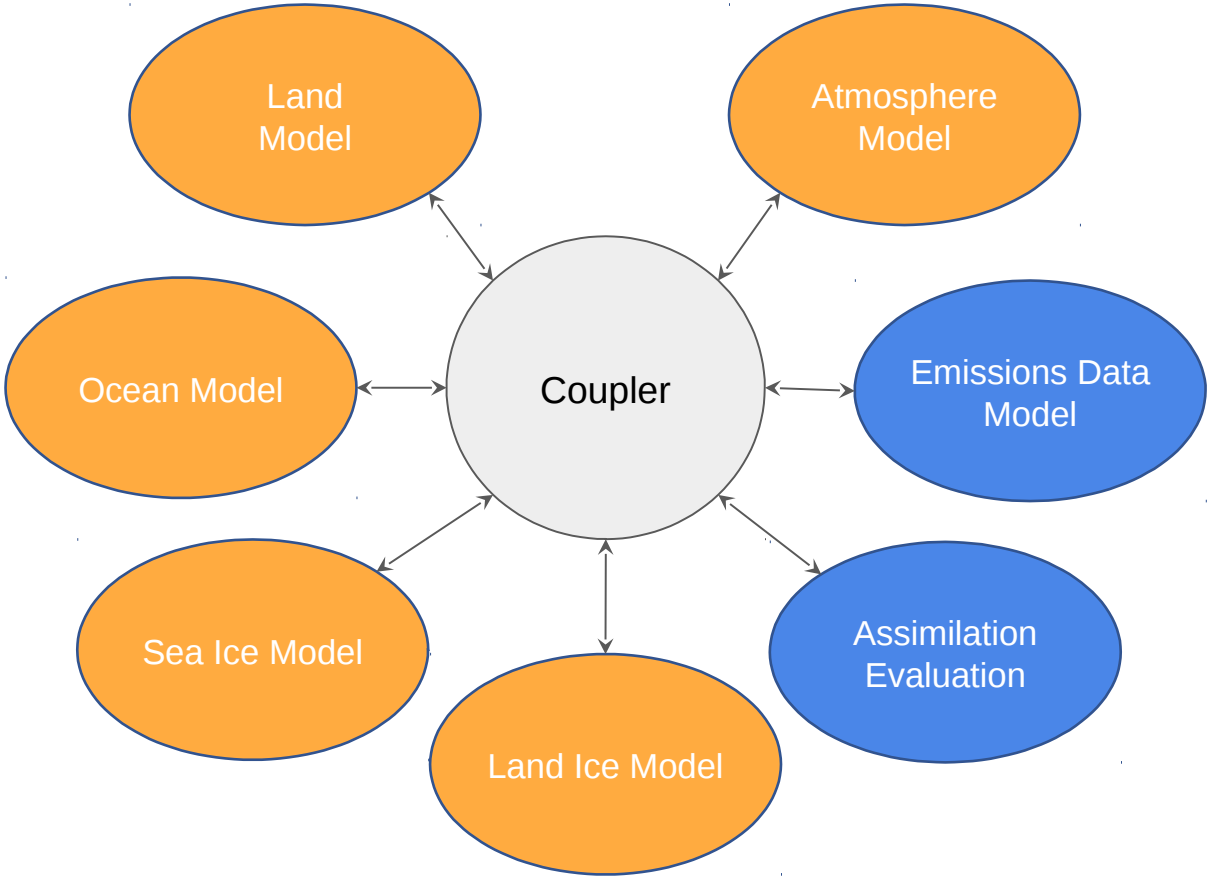
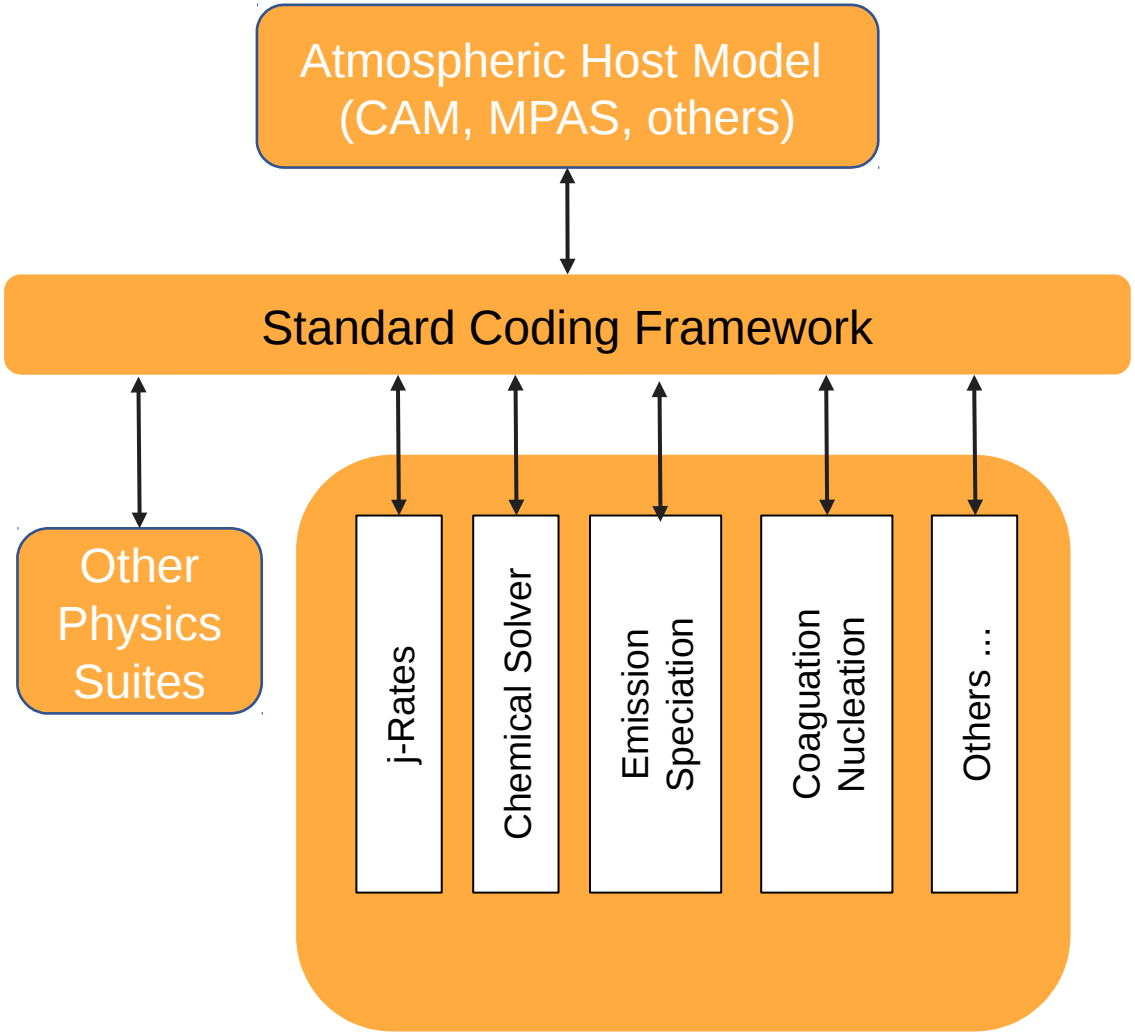
Intent of Chemistry Infrastructure

- User-friendly
  - Less code editing for each experiment
  - Fewer hidden side effects (WSM6 doesn’t work with Aerosol Indirect?)
  - User can add reaction without having to install some unix tool (yacc)
- Explicit
  - Data describes what chemicals are present and their properties
  - Data describes chemical interactions
  - No code choices about configuration (“if MAM”) or code choices based on name (“if hno3”)
- Flexible
  - User can add a species to aerosol without rewriting aerosol scheme code
  - User can add a reaction without a complicated user process
- Separated concerns
  - Radiation code is ignorant of which aerosol is being implemented
- Traceable
  - What was the chemistry specified in that experiment?
  - Which emissions did we use?

Generalize interaction of model with external data




Atmospheric Host Model
(CAM, MPAS, others)
Standard Coding Framework
Other
Physics
Suites
j-Rates
Chemical Solver
Emission
Speciation
Coaguation
Nucleation
Others ...

Atmosphere Host Models (CCPP)

- CAM (part of CESM, using coupler to surface models) [FV, MPAS, FV3, SE, SE-RR]
- MPAS-A (Includes MPAS, and surface models)
- WRF
- NOAA models

Reaction Type: Arrhenius

Number of Reactants (Excluding M)

Reaction Rate:

$$Ae^{(\frac{-C}{T})}\left(\frac{T}{D}\right)^{B}(1.0+E*P)$$

Standard Arrhenius, including (1 + E*P) factor from some pollution modeling

Parameter	Value	Default	Units	Comment
A	Number	1e-8	1/sec*(1/ndens)^(n_react-1)	Always positive number
C	Number	0	K	typical ranges: -1500:1500
D	Number	300	K	typically 300
B	Number	0	none	Sometimes called -n
E	Number	0	1/Pa	Almost always 0

Chemical Potential Heating Rate: cph

Reactants: CLm + H

Products: HCL + e

ajc : 2019-12-13 : Add A Comment. Your initials and date will be prepended automatically.

Musica Development Pathways

MICM (box model) with CCPP

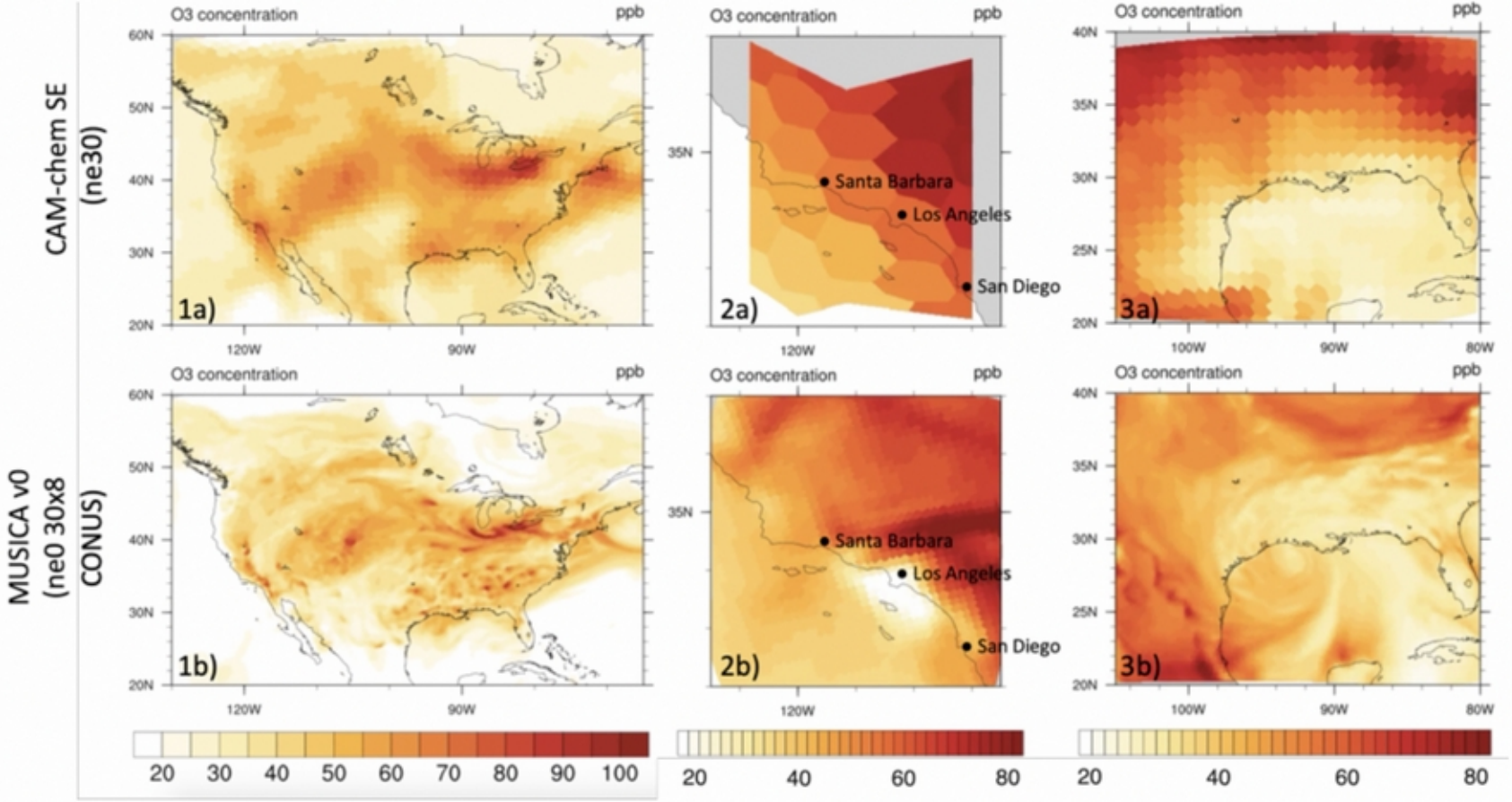
- Photodecomp (j-rates)
- Actinic flux
- Reaction kinetics
- no emissions
- gas phase only
- Database-driven
- -> aerosols

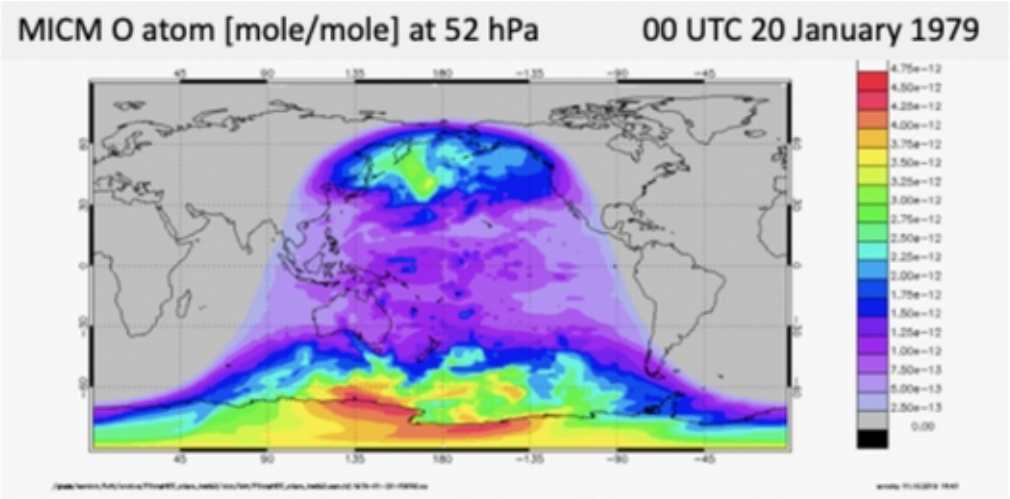
MICM in CAM/CESM without CCPP

CCPP into CAM (or rebuild CAM around CCPP and new versions of physics packages)

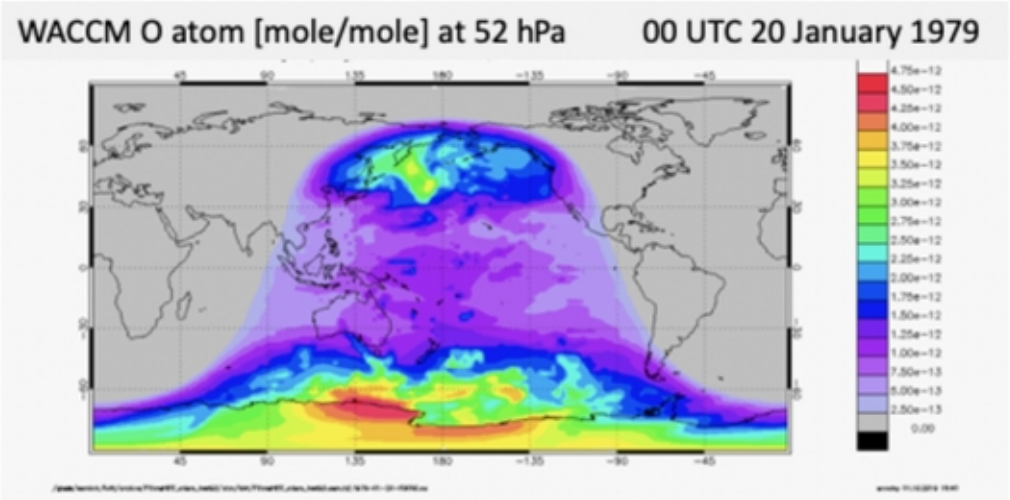
CAMP: Combined Aerosol/gas phase solver

Others: Emissions, Evaluation, Assimilation


CAM-chem SE
(ne30)
MUSICA v0
(ne0 30x8
CONUS)
O3 concentration
ppb
1a)
2a)
3a)
1b)
2b)
3b)
Santa Barbara
Los Angeles
San Diego
60N
50N
40N
30N
20N
35N
25N
120W
90W
100W
80W
20 30 40 50 60 70 80 90 100
20 40 60 80
20 40 60 80



MICM/Chapman in CAM



Full WACCM

MUSICA Status

Musica v0 is cam-chem running with a spectral element dynamical core including regional refinement.

- Improved ozone over (CONUS) regionally-refined region

(Forrest)

Box chemistry solver with CCPP: “MICM” https://github.com/NCAR/MusicBox

- MICM scheme:
  https://github.com/NCAR/MICM_chemistry/blob/master/src/chemistry_driver.meta
  https://github.com/NCAR/MICM_chemistry/blob/master/src/chemistry_driver.F90
- Incorporated (MICM-chapman) in atmosphere model
- Works with a web-service preprocessor
- Will replace this with a combined gas/aerosol multiphase solver (CAMP) without a preprocessor. Allows runtime specification of chemistry.

Both MICM and CAMP use (very similar) specification of molecular properties and chemical reactions
CCPP in CAM has some ways to go.