Impact of Horizontal Resolution on Ozone Atmospheric Chemistry in Southeast Michigan during MOOSE

2024 CESM Workshop

June 12th, 2024

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WAYNE STATE UNIVERSITY

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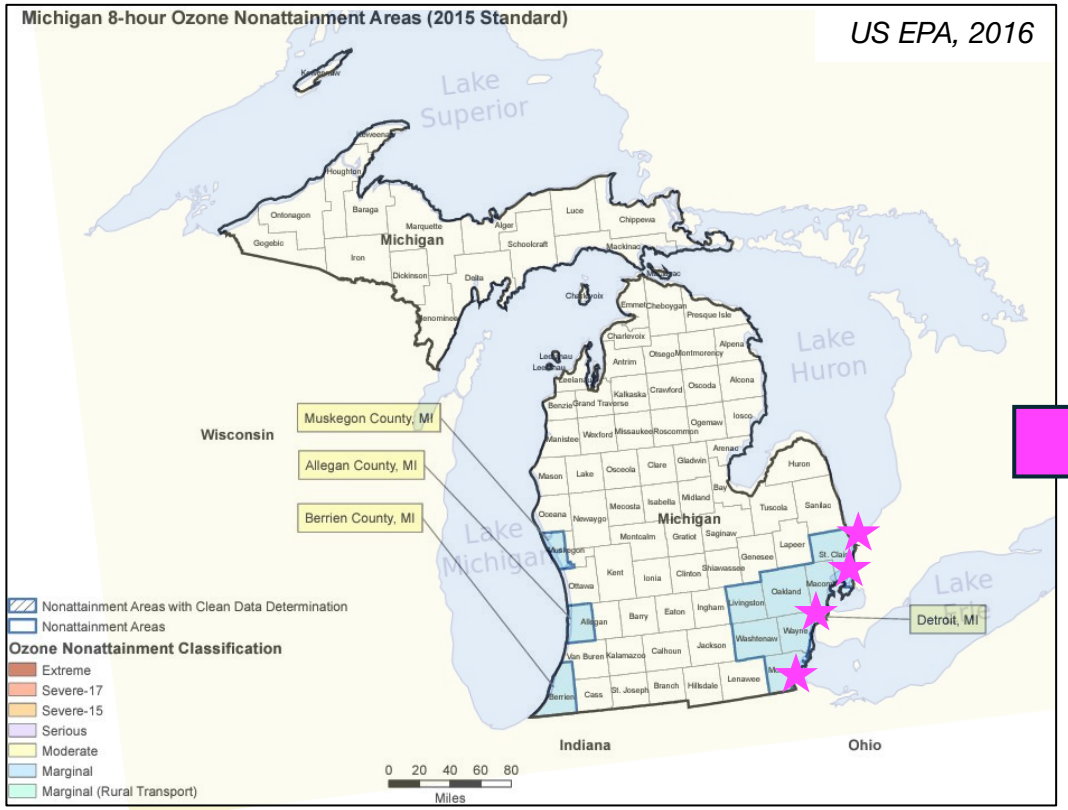
Ozone in Southeast Michigan



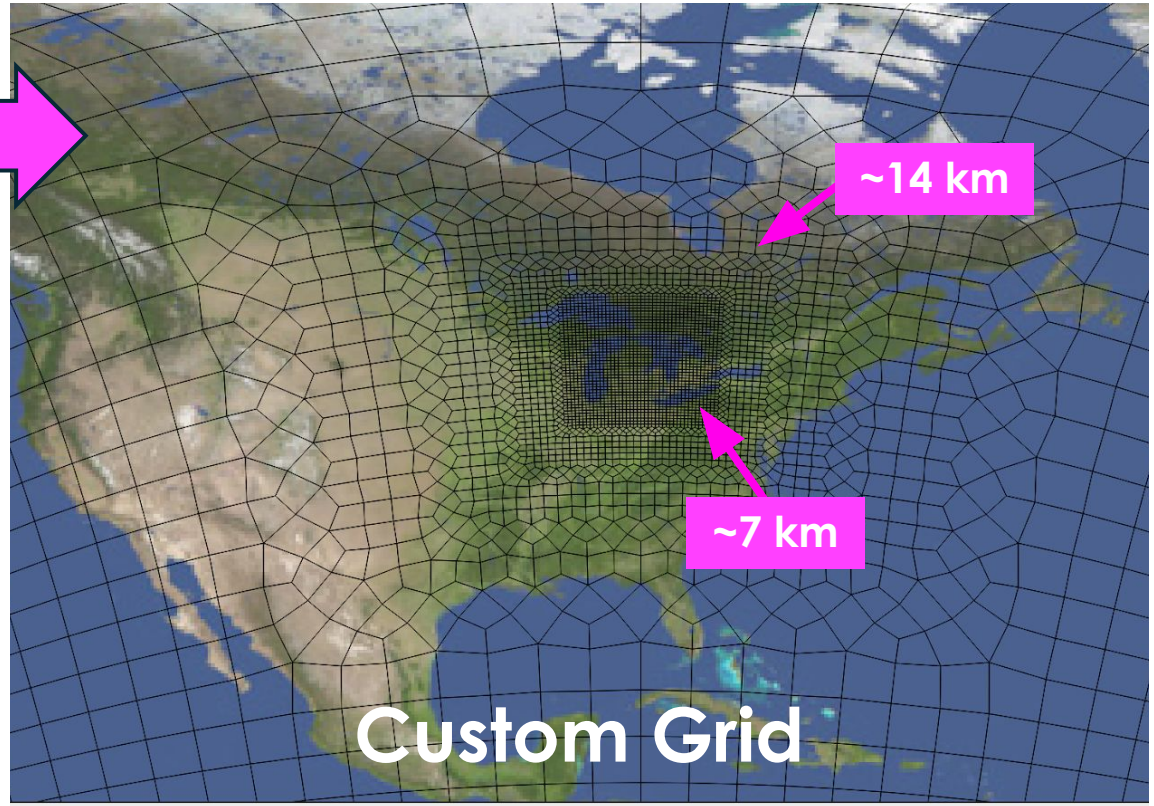
Monroe, MI

Detroit, MI

East China, MI

Sarnia, ON

- **MUSICAv0** is a configuration of CESM/CAM-Chem using the **Spectral Element Dynamical Core** and **Regional Refinement** capabilities.



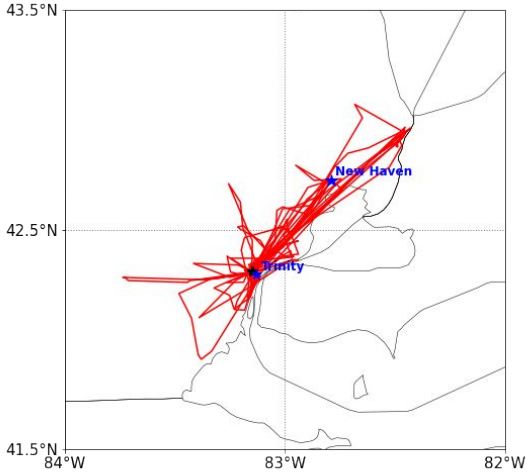
1/16˚ over Michigan

Model Simulation Period & Setup

Michigan-Ontario Ozone Source Experiment (MOOSE)

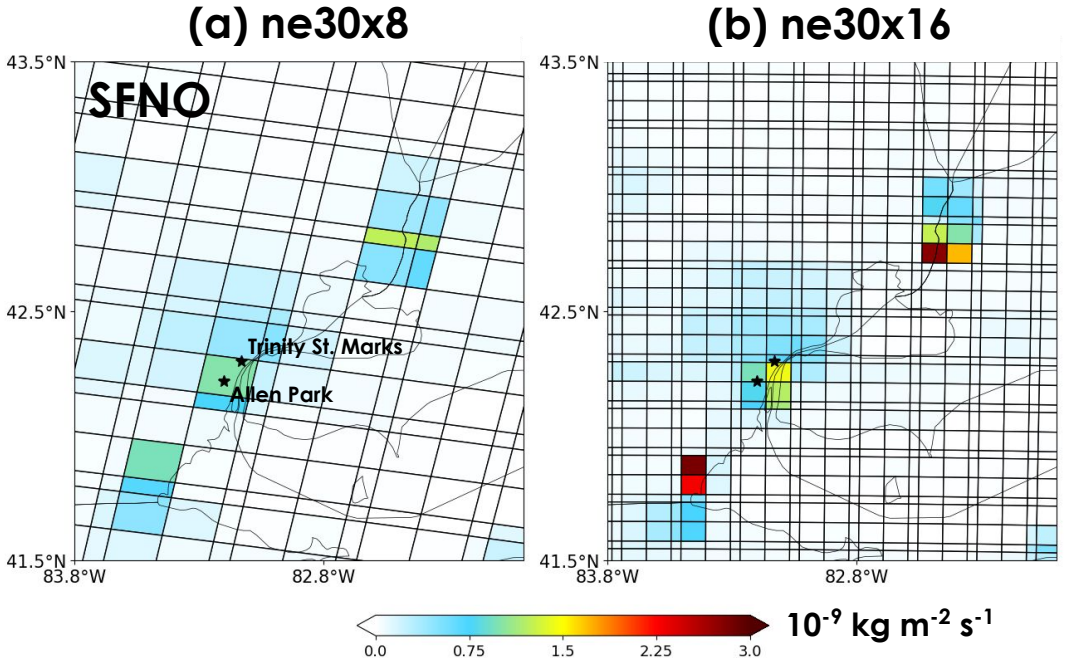
- Goal: Define potential attainment strategies & understand excess O_3 in SEMI.
- **Phase I: May 24 – June 30, 2021** (*Xiong et al., JGR, 2023*)
- Phase II: June 6-28, 2022
- Varied, High-Resolution Measurements
  - Aircraft (NASA G-III), Mobile Lab (Aerodyne), Stationary, Pandora

AML Track



Trinity St. Marks

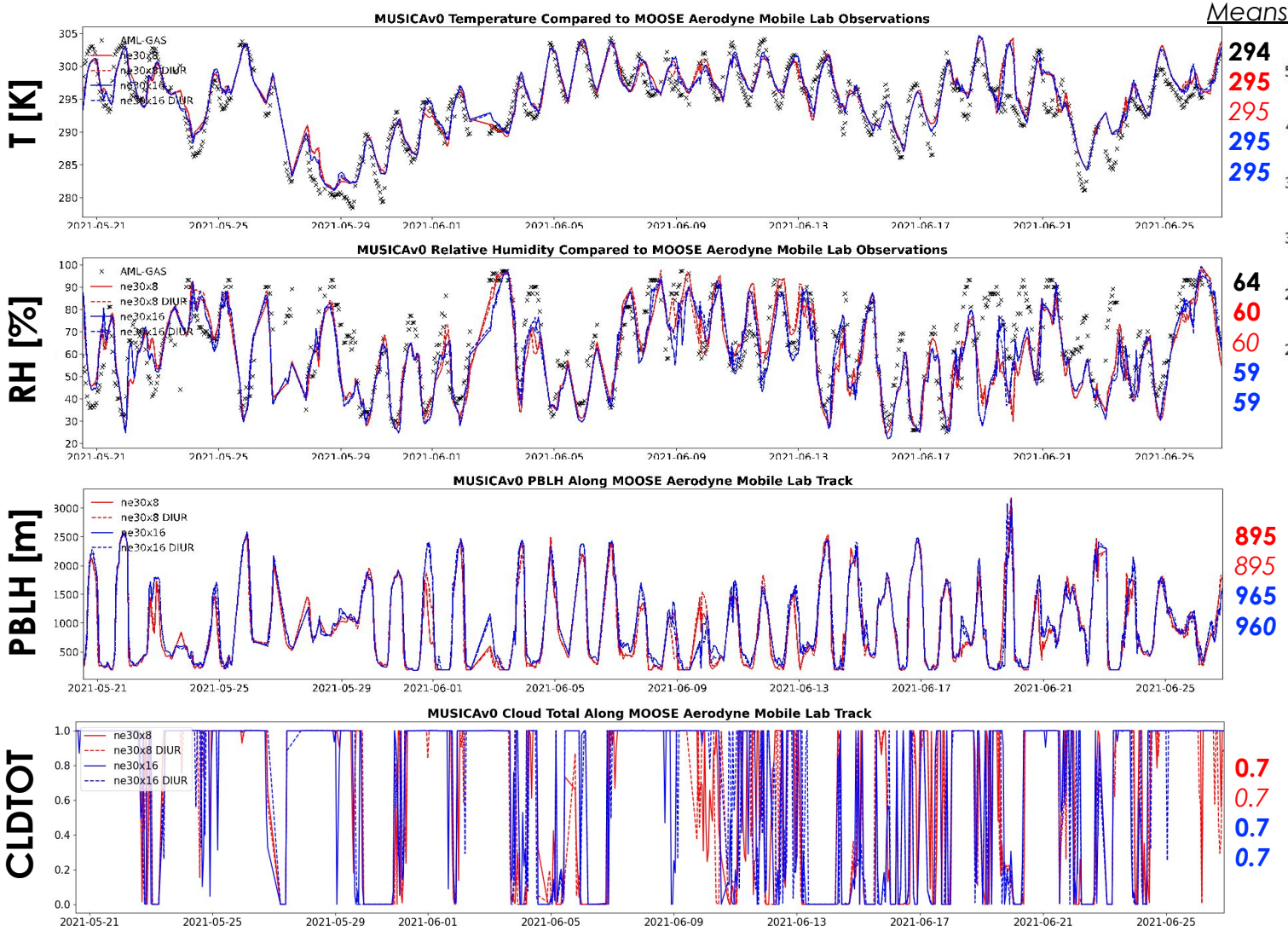
New Haven



Model Simulations

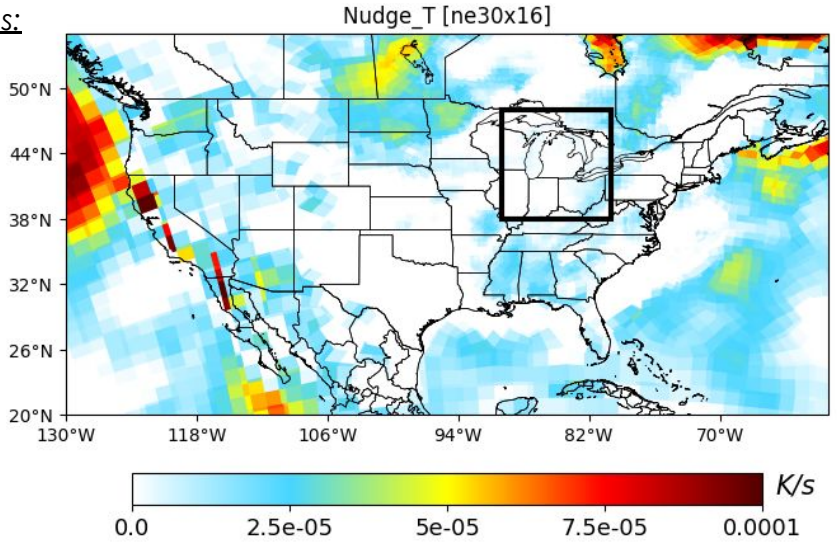
- Two different resolutions (~14 km & ~7 km)
- Implementation of diurnal cycles of nitric oxide anthropogenic emissions
- MOZART-TS2 Chemical Mechanism
- NASA MERRA2 (0.625˚ x 0.5˚ every 3 hours)
- CAMS-GLOB-ANTv5.1, CAMS-GLOB-AIRv2.1, QFED, MEGANv2.1

Meteorological Consistencies

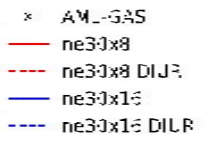


Means:

T [K]	294
	295
	295
	295
	295
RH [%]	64
	60
	60
	59
	59
PBLH [m]	895
	895
	965
	960
CLDTOT	0.7
	0.7
	0.7
	0.7



- NASA MERRA-2 (Resolution: 0.625˚ x 0.5˚ every 3 hours)
  - **No nudging** within the state of Michigan, but a 50-hr relaxation time over the rest of the globe.

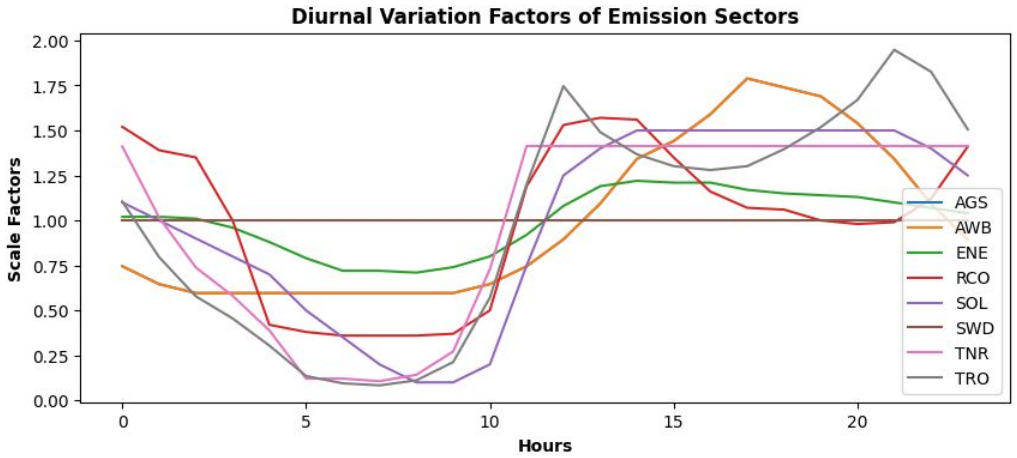


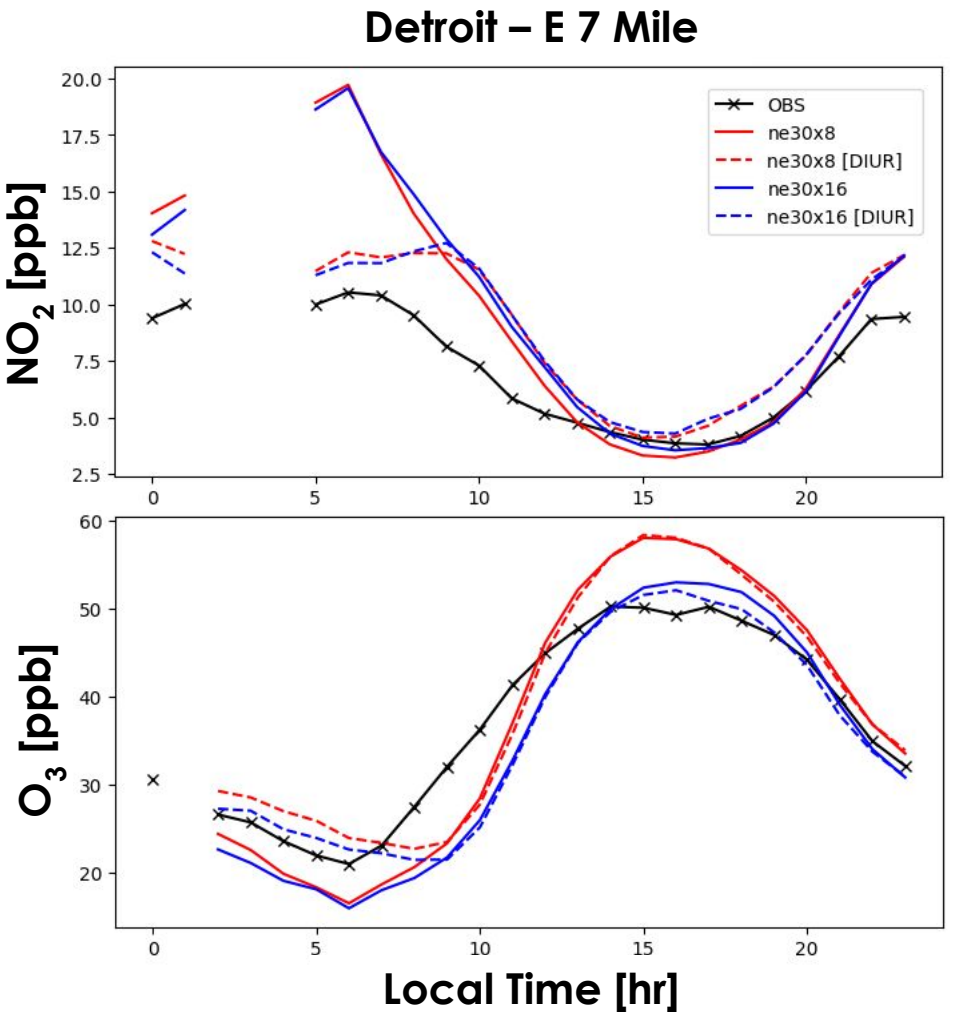
Meteorology is generally consistent in all MUSICAv0 simulations.

Importance of Diurnal Cycles in the Model

- Diurnal variations for anthropogenic emissions are NOT generally considered in CESM2.
- Used sector- and country-specific temporal profiles from Crippa et al (2020)
- Hourly profiles based on downscaling of annual emissions to hourly per grid

	MICH [kt]	SEMI [kt]	SEMI/MICH
AGS	0.46	0.04	9.0%
AWB	0.10	0.01	10.8%
ENE	9.44	2.86	**30.3%**
RES	1.03	0.48	**47.1%**
TNR	1.99	0.36	**18.1%**
TRO	15.13	3.50	**23.2%**





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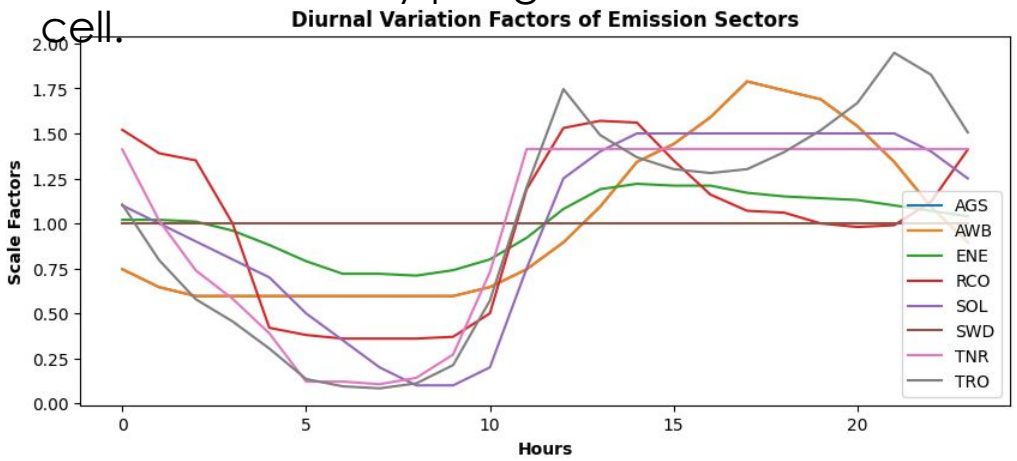
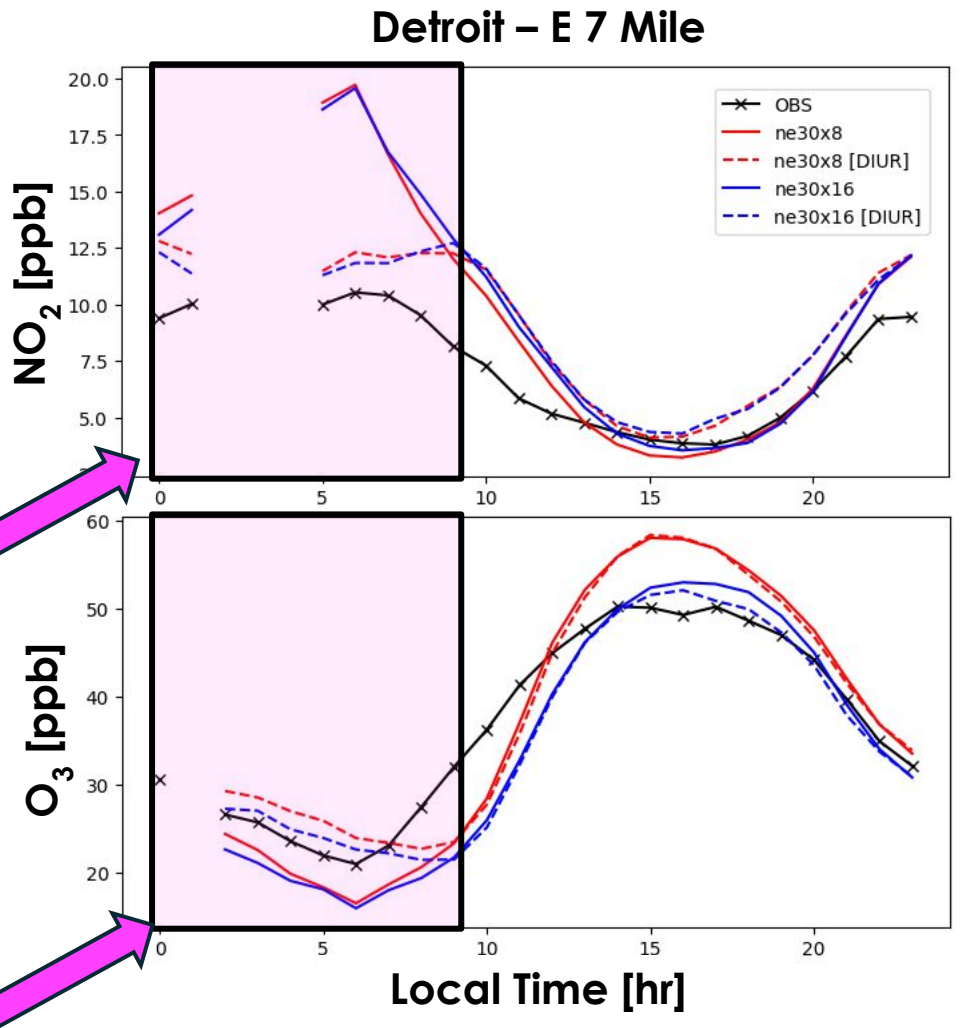


Addition of diurnal cycle improved NO_2 simulation during 0-10 EDT.

Improvement in O_3 bias during 0-10 EDT as a result of better NO_2 simulation.



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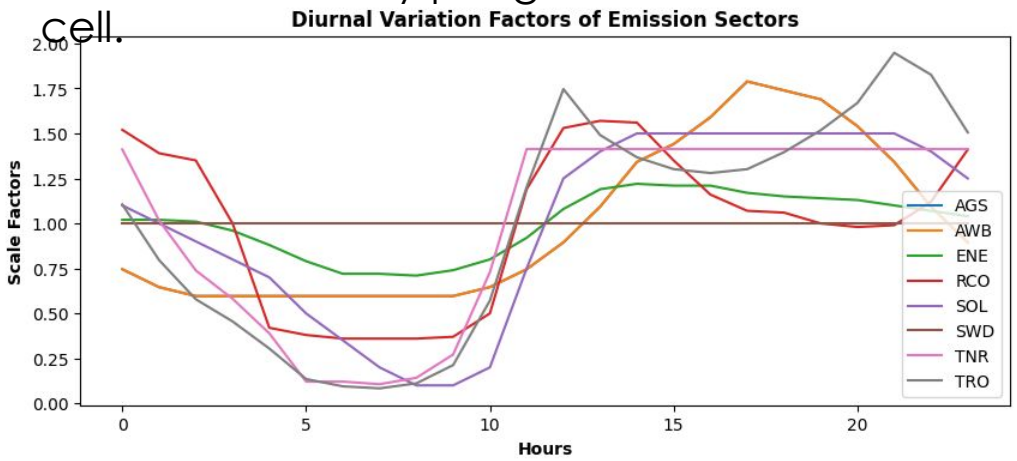
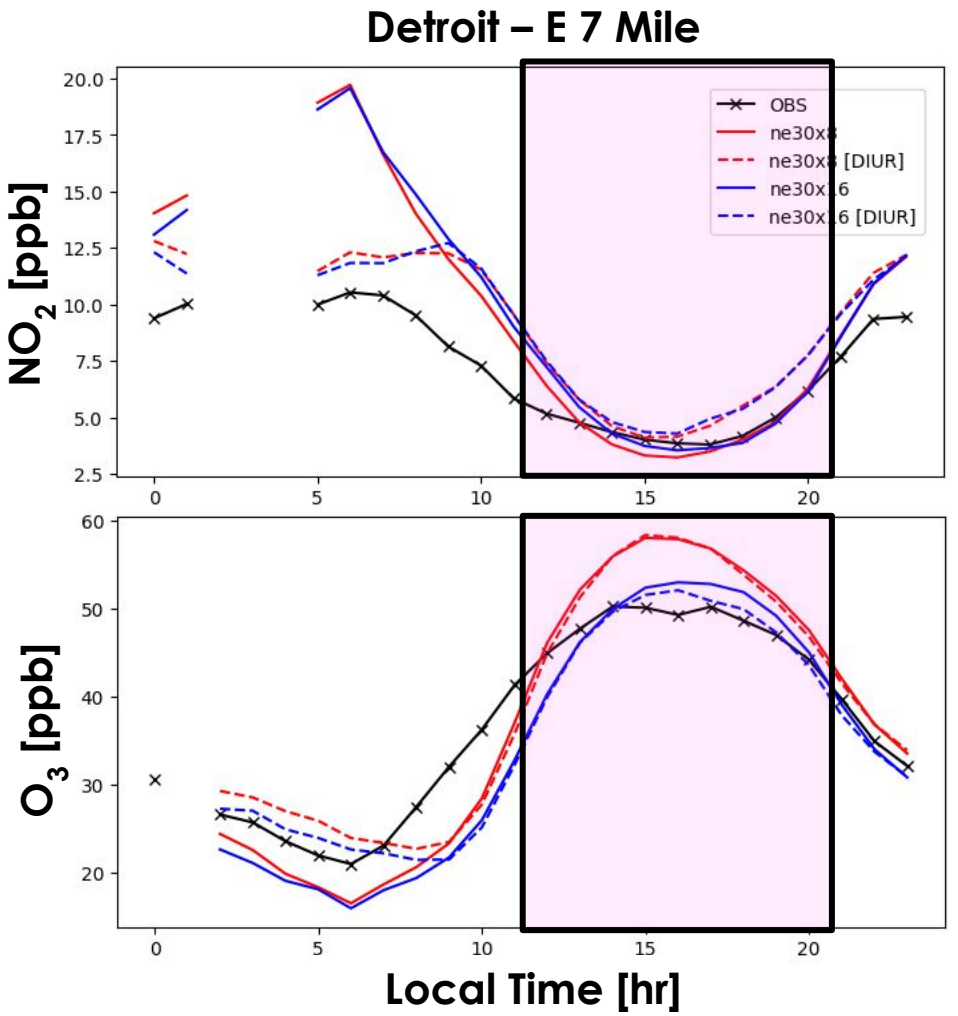
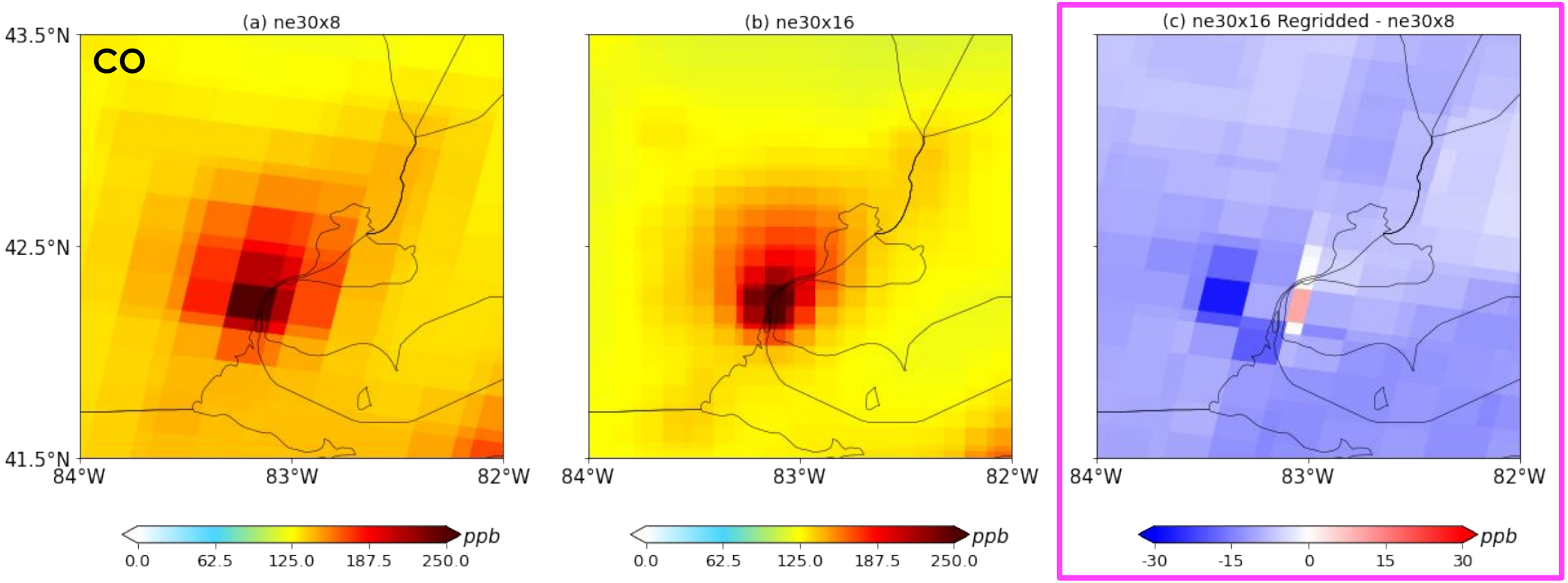


Little to no change during peak O_3 times when adding diurnal cycle.



Carbon Monoxide Concentrations at the Surface

ne30x16 Regridded – ne30x8



- Carbon Monoxide (CO) **fine-scale features captured in regional refinement grids**, with point sources better resolved in the ne30x16 (7km resolution).
- CO is relatively chemically inactive, so low chemistry effects due to horizontal grid resolution.

Ozone Concentrations at the Surface

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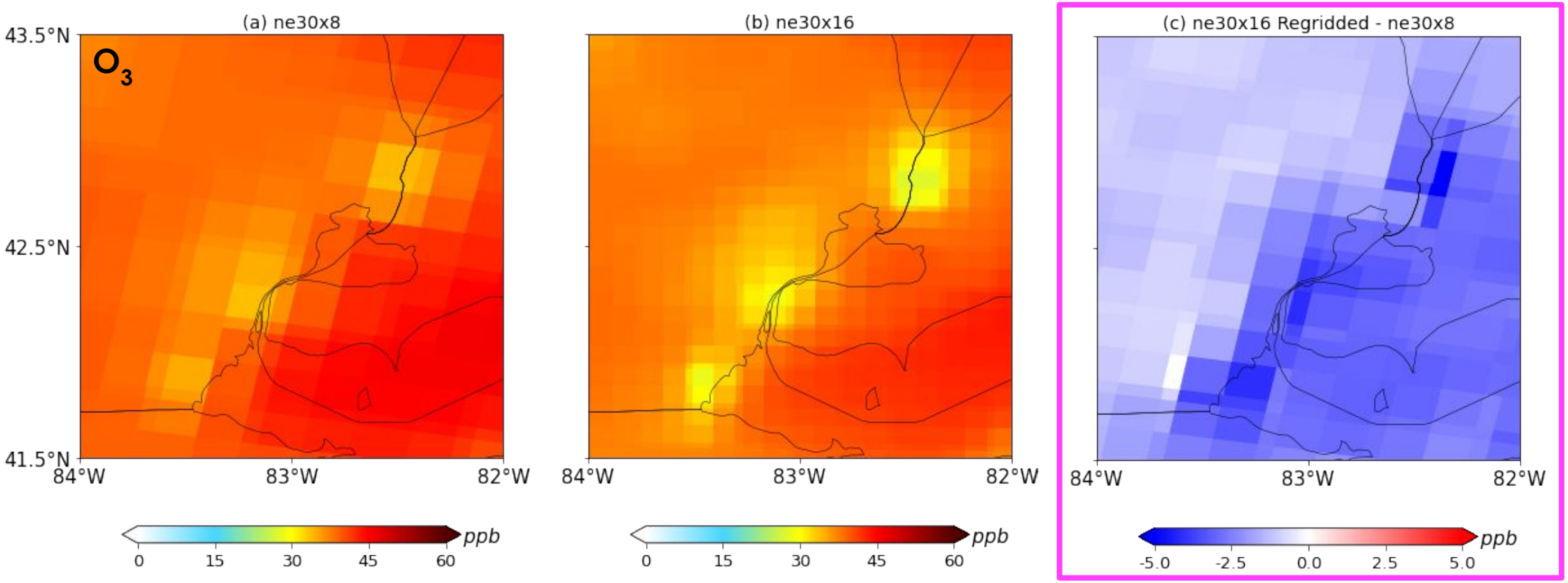
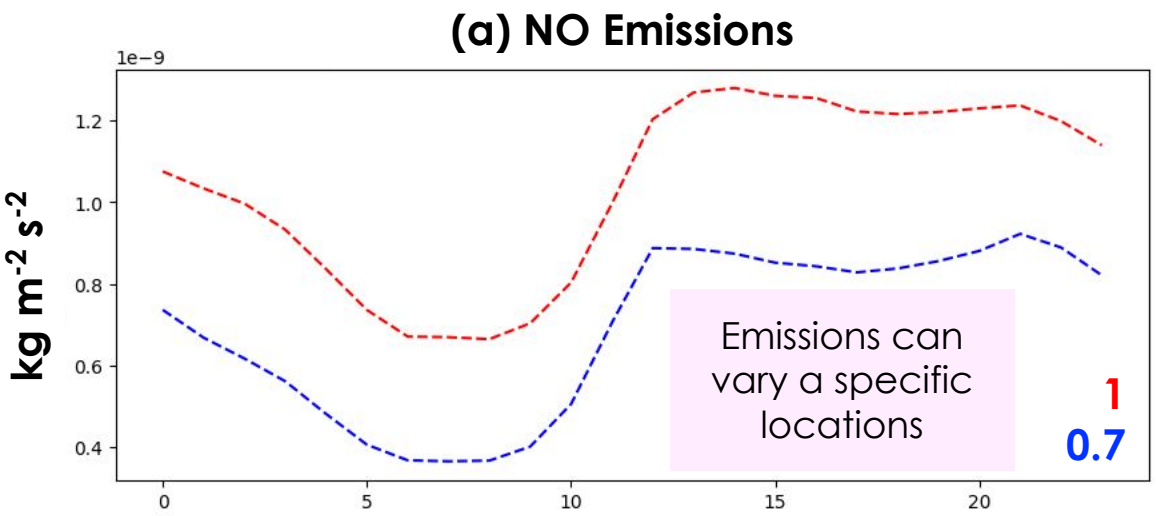
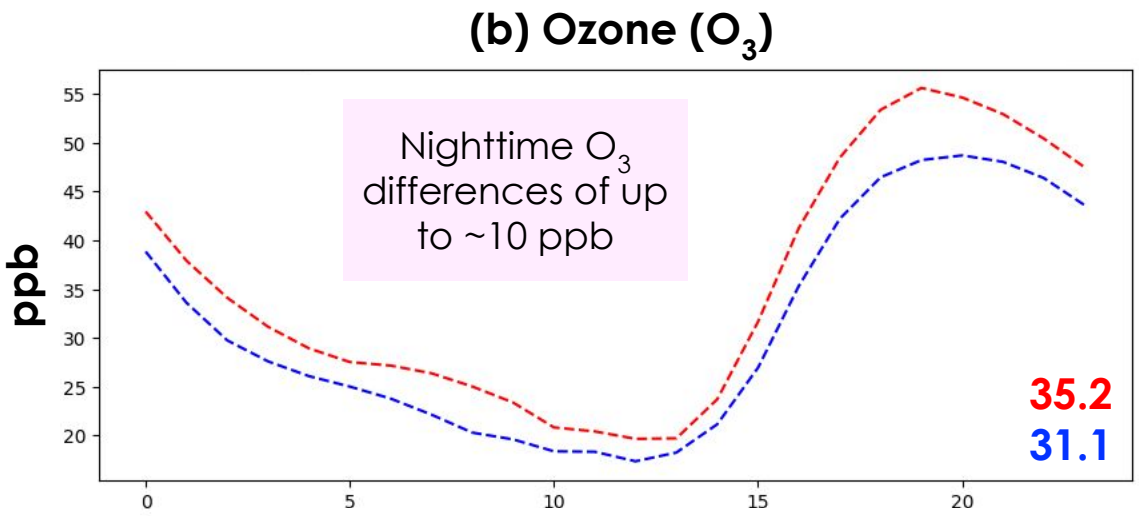


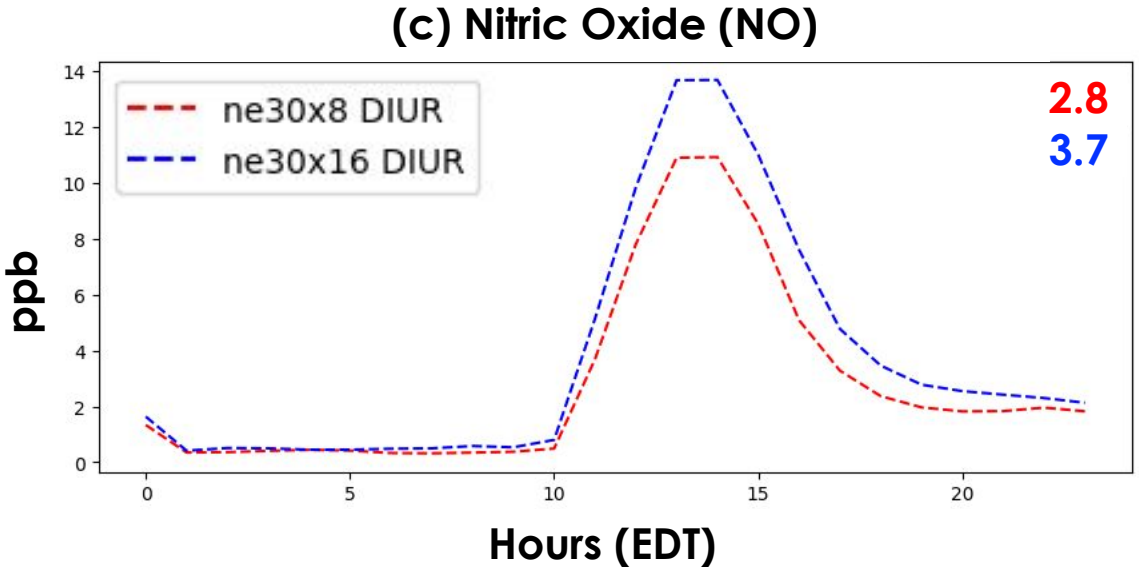
- ne30x16 grid captures more NO_x titration over urban areas due to **less artificial mixing** of NO_x over urban areas.
- Regridding of ne30x16 to ne30x8 resolution does not reproduce the same results the ne30x8 simulation output.

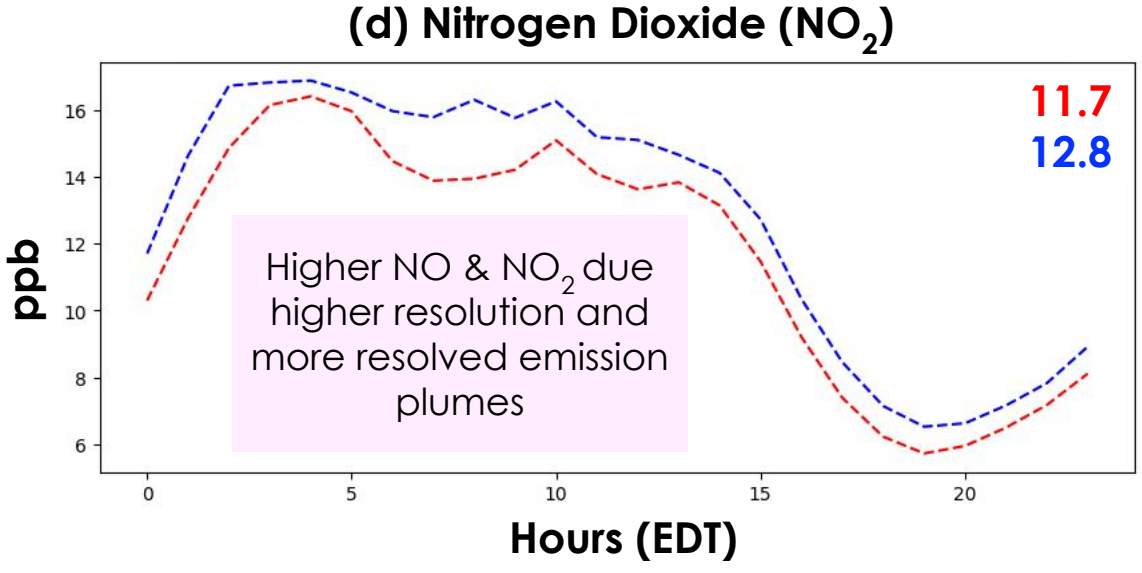
Changes in Ozone

*Urban (Trinity) Reference Site





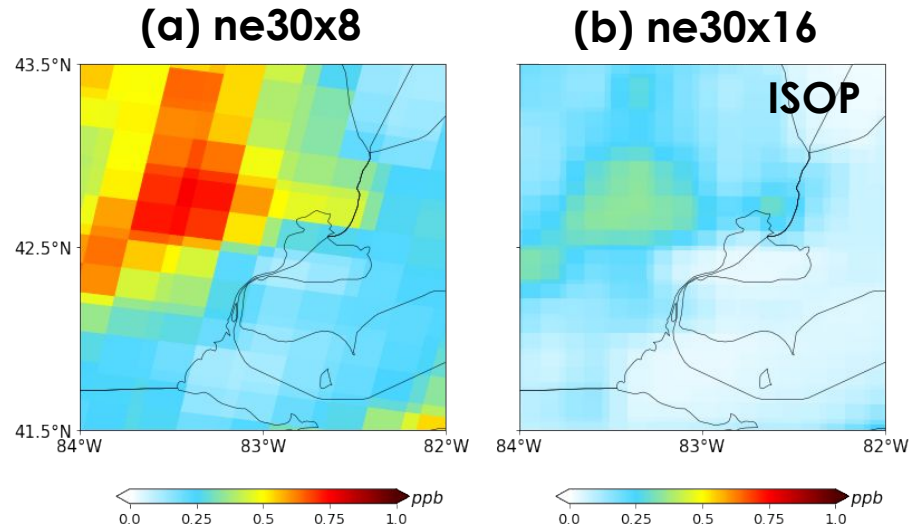


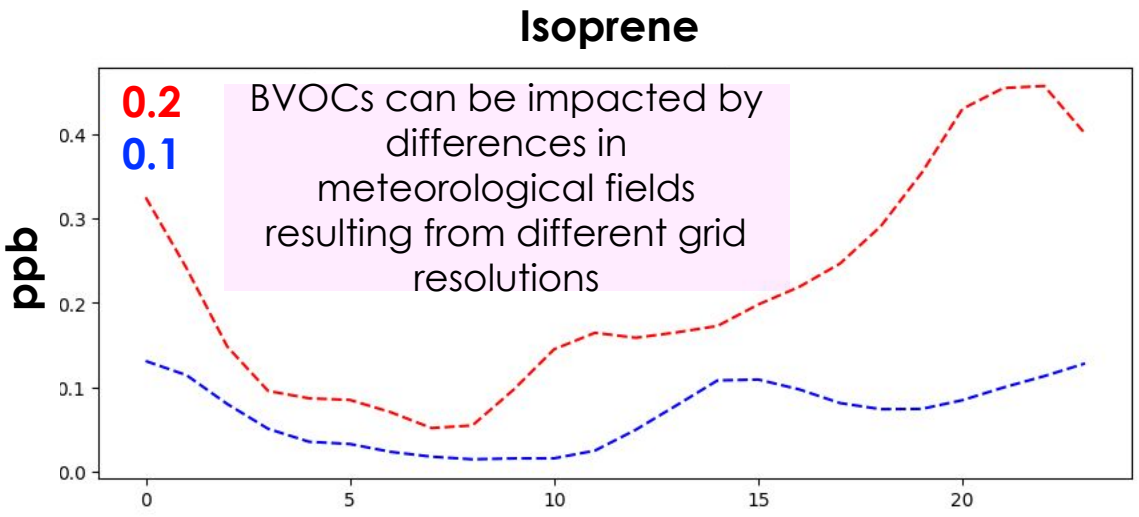


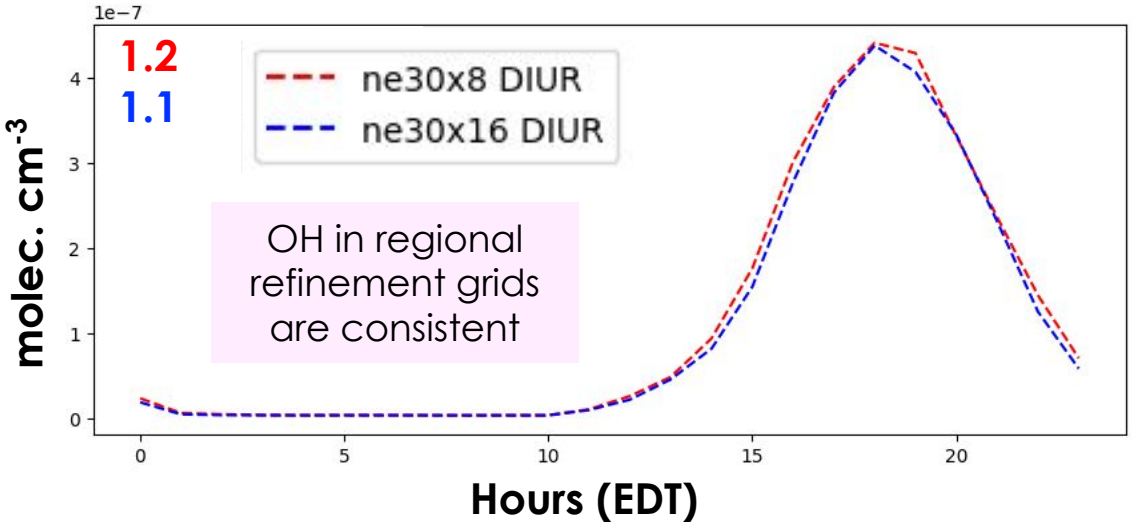
Biogenic VOCs Dependent on Grid Resolution

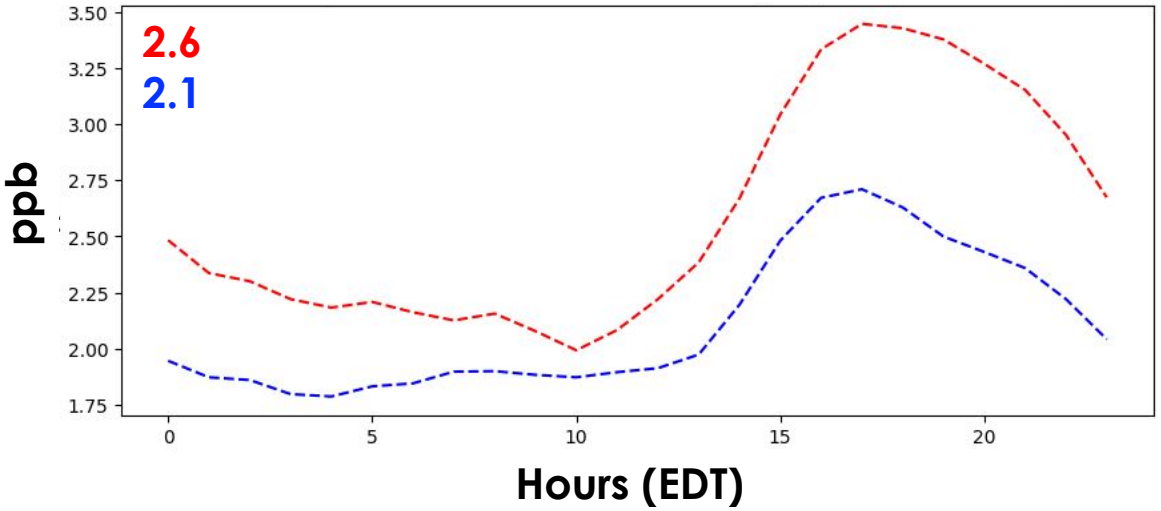
*Urban (Trinity) Reference Site

BVOCs calculated online via MEGANv2.1 in CLM

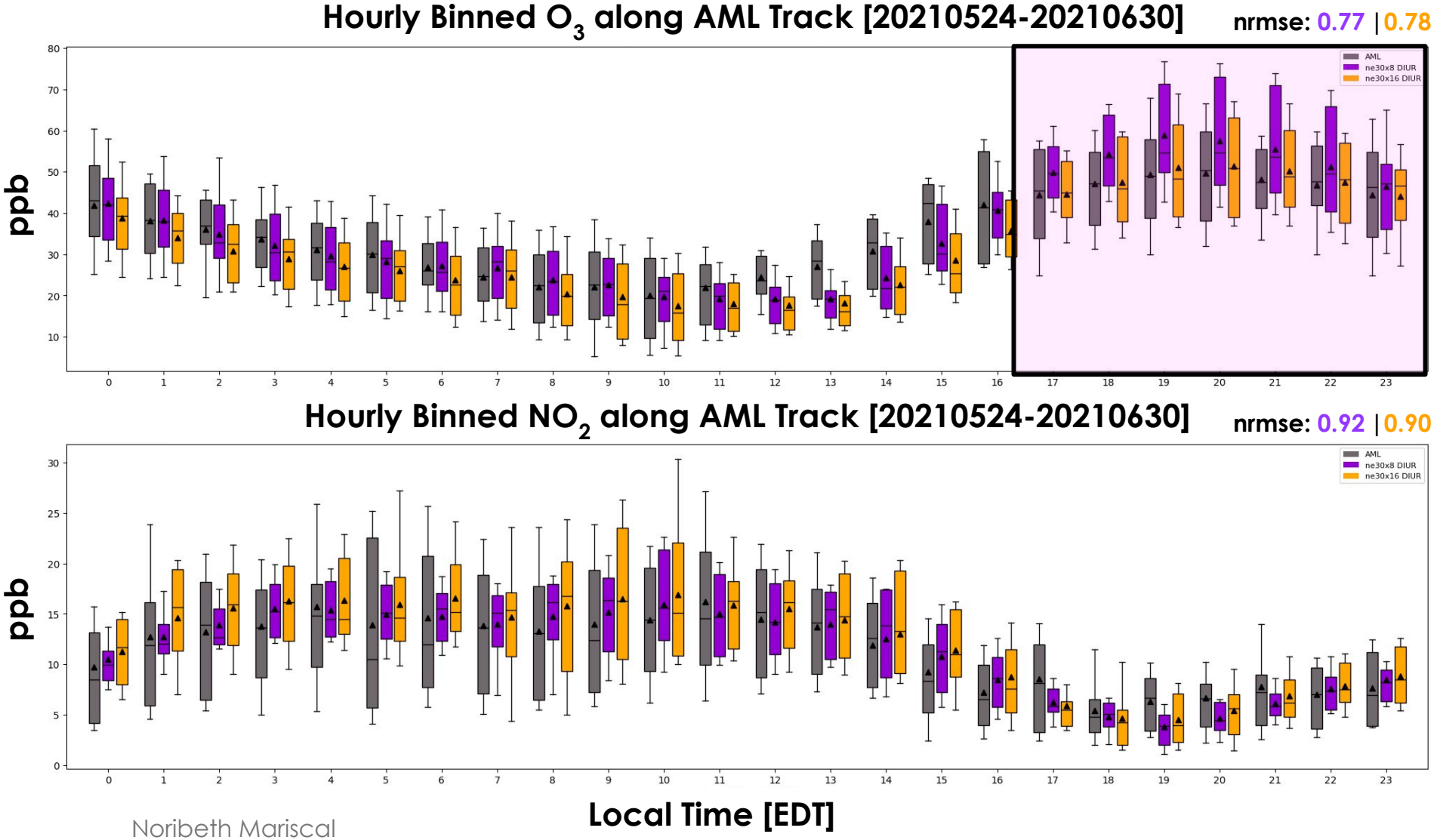








Model Evaluation with Aerodyne Mobile Lab

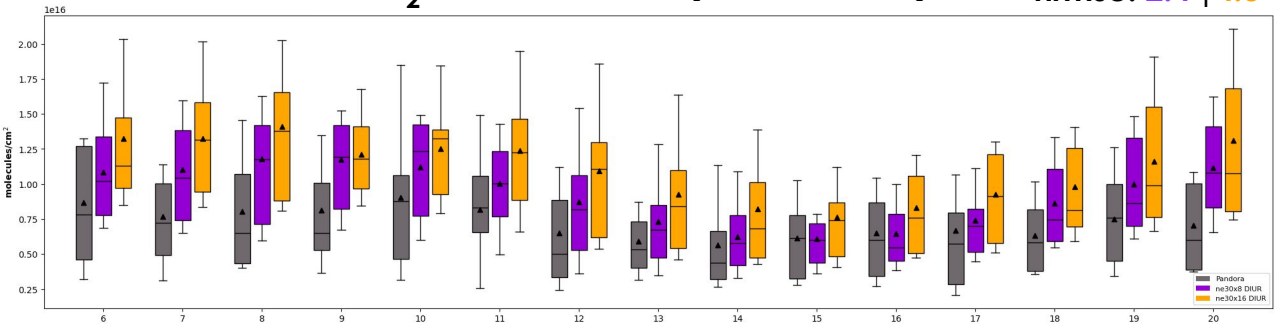


- Both O_3 and NO_2 are represented well at the ne30x8 and ne30x16 resolutions.
- O_3 in the ne30x16 simulations performs best during peak O_3 times.

Model Evaluation with Pandora (in molecules/cm^2)

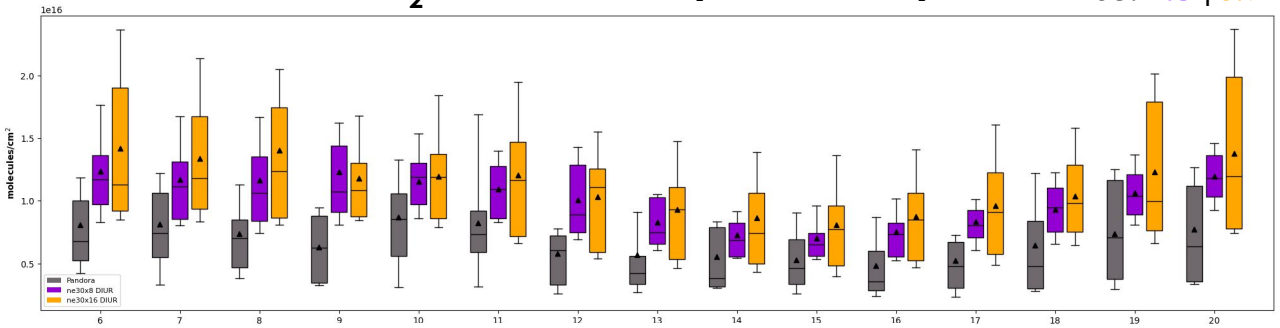
NO_2 VCD @ 3.4 km (SWDetroitMI)

nrmse: 2.4 | 4.0



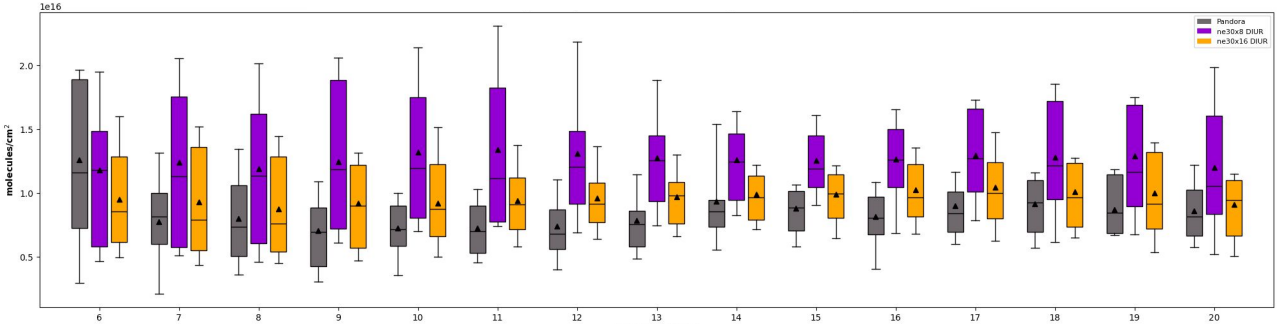
NO_2 VCD @ 3.4 km (DearbornMI)

nrmse: 2.8 | 3.7



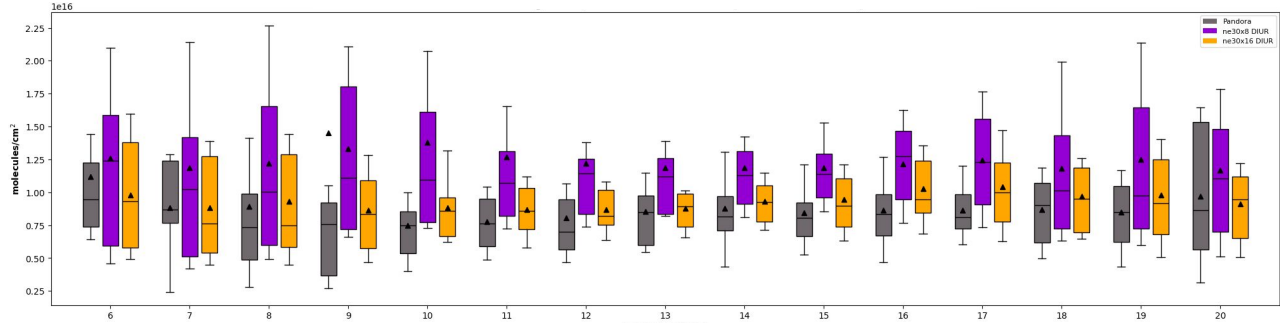
HCHO VCD @ 3.4 km (SWDetroitMI)

nrmse: 3.4 | 1.3



HCHO VCD @ 3.4 km (DearbornMI)

nrmse: 2.2 | 1.1



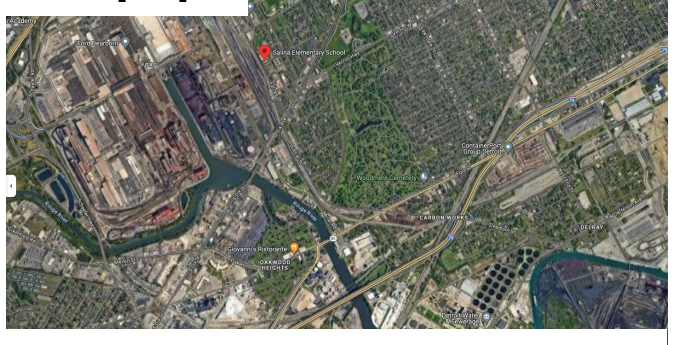
Local Time [EDT]

Local Time [EDT]

Pandora
ne30x8 DIUR
ne30x16 DIUR

- NO_2 VCD model calculations generally perform well compared to observed NO_2 VCDs from Pandora.
- HCHO VCD better reproduced by ne30x16 simulations.

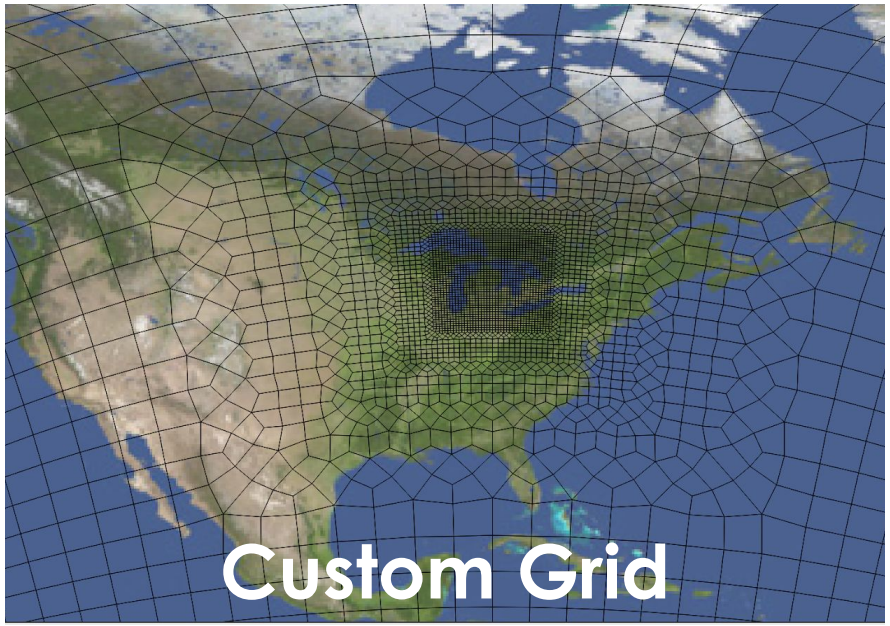
SWDetroitMI

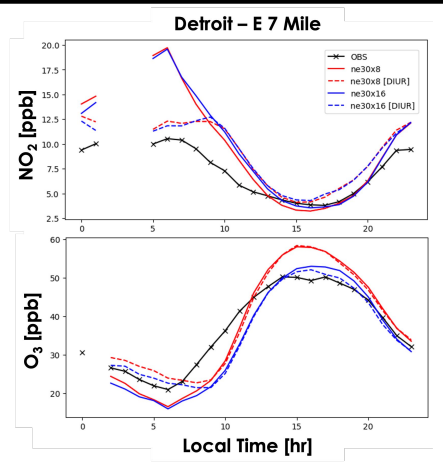


DearbornMI

Summary

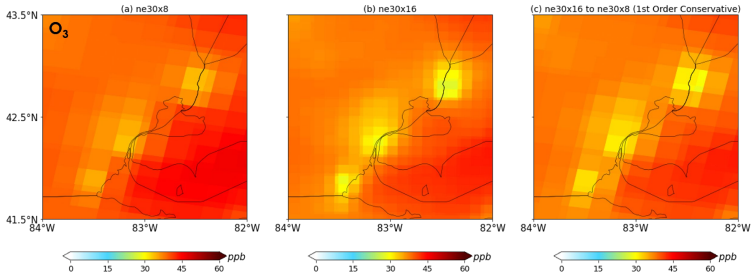
MUSICA
Multiscale Infrastructure for Chemistry and Aerosols

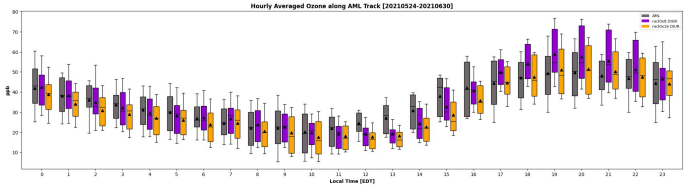




- Application of the diurnal cycle for CAMSv5.1 NO anthropogenic emissions improved simulation of NO_2 and O_3 during 0-10 EDT, with little to no change in peak O_3.

- Changes due to grid resolution result from artificial mixing & misclassification of sources





- Similar performance, but slightly better representation in ne30x16 during peak O_3 times.

thank you!

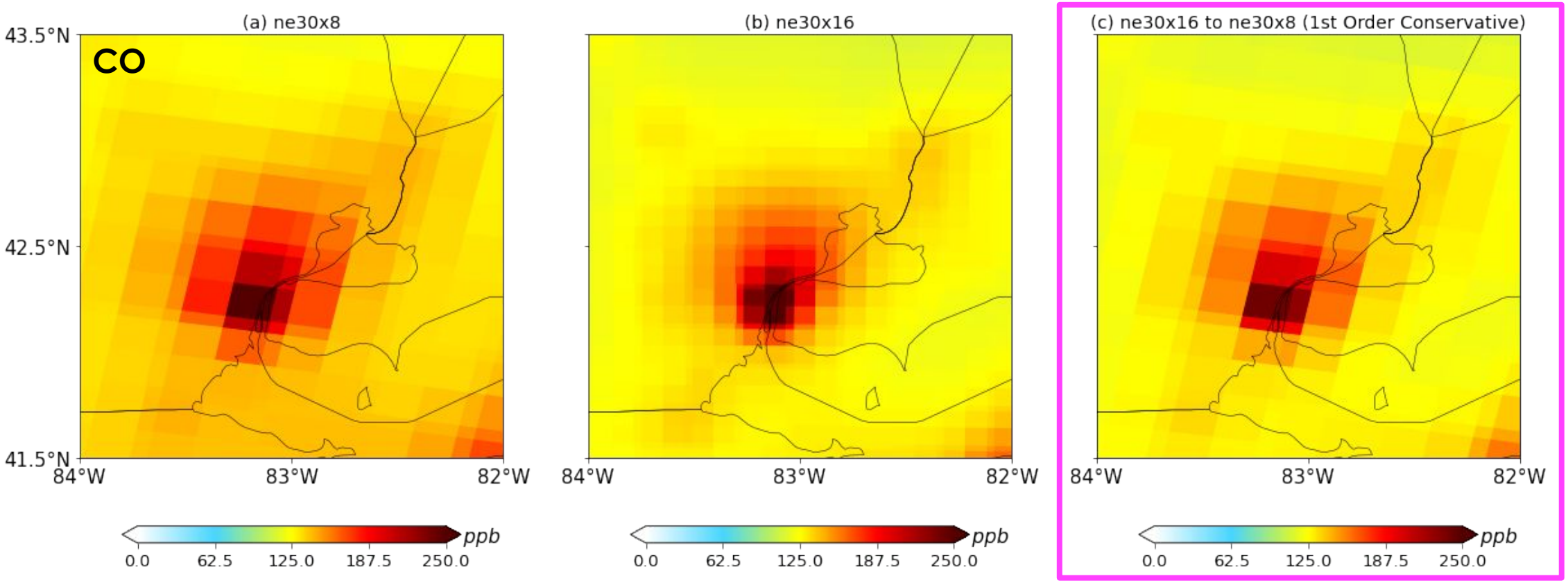
questions?

Contact: nmariscal@wayne.edu

backup slides.

Carbon Monoxide Concentrations at the Surface

Regridded



- Carbon Monoxide (CO) **fine-scale features captured in regional refinement grids**, with point sources better resolved in the ne30x16 (7km resolution).
- CO is relatively chemically inactive, so low chemistry effects due to horizontal grid resolution.
- Regridding model output does not give the same results.

Ozone Concentrations at the Surface

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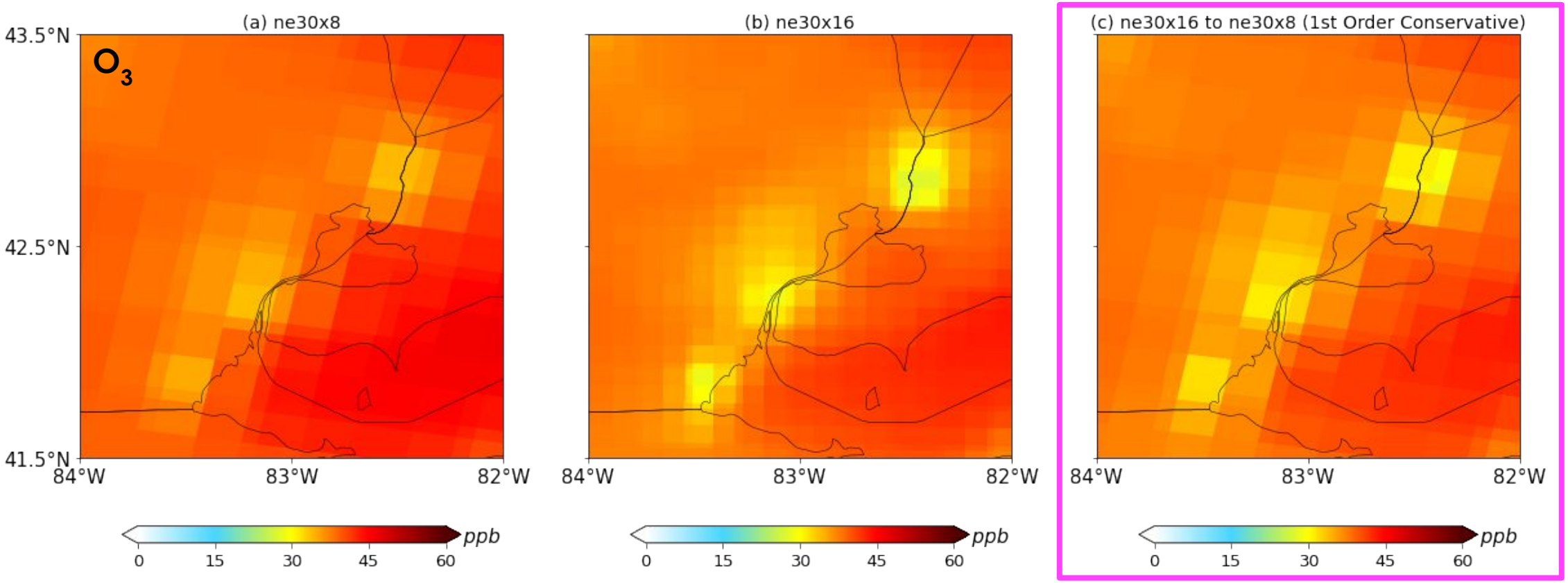

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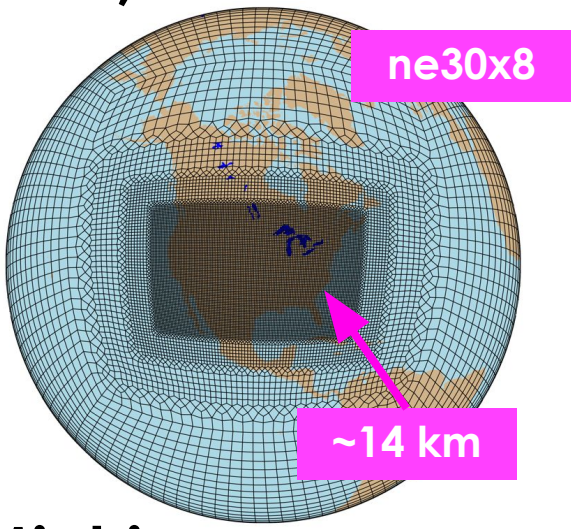
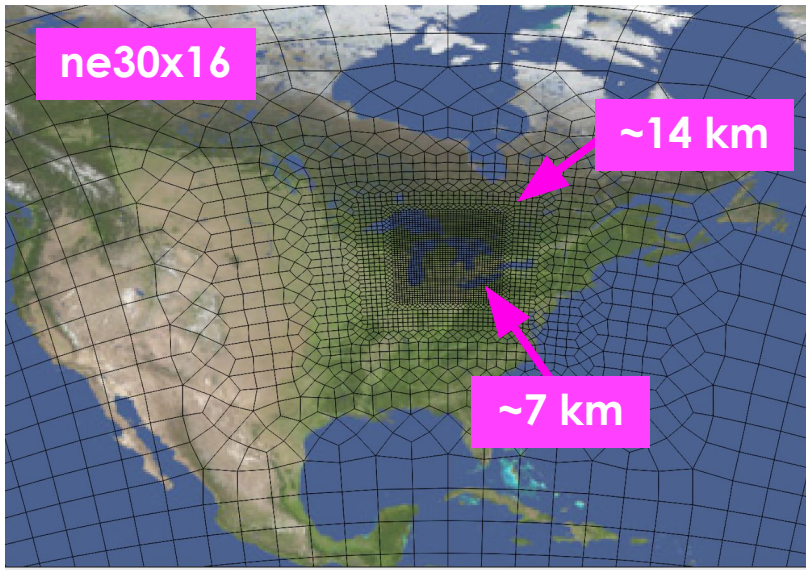
- Regridding of ne30x16 to ne30x8 resolution does not reproduce the same results the ne30x8 simulation output.

MUSICAv0

MUlti-Scale Infrastructure for Chemistry & Aerosols, Version 0

- Configuration of CESM/CAM-Chem
- Spectral Element Dynamical Core Regional Refinement
- Default Resolution:
  - ~14 km Latitude x ~14 km Longitude (1/8˚) over CONUS
  - 32 Vertical Layers (~40 km Model Top)
  - ~28,000 core-hr/sim-month





Regional Refinement over Michigan

- *Community Mesh Generation Toolkit*
- ne30x8 CONUS **ne30x16 MICH**
- **~7 km Latitude x ~7 km Longitude over Michigan**
- Smooth transition (halo) between resolutions to mitigate potential errors
- Time Step: 3.75 mins
- ~18,000 core-hr/sim-month

GRID SETUP

Regional Refinement over Michigan

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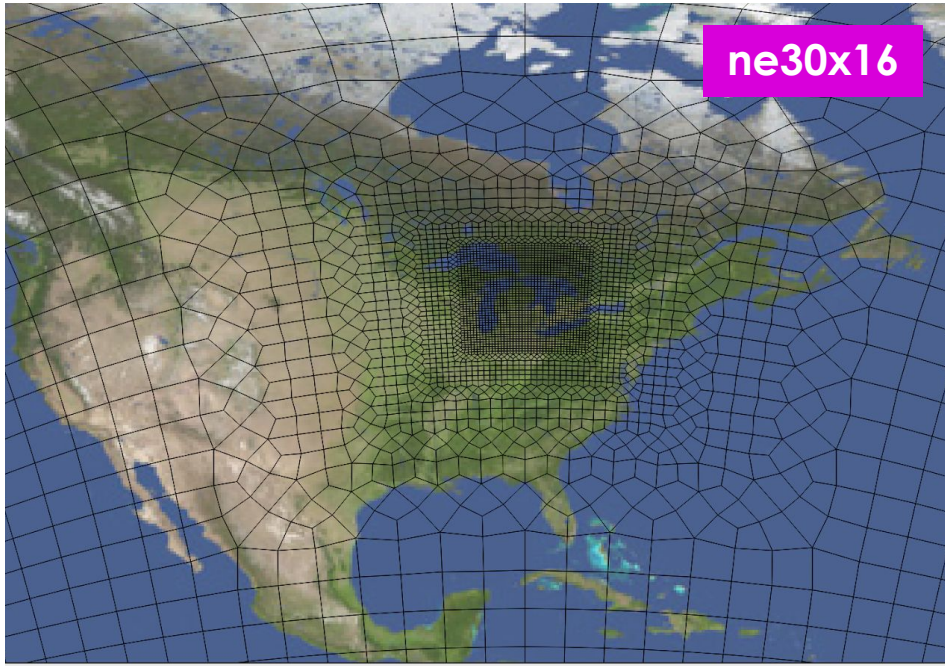

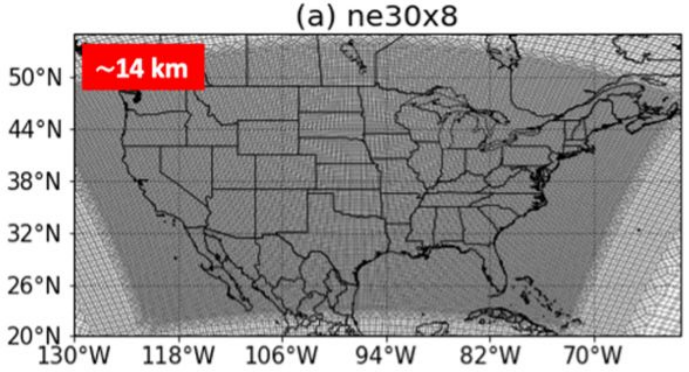

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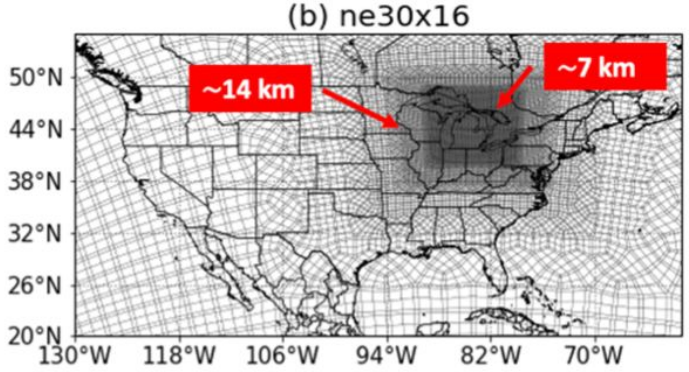

~18,000 core-hr/sim-month

MODEL CONFIGURATION

- April-August 2021
  - April used as a spin up
- Initial conditions based on SE 1˚ CAM-Chem run
- NASA MERRA-2 (Resolution: 0.625˚ x 0.5˚ every 3 hours)
  - Meteorological nudging not applied to Michigan [41˚N, 272.5˚W]
- **MOZART-TS2**
  - Comprehensive representation of tropospheric and stratospheric chemistry with updated gas-phase chemistry for isoprene and terpene species
  - **MAM4**: Spatial distribution of aerosols
  - **VBS-SOA**: secondary organic aerosols separation

EMISSIONS

Anthropogenic and biomass burning emissions are generated offline and regridded to corresponding resolution.

- **Copernicus Atmosphere Monitoring Service Version 5.1 (CAMS-GLOB-ANTv5.1)**
  - Global anthropogenic emissions based on monthly emissions from EDGARv5 and CEDSv2
  - Resolution: 0.1˚ x 0.1˚
  - Sectors: ENE, RCO, TRO, TNR, FEF, IND, SLV, AGR, MMA, SHP, SWD
- **CAMS-GLOB-AIRv2.1**
  - Aircraft emissions
  - Resolution: 0.5˚ x 0.5˚

EMISSIONS

- **Biomass Burning**
  - Quick Fire Emissions Dataset (QFED)
    - Resolution: 0.25˚ x 0.25˚
  - Fire INventory from NCAR (FINN)
    - Provides emission factors for aerosols and trace gases
    - Resolution: 0.9˚ x 1.25˚

NASA NCAR

EMISSIONS

- **Biogenic Emissions**
  - Model of Emissions Gases and Aerosols from Nature, Version 2.1 (MEGANv2.1)
  - Based on plant functional types (PFT) distributions and leaf area index (LAI) from MODIS
  - Calculated online **horizontal resolution affects meteorological fields and resolves topography**.

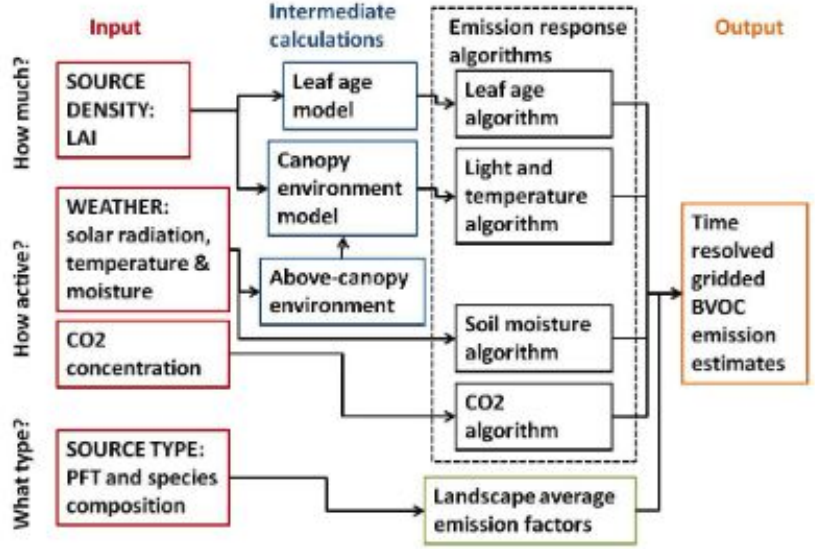

Fig. 1. Schematic of MEGAN2.1 model components and driving variables.

Guenther et al., 2012