Advancing Ultra-High Resolution & Complex Chemistry Capabilities in CAM

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System for Integrated Modeling of the Atmosphere (SIMA)
Project Activities

June 11, 2024, CESM Workshop

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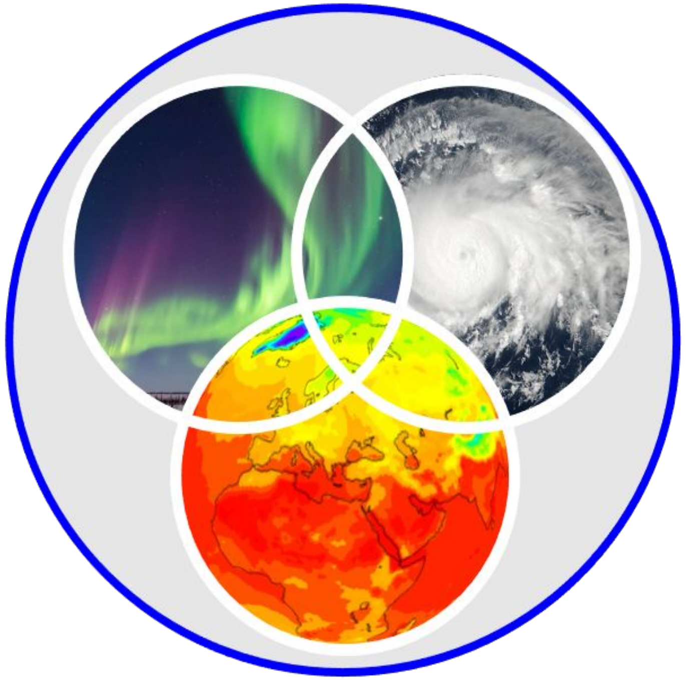
Towards integrated atmospheric modeling capabilities

SIMA Project aims to enhance frontier science simulations with one modeling system

- Earth system modeling for climate, weather, atmospheric chemistry, geospace, and cross-discipline research
- Surface to ionosphere
- Storm resolving to climate applications

Two Major Activities

- Developing software infrastructure
- Demonstrating science of new configurations

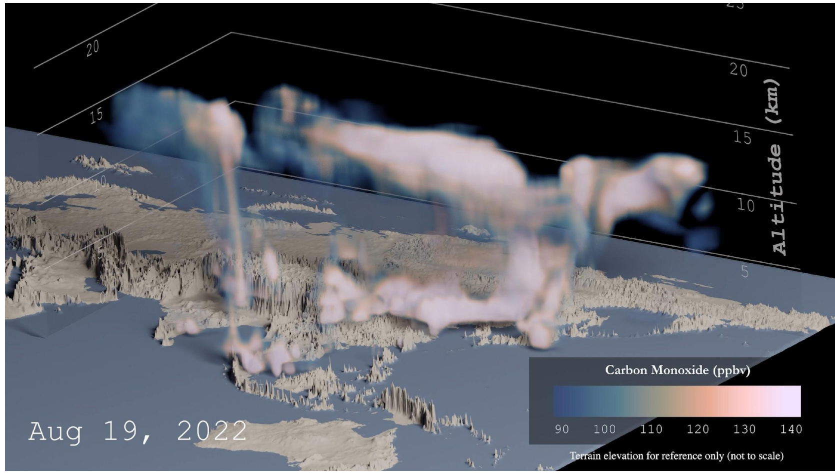


SIMA = System for Integrated Modeling of the Atmosphere
sima.ucar.edu

Emerging Capabilities for Complex Chemistry and Global Storm-Resolving Simulations

Simulations with Complex Chemistry [Mary]

- Asian summer monsoon and composition: CAM-chem with the MPAS dynamical core
- Extreme weather events: Global-to-local scale WACCM with the MPAS dynamical core



Lofting of CO (carbon monoxide) by deep convection as simulated by CAM-SE using regional refinement (~100km - ~27km over eastern Asia).
Credit: Ren Smith, Jun Zhang

Capability for Global Storm-Resolving Simulations [Brian]

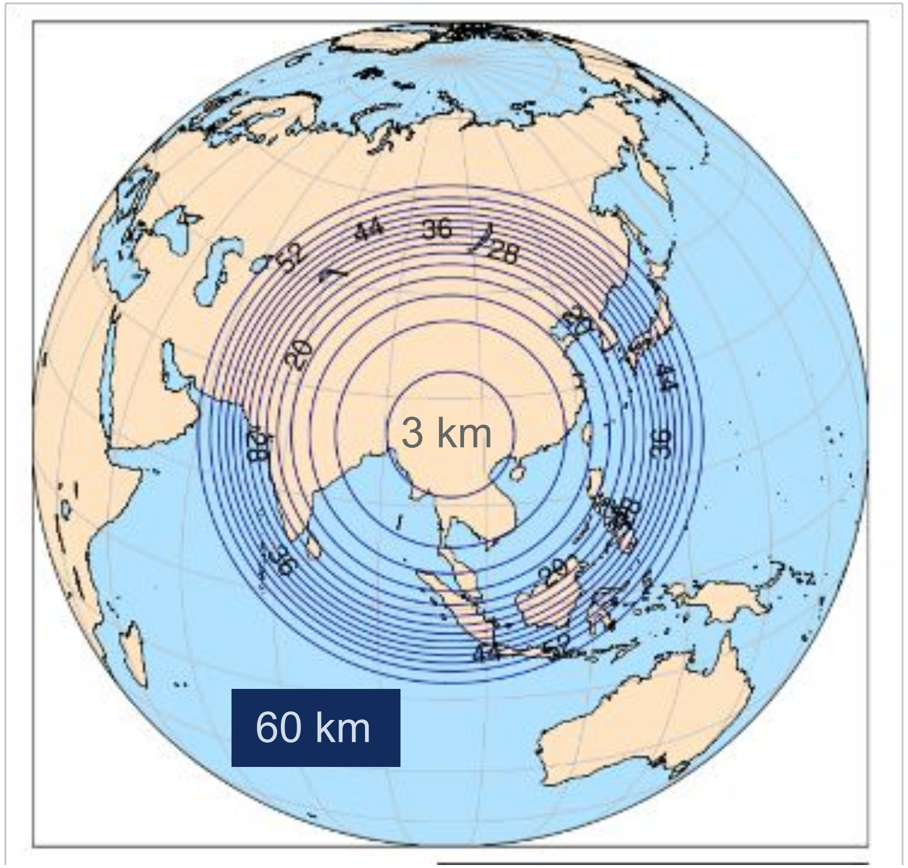
- Update on the computational capabilities

Tests of CAM-MPAS with full chemistry

Asian Summer Monsoon

- Grid mesh centered over SE Asia

1) 60 - 3 km grid mesh (840,000 columns)
    1) 32 vertical levels, mpas_dt=20s, dt_phys=30m
    2) 58 vertical levels, mpas_dt=20s, dt_phs=30m
2) 60 km uniform grid mesh
    1) 32 vertical levels, mpas_dt=300s, dt_phys=30m
    2) 58 vertical levels, mpas_dt=300s, dt_phs=30m
    3) 32 vertical levels, mpas_dt=20s, dt_phys=30m
    4) 32 vertical levels, mpas_dt=20s, dt_phys=20s



- Troposphere-Stratosphere (TS1) chemistry (168 trace gases & aerosols)
- Emissions: CAMS 0.1deg emissions inventory
- No nudging (i.e., free running)

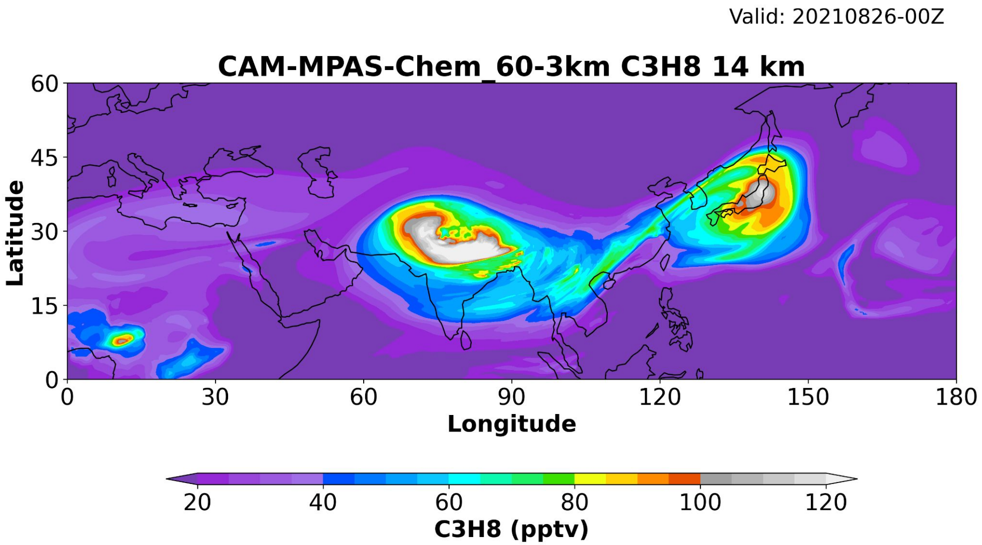
Case study: 23-28 August 2021

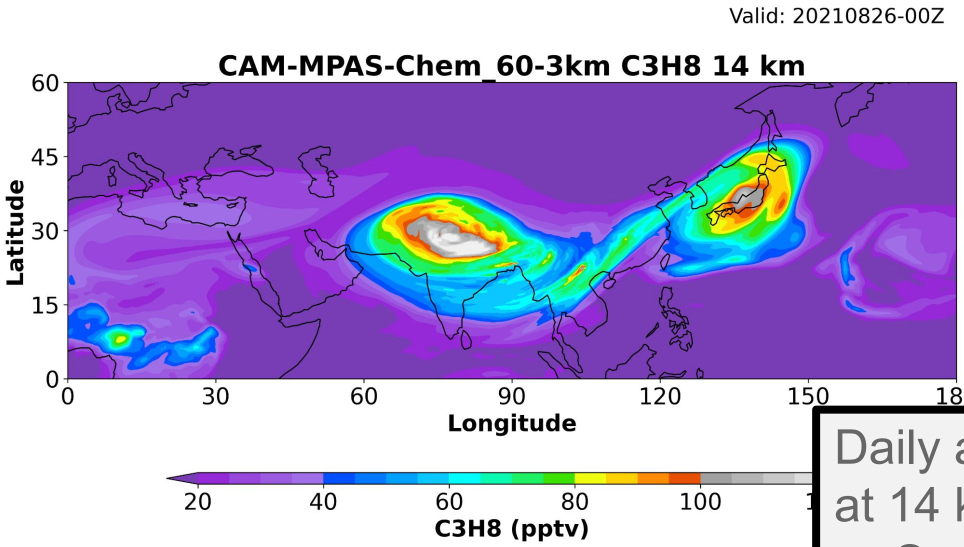
- Examine impacts of spatial and temporal grid resolution on convective transport of trace gases

Convective Transport of Propane, a tracer of transport

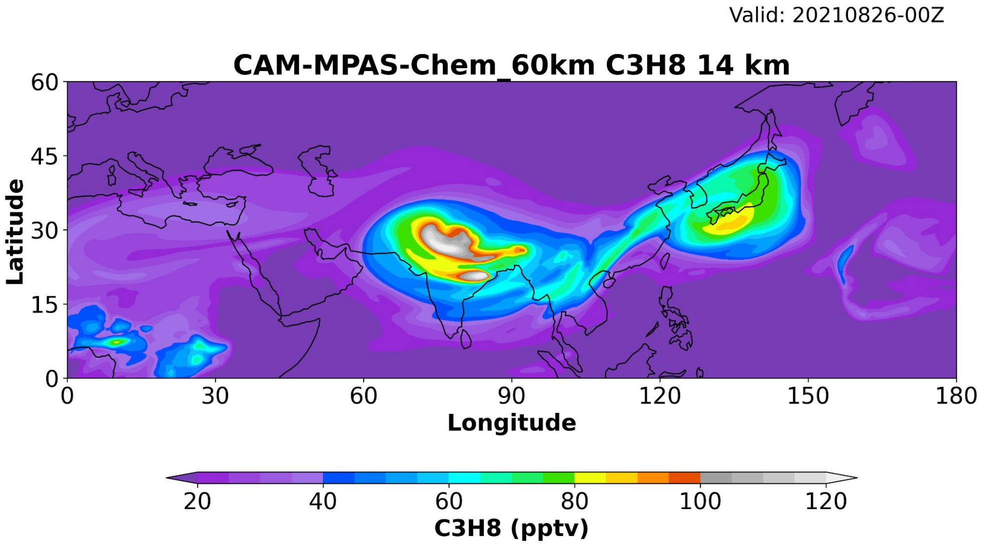
32 Levels | **58 Levels**

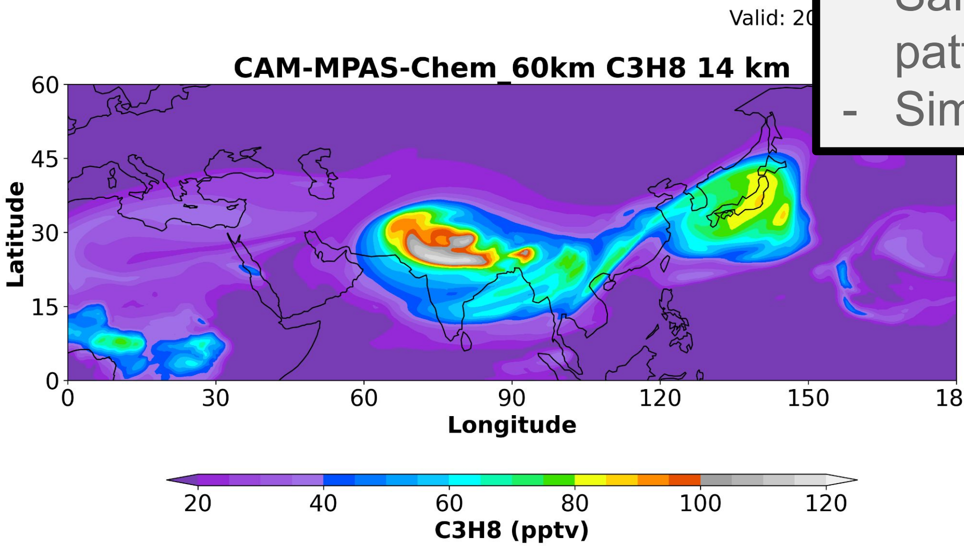
Regionally Refinement

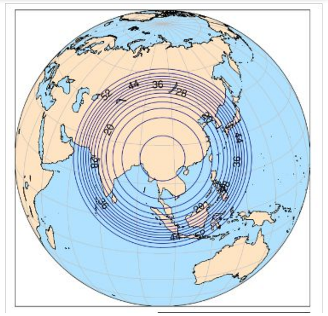




Uniform Grid



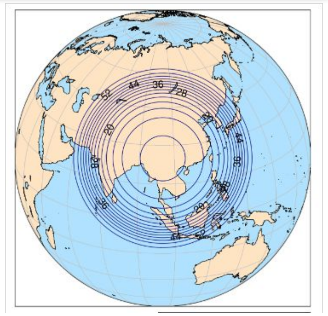




Daily average propane at 14 km altitude

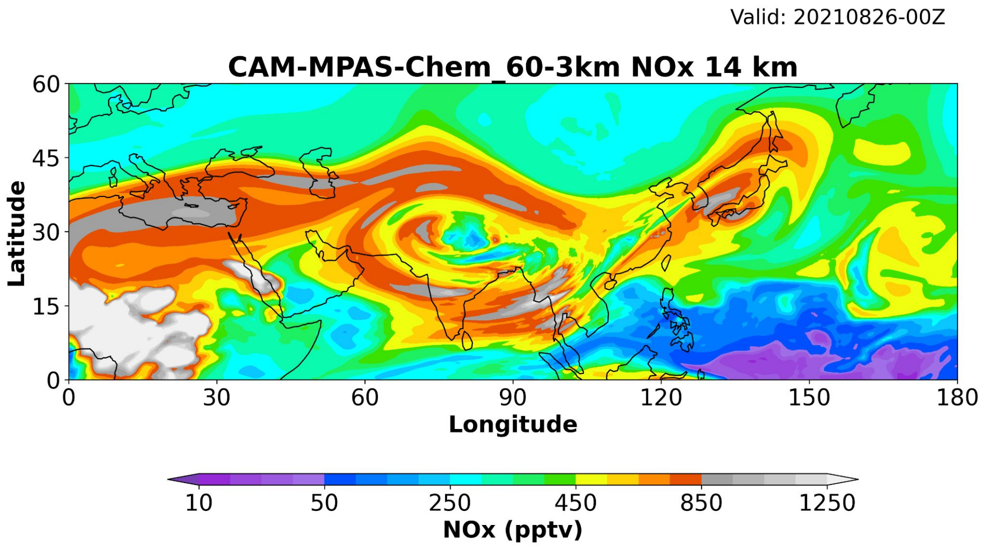
- Same large scale patterns
- Similar magnitude

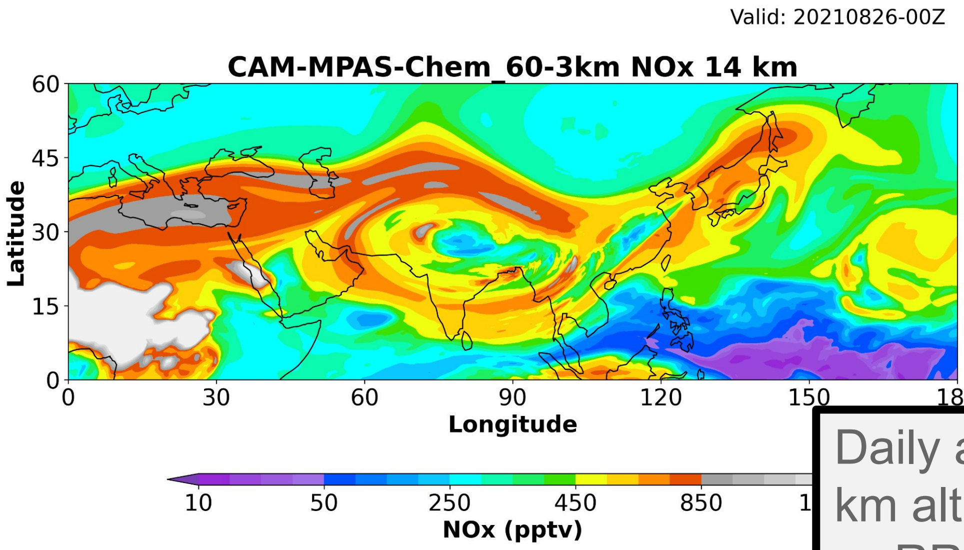
NO_x – affected by lightning, transport, chemistry



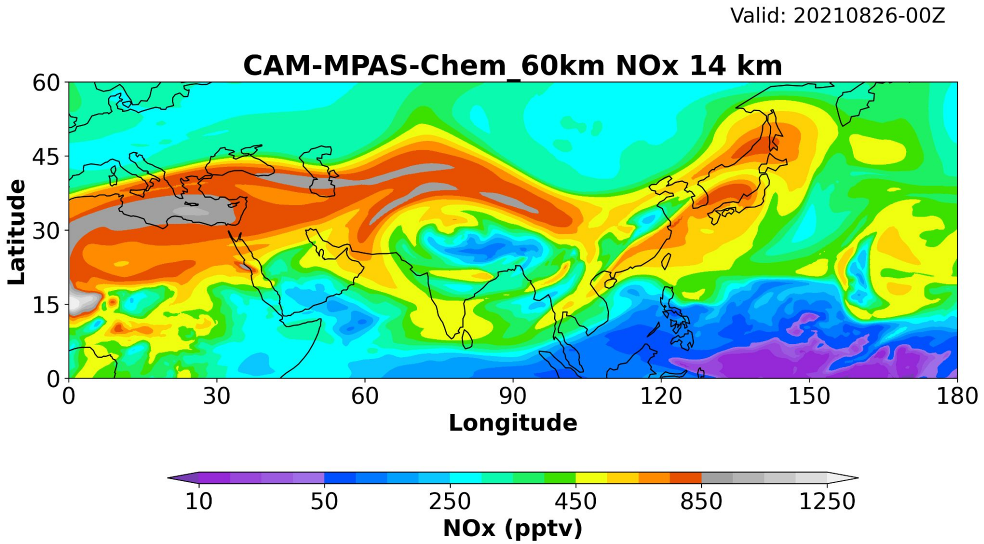
32 Levels | 58 Levels

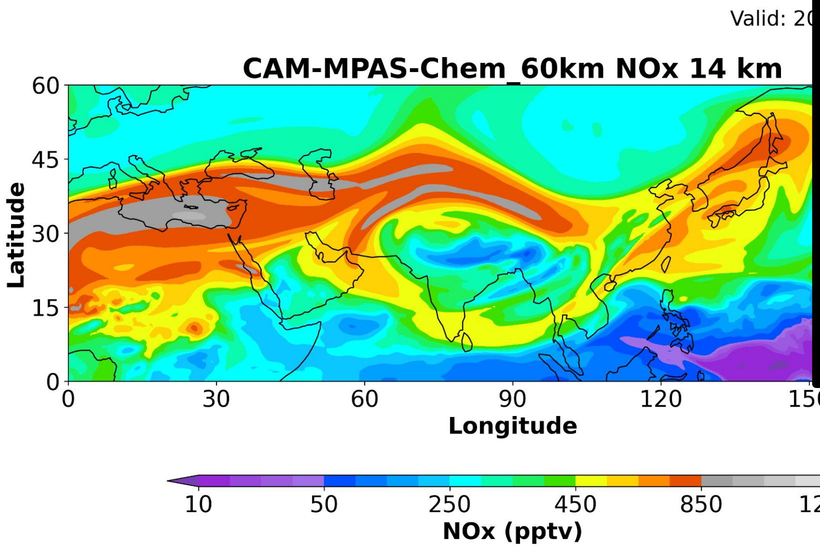
Regionally Refinement





Uniform Grid

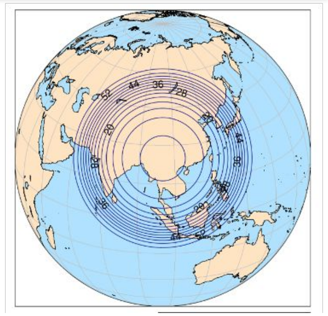




Daily average NO_x at 14 km altitude

- RR NOx much higher over Africa and southern India
- Does shorter time step affect answers?
- Is it lightning-NOx production?

NO_x – effect of time step for 60km, 32L grid mesh

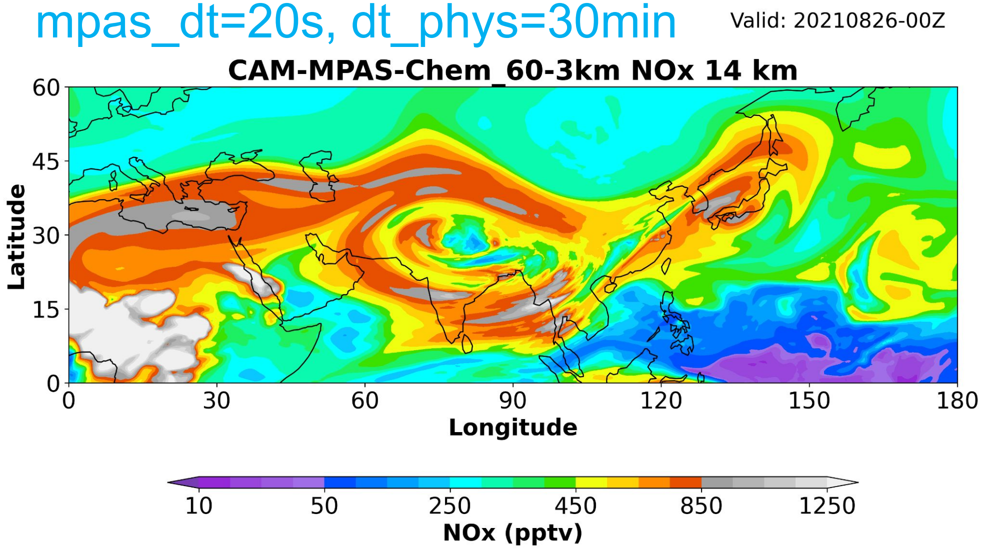


Original Runs

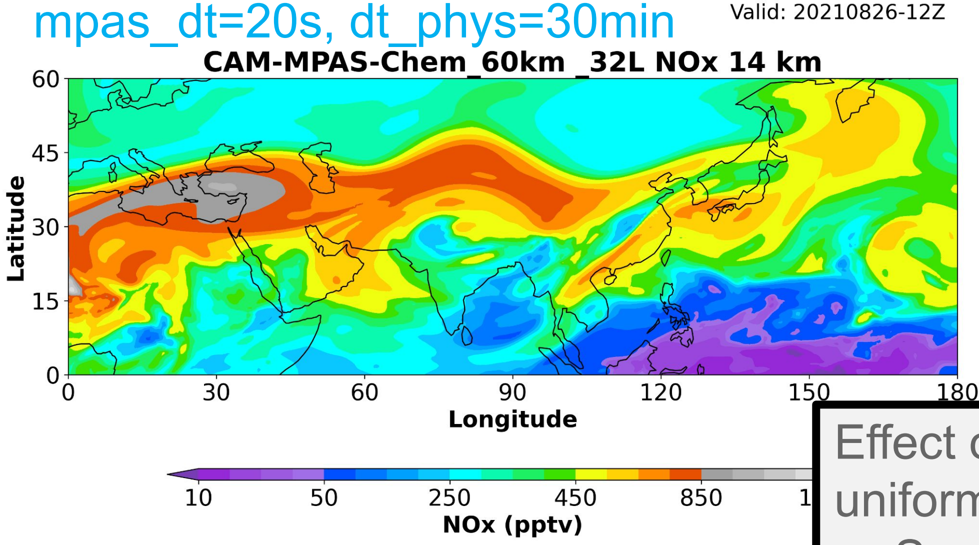
Uniform Grid

Regionally Refinement

mpas_dt=20s, dt_phys=30min

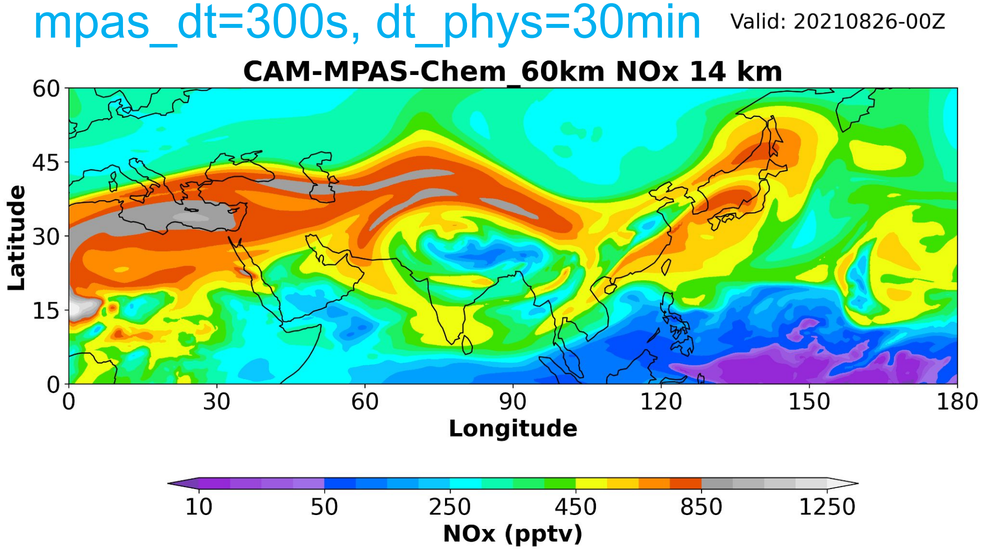


mpas_dt=20s, dt_phys=30min

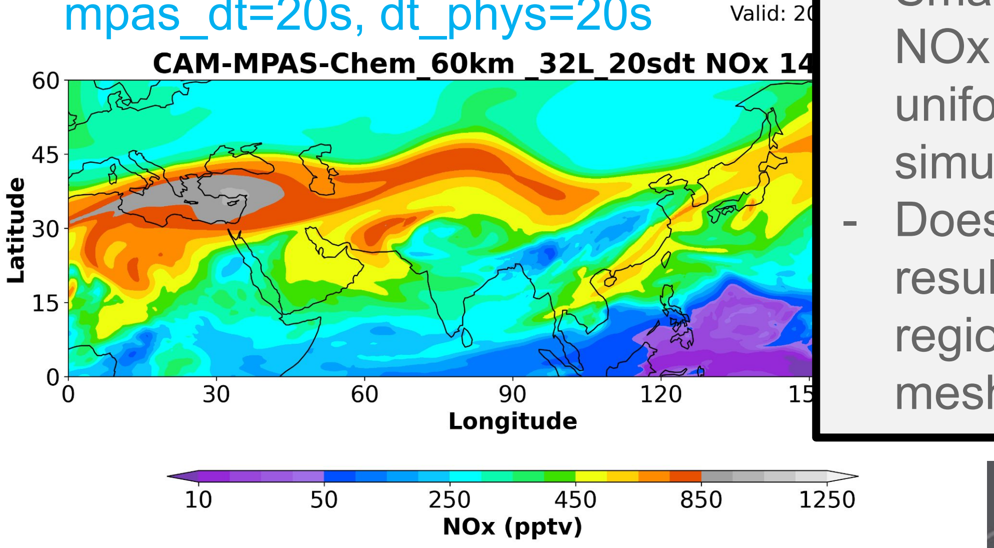


Uniform Grid

mpas_dt=300s, dt_phys=30min



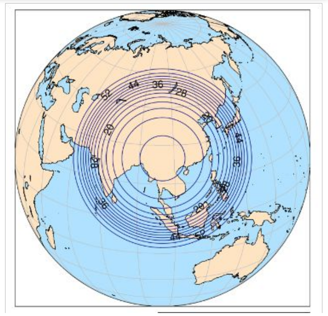
mpas_dt=20s, dt_phys=20s



Effect of time step on uniform grid

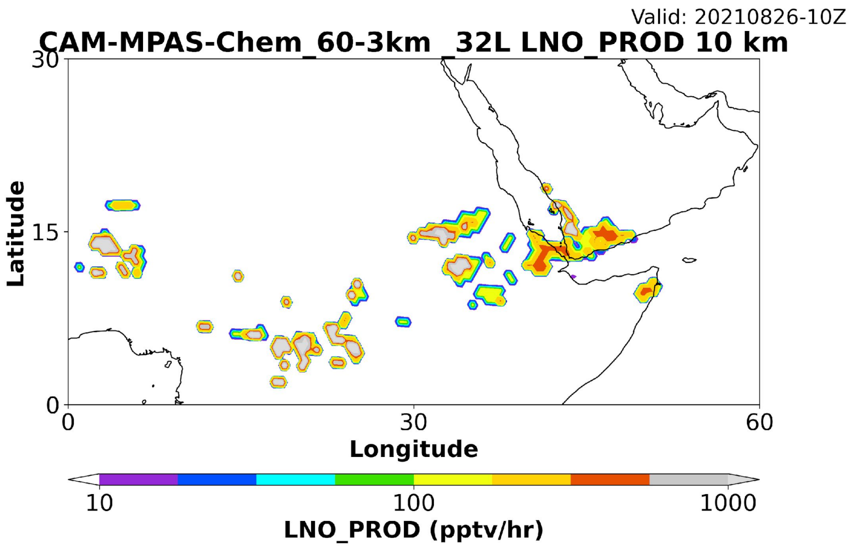
- Small differences in NOx between 60km uniform, 32L simulations
- Does not explain the results in the regionally-refined mesh

Lightning NO Production & Flash Rate

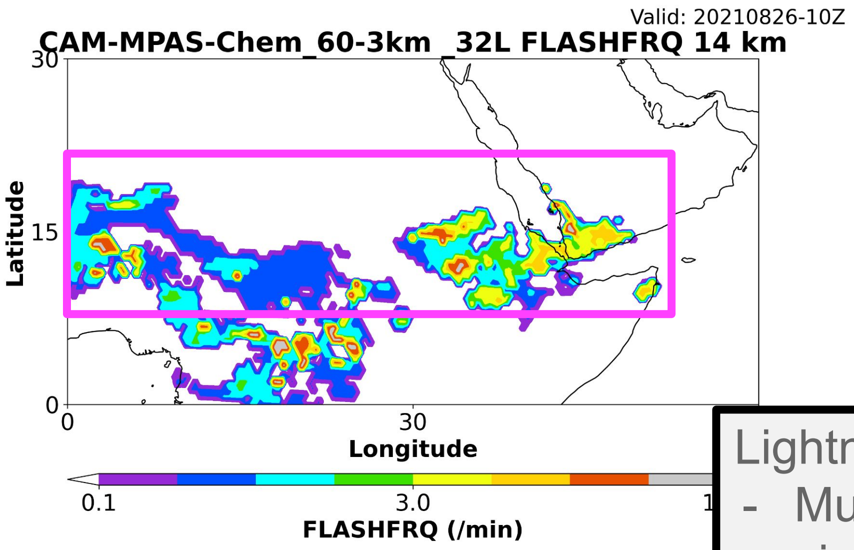


Regionally Refinement

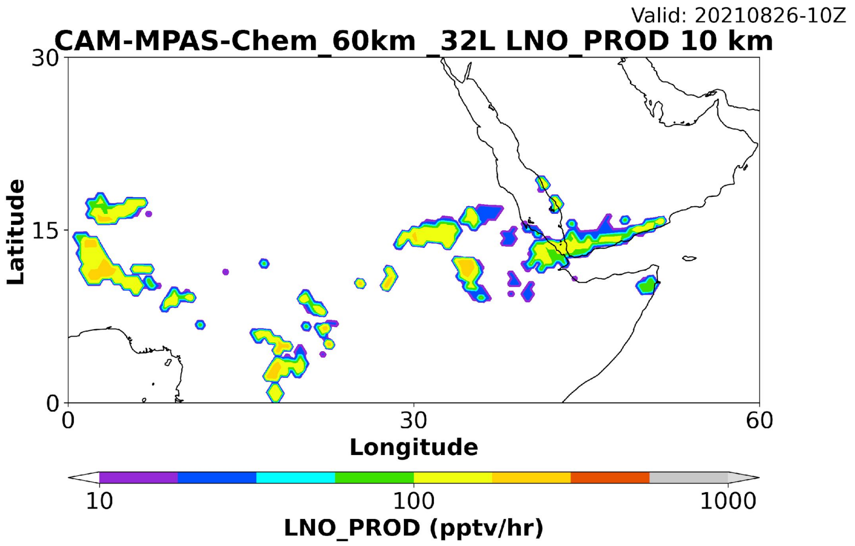
LNO_PROD (pptv/hr)

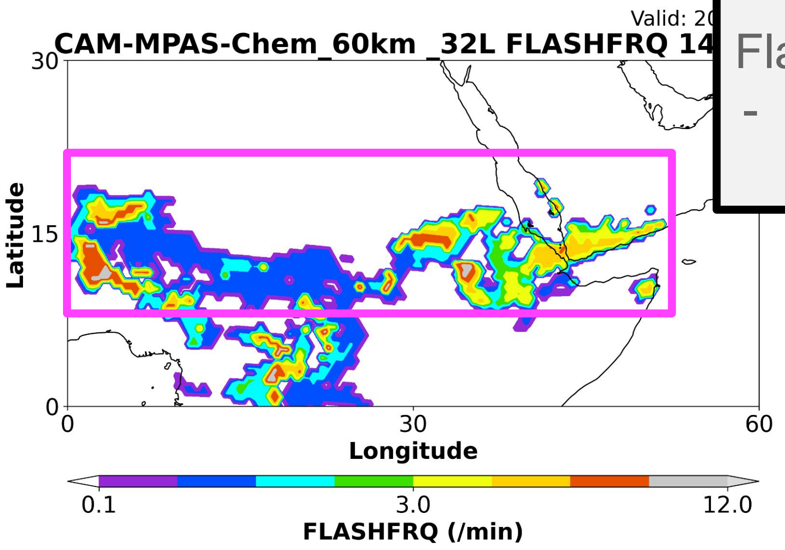


Flash Rate (/min)



Uniform Grid

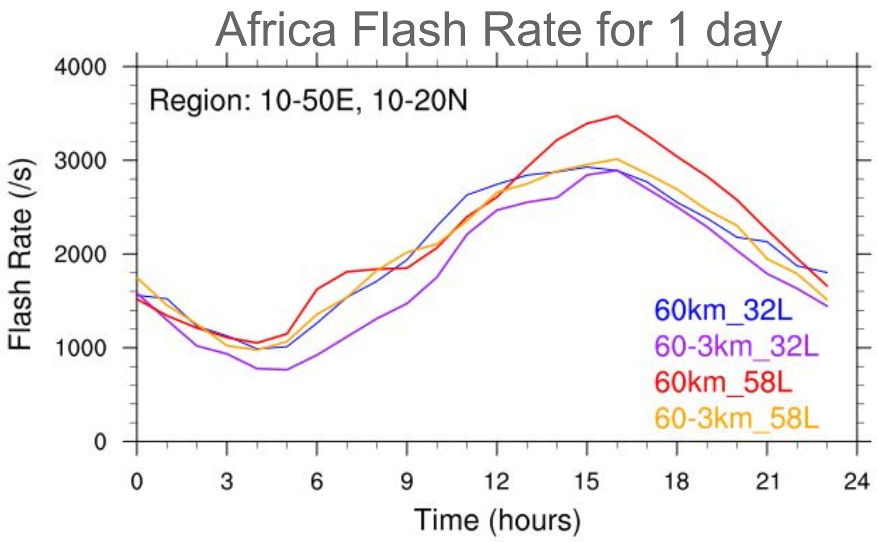


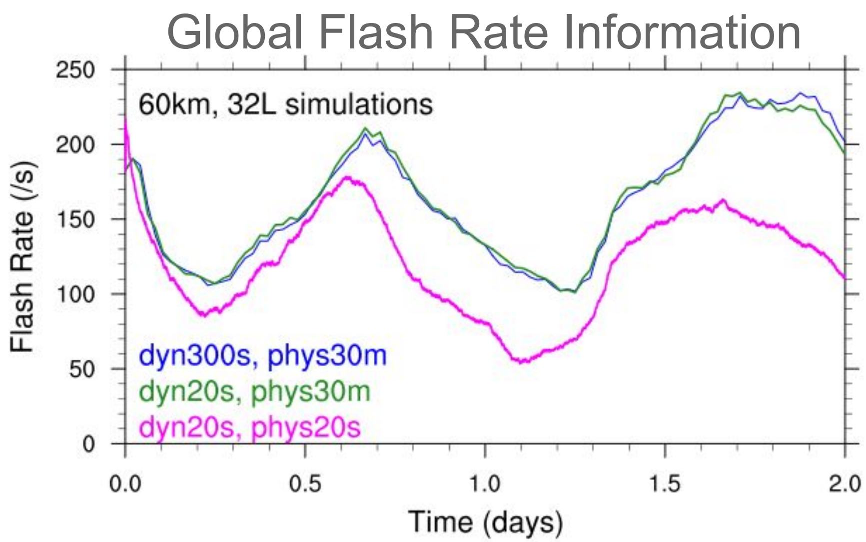


Lightning NO Production
- Much greater in RR simulation

Flash Rate
- May be slightly less in RR simulation

Flash Rate





Flash Rates are smaller in RR simulations

- 58L simulations have higher flash rates

Flash Rate = f(Convective Cloud Top Height)$^{4.9}$

LNOx = f(flash rate) and is scaled to area of grid box

Yet, it appears LNOx production is different

Global Flash Rates are smaller in simulation with shorter physics time step

- Physics time step affects the cloud top height

Note: **Convective parameterization is active in the 3-km region** allowing lightning-NOx to be produced

 Adjustments must be made for a scale-aware convective scheme

Extreme weather events: WACCM with the MPAS dynamical core

Subseasonal-to-Seasonal, Sun-to-Surface (S2S^2) Prediction System

PI: Hui Li (NCAR/CGD)
P. Callahan, J. Richter, S. Yeager, I. Simpson, N. Pedatella, J. Berner, A. Prein, G. Danabasoglu

Science Goals

- Evaluate role of small-scale processes on extreme weather events
- Quantify the value of refined resolution of events, their surface impacts, and coupling to the upper troposphere

CESM Configuration

- CAM-MPAS with CAM7 physics
- WACCM-MPAS with TSMLT chemistry and CAM7 physics
- Simulations
  - Initially with 58L vertical levels to stratosphere
  - 135L to lower thermosphere

Extreme weather events: WACCM with the MPAS dynamical core

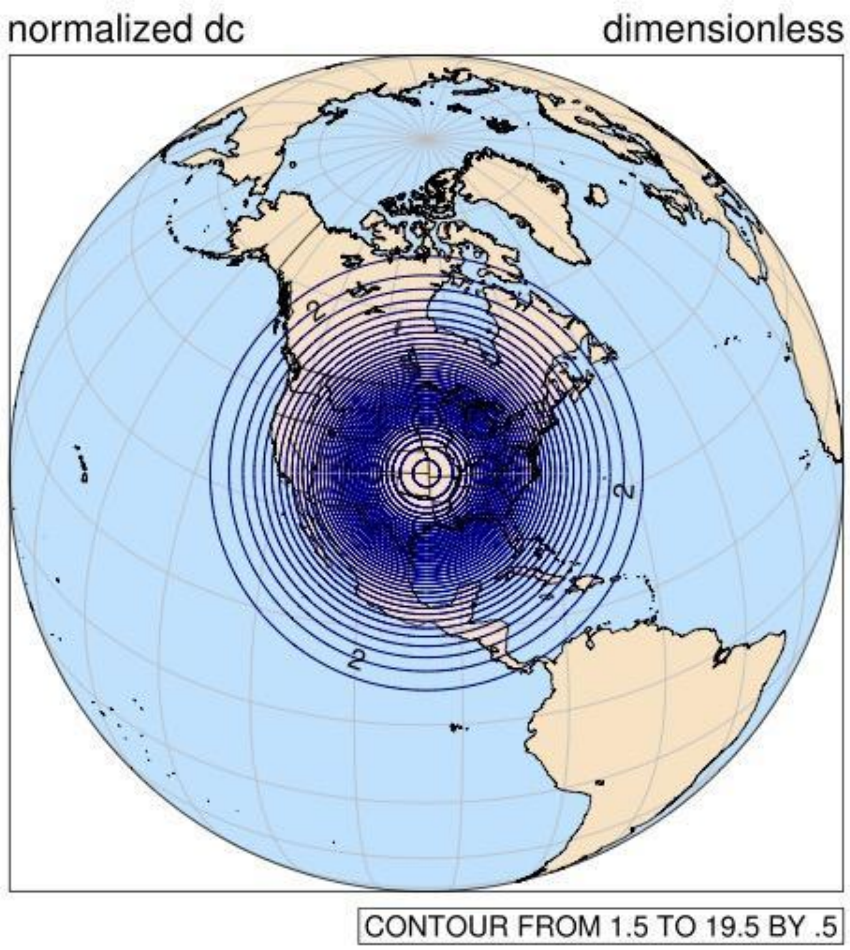
Extreme Weather Events

Cold Air Outbreak in February 2021 in southern US

- 10-member ensemble simulations

Heatwave in June 2021 in Pacific Northwest

- 10-member ensemble simulations



Updates and Highlights:

- Successful development of high-resolution land initialization tools and workflows.
- **Successful test of CAM 58L configuration with desired grid configuration** (60km uniform mesh and RR)
- Progress in developing initialization tools and dataset.
- Outcomes will include streamlined workflow, user repository, and **step-by-step guide for running initialized ensemble forecast with SIMA framework**.

SIMA Ultra-High Resolution Target: Global 3.75km (FMTHIST)

Relative Cost vs Workhorse CESM2	
Δx	32
Δy	32
Δz	2.9
Δt	30
Δphysics	1.1
Total	**~100K**

Derecho is ~*3.5x* faster than Cheyenne.

So, optimistically, just 28,600x to go!

NWSC11 in 2063? (22,500x, @3.5x / 5-yrs)

Current Successes

Milestones start from simple to complex; lots of recent progress!

- ✓ FKESSLER (32L)
- ✓ QPC4 (32L)
- ✓ QPC6 (32L)
- ✓ I2000Clm50Sp
- ✓ F2000climo (32L)
- ✓ QPC6 (93L)
- ✓ *Current Testing: FLTHIST (58L)*

Performance Tests from 41K cores – 164K cores.

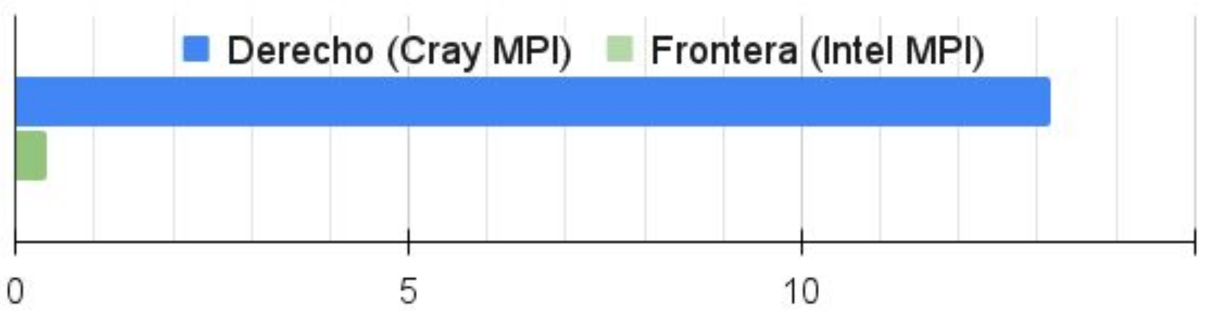
(Some) Identified Software Challenges

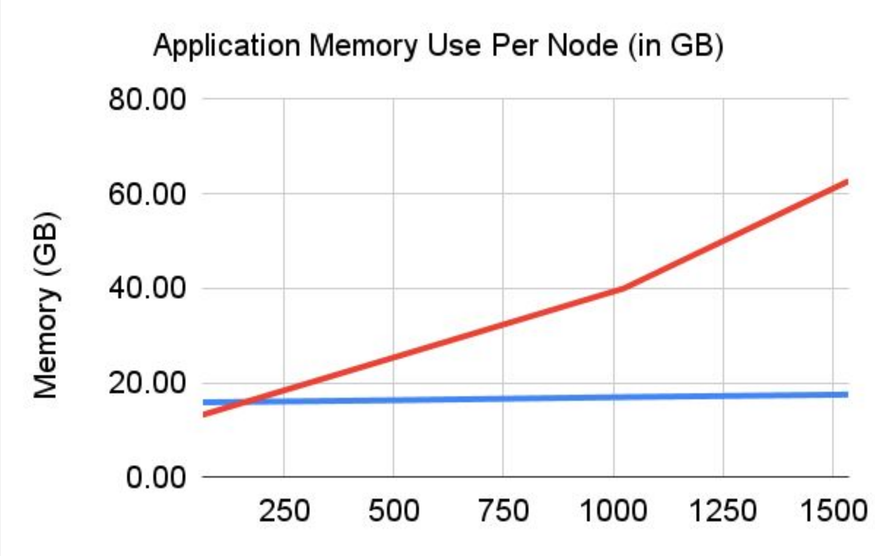
Initialization	ESMF init routines scaling at O(N^2) by core count
I/O	Issue with large writes in PNetCDF; *huge* model states
Low-Res Data	Interpolation issues when processors > points!
Testing, Tracing & Error Checking	Inability to test specific routines; lack of clarity on crashes

Software is not *magic*; it operates within a specific *design space*;
moving outside that space requires *redesign.*

(Some) Identified System Challenges

MPI_Alltoallv Performance
(1 byte, 1280 nodes)





NCAR : 2 GB/core

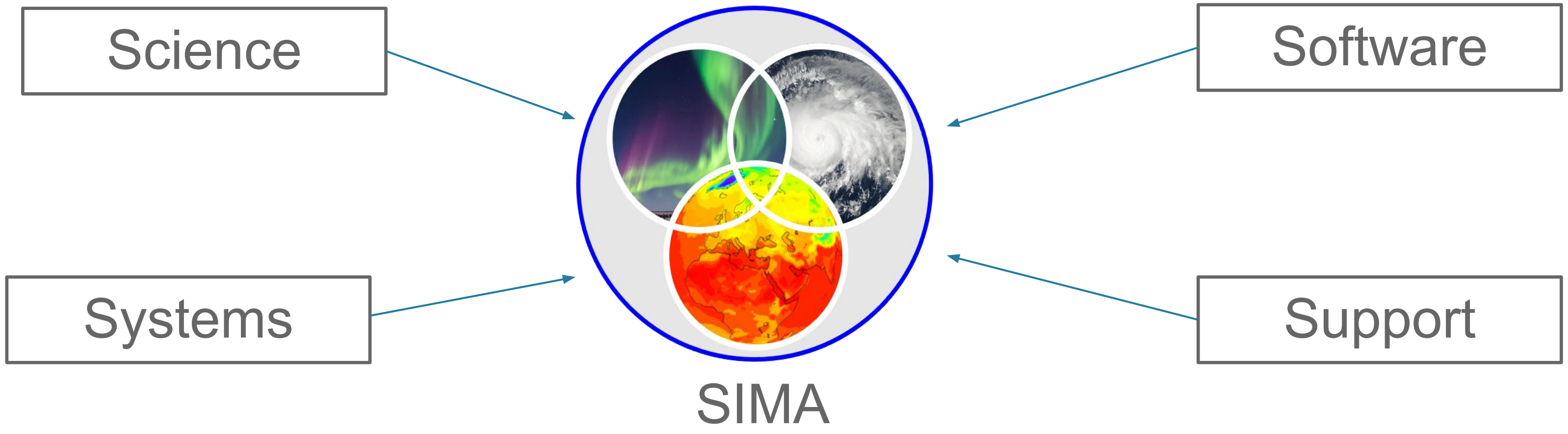
Max Planck : 3.6 GB/core

NASA : 8 GB/core

At the '*capability*' scale, system design is also critically important!

Co-Design: Science, Software, Systems & Support

"Space is big. You just won't believe how vastly, hugely, mind-bogglingly big it is. I mean, you may think it's a long way down the road to the chemist's, but that's just peanuts to space."
- Douglas Adams



"Ultra-High Resolution" is a milestone for SIMA…

… but a complex, all-encompassing *co-design* issue for NCAR & the community

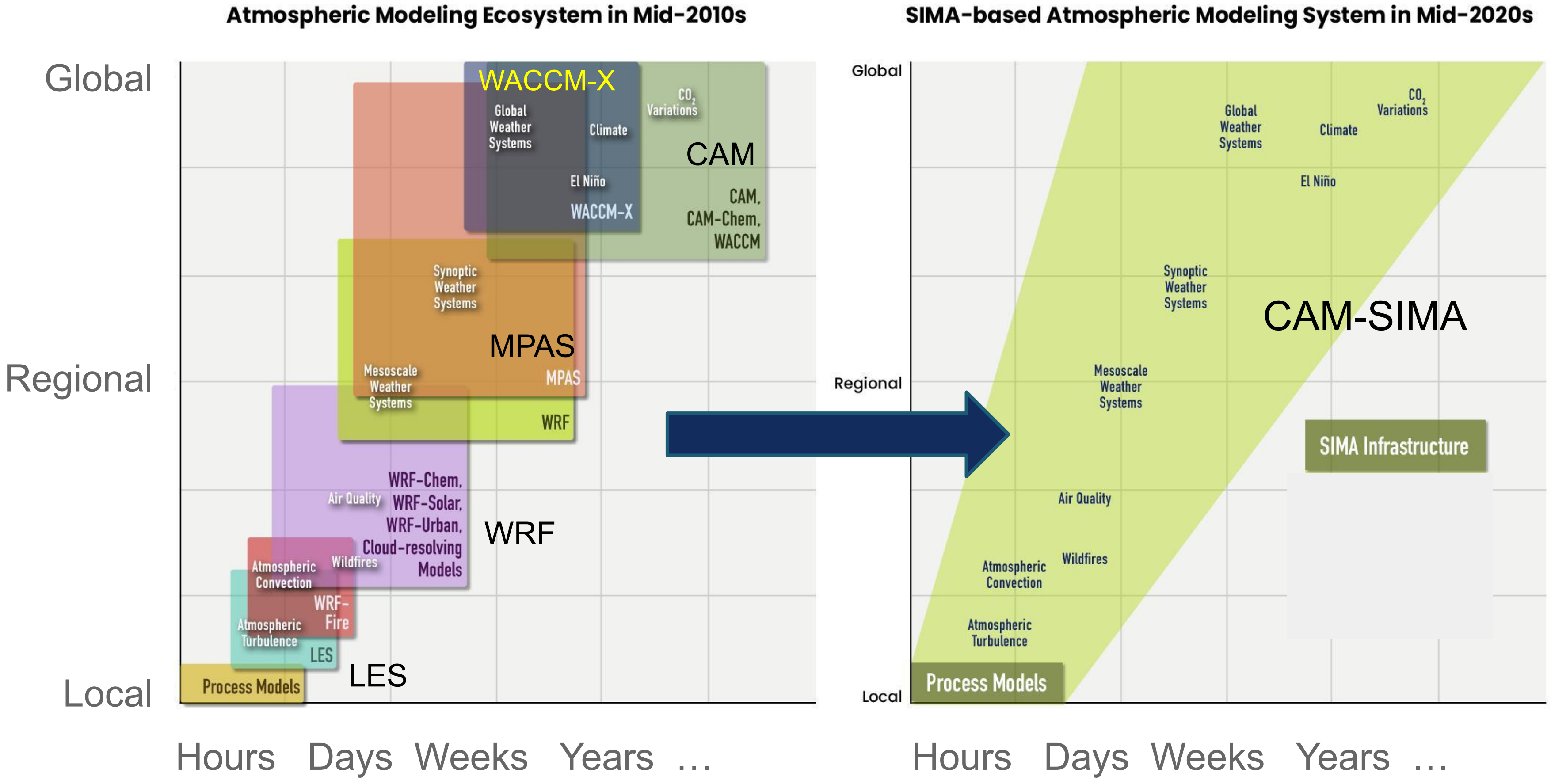
Summary

Simulations with Complex Chemistry [Mary]

- Asian summer monsoon and composition: CAM-chem with the MPAS dynamical core
  - Convective transport of trace gases give similar results for uniform and regionally-refined grid meshes
  - Upper troposphere NO_x in some regions are much greater in the regionally-refined grid mesh simulations than the in the uniform grid simulations likely due to lightning-NO production which depends on convective cloud top height
    - Flash rates vary somewhat with the physics time step and grid mesh
    - Convective parameterization is active in the 3-km region
- Extreme weather events: Global-to-local scale WACCM with the MPAS dynamical core
  - Successful test of CAM-MPAS 58L with regional refinement

System for the Integrated Modeling of the Atmosphere (SIMA)

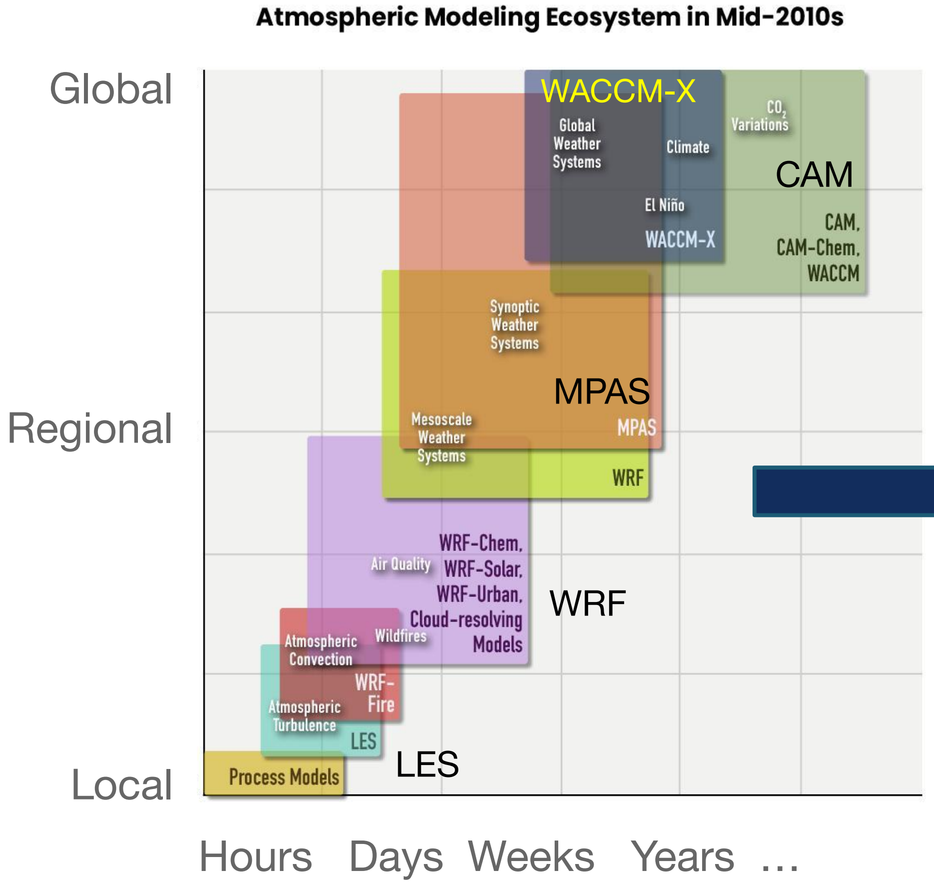
Transition from multiple atmosphere models towards an integrated atmosphere model within CESM

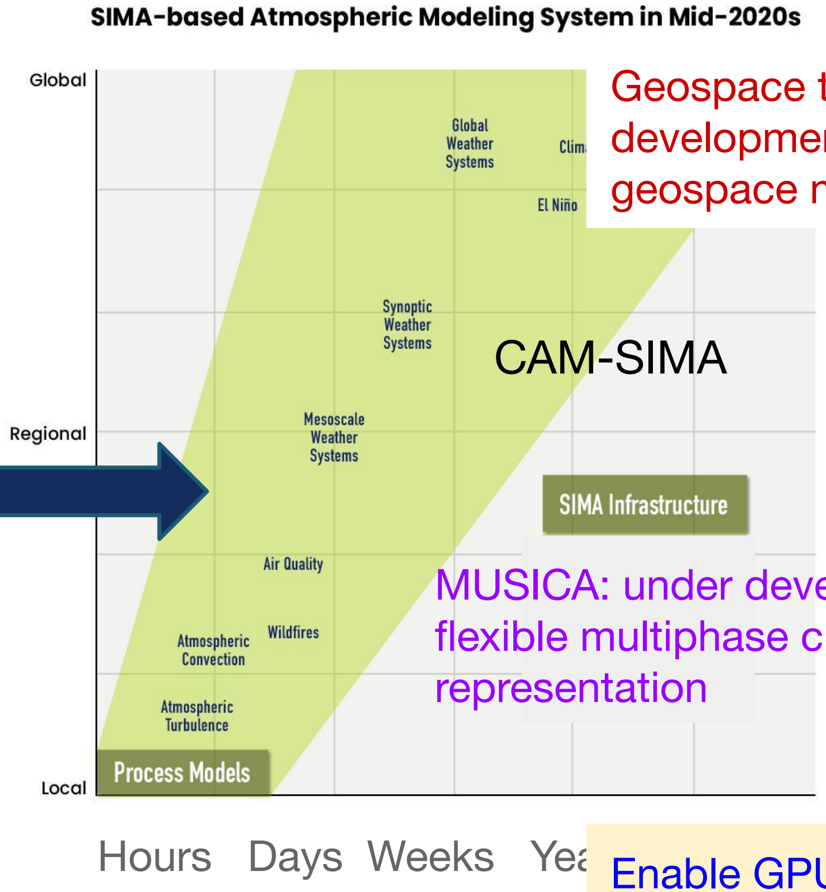


Atmospheric modeling ecosystem in the mid-2010s and anticipated structure in mid-2020s

Software Development Related to the SIMA Project

Transition from multiple atmosphere models towards an integrated atmosphere model within CESM





Geospace tools: under development to have whole geospace modeling capabilities

MUSICA: under development to provide flexible multiphase chemistry and aerosol representation

Enable GPU capabilities in the atmospheric modeling system