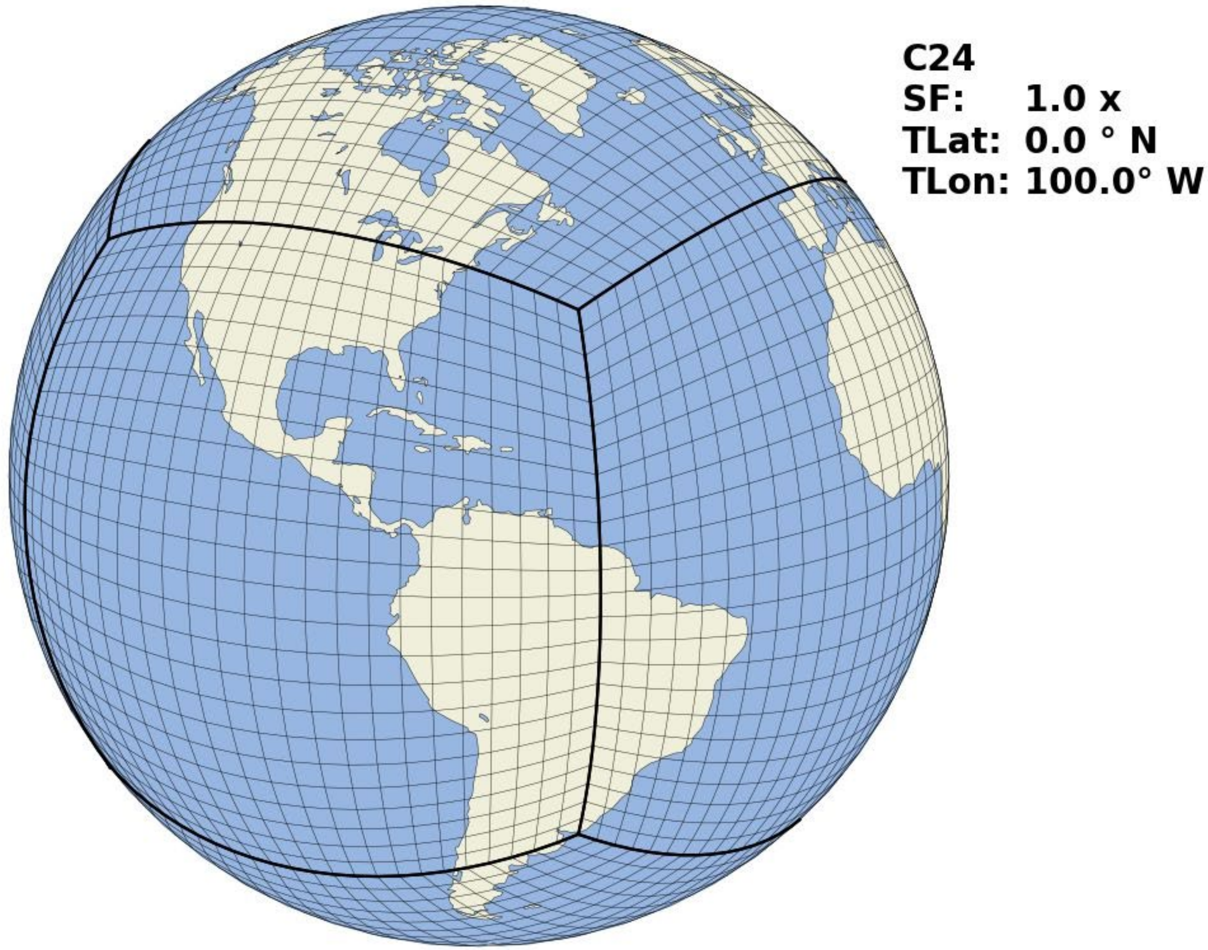


Martin et al., 2021

GCHP enables higher-resolution simulations than previously possible

Full chemistry at C360 (~25km) resolution: Junwei Xu and Aaron van Donkelaar

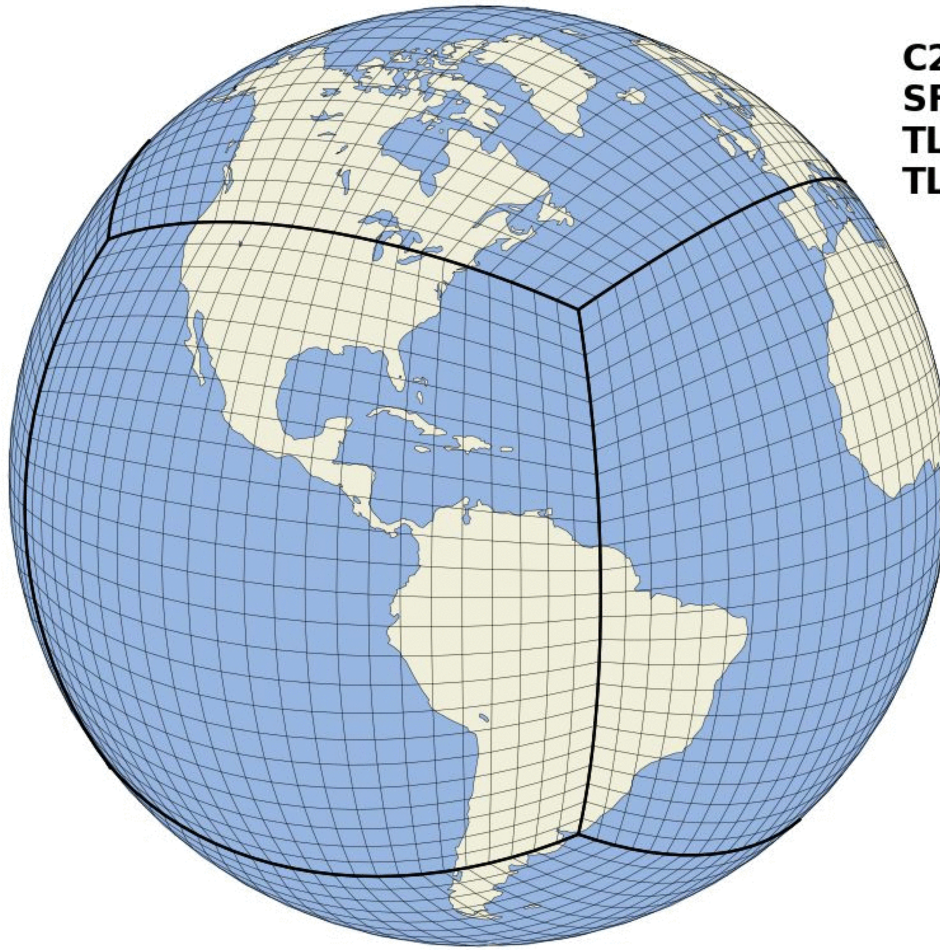
Stretched-grid capability for targeted high-resolution simulations using GCHP



Bindle et al., 2021

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 cost**



Bindle et al., 2021

Stretched-grid simulation with C720 (12 km) resolution

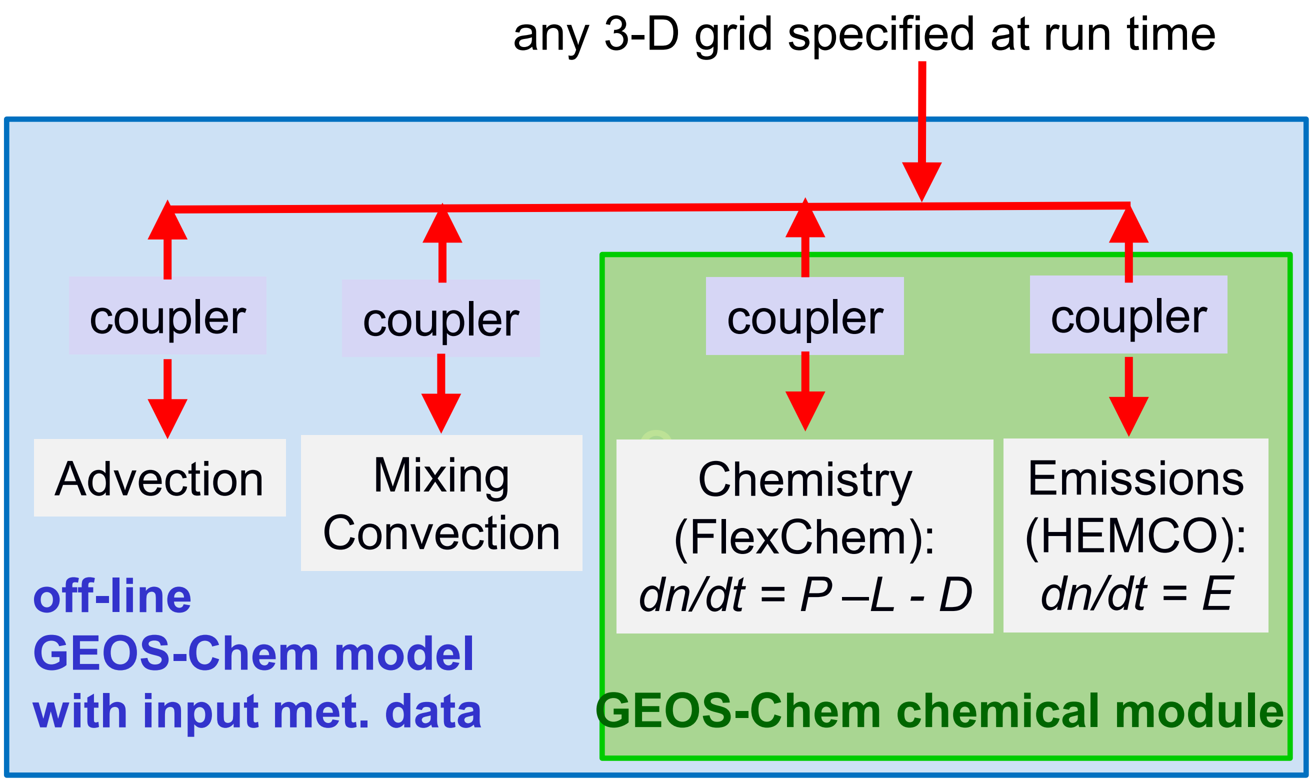
Full chemistry simulation over California (surface ozone)

Liam Bindle, WashU

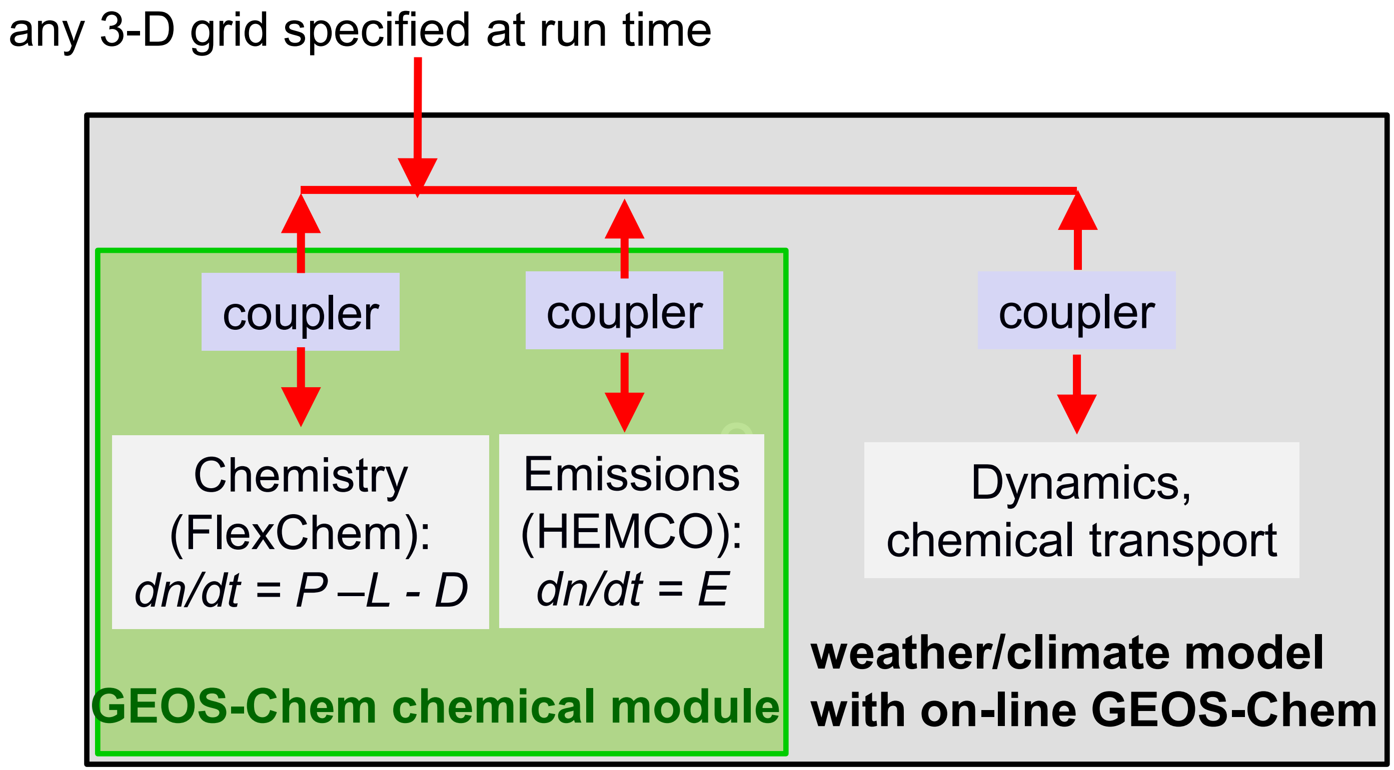
Complex topography and source structure better represented at fine resolution

Implicit 2-way ‘nesting’

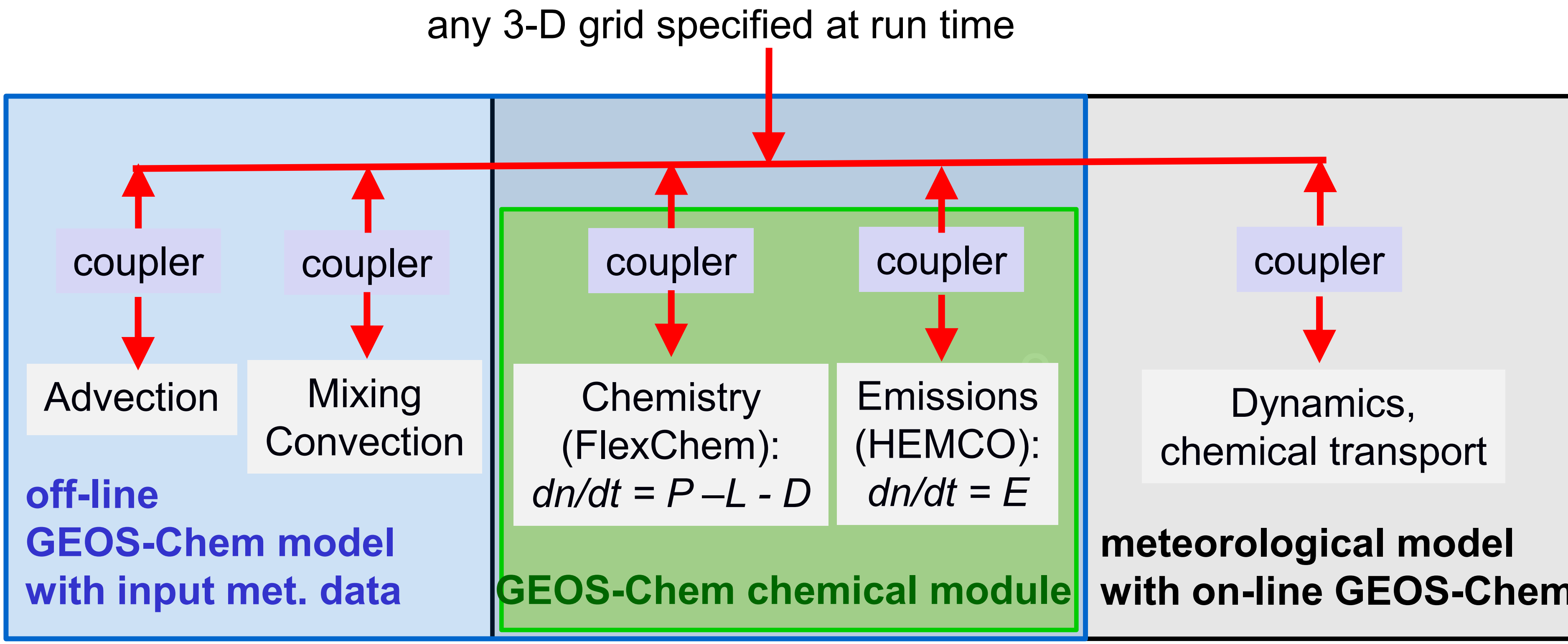
GEOS-Chem as chemical module for weather/climate models



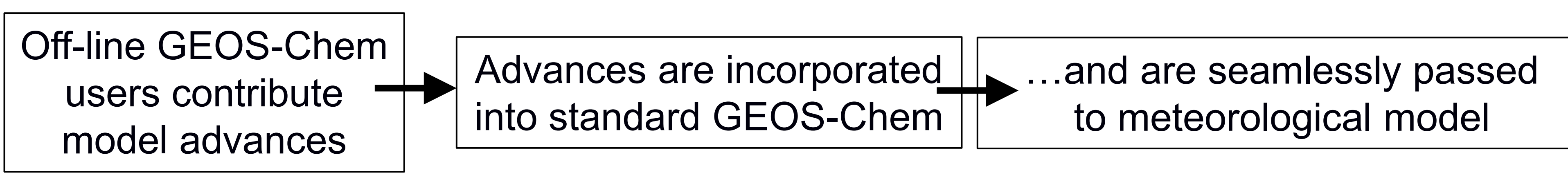
GEOS-Chem as chemical module for weather/climate models



GEOS-Chem as chemical module for weather/climate models



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



Global composition analyses and forecasts at NASA GMAO (GEOS-CF)

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

Keller et al., 2021

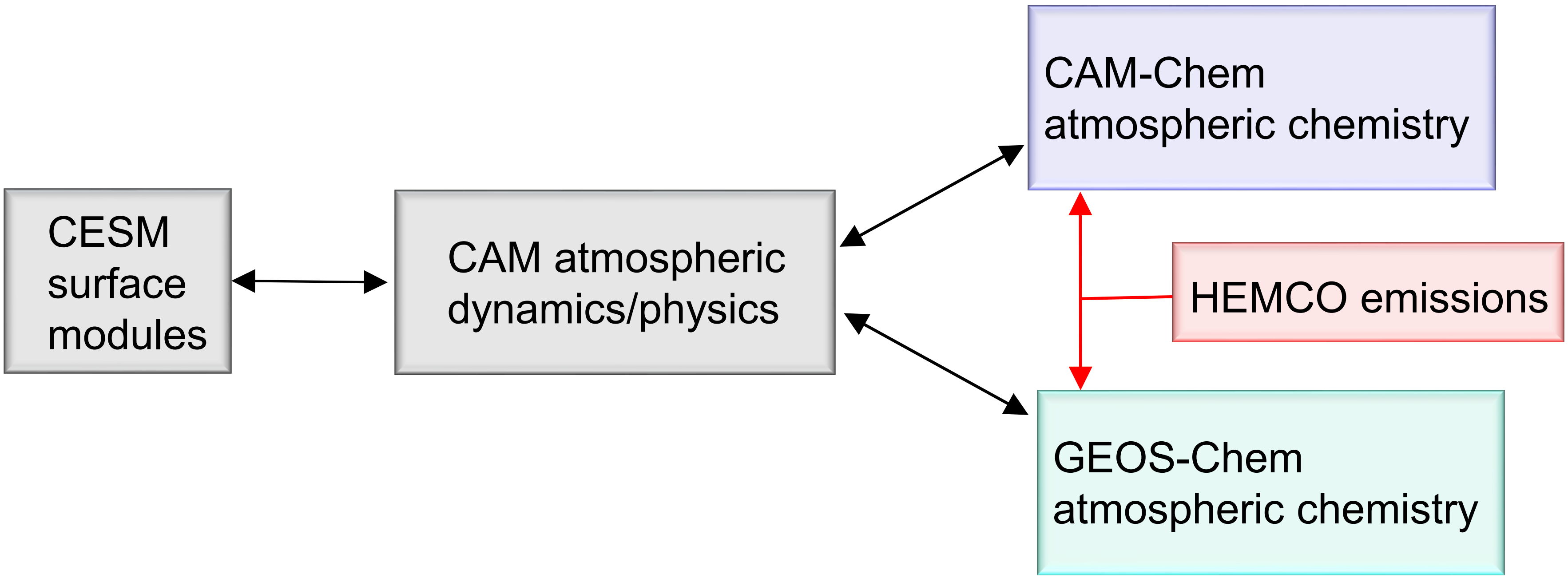
Coupling of GEOS-Chem with WRF (WRF-GC)

- 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

Lin et al., 2020; Xu et al., 2021

GEOS-Chem chemical module implemented in NCAR CESM



- GEOS-Chem is now an option in CESM as alternative to CAM-Chem
- HEMCO module serves the same emissions to both
- GEOS-Chem source code in CESM is exact same as standard offline GEOS-Chem

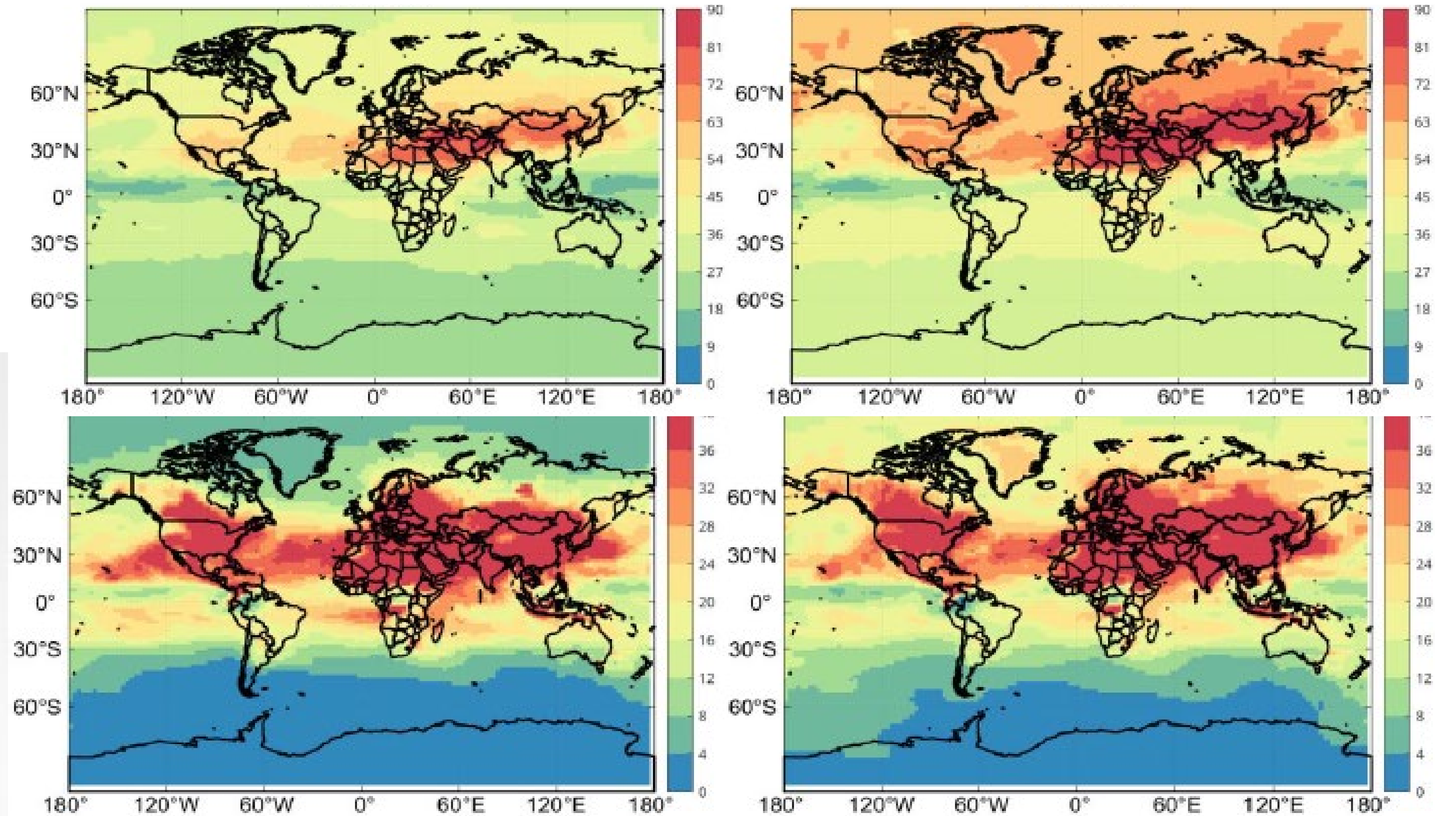
Lizzie Lundgren, Haipeng Lin, Daniel Jacob (Harvard)
Seb Eastham, Thibaud Fritz (MIT)
Louisa Emmons (NCAR)

Comparing GEOS-Chem and CAM-Chem within CESM

GEOS-Chem CAM-Chem

500 hPa ozone, July 2016

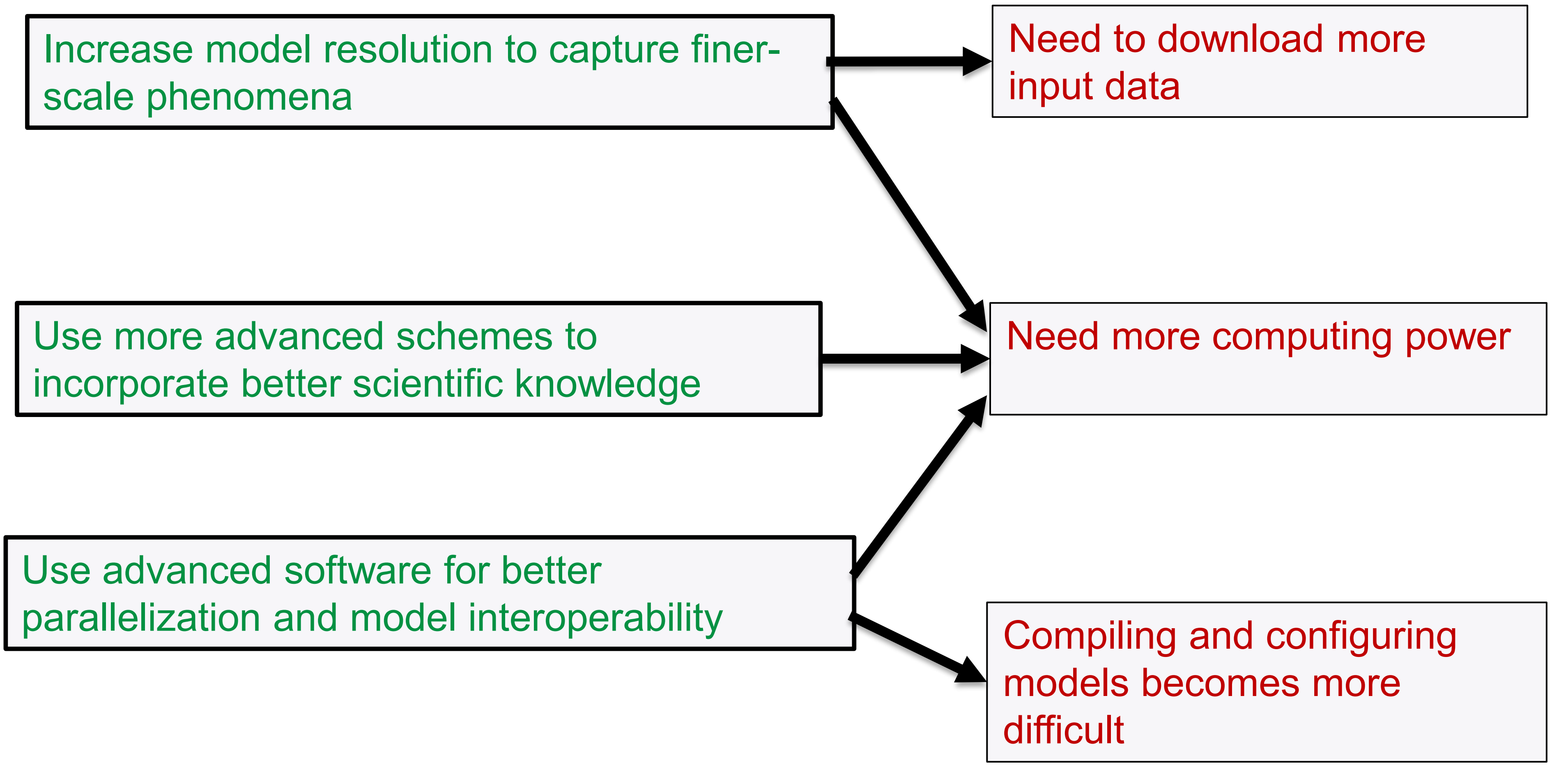
500 hPa NO_x, July 2016



- GEOS-Chem ozone in CESM is consistent with standard offline GEOS-Chem and 10-20 ppb lower than CAM-Chem
- Ozone difference with CAM-Chem is not driven by cross-tropopause transport or NO_x; major difference is lack of tropospheric halogen chemistry in CAM-Chem

Haipeng Lin, in prep.

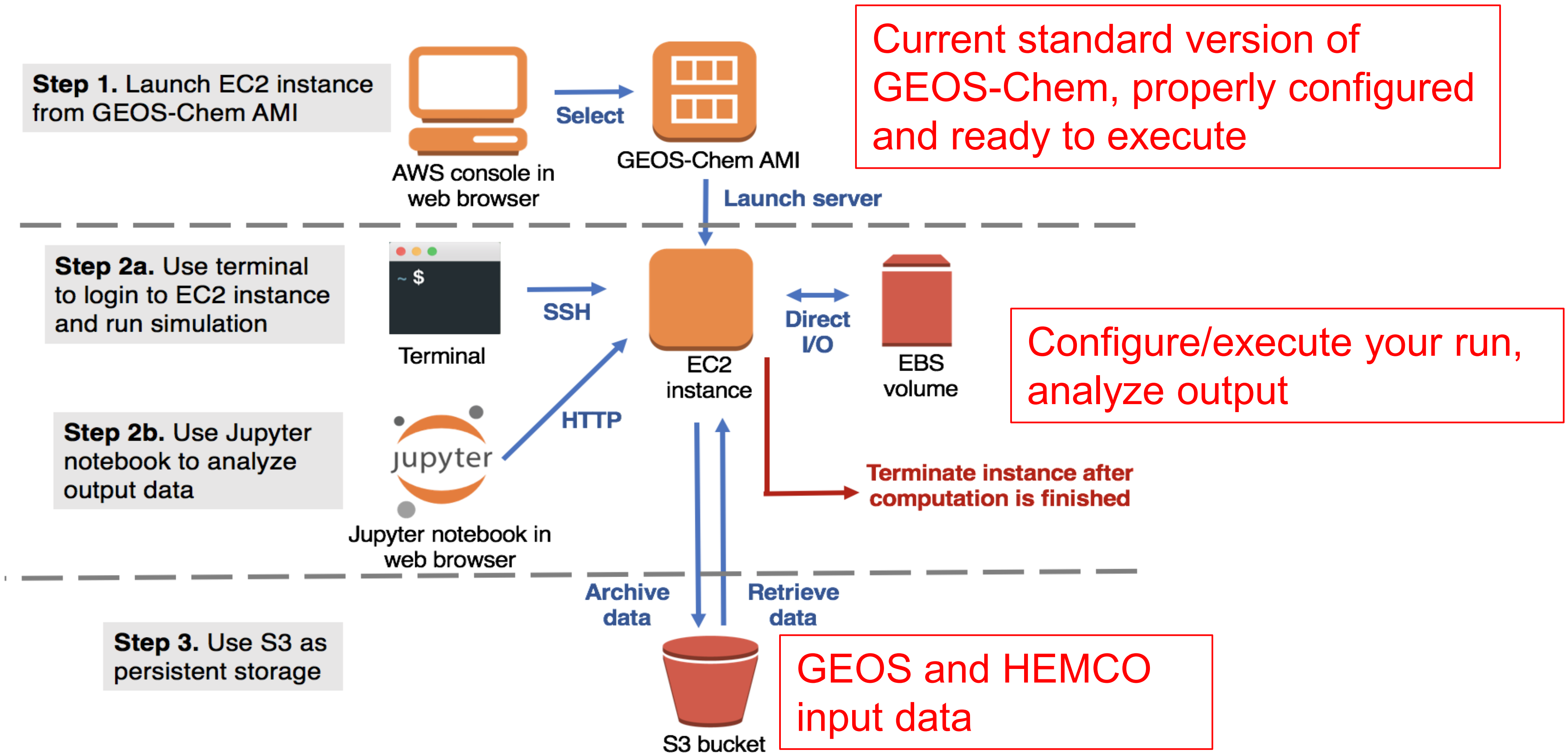
The better a model becomes, the less accessible it is



GEOS-Chem on the AWS cloud

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

GEOS-Chem research workflow on the AWS cloud



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

off-line

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

off-line

GEOS-Chem high performance (GCHP)
- Parallelization on over 1,000 cores
- More accurate advection

on-line

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