Fast Chemistry Mechanisms for Climate Applications

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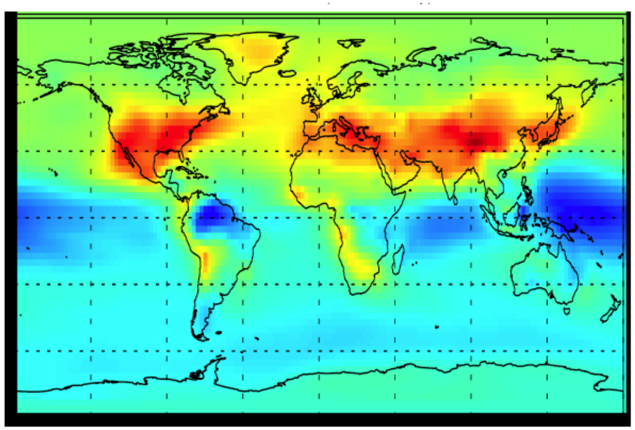
Our **fast** & super-fast mechanisms increase GCM computational cost by 100% and 40%.

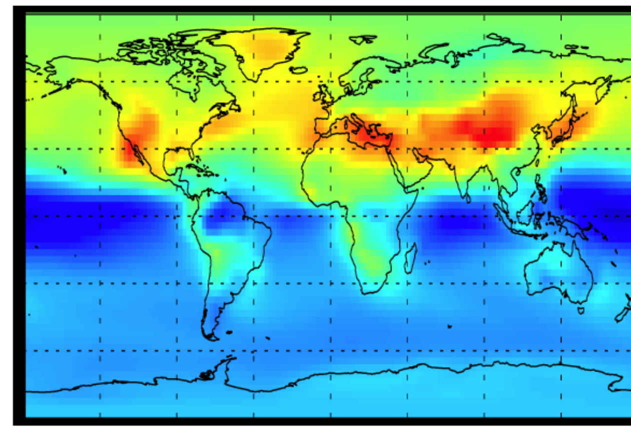
(1) O_3
(2) O
(3) $O(^1D)$
(4) OH
(5) HO_2
(6) H_2O_2
(7) N
(8) N_2O
(9) NO
(10) NO_2
(11) NO_3
(12) N_2O_5
(13) HONO
(14) HNO_3
(15) HO_2NO_2
(16) CO
(17) CH_4
(18) CH_2O
(19) HCOOH
(20) CH_3O_2
(21) CH_3O_3
(22) CH_3OOH
(23) $CH_3O_2NO_2$
(24) DMS
(25) H_2S
(26) MSA
(27) SO_2
(28) SO_4

Super-fast captures 70-80% of O3 & OH large-scale amplitude AND sensitivity.

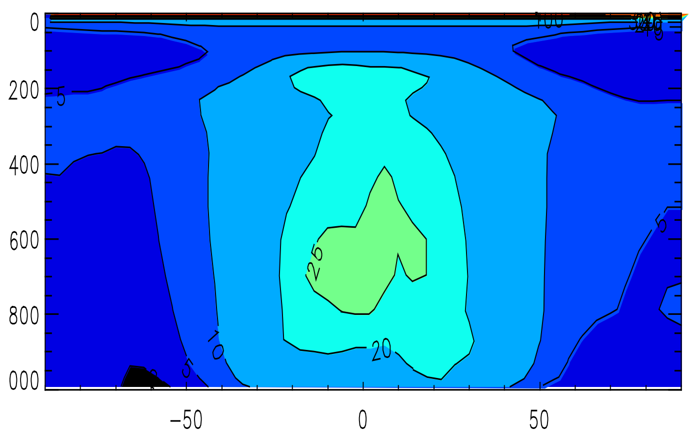
Full Chemistry | Super-fast Chemistry

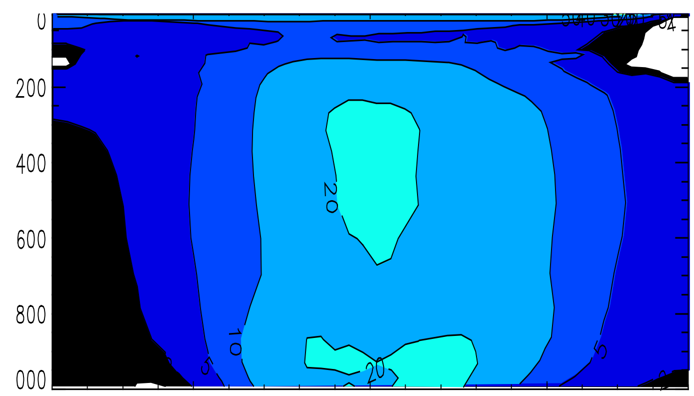
Surface $[O_3]$ ppb





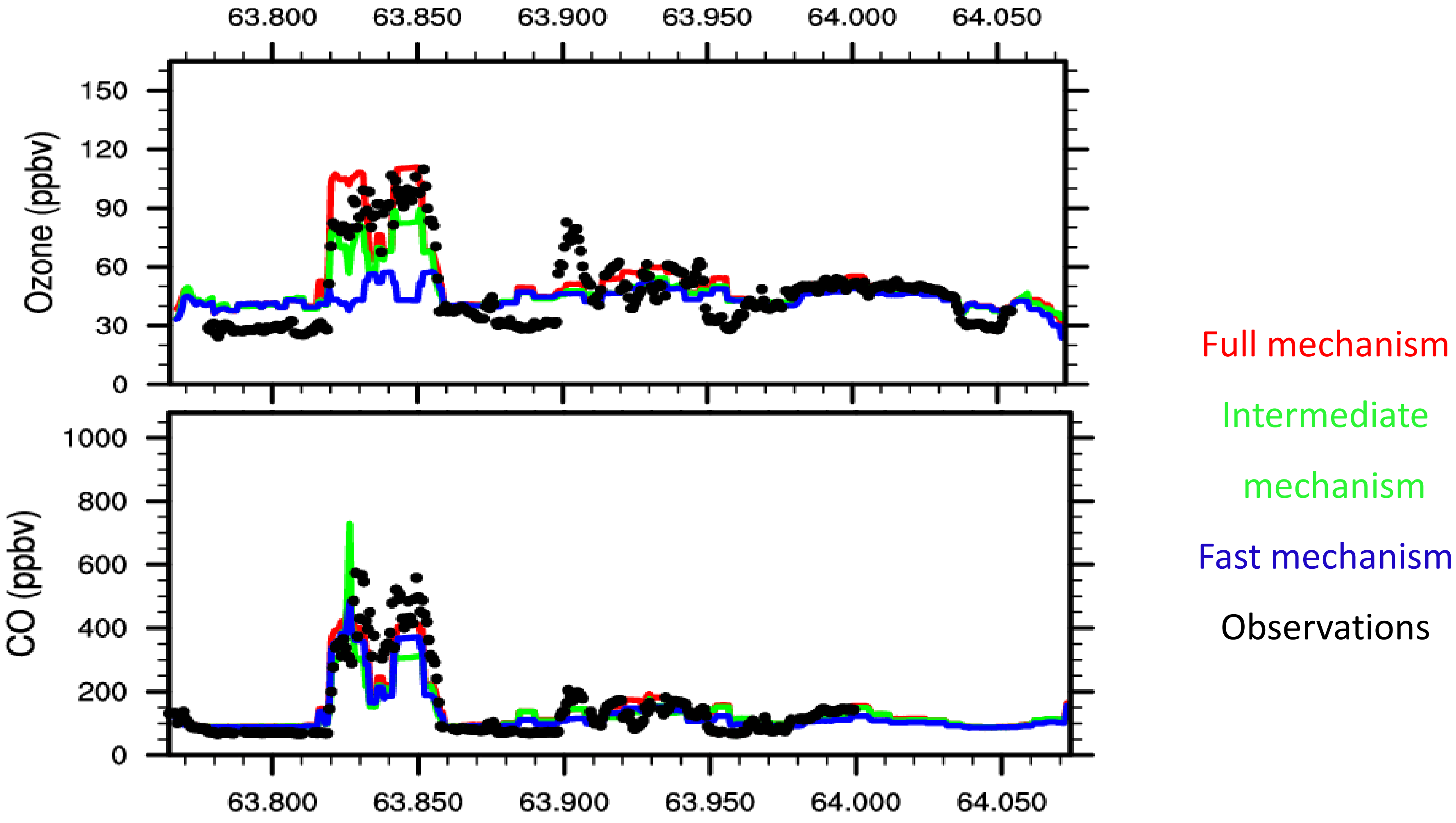
Zonal mean [OH] 10^5mol/cm^3





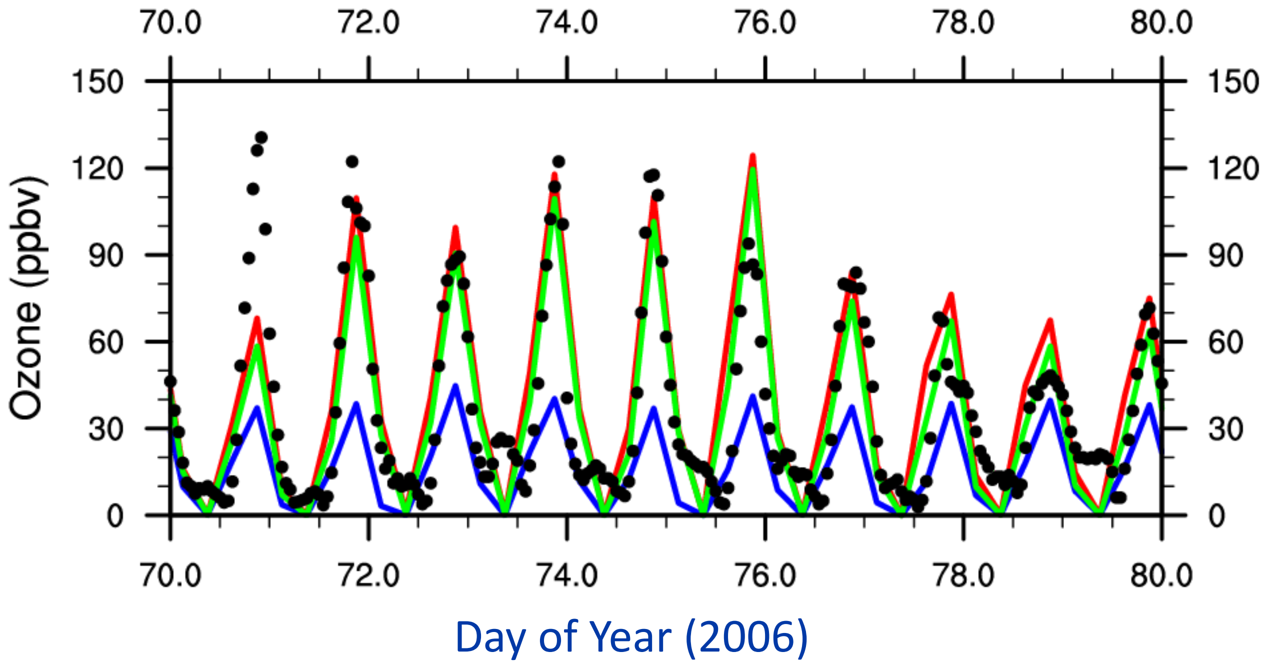
Philip Cameron-Smith, LLNL, LLNL-PRES-4

Mexico City aircraft obs. confirm good background, but weak pollution plumes.



Day of Year (2006)

Mexico City surface observations confirm weak response to urban diurnal cycle.



Red: Full mechanism

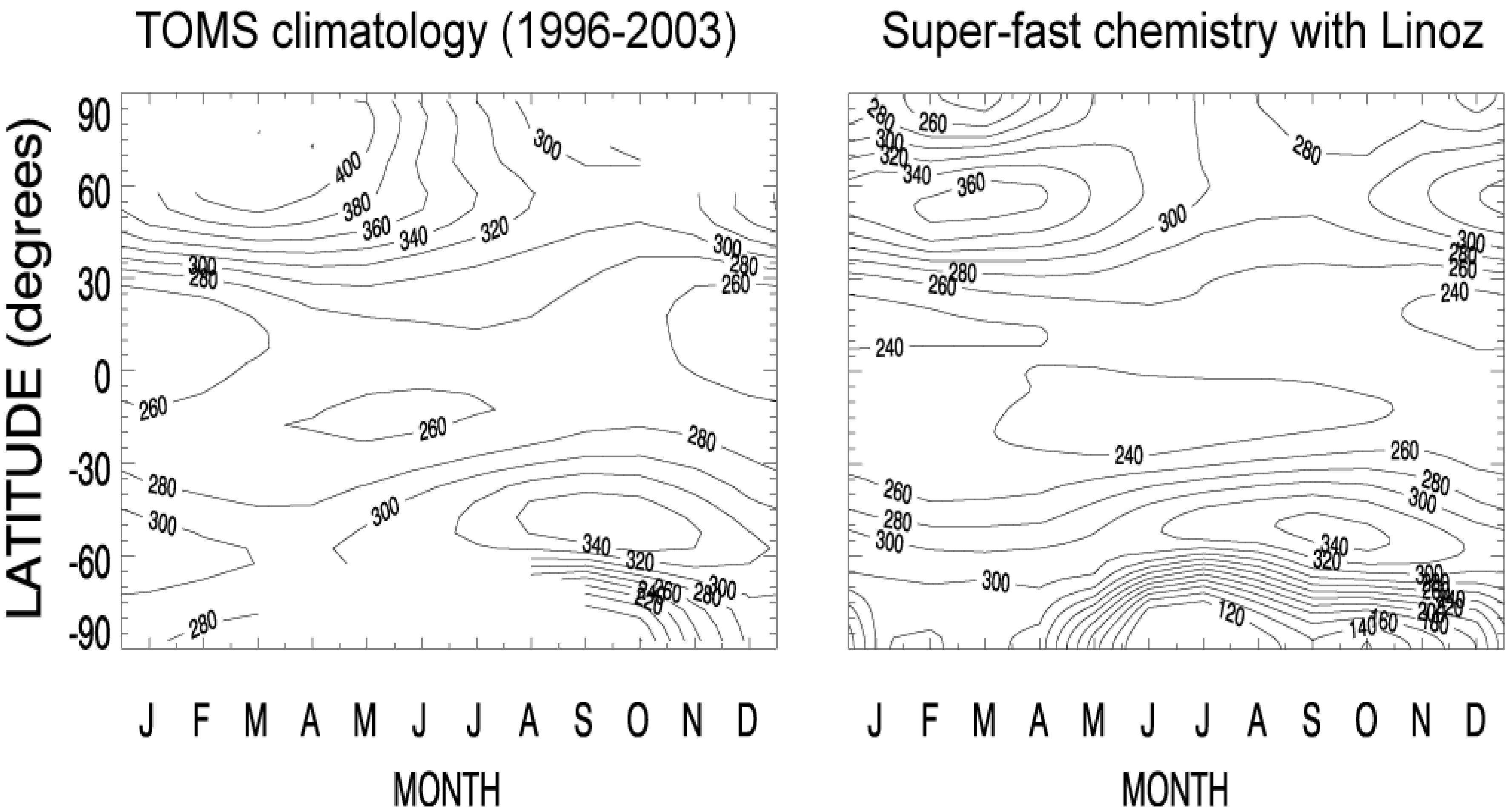
Green: Intermediate mechanism

Blue: Fast mechanism

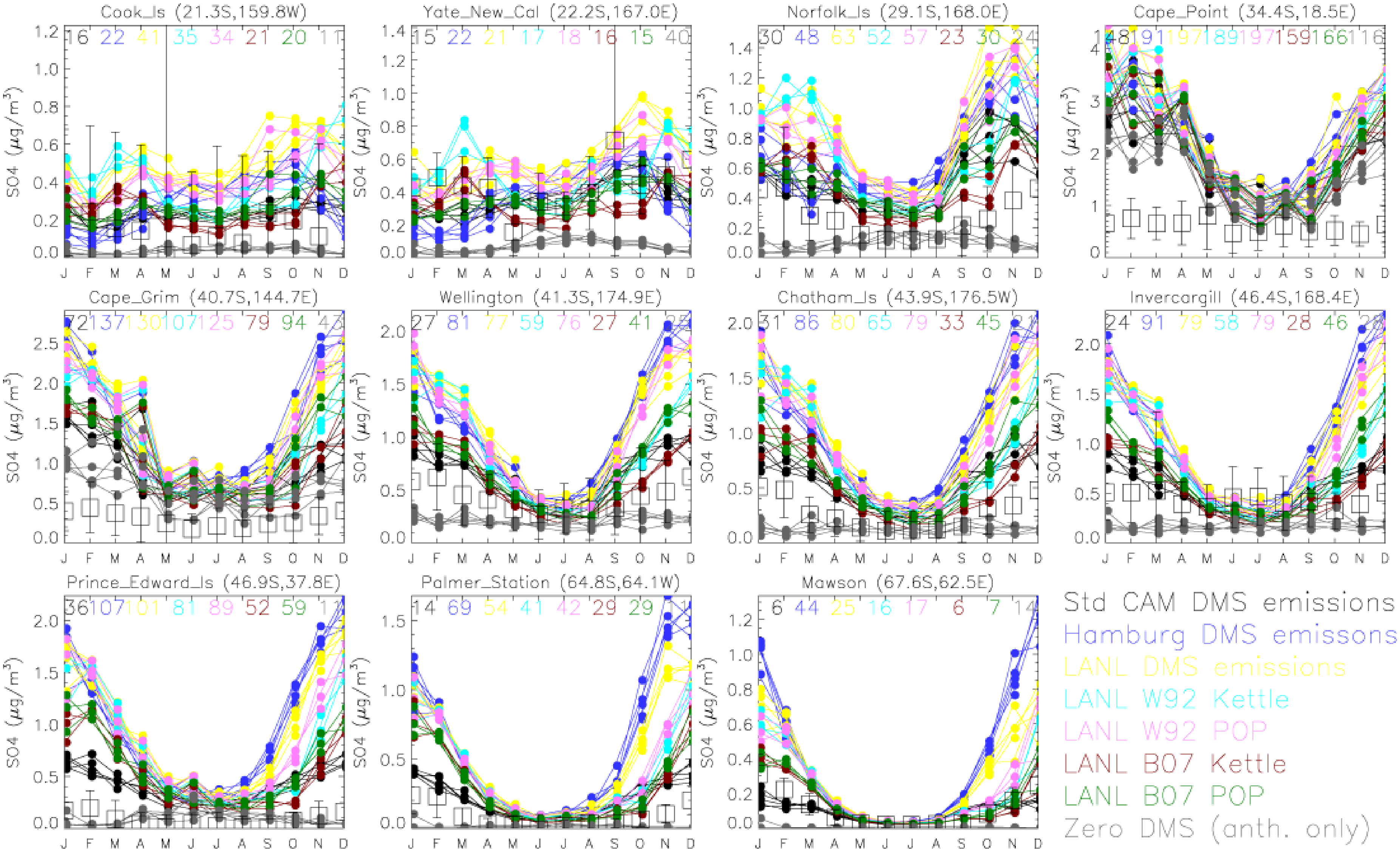
Dots: observations

On most days, full and intermediate capture well the diurnal cycle and amplitude; the fast mechanism is much lower

Linoz only needs 1 tracer. Its stratospheric columns compare well with observations.



Sulfate aerosols validate well against surface observations.



Philip Cameron-Smith, LLNL, LLNL-PRES-4

Fast mechanisms maintain sensitivity of methane lifetime to perturbations.

	Full mechanism	**Fast**	**Super-fast**
Control	7.03	7.16	8.45
Increase NO_x 10%	6.83 (-0.199 = -2.83%)	6.96 (-0.205 = -2.87%)	8.24 (-0.211 = -2.50%)
Increase CO 10%	7.11 (+0.086 = +1.22%)	7.26 (+0.100 = +1.40%)	8.56 (+0.110 = +1.30%)
Increase CH_4 10%	7.26 (+0.231 = +3.29%)	7.43 (+0.267 = +3.73%)	8.72 (+0.264 = +3.12%)

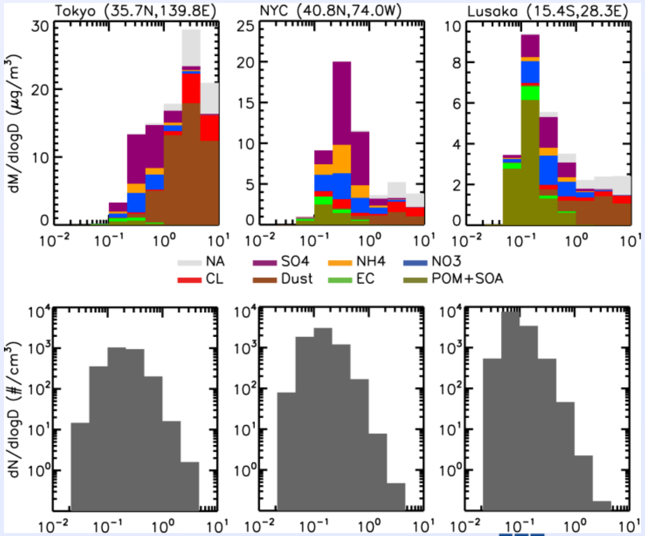
Methane lifetime in years. In parentheses, the change in lifetime due to the change in emission relative to the control.

LLNL is adding sectional aerosol scheme to CAM, including SOAs.

Cathy Chuang, Dan Bergmann, Cameron-Smith.

- Implement an aerosol microphysics model (MADRID) and an online biogenic emission system (MEGAN) into LLNL IMPACT model
  - MADRID predicts the chemical compositions, *number, and mass* size distributions of *inorganic* and *organic* aerosol components.
  - MEGAN calculates the hourly emissions of 20 compound classes, representing 138 compounds, which can be grouped into various chemical mechanism.
- Perform our first global simulation of size-resolved aerosol concentrations and mixing, including the secondary organic aerosols (SOAs)
  - Compare the simulated PM1 to measurements from Aerosol Mass Spectrometer in 37 field campaigns.
  - Assess the predictions of aerosol concentrations with IMPROVE network at 156 national parks.
- Incorporate the SOA chemistry and MADRID into the NCAR Community Climate System Model
  - Chemistry mechanism installed in CAM with 8 size bins for aerosols and > 300 total species
  - Land model (CLM) modified to accommodate a more detailed version of MEGAN
  - Installation of MADRID in progress

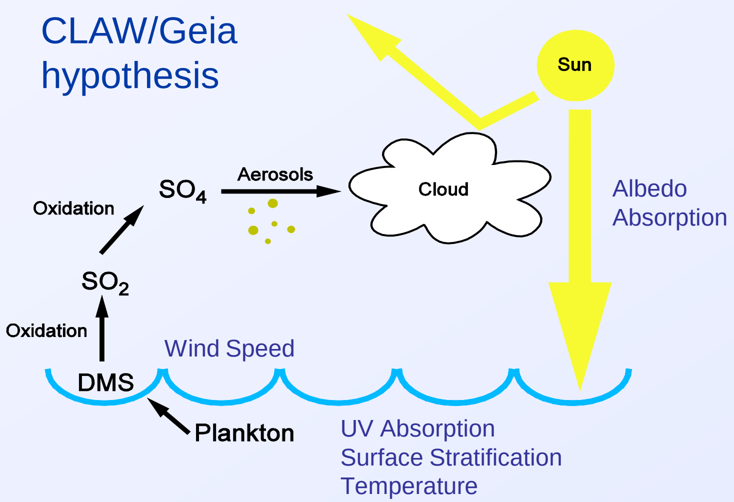
Simulated aerosol mass and number distributions in regions of Tokyo, New York City, and Lusaka.

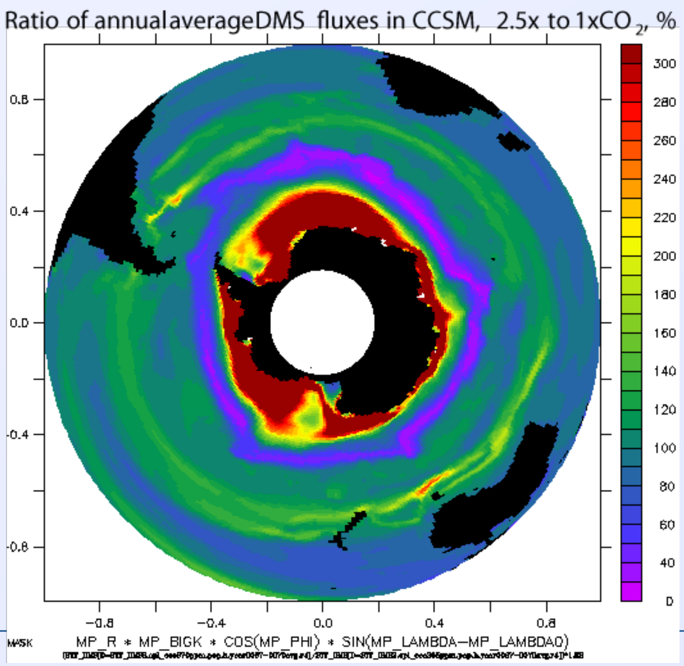


We are developing an Earth System Model (ESM): biosphere-atmosphere-chemistry coupling in CCSM.

P. Cameron-Smith, S. Elliott, M. Maltrud, R. Jacob, D. Bergmann, D. Erickson, M. Ham.

- The biosphere and atmospheric chemistry interact to affect climate.
- We are combining our atmospheric chemistry with the state-of-the-art ocean sulfur cycle from LANL in CCSM.
- We have run 50 year simulations of ocean sulfur cycle for present-day and 2100.
- End goal is to test the CLAW/Gaia climate stabilization hypothesis.

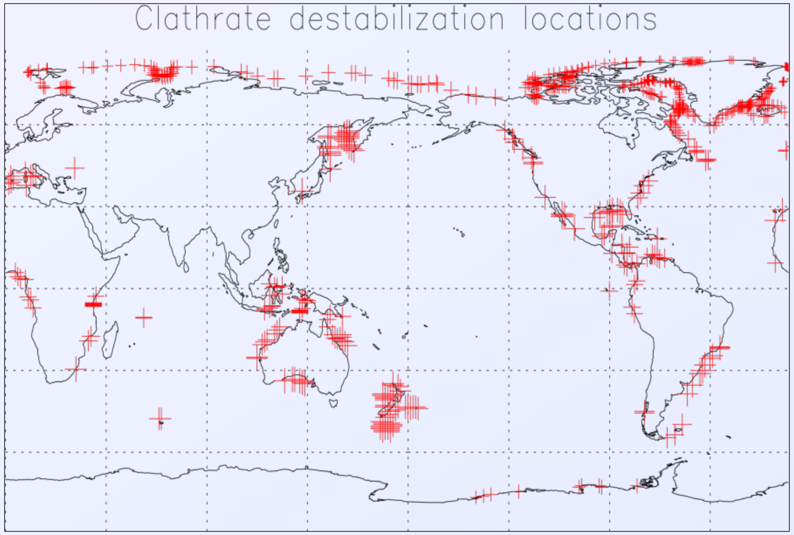


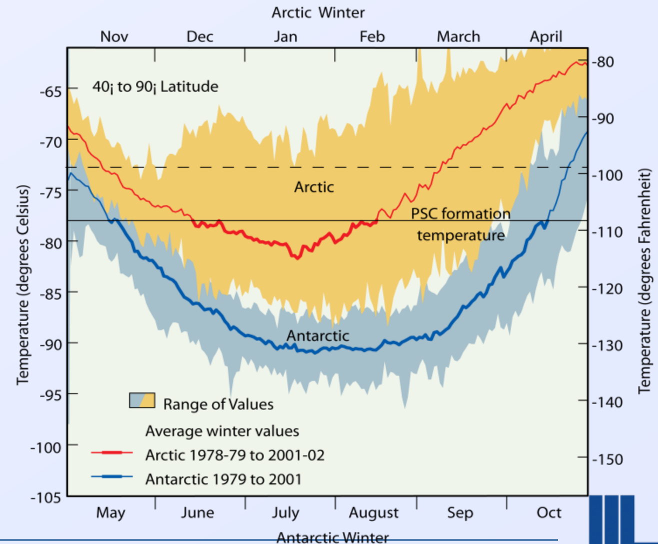


Ratio of DMS flux: 2100 to 2000

IMPACTS: Climate impact of methane clathrate releases

- Matthew Reagan (ocean sediments, LBNL),
- Scott Elliott & Mat Maltrud (oceans, LANL),
- Philip Cameron-Smith (atmosphere, LLNL)
- A vast quantity of methane is locked in icy clathrates in ocean sediments, (as much carbon as all other fossil fuels combined).
- Rapid destabilization of the clathrates due to climate warming would significantly increase methane releases, potentially causing:
  - ocean dead-zones (hypoxia),
  - strong greenhouse heating,
  - increased surface ozone (ie, poorer air-quality),
  - reduced stratospheric ozone,
  - intensification of the Arctic ozone hole,
- Connects to IMPACTS-Boreal project, through terrestrial methane releases.





Status of Track 1 (slide A)

- Super-Fast mechanism implemented in CAM & CCSM.
  - Both track 1 & 5 (not connected to MAM or indirect effects, yet).
- TUV occasionally produces negative photolysis rates:
  - Can kill simulation.
  - Not numerical precision.
  - Approximately once every 4 days.
  - Always at evening terminator (sza 84-90 degrees).
  - Always over Europe and Bangladesh.
  - In CCSM, but not CAM.
- Possible solutions.
  - Zero negative emissions
  - Fix TUV.
  - Switch to look-up table.
  - Implement Fast-J.

Status of Track 1 (slide B)

- How to implement methane:
  - Fixed, from Jean-Francois's transient CAM simulation.
  - Surface & stratosphere boundary conditions.
  - Emissions.
- How best to derive methane lifetime?
  - Diagnose from monthly output.
  - Accumulate within chemistry solver (explicit).
  - Accumulate in dummy product for CH_4 reaction (not advected).
- Tropopause definition (for Linoz)? [student??]
  - 0< lapse rate < -2 K/km [many wrong values].
  - Lapse rate < -2 K/km.
  - O3 < 100, 150, 200 ppb .
  - Stobie.
  - Reichler [interpolates lapse rates. Diagnoses fractional layer].

Status of Track 1 (slide C)

- Aerosols with super-fast:
  - Super-fast calculates SO_4 mass.
  - Possible options:
    - Prescribed aerosols (except SO_4).
    - BAM (also could handle aqueous oxidation rather than chemistry).
    - MAM3 or MAM7
- What output?
  - Monthly mean:
    - Concentrations.
    - Dry deposition.
    - Wet deposition.
    - Net chemical tendency.
    - Methane loss-rate.
    - ……
- Standard diagnostic suite?

The end.

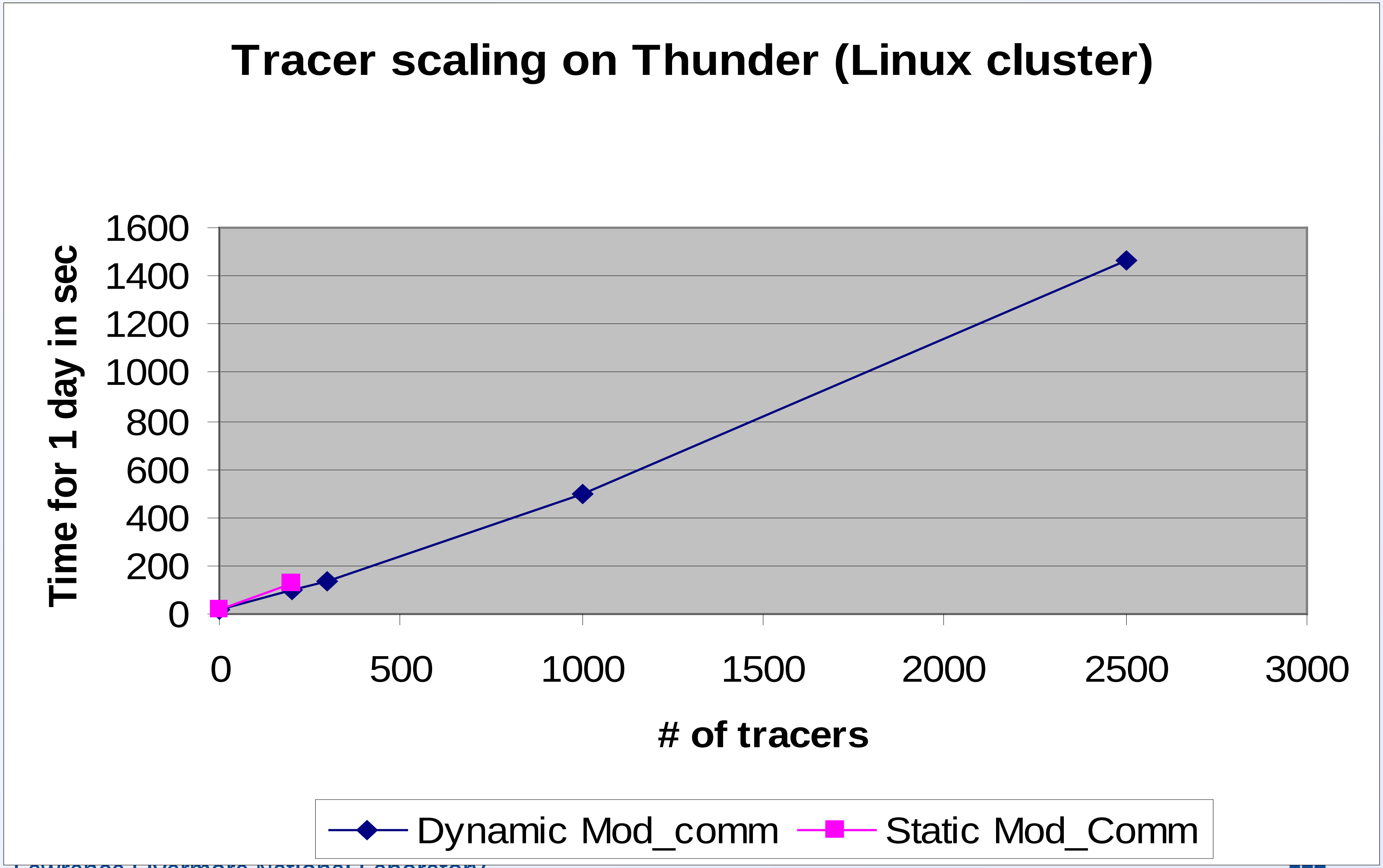
Interactive chemistry brings many benefits to climate simulations.

1. Provides consistent distribution of greenhouse gases (troposphere and stratosphere), including the effects of:
   i. Changes in stratosphere-troposphere exchange (STE),
   ii. Feedback on climate through the GHGs and aerosols.
2. Provides consistent distribution of oxidants for:
   i. Aerosol production, including sulfate & secondary-organic aerosols,
   ii. Lifetimes of many species of interest, including methane.
3. Provides distribution of air quality (background).
4. Provides interaction with biogeochemistry: nitrogen deposition, ozone damage, dimethyl sulfide (CLAW).

Interactive chemistry brings many benefits to climate simulations.

5. Provides statistics from IPCC simulations on:
   i. O_3 columns,
   ii. tropospheric O_3 (radiative forcing),
   iii. tropospheric OH (CH_4 & HCFC lifetimes).
6. Tracers good for diagnosing and validating GCM:
   i. Interhemispheric mixing time,
   ii. Stratospheric lifetime,
   iii. Convective massfluxes.
7. Offline chemical fields take human & computer time too.

Half of chem time is advection. Tracers scale as 2-3% of CAM/tracer

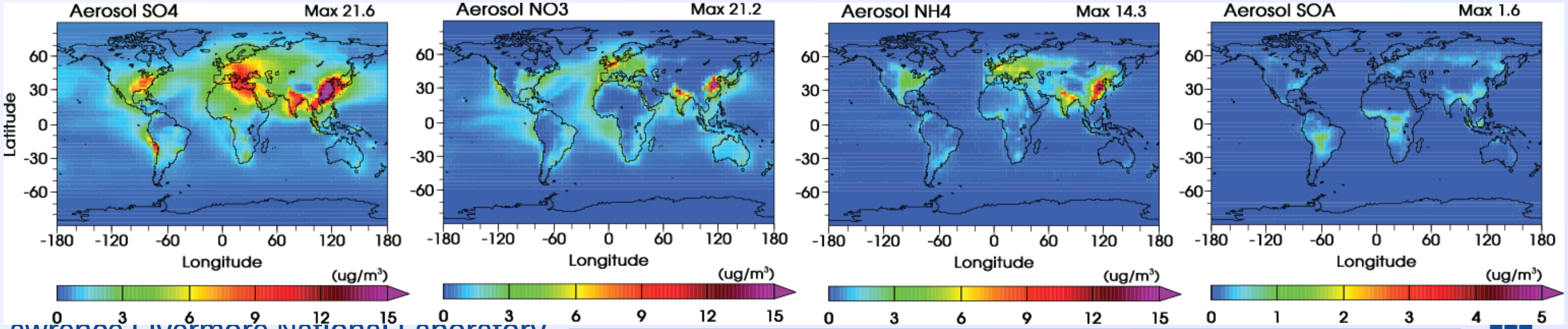


We have developed a sectional aerosol capability for CCSM, building a bridge between CCPP/SciDAC, ASP, and ARM.

C. Chuang, D. Bergmann, P. Cameron-Smith.

- Sectional aerosol microphysics schemes are the ‘gold standard’:
  - They resolve size distributions and composition explicitly.
- We have developed a sectional aerosol capability for global models based on the MADRID code.
  - We are currently implementing it into CCSM.
  - Includes atmos. chemistry for secondary organic aerosols.
  - The # of size bins is variable (currently 8 bins and 350 tracers).
- This will facilitate interaction between CCPP/SciDAC, ASP, and ARM (each program is supporting part of this work).

Secondary aerosol components at the surface (IMPACT)



Conclusions

- Our fast mechanisms validate well for present day.
- Chemical *sensitivities* of fast mechanisms compare well to full mechanism.
- Fast mechanisms provide:
  - Consistent greenhouse gas and aerosol fields,
  - Climate feedbacks,
  - Interaction with biogeochemistry,
  - Only background air-quality calculated.
- These mechanisms are fast enough (1.4x) for inclusion in main IPCC simulations:
  - Provides statistics on these effects from main IPCC simulations.
- ESM simulations for CLAW hypothesis are underway.
- Studying risk of methane clathrates.