Chemistry -Climate Working Group Status – February 2021

Louisa Emmons (NCAR) – co-chair

Xiaohong Liu (Texas A&M University) – co-chair

Simone Tilmes (NCAR) - liaison

Francis Vitt (NCAR) – Software Engineer

8 February 2021

New Features in 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*** → *presentations Thurs AM*
- 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: TS1.1 and TSMLT1.1 mechanisms
- Compset for MOZART-T2 (expanded isoprene & terpene oxidation) [R. Schwantes et al., *ACP*, 2020]
- Aerosol convective scavenging in CAM-chem [Shan et al., in prep.; P. Yu, 2019]

See past CESM workshop and WG presentations for more details

Developments for CESM2.3

Corrected Bugs:

- Surface Area Density – was missing pom_a1
- Simple SOA in CAM - removed erroneous reassignment of molecular weight in code

Being evaluated further and tuning model for climate simulations:

- MOSAIC gas-aerosol exchange – allows simulation of ammonium and nitrate aerosols
  - description paper: Rahul Zaveri, JAMES, in review
  - with MAM4 in CESM2: Zheng Lu et al., JGR, in review
- MAM5: additional mode for coarse sulfate in stratosphere → ***Ziming Ke's talk on Tuesday***
- New dust emissions scheme [Li, Mahowald, et al., in prep.] {see past CESM presentations}
- Brown Carbon radiative impacts → ***Hunter Brown's talk on Tuesday***
- Aerosol convective scavenging for CAM and WACCM (in only CAM-chem in CESM2.2)

Compsets for online ocean emissions from OASISS (acetone, acetaldehyde, DMS) [Siyuan Wang]

Very short-lived halogen chemistry → ***Rafa Fernandez's talk on Thursday***

Additional developments

- Connecting GEOS-Chem module and HEMCO emissions module to CESM2 (MIT & Harvard)→ ***Haipeng Lin's talk on Thursday***
- TUV online photolysis rate calculation
- Simpler chemistry for climate applications
- More complex chemistry (e.g., speciated larger alkanes)
- CARMA
- Coupling fire emissions from CLM to CAM-chem:
  evaluation with FIREX-AQ & WE-CAN, climate feedbacks, plume rise
- Soil NO, NH_3, N_2O emissions in CLM (Maria Val Martin, Sheffield U.)
- Air quality impacts of online Soil NO, NH_3 emissions (Anthony Wong, Jeff Geddes, Boston Univ.)
- MEGAN3 – biogenic emissions (Alex Guenther et al., UC-Irvine)

MUSICA
Multiscale Infrastructure for Chemistry and Aerosols

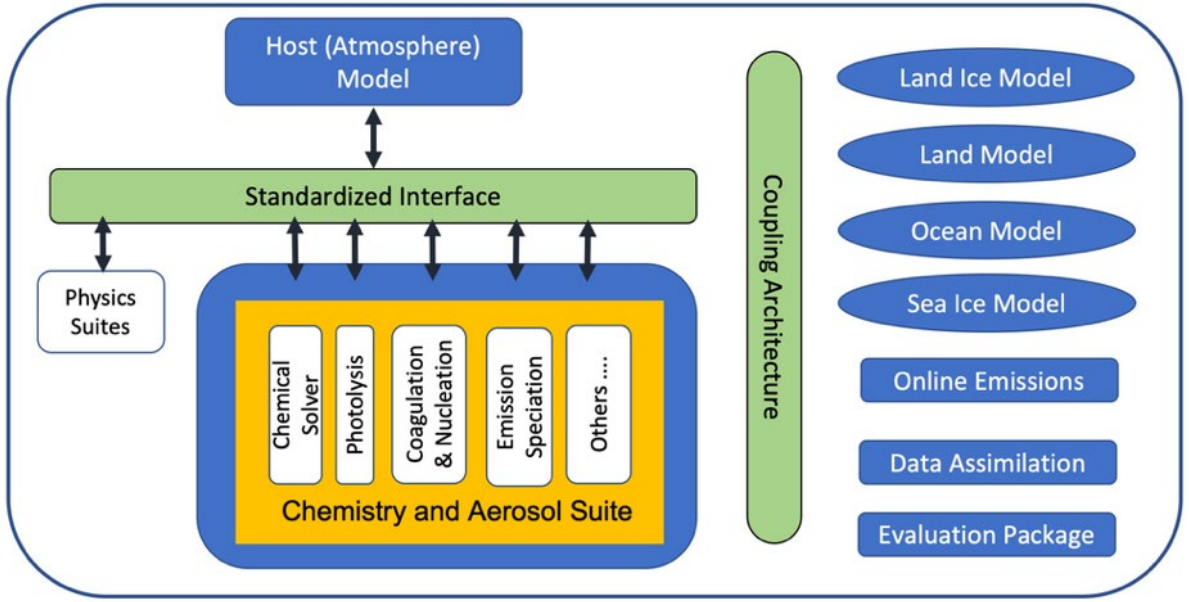
MUSICA: MUlti -Scale Infrastructure for Chemistry & Aerosols

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 in 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 being developed in partnership with SIMA: System for Integrated Modeling of the Atmosphere
  https://wiki.ucar.edu/display/SIMA/

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



MUSICA working groups

Model Architecture	Andrew Conley, Seb Eastham, Steve Goldhaber
Emissions & Deposition	Louisa Emmons, Claire Granier, Marc Guevara
Chemical Schemes	Bernard Aumont, Kelley Barsanti, John Orlando
Aerosols	Jerome Fast, Alma Hodzic, Xiaohong Liu
Physics, Transport, Subgrid	Mary Barth, Karen Rosenlof, Allison Steiner
Whole Atmosphere	Nick Davis, Lorenzo Palvani, John Plane
Evaluation & Data Assimilation	Ave Arellano, Ben Gaubert, Daven Henze, Simone Tilmes

Leads of each WG are writing implementation plans

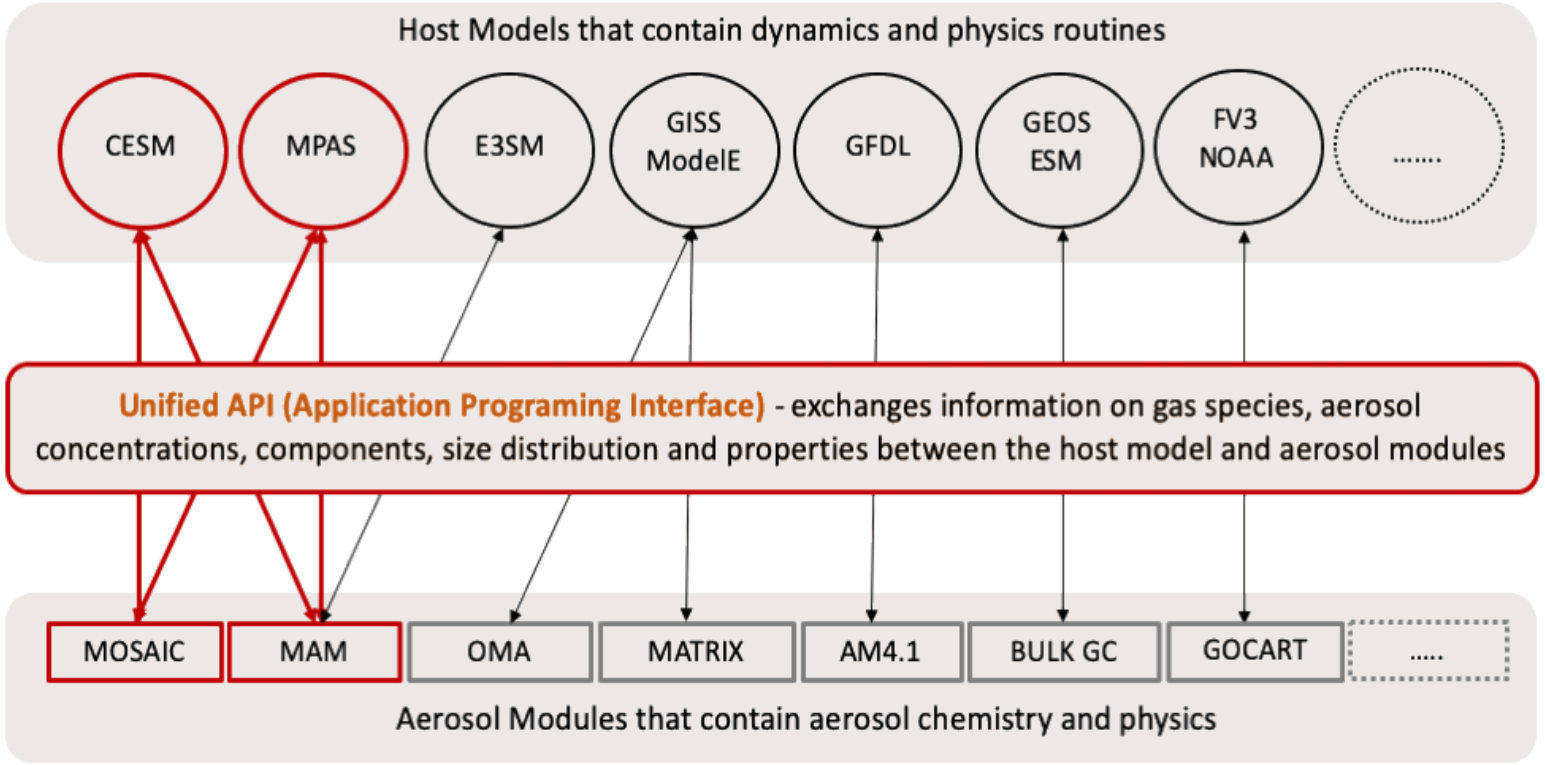
Outline software engineering plans for each WG

Bring together individual WG plans into one overall MUSICA implementation plan

Community Participation Invited

MUSICAL - Leveraging MUSICA to innovate on aerosol science in community models

- Community effort to build a generalized **aerosol programing interface** for use in weather/climate models.
- Facilitate the interchange of aerosol–chemistry models across current models, model updates and model intercomparisons.
- White paper drafted and being brought to attention of funding agencies.
- Participants: modelers from NCAR, Cornell, PNNL, NASA/GISS, GEOS-Chem, NOAA/GFDL, TAMU, U. Illinois



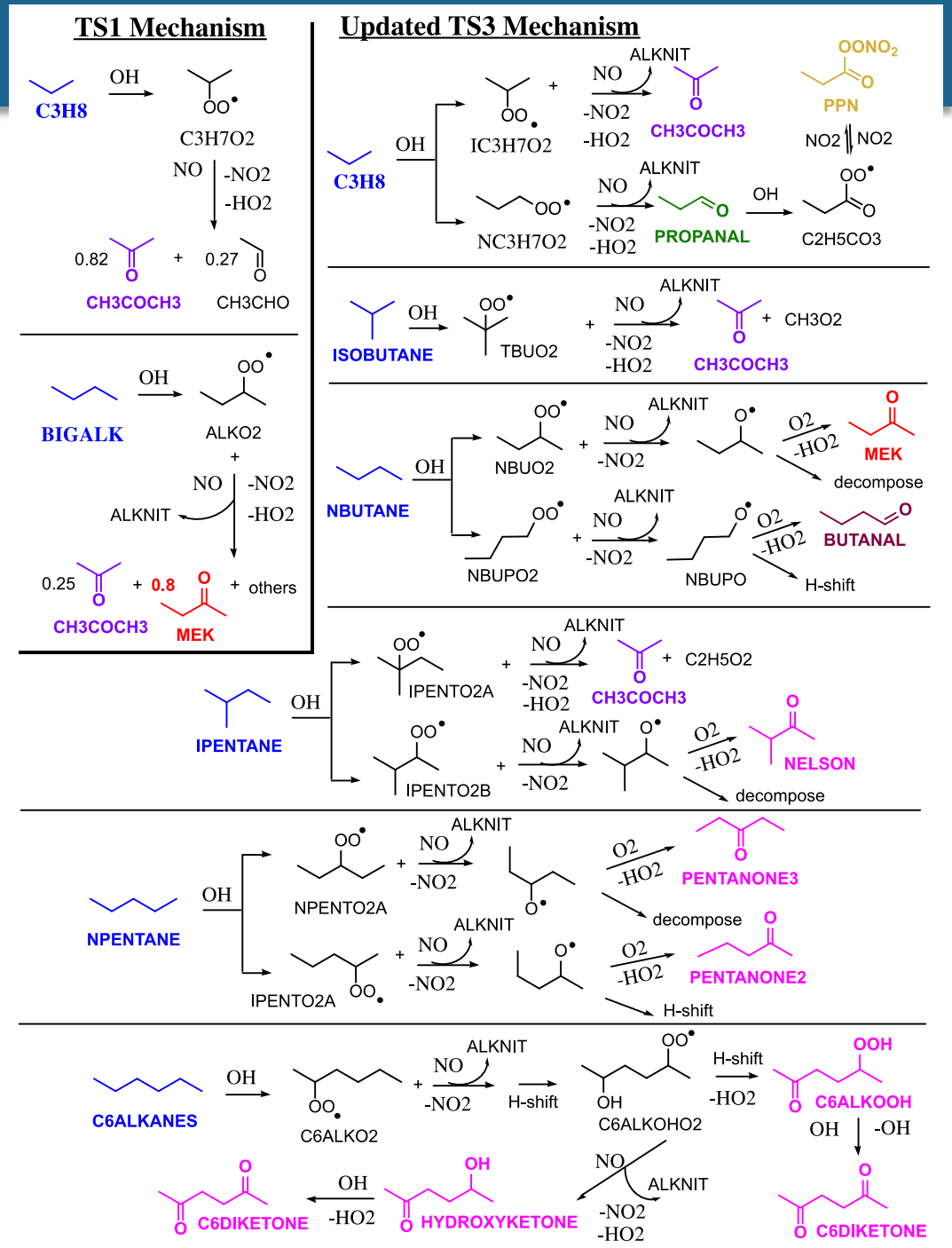
Please join the effort!

PIs : Natalie Mahowald (Cornell), Alma Hodzic (NCAR)

MOZART-TS3 Mechanism Development

Becky Schwantes - NOAA

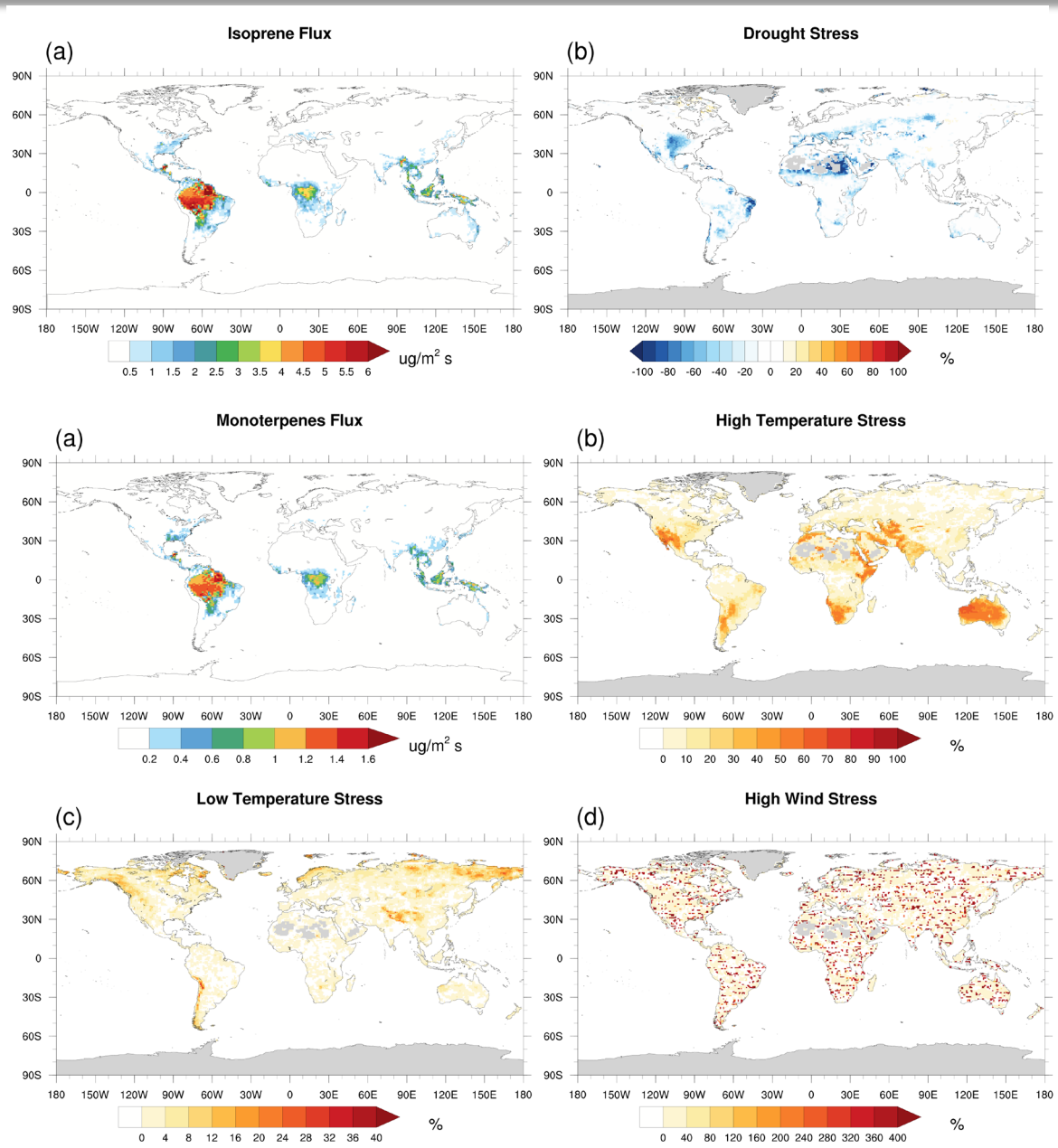
- MOZART-TS3 includes updated and more complex alkane oxidation chemistry
- Currently evaluating whether MOZART-TS3 improves alkanes and their oxidation products in the remote atmosphere against the ATom campaign



MEGAN3.1-CLM5

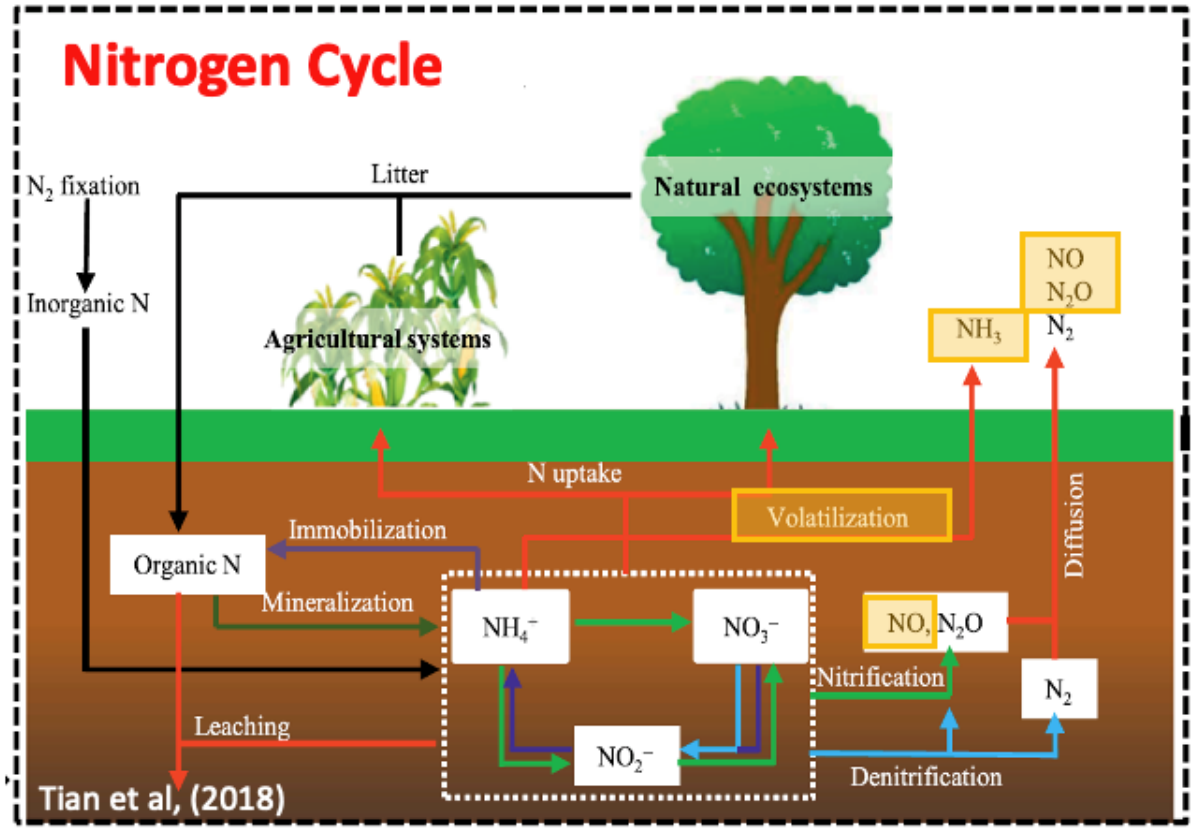
Hui Wang, Alex Guenther – UC-Irvine

- Expanded BVOC species from 150 compounds to **201 compounds**
- Accounts for response of isoprene emission to **drought stress** (Jiang et al. 2018);
- Accounts for the responses of monoterpenes and sesquiterpenes emissions to **environmental stresses** including:
  - High temperature (heat wave)
  - Low temperature
  - High wind
  - Air quality (ozone)
- Next steps:
  - Updated emission factors
  - Improved drought+heat response
  - Improved seasonal variations
  - Improved Arctic and Tropical responses



Nitrogen Emissions from Soil

Maria Val Martin – University of Sheffield



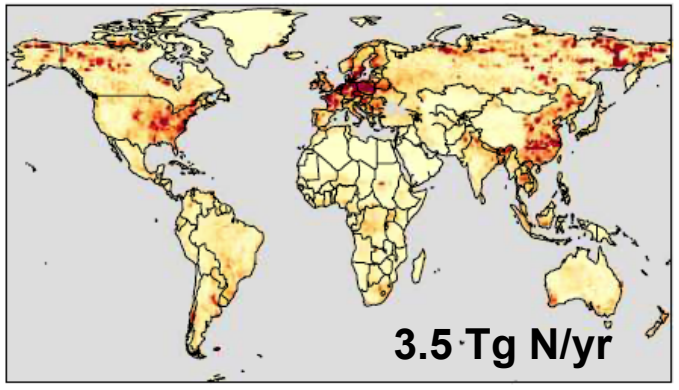
New Implementations

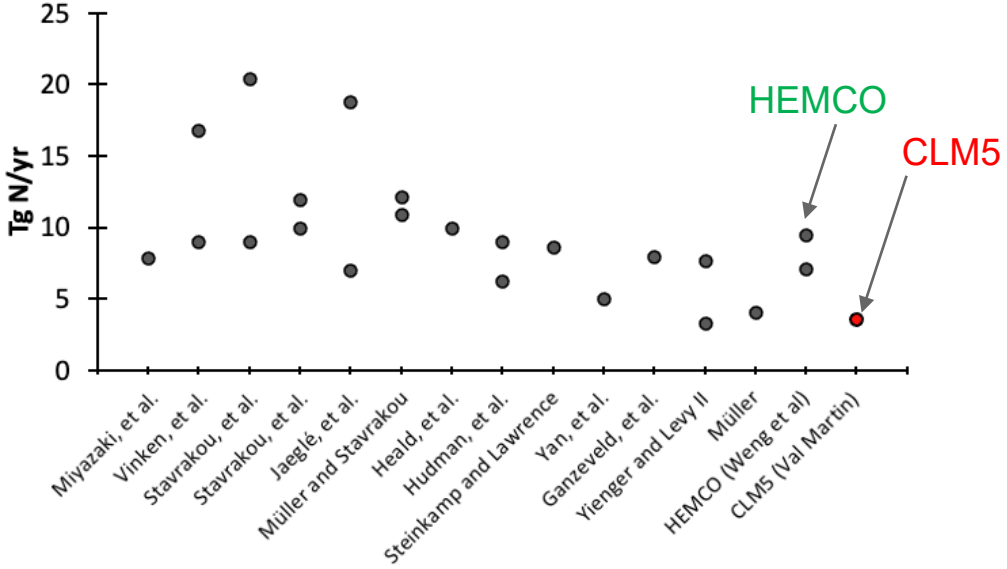
- Soil NO and NH_3 schemes implemented within the CLM5 N Cycle:
  - **Soil NO** based on DayCent (M Val Martin, Univ of Sheffield)
  - **Soil NH_3** (K M Fung, CUHK/MIT)
- **Bidirectional approach**: soil N_2O, NO and NH_3 are driven by soil properties and fertilization and N losses affect the remaining terrestrial N cycle
- **Bidirectional coupling**: soil nitrogen fluxes are coupled to CAM-chem and can be driven from N deposition from CAM-chem (F Vitt)

Nitrogen Emissions from Soil

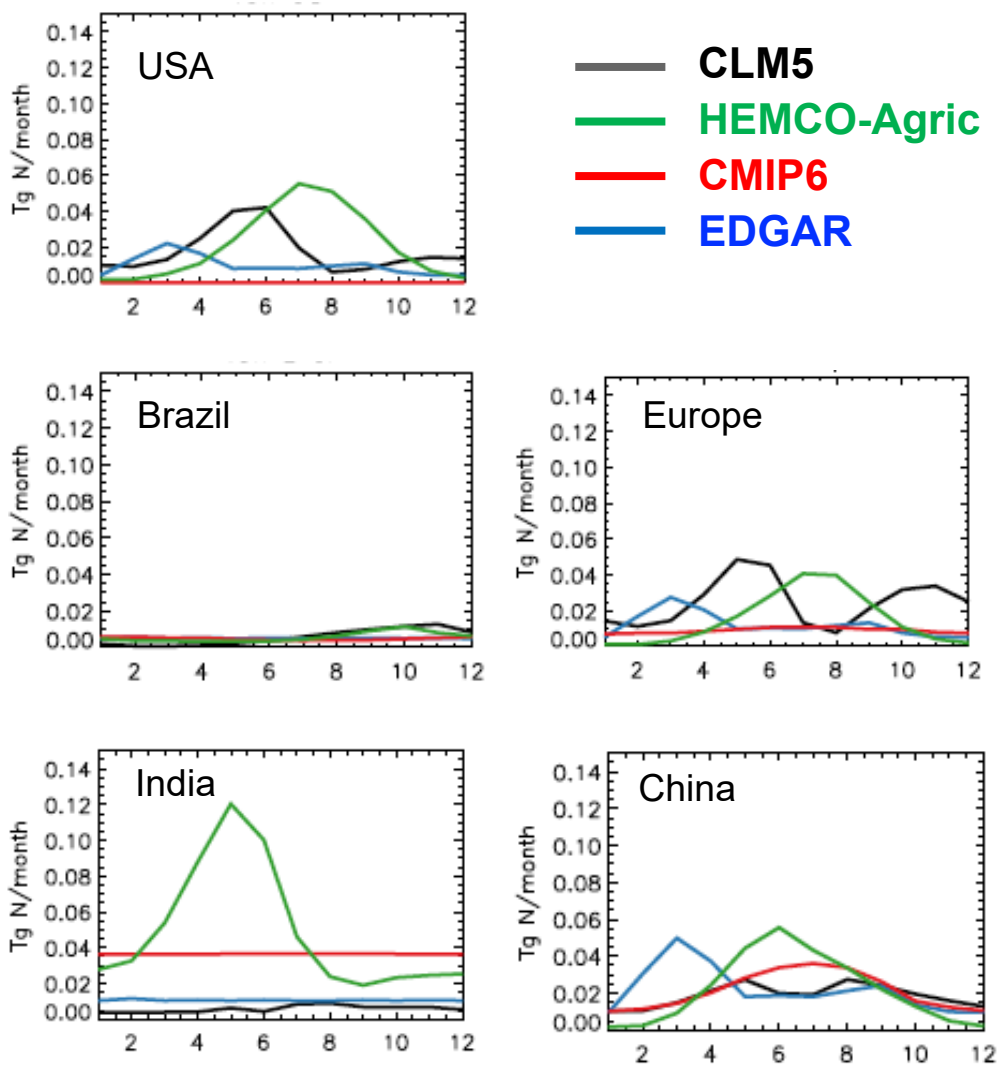
(Maria Val Martin, U. Sheffield)

Global soil NO emissions are at the lower end of previous estimates





Agricultural NO emissions in major crop regions are within estimates



Role of Reactive Soil Nitrogen Emissions in the Coming Century

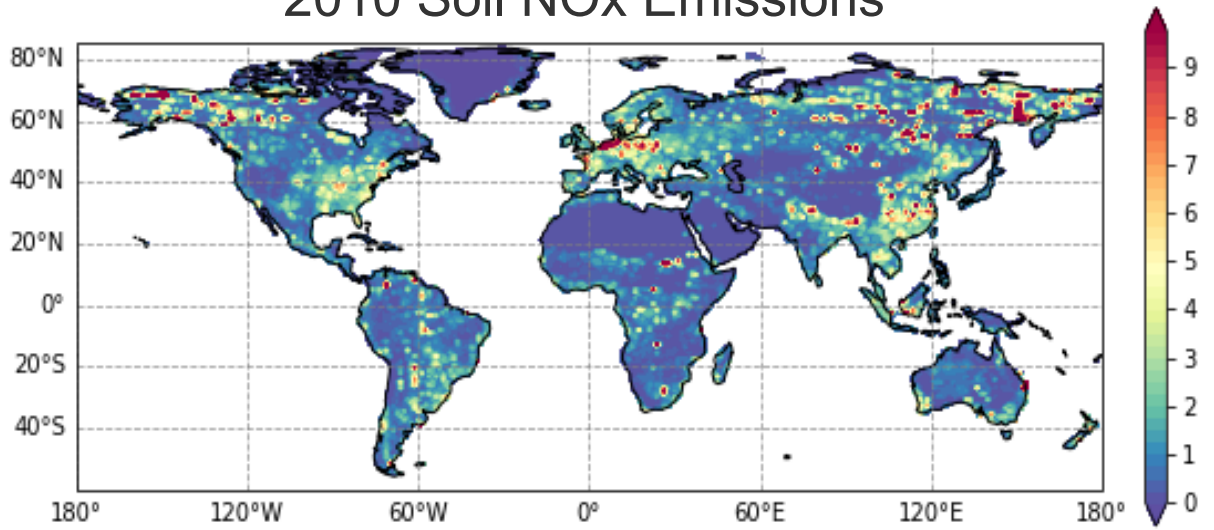
Anthony Wong, Jeffrey Geddes – Boston University

- Building on Maria's and Ka Ming Fung's development of soil NO and NH3 emissions
- Adding effect of emissions pulsing after rain
- Studying impacts of future climate and land use change

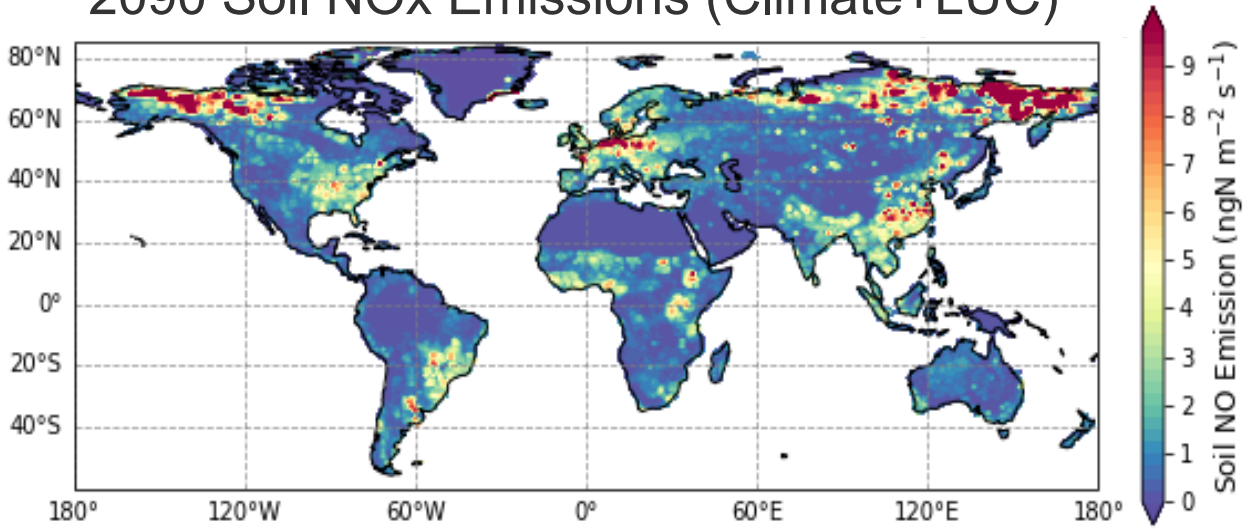
Comparable (and competing) climate and land use effects on reactive soil nitrogen emissions

Potentially missing air quality "climate penalty"?

2010 Soil NOx Emissions



2090 Soil NOx Emissions (Climate+LUC)



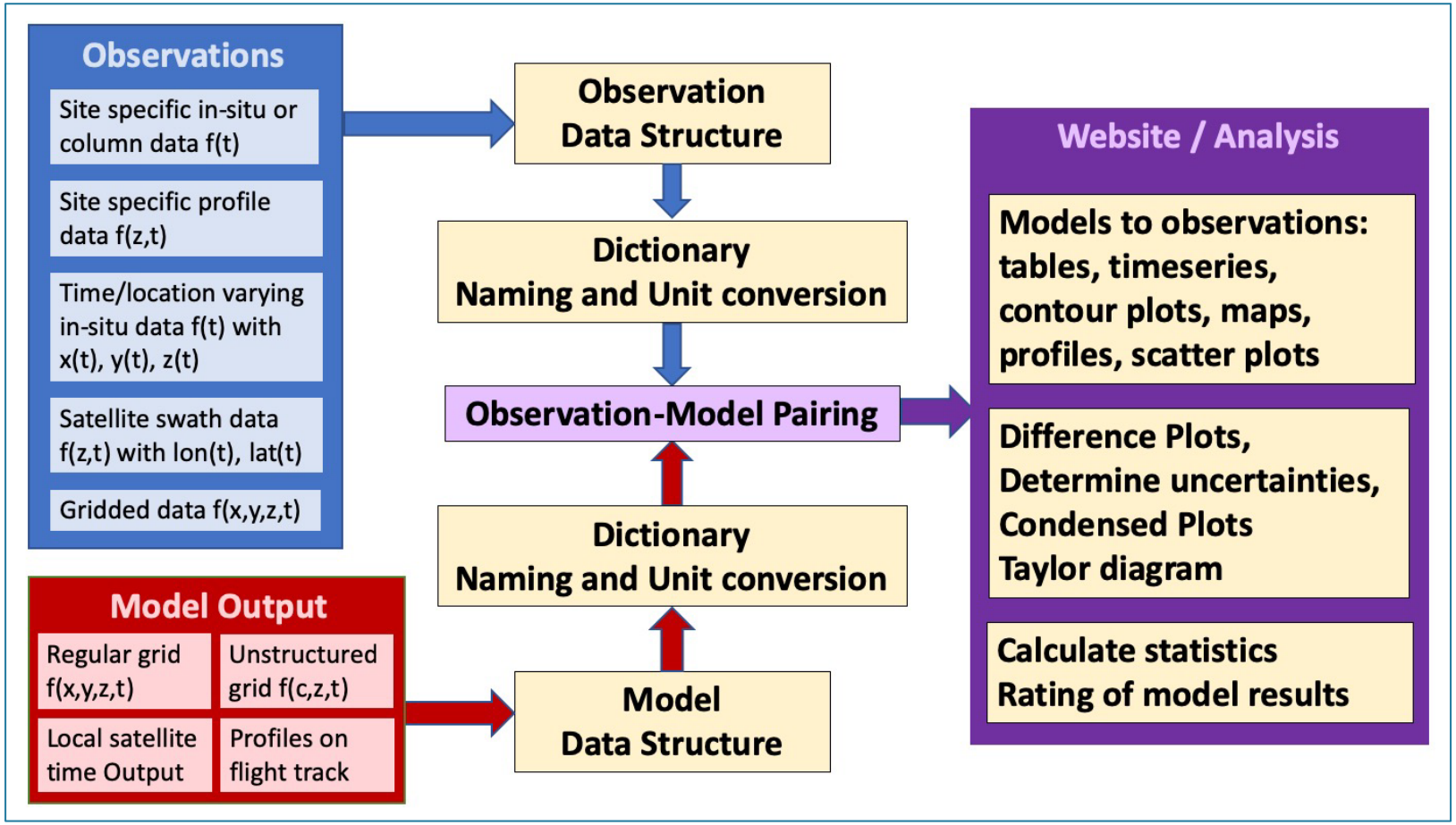
MELODIES for MUSICA

A modular framework to compare model results and observations of atmospheric chemistry

Proposal funded by NSF Earthcube, Aug 2020 – Aug 2023

MELODIES: Model EvaLuation using Observations, DIagnostics and Experiments Software

MUSICA: Multi-Scale Infrastructure for Chemistry and Aerosols



- Modular framework
- User-friendly interface
- Community input
- User Guides will be produced
- Tutorial for community, targeting students and postdocs

https://www2.acom.ucar.edu/modeling/model-evaluation-using-observations-diagnostics-and-experiments-software-melodies

Questions?

Email me: emmons@ucar.edu

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

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

MUSICA wiki:
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