Chemistry-Climate Working Group Status

Louisa Emmons (NCAR) – co-chair

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Simone Tilmes (NCAR) - liaison

Francis Vitt (NCAR) – Software Engineer

15 June 2020

Status of CESM2 chemistry and aerosols

Papers describing chemistry and aerosols in CESM2 for CMIP6

- MOZART-T1 chemistry (Emmons et al., *JAMES,* 2020)
- Secondary organic aerosols (VBS-SOA) (Tilmes et al., *JAMES*, 2019)
- WACCM6 (Gettelman et al., *JGR-Atmos*, 2019)

AerChemMIP

Atmos. Chem. Phys. Special Issue:

Allen, R. J., et al., Climate and air quality impacts due to mitigation of non-methane near-term climate forcers, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2019-1209, in review, 2020.

Griffiths, P. T., et al., Tropospheric ozone in CMIP6 Simulations, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2019-1216, in review, 2020.

Stevenson, D. S., et al., Trends in global tropospheric hydroxyl radical and methane lifetime since 1850 from AerChemMIP, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2019-1219, in review, 2020.

Thornhill, G. D., et al., Effective Radiative forcing from emissions of reactive gases and aerosols – a multimodel comparison, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2019-1205, in review, 2020.

Turnock, S. T., et al., Historical and future changes in air pollutants from CMIP6 models, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2019-1211, in review, 2020.

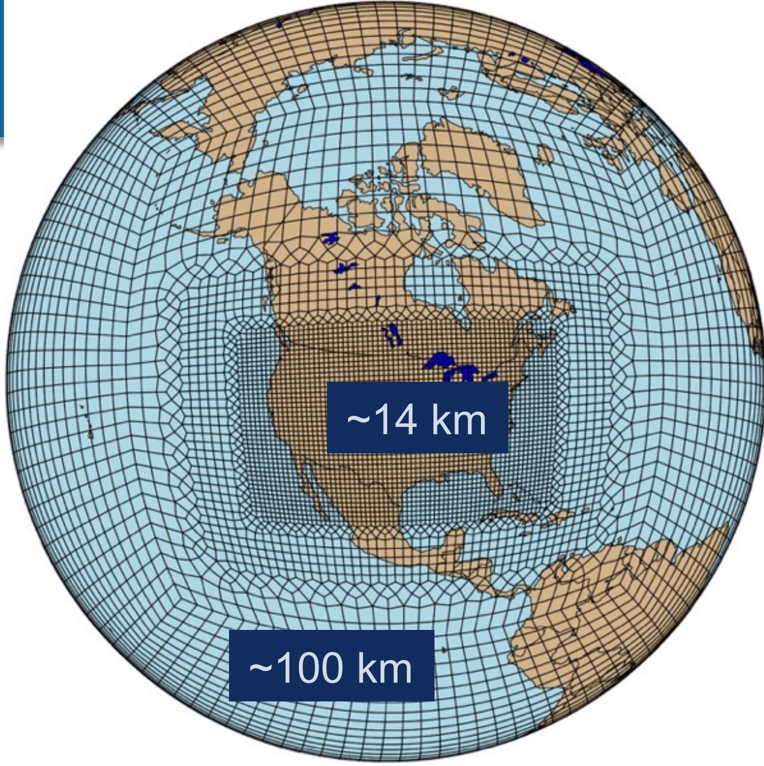
CESM2-WACCM simulations available on /glade/ and EarthSystemGrid
-- many opportunities for more analysis!

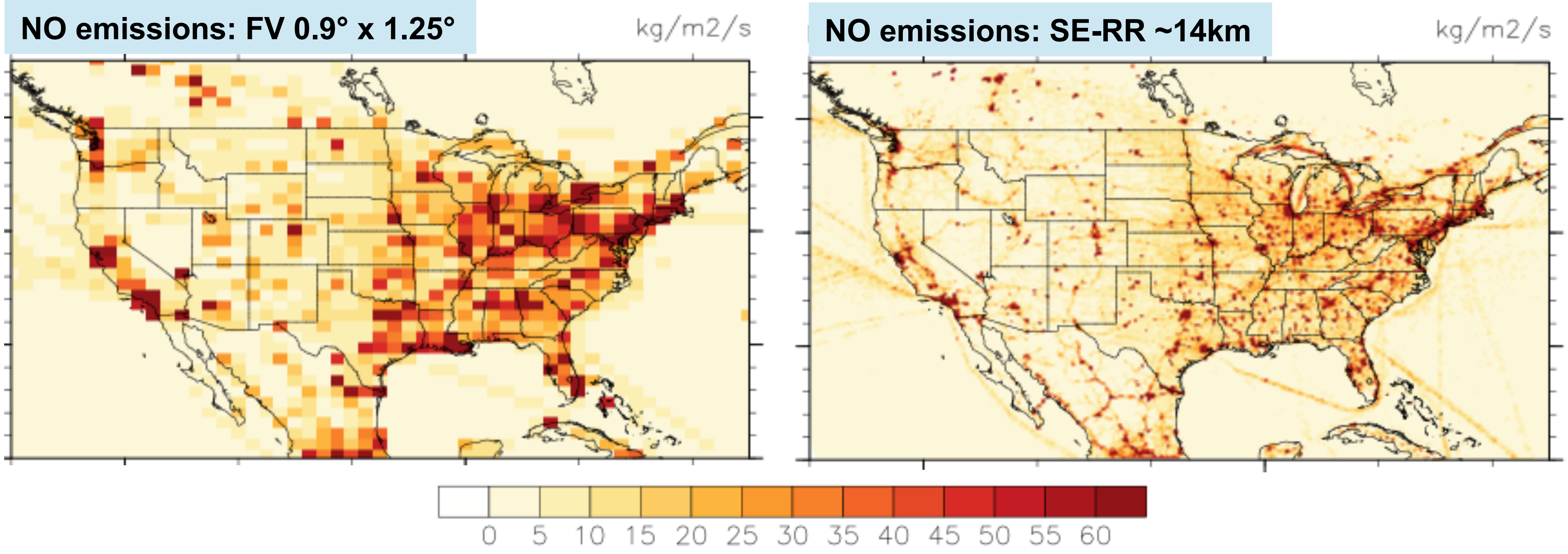
Updates for CESM2.2

- Functionality of spectral element (SE), and CSLAM compsets in CAM-chem -- still being evaluated and scientifically validated
- Compset for Regionally Refined configuration of Spectral Element in CAM-chem CAM-chem-SE-RR(conus), aka ***MUSICA-V0***
- Compsets for nudging to observed meteorology on model levels, for FV, SE, SE-RR configurations (replacing Specified Dynamics on GEOS/MERRA levels)
- Update to secondary organic aerosols (SOA): NOx-dependent VBS-SOA formation (in TS1 and TSMLT1 chemistry)
- Compset for MOZART-T2 (expanded isoprene & terpene oxidation) [R. Schwantes et al., *ACP*, 2020]
- Online ocean emissions (OASISS) of DMS, VOCs [S. Wang: *GRL*, 2019; *JGR* in rev.]

MUSICA-V0: CAM-chem-SE-RR(conus)

- Spectral Element dycore permits variable resolution (regional refinement)
- Simulations of CAM-chem with CONUS RR are being evaluated for resolution impacts on chemistry and air quality
- Anthropogenic emissions at 0.1 degree horizontal resolution are conservatively regridded to standard CESM 1 degree and SE Regionally Refined approximately 1/8 degree (14 km)





Impact of resolution on chemistry

Comparison of 1-degree (ne30) Spectral Element grid to 1/8-degree (~14km) regional refinement over continental US

Hourly output of surface ozone – Aug 9, 2013 18Z

Shows more resolved urban pollution

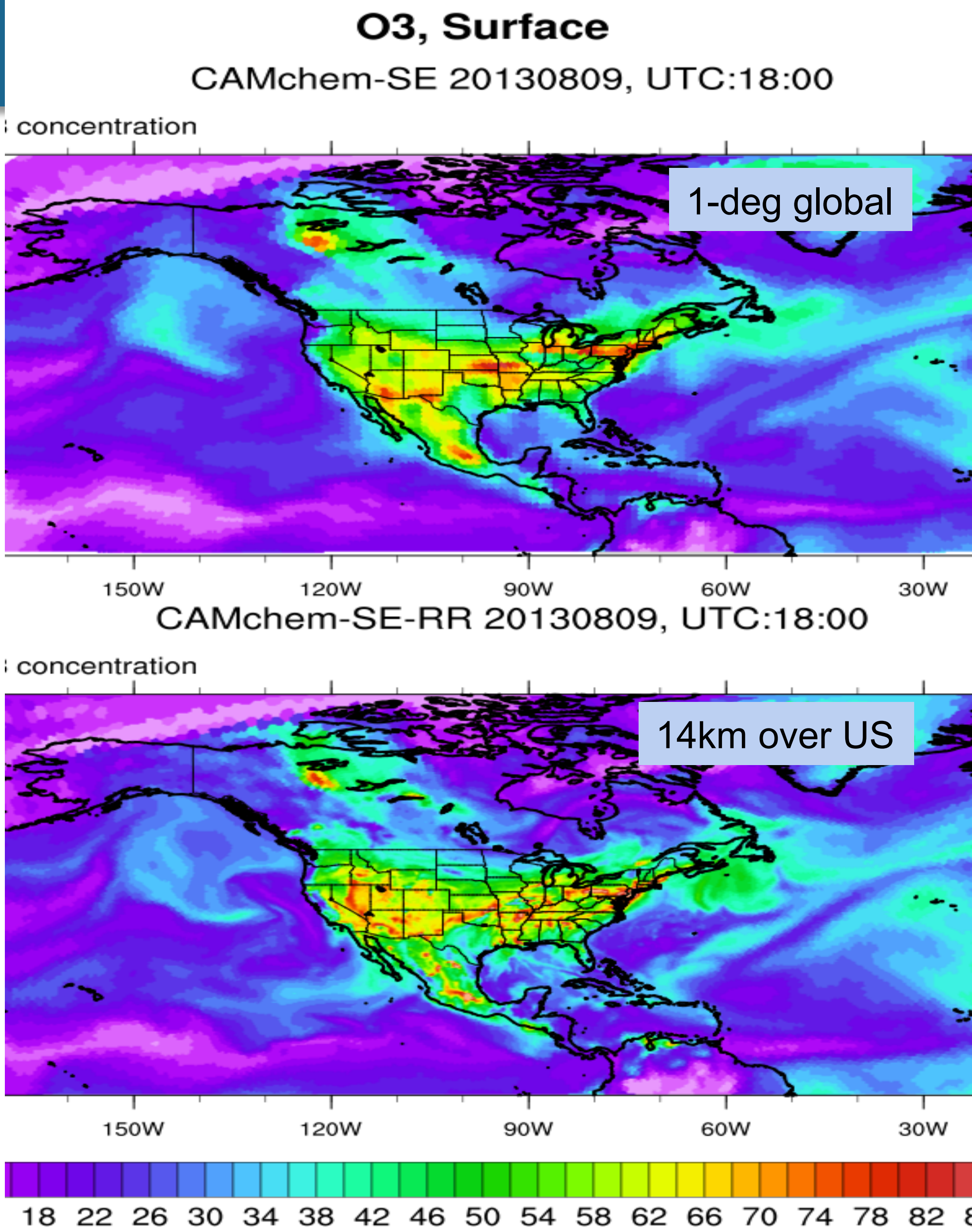
General features of distribution the same, but higher ozone mixing ratios in RR(conus) over Atlantic and Gulf of Mexico in continental outflow

Model description and evaluation papers in prep. by Becky Schwantes and Forrest Lacey

Compset in CESM2.2 for this configuration

Online tutorial is being developed:

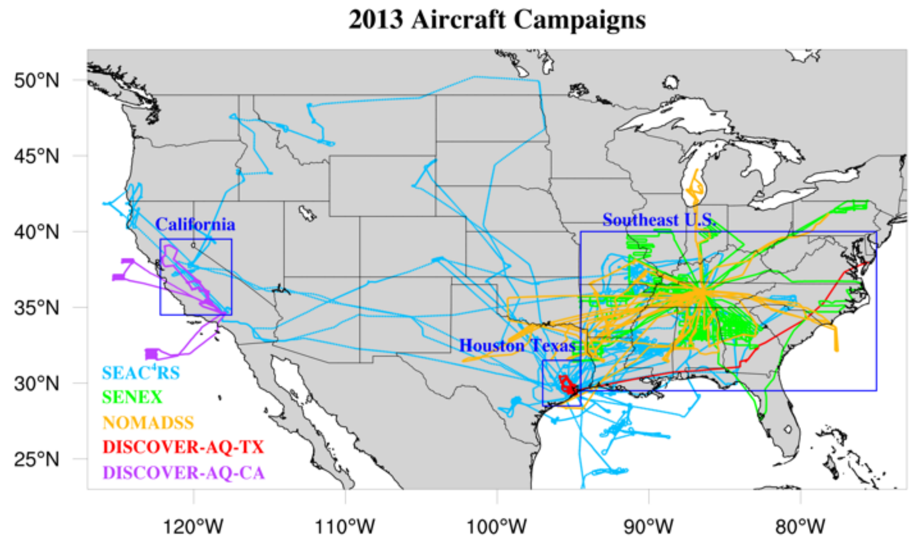
https://www2.acom.ucar.edu/workshop/musica-tutorial-2020

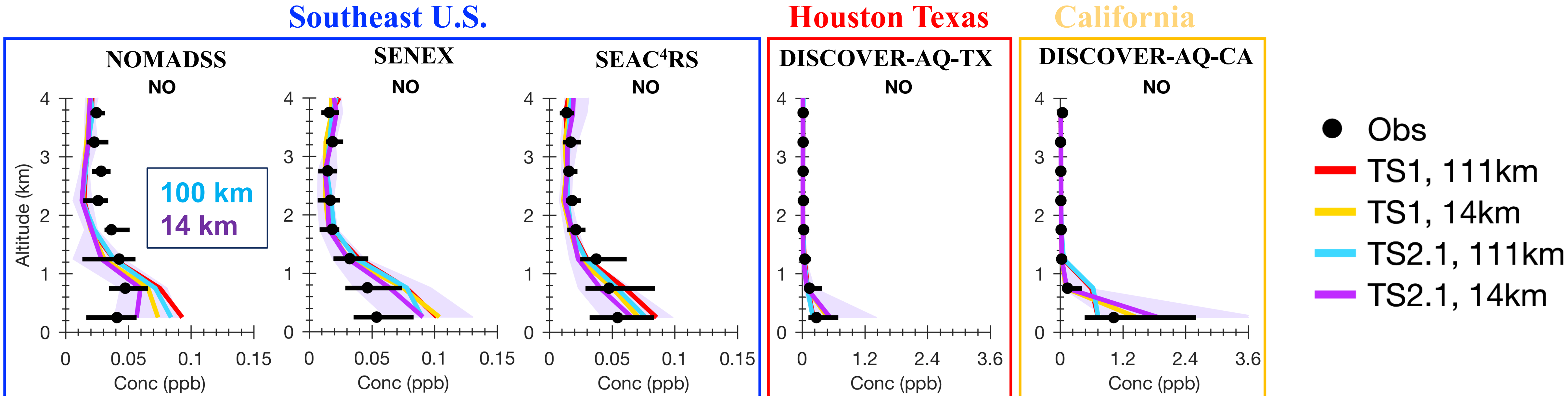


MUSICA-V0 evaluation with aircraft observations

Detailed comparisons against 5 field campaigns over the US are in progress

Ozone precursors NO_x, CO, and VOCs are generally better represented at the finer horizontal resolution of 14 km (purple) compared to the coarser resolution of 111 km (blue).



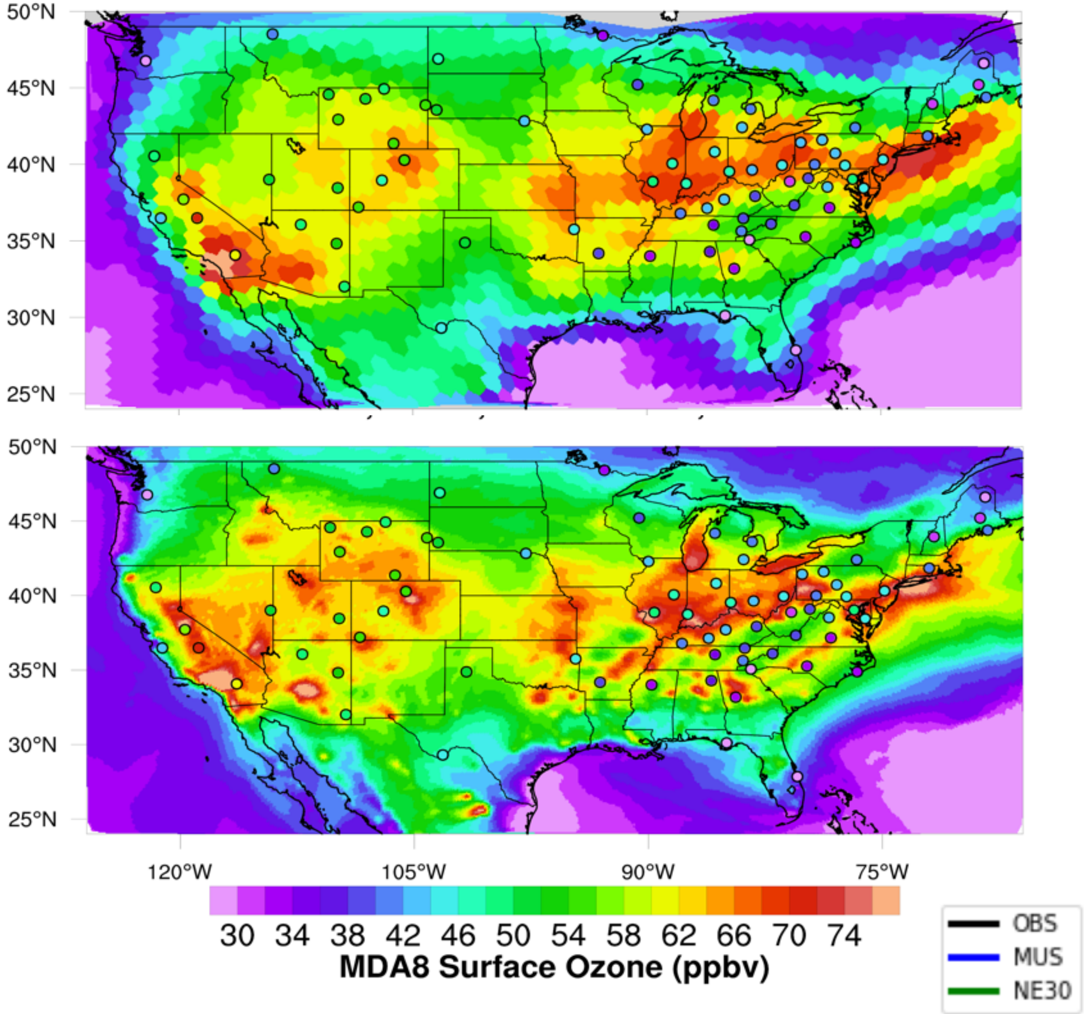


(Schwantes et al., 2020 - in preparation)

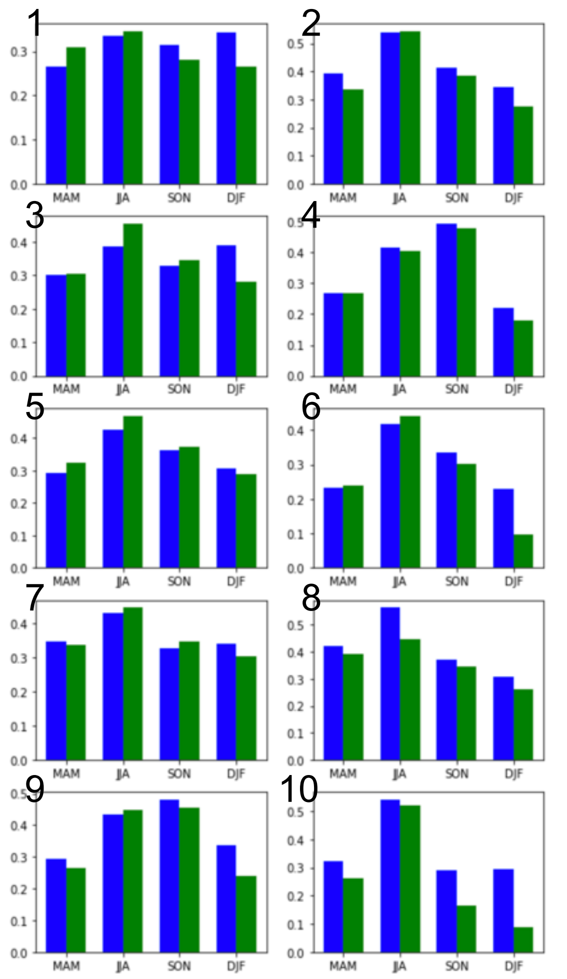
MUSICA-V0 evaluation with surface observations

Surface comparisons of ozone also show regions of improvement (using CASTNET and EPA AQS sites) especially in regions with spatially diverse emissions and meteorology

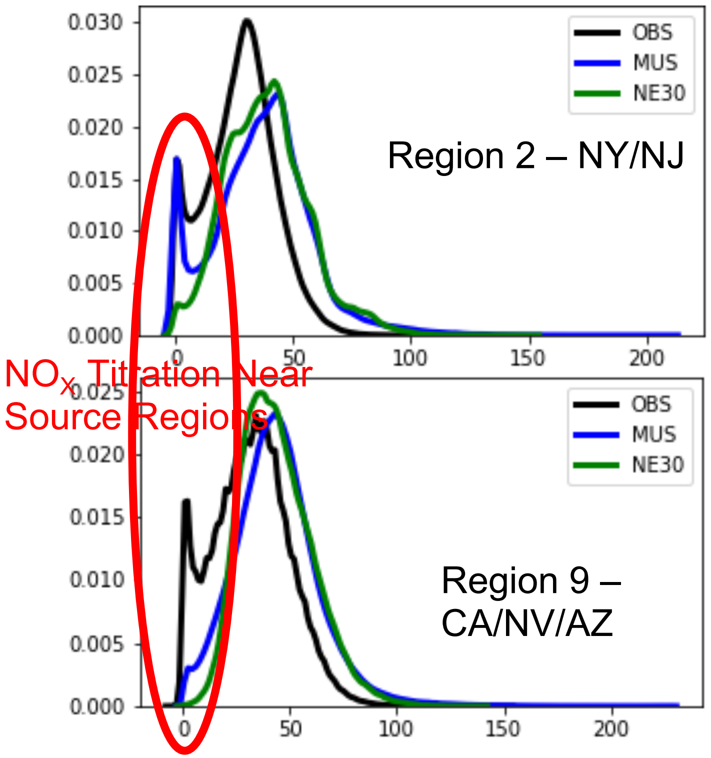
Summertime MDA8 CASTNET Comparison



EPA AQS Region Observation R^2



Region Specific Frequency Distributions



In particular localized O_3 production and loss in urban-dominated regions is improved

(Lacey et al., 2020 - in preparation)

CESM Nudging Module

Patrick Callahan, CGD

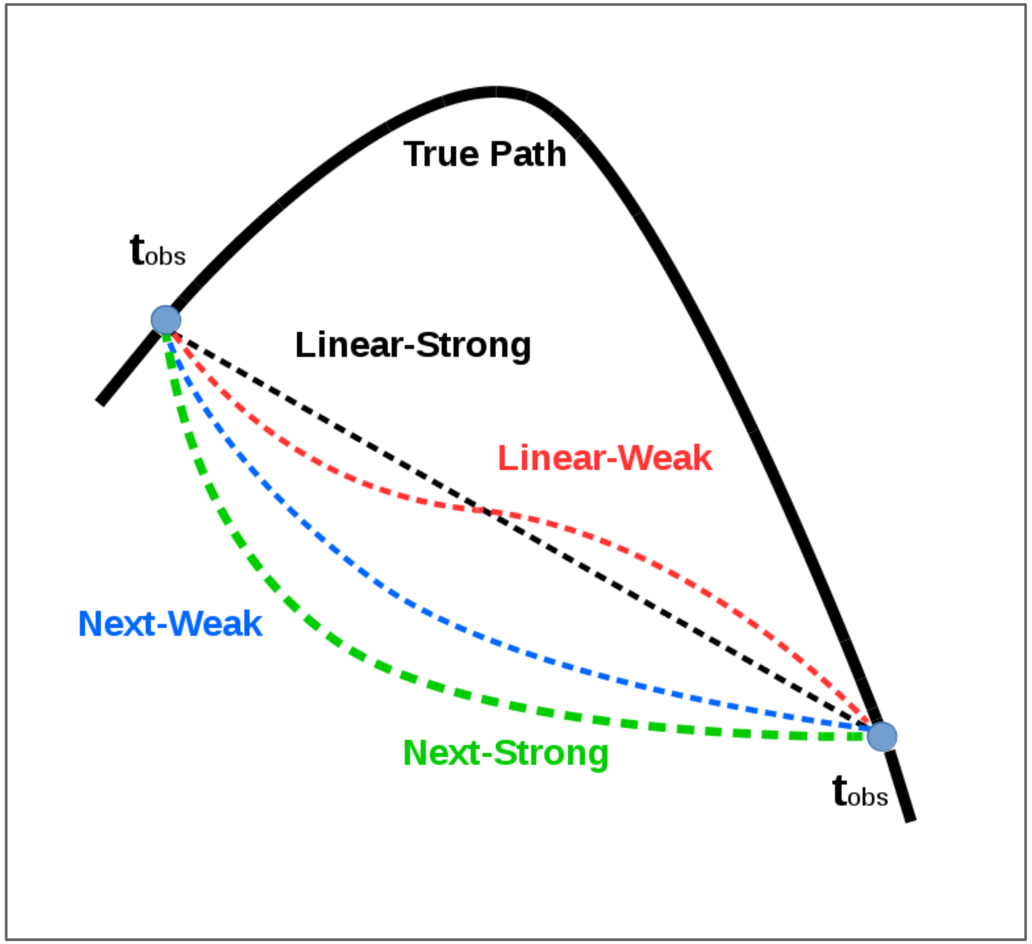
Nudge model toward observed (reanalysis) T, U, V, Q on CESM model levels

Implementation:

- Nudging is implemented as a relaxation tendency.

$$N_x = \frac{\propto}{\Delta T_{nudge}}\left(X_{target} - X_{model}\right)$$

- $\propto$ = Normalized relaxation coefficient between [0.,1.]
- Target data X_{target} is either:
  - **NEXT**: Target are the OBS values at the next OBS time.
  - **LINEAR**: Target is a linear interpolation of nearby OBS values to the current model time.
- The strength of the nudging time scale ΔT_{nudge} is either:
  - **WEAK:** The nudging time scale is equal to the time step between OBS values.
  - **STRONG:** The Nudging time scale is equal to the difference between the next OBS time and the current model time.



Reanalysis data are pre-processed onto model grid (horizontal and vertical)

Nudging settings are specified in CAM run-time namelist

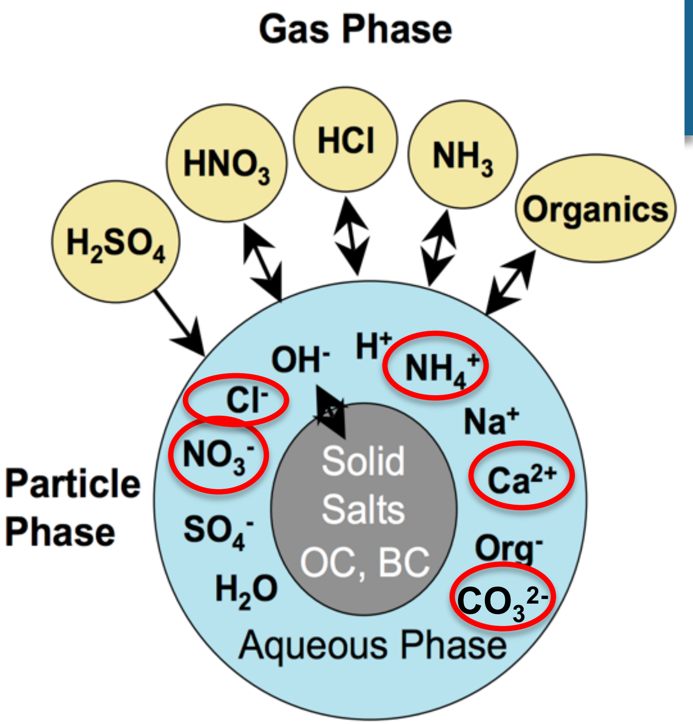
Developments for CESM2.3

Being evaluated further and tuning model for climate simulations

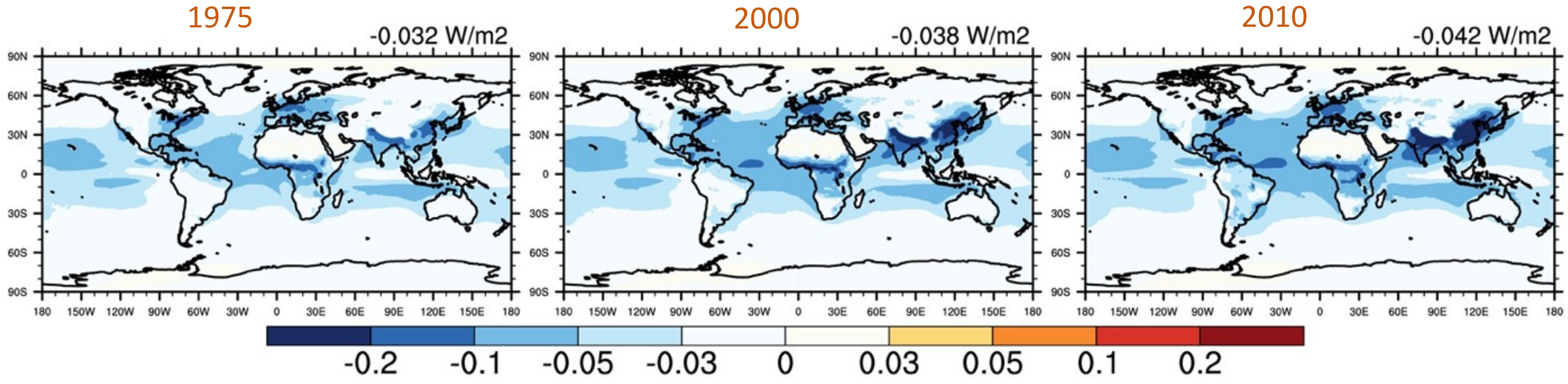
- MOSAIC gas-aerosol exchange – allows simulation of ammonium and nitrate aerosols [with MAM4 in CESM2, Lu et al., JGR, in review]
- MAM5: additional mode for coarse sulfate in stratosphere
- Aerosol wet scavenging improvements – improves aerosol distributions at high altitudes, high latitudes [Shan et al., in prep.; P. Yu, 2019]
- Brown Carbon radiative effects – locally important [Brown, ACP, 2018]
- New dust emissions scheme [Li, Mahowald, et al., in prep.]

Nitrate Aerosols in CESM2

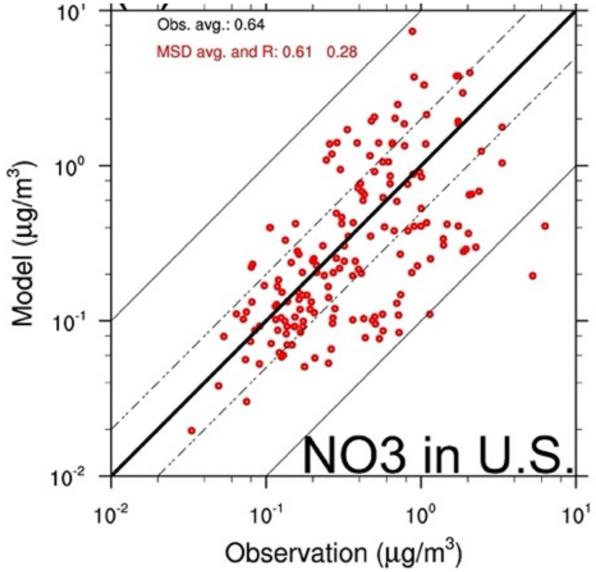
- Model for Simulating Aerosol Interactions and Chemistry (MOSAIC) module [Zaveri et al., 2008] is coupled with MAM4 in CESM2 to treat gas-particle partitioning of nitrate.
- The code is currently being polished (i.e. removing CPP macro)
- A paper on nitrate simulated by MOSAIC/CESM2-MAM4 is under review [Lu et al., JGR, 2020].



Red circles: new aerosol species



Direct radiative effect of nitrate as modeled by CESM2-MAM4-MOSAIC : significantly increasing especially over developing countries, like China and India from 1970s to 2010s (Lu et al., 2020)

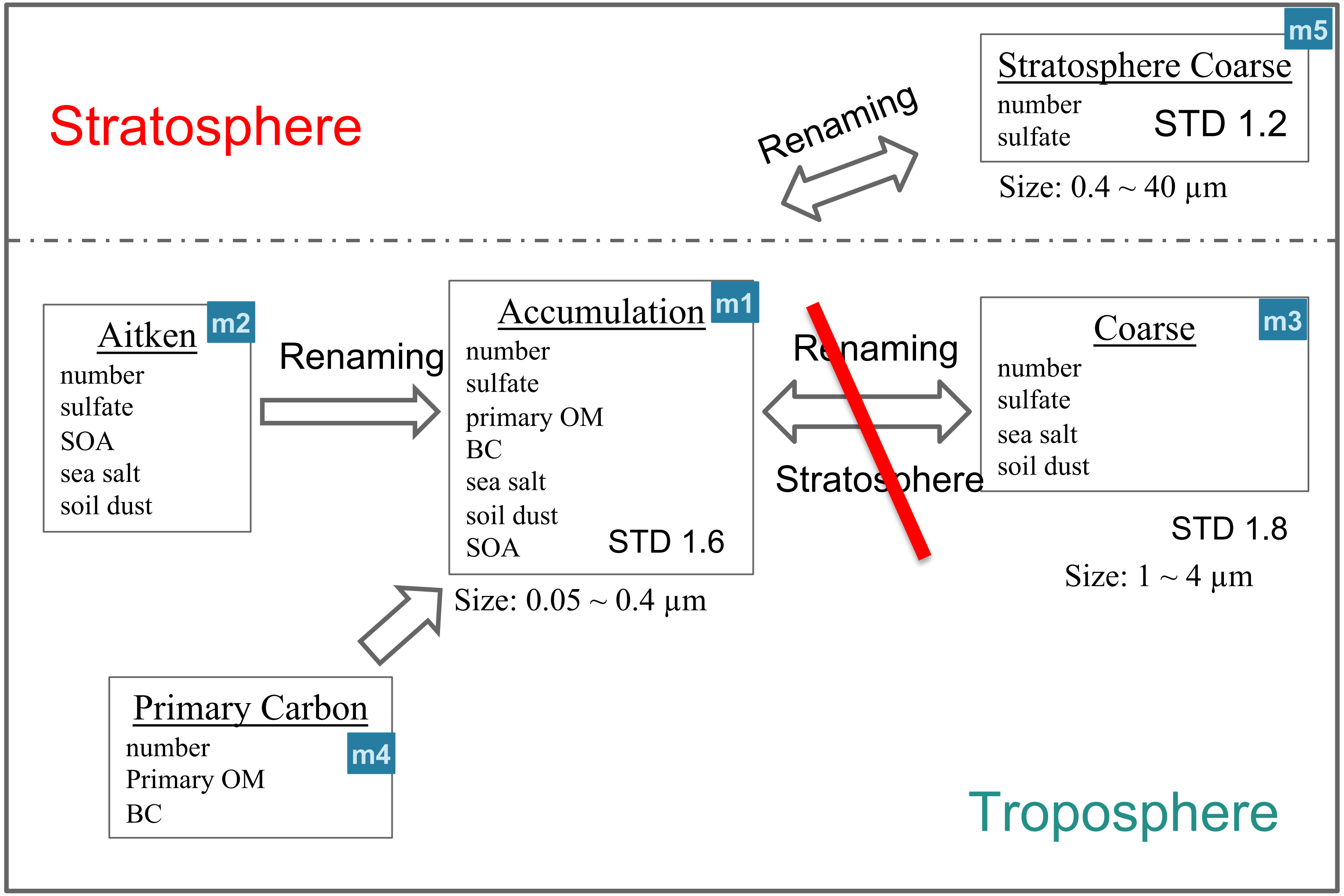


Modeled nitrate mmr agrees well with observations

Z.Lu and X.Liu

WACCM-MAM5 Schematic Chart

Ke and Liu



Purpose: maintaining sulfate aerosol in the stratosphere with minimum increase in computational cost

Motivation:

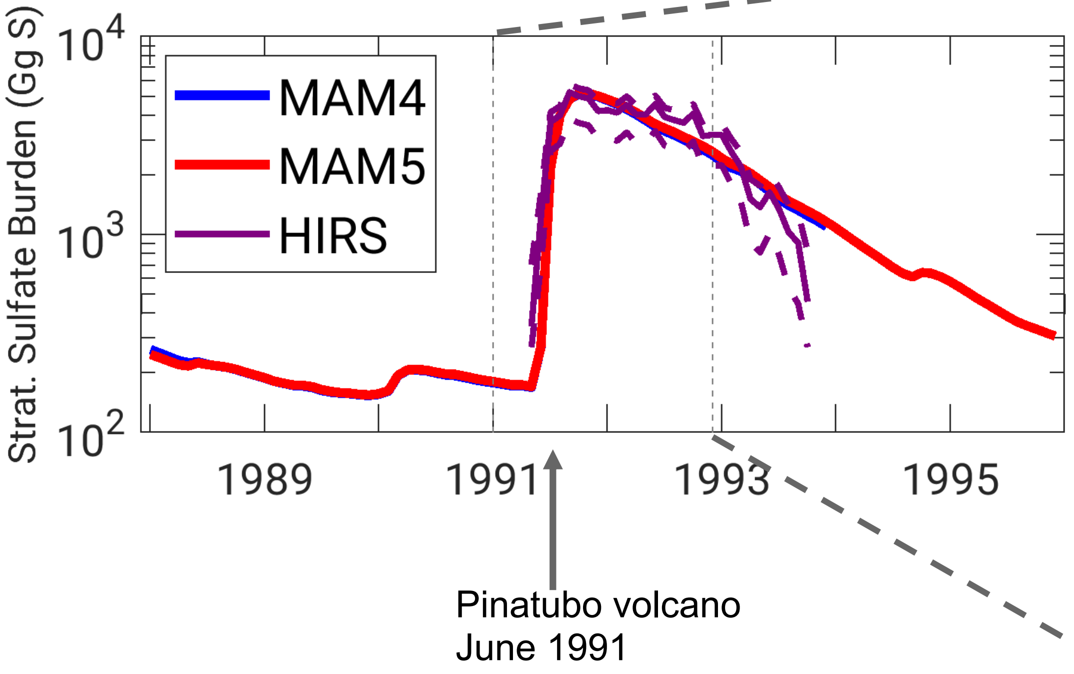
- Current MAM4 coarse mode uses a low STD (1.2) and small sizes to maintain the stratosphere sulfate burden, which causes biases of dust and sea salt in the troposphere

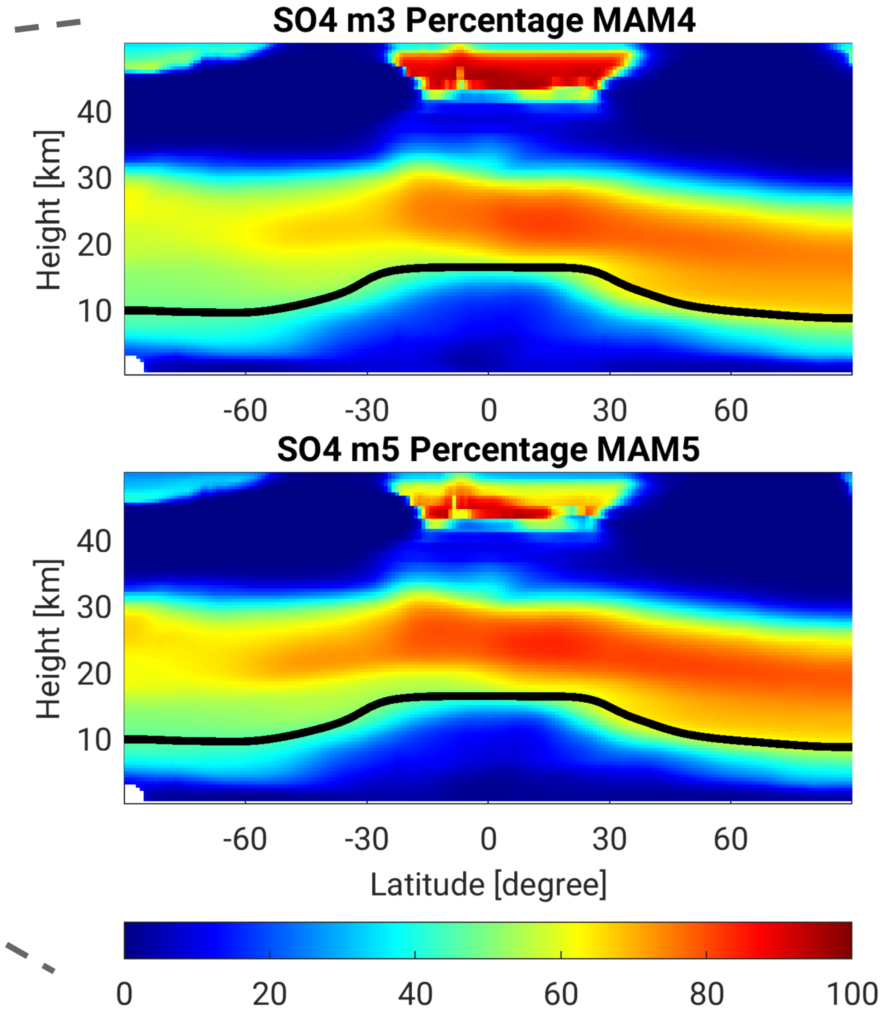
Changes:

- Add the stratospheric coarse mode (Mode 5) for stratospheric sulfate aerosol
- Set tropospheric coarse mode STD and size range back to those used in CAM5

Stratospheric Sulfate Aerosol Burden Comparison

Ke and Liu



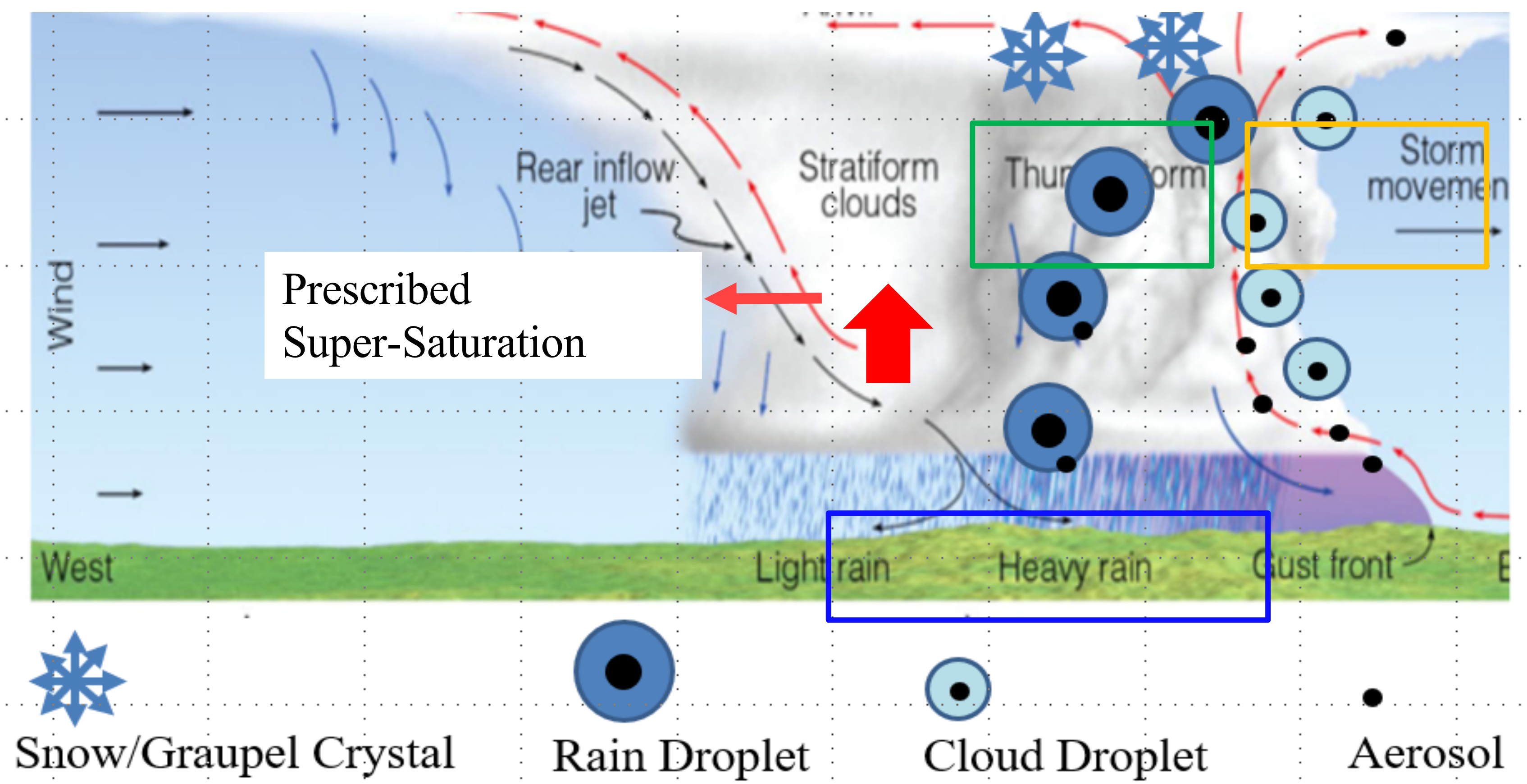


1991-1992 mean sulfate burden in modes

MAM5 reproduces the stratospheric sulfate aerosol burden compared to MAM4 by adding Mode 5

Improvement in aerosol scavenging in convective clouds

Shan and Liu



$$\left(\frac{\partial q_{ec}}{\partial t}\right)_{up} = \frac{\partial(M_u q_{uc})}{\partial p} - \frac{\partial(M_u q_{ec})}{\partial p} + ACT \cdot q_{ei} - WET \cdot q_{ec} + RES \cdot q_{ec}$$

Cloud-borne Aerosol conc. | **Sub-grid transport budget (coming-in minus -out)** | **Activation** | **Scavenge** | **Resuspension**

Aerosol resuspension by Bergeron process

$$WET = \frac{PREC - RBERG}{PREC + CLDM}$$

Aerosol secondary activation in cumulus

Convective cloud-borne aerosol detrainment

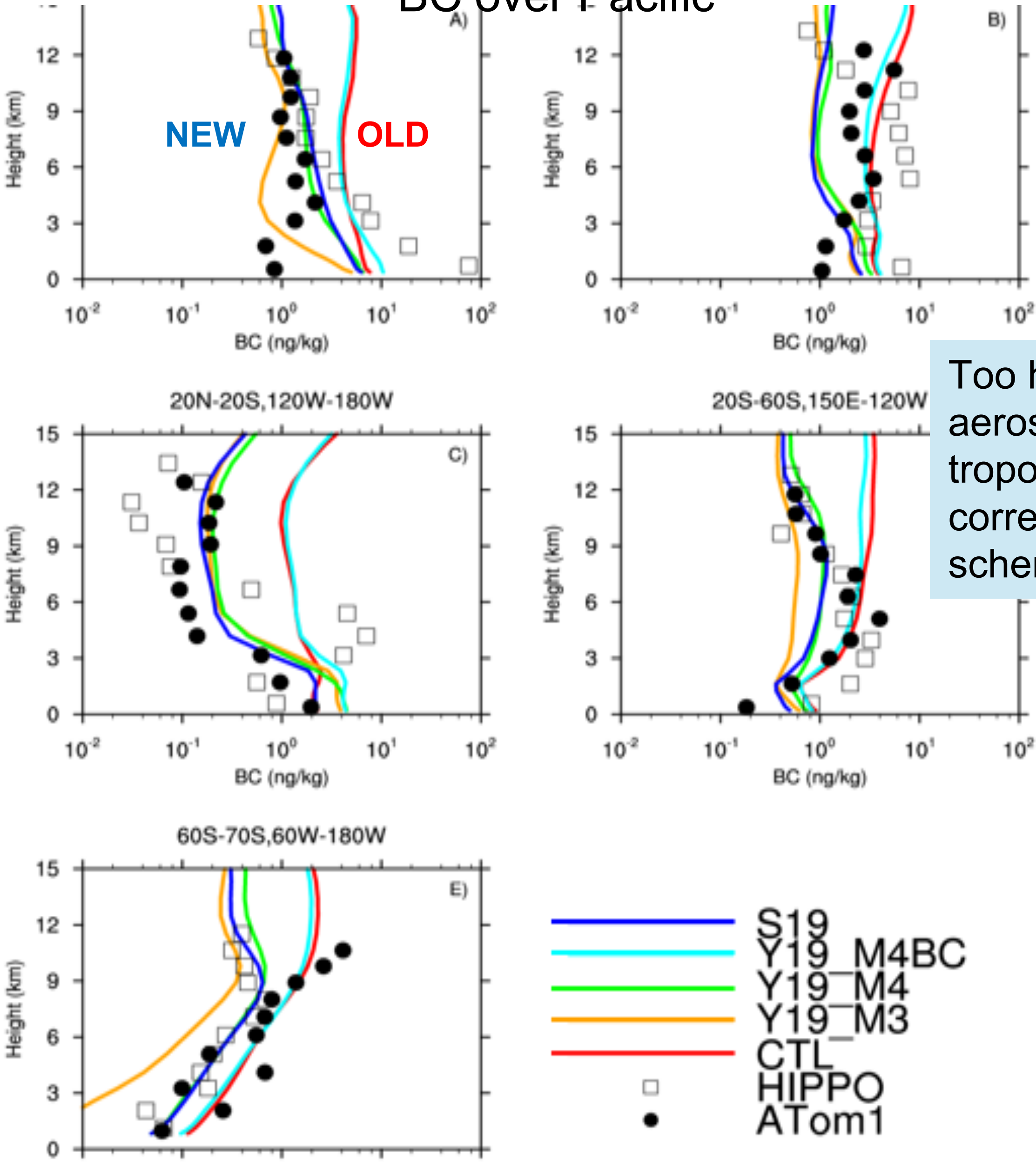
Resuspension by rain-water total evaporation

$$RES = -\frac{REVA}{PREC + CLDM}$$

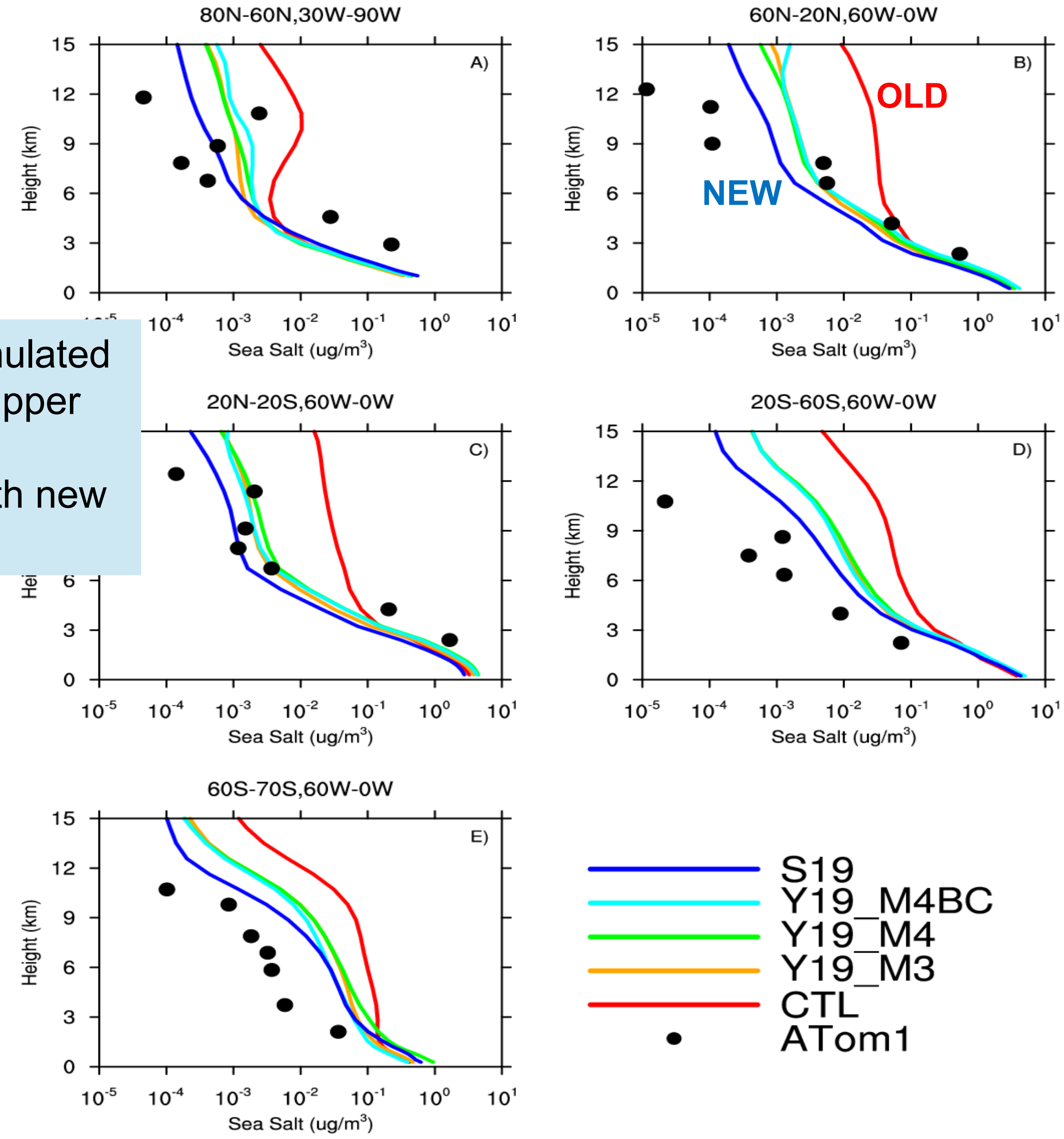
Improvements in simulated BC & sea salt profiles

Shan and Liu

BC over Pacific



Sea salt over Atlantic



Too high simulated aerosols in upper troposphere corrected with new scheme

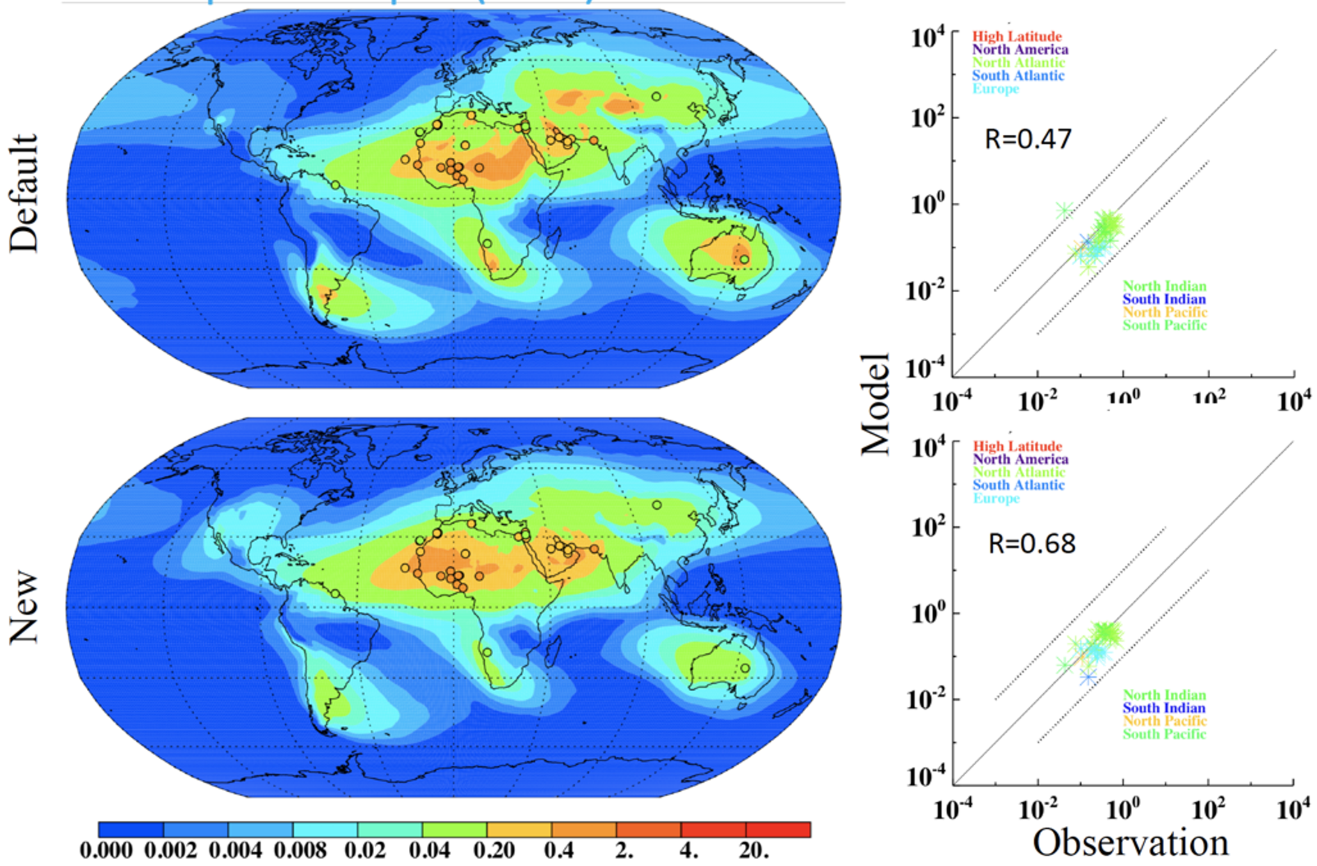
Improvements in desert dust algorithm

Li, Mahowald - Cornell

3 main improvements:

1. return of coarse mode size to CAM5 sizes
   a. Default coarse mode is too small in CAM6
   b. important for radiative forcing estimates for dust and seasalts
2. Introduction of Kok et al., 2014 scheme.
   a. Improves comparison with obs.
   b. Does not require soil erodibility map
3. Inclusion of dust asymmetry effects into optics --> better comparison with obs.

Dust Aerosol Optical Depth (AOD)



Longlei Li, Natalie Mahowald, Jasper Kok and others…..

Li et al., in prep.

Also possible to calculate dust mineral impacts on radiation, iron oxides, etc. (Li et al., 2020; Hamilton et al., 2019; etc.)

Additional developments

- Connecting GEOS-Chem module and HEMCO emissions module to CESM2 (MIT & Harvard)
- Soil NO, NH_3, N_2O emissions in CLM (Maria Val Martin, Sheffield U.)
- Soluble iron from dust, fires, anthropogenic sources, deposited for marine and terrestrial biogeochemical response (D. Hamilton & N. Mahowald, Cornell U.)
- TUV online photolysis rate calculation
- Simpler chemistry for climate applications
- More complex chemistry (speciated larger alkanes, very short-lived halogens)
- Coupling fire emissions from CLM to CAM-chem:
  evaluation with FIREX-AQ & WE-CAN, climate feedbacks, plume rise

Coupling GEOS-Chem to CESM – Harvard & MIT

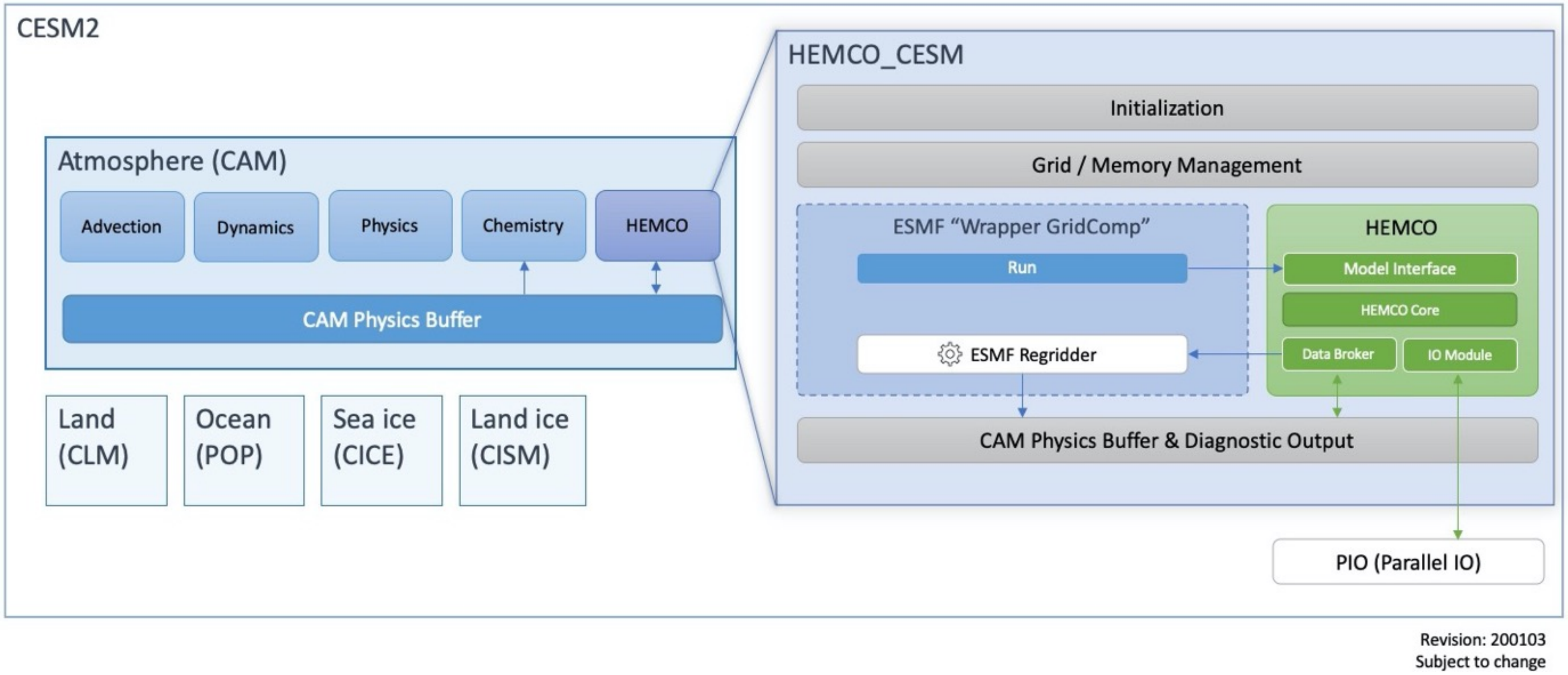
Coupling of GEOS-Chem to CESM is underway, with a functioning prototype in place

The project is being used as an opportunity to address “invisible” interdependencies in CESM

Enabling greater modularity – including (for example) the option to select either static (data) or dynamic (CLM) land surface data for dry deposition

HEMCO-CESM Architecture

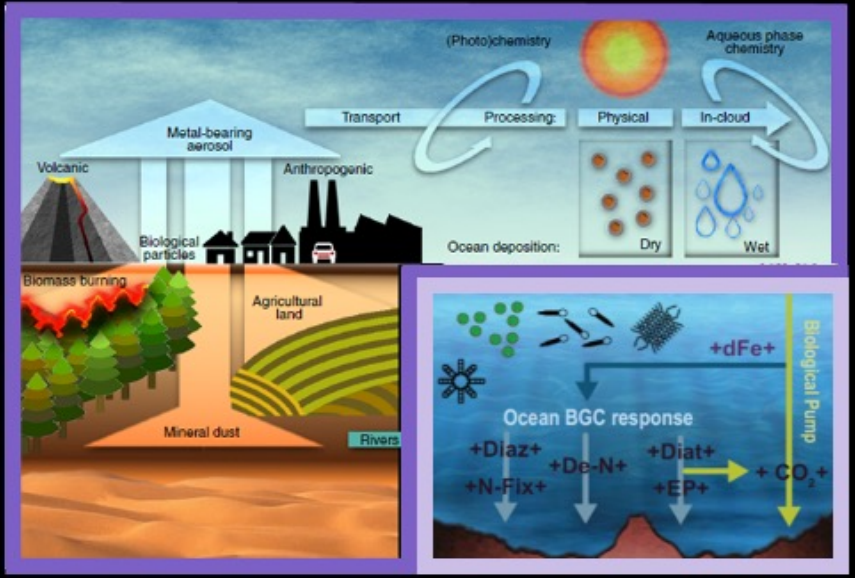
This includes implementation of HEMCO in CESM, enabling emissions (or other) data to be acquired from disk at arbitrary resolution, conservatively regridded, and passed to any module – including CAM-chem and GEOS-Chem



Mechanism of Intermediate complexity for Modelling Iron (MIMI v1.0)

Hamilton et al. (2019) GMD

Iron is an essential component of the Earth system which requires more study on climate, health, and biogeochemistry impacts. Aerosol soluble iron is a new source to marine ecosystems and fuels primary productivity where it is the limiting micronutrient.

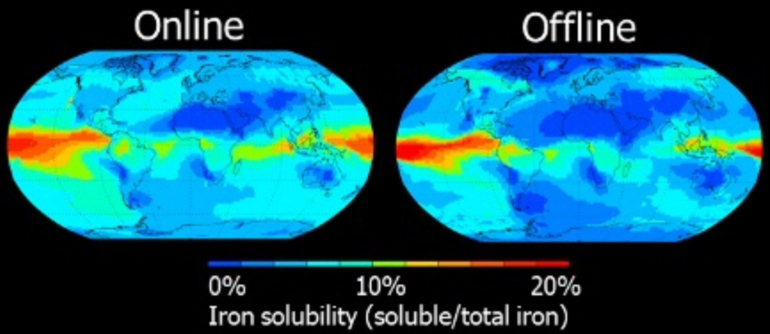


MIMI does this:

- Natural iron emissions with dust and fires: both of which are coupled/online;
- Anthropogenic activity iron emissions: offline from inventory;
- Further dissolution of iron to a soluble(bioaccessible) form during transport;
    - Acid processing of interstitial aerosol;
    - Organic-ligand (oxalate) processing of cloud-borne aerosol;
- and requires minimal core-cores to run for CAM6.

So as to better quantify the marine (and terrestrial) biogeochemical response

MIMI is an intermediate complexity iron aerosol module, originally designed for the DoE E3SM model, and now coupled to CAM(4-6)
MIMI has been tested against observations and has provided fields to the ocean BGC model (Hamilton et al. 2020)



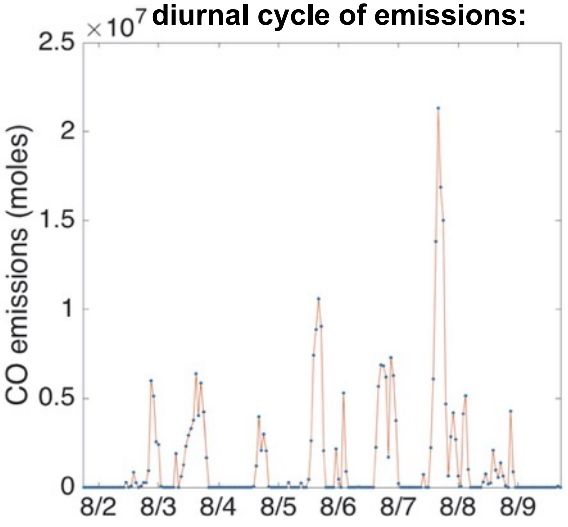
Coupling MIMI is important as simulated iron solubility (percent iron bioaccessible) is sensitive to temporal resolution. Coupling at every model time-step (online) has a very different spatial pattern than forcing using monthly mean (offline) estimates.

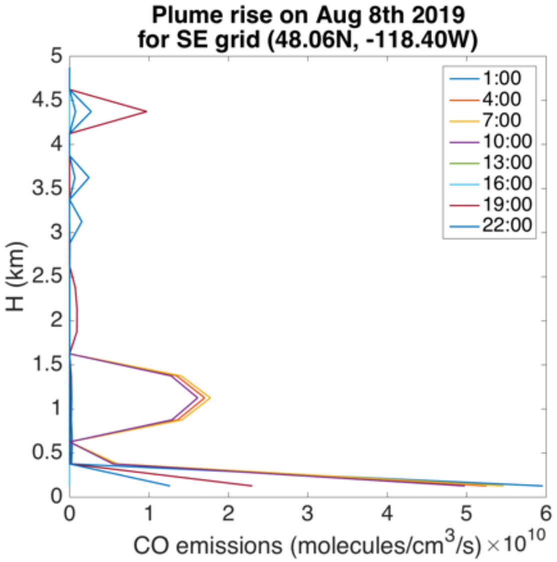
Interactive fires in CLM coupled to CAM-chem

- Testing and evaluating climate simulations with CLM fires generating emissions for atmospheric chemistry
- Adding diurnal cycle and plume rise to fire emissions in CAM-chem
- Evaluating the improvement with observations from the 2019 FIREX-AQ field campaign

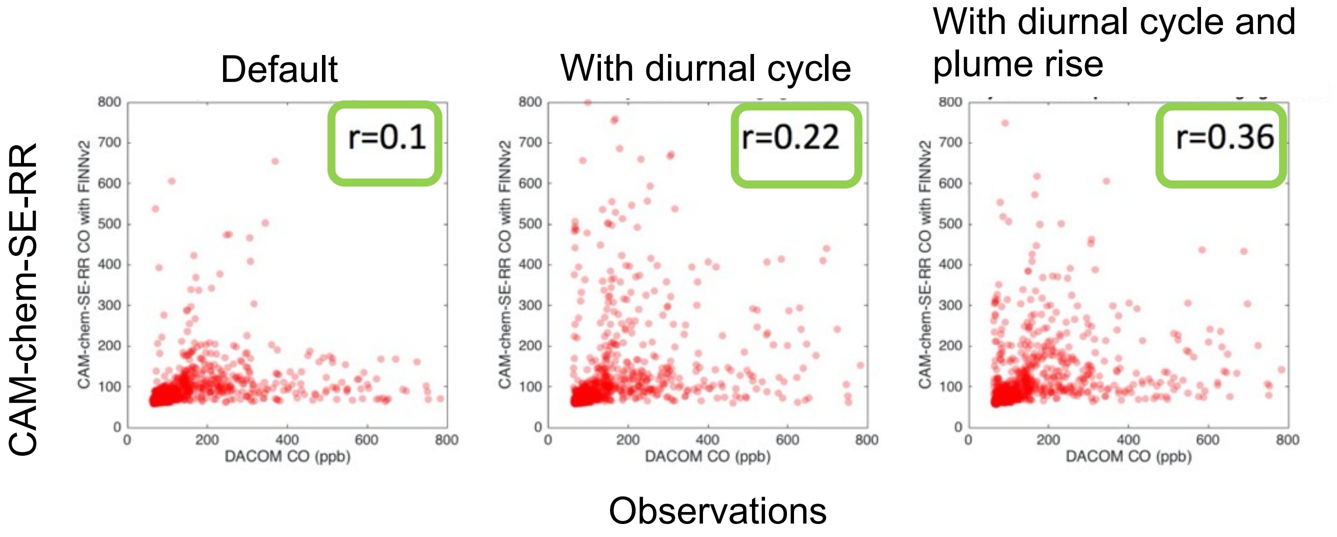
Example: Williams Flats fire (Aug 2-10, 2019; 47.94N, -118.62W)

Demonstration of diurnal cycle and plume rise of fire emissions





Preliminary model results



Wenfu Tang – ASP postdoc, NCAR/ACOM

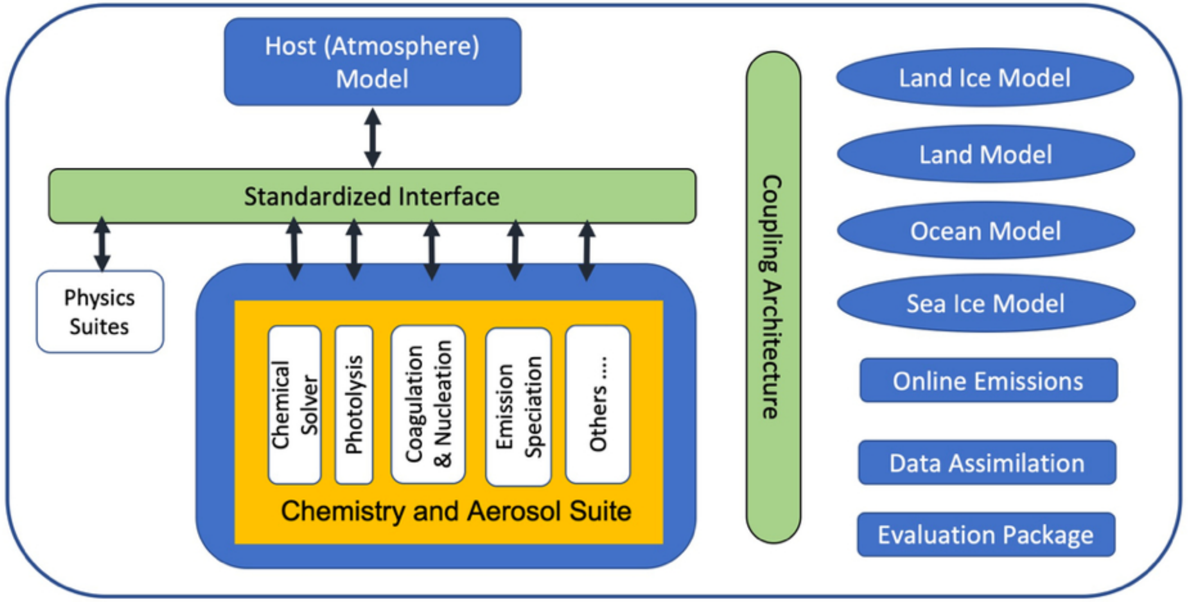
MUSICA: MUlti-Scale Infrastructure for Chemistry & Aerosols

A new model-independent infrastructure, which will enable chemistry and aerosols to be simulated at different resolutions in a coherent fashion

https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica

- MUSICA Vision paper accepted by BAMS (Pfister et al., 2020)
- Developing an Implementation Plan – ***community participation invited***
- Join a working group: https://www2.acom.ucar.edu/sections/musica-governance
  (chemical schemes, aerosols, emissions, multi-scale physics, whole atmosphere, data assimilation, model architecture)
- MUSICA is connected to SIMA,
  part of the upcoming SIMA workshop
  https://cpaess.ucar.edu/meetings/sima-2020

MUSICA-V0 (CAM-chem-SE-RR) being released as a compset in CESM2.2



Questions?

Please join the Whole Atmosphere & Chemistry-Climate WG session Tuesday afternoon

Email me: emmons@ucar.edu

Visit Chemistry-Climate WG webpage:
http://www.cesm.ucar.edu/working_groups/Chemistry/