Towards the next generation integrated meteorology and atmospheric chemistry model

Jonathan Pleim
Atmospheric Model Development Branch
USEPA

2016 Air Quality Modeling Research Needs Workshop
February 9-10, 2016

A brief history of AQ modeling

- Eulerian grid chemical transport models
  - Emission, advection, diffusion, chemistry, deposition
- First generation AQ models - e.g. UAM, ROM
  - Gas-phase photochemistry
  - Single mixed layer with diurnal evolution, another layer aloft
  - Meteorology interpolated from observations
- Second generation – e.g. RADM, ADOM, STEM
  - Multi-layer terrain following coordinates
  - Meteorology from prognostic model (e.g. MM4)
  - Include cloud processes – convective transport, aq chem, wet dep
- Third generation – e.g. WRF-Chem, WRF-CMAQ, GEM-MACH
  - Integrated or coupled Met – Chem
  - Include aerosol with feedback to meteorology

Why Next Gen Model?

- Much of the code dates back to the 1990's.
- Needs thorough redesign for:
- Greater efficiency, less buggy, more flexible, more extensible
- Need global multi scale system
- Need online or coupled Met-Chem system
- Need earth system linkages
- Need AQ-climate linkages
- Multiple configurations for different applications

Model Development Needs

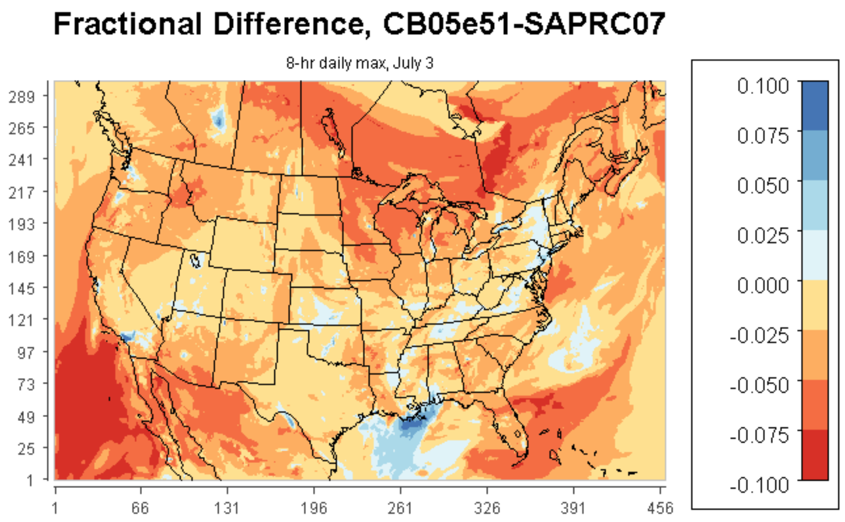
- Multi-scale global
- Integrated meteorology – chemistry
- Improved integrated physics
  - Cloud processes (resolved and subgrid)
  - Land surface, dry deposition, bi-directional flux
  - Consistent radiation and photolysis – cloud effects, aerosol effects, surface albedo
- Emission modeling
  - Wind-blown dust
  - Sea salt
  - Biogenics
- Closer integration of gas – aerosol – aqueous - heterogeneous
  - Condensed chemical mechanisms derived from detailed mechanisms
  - Improved organic aerosol models

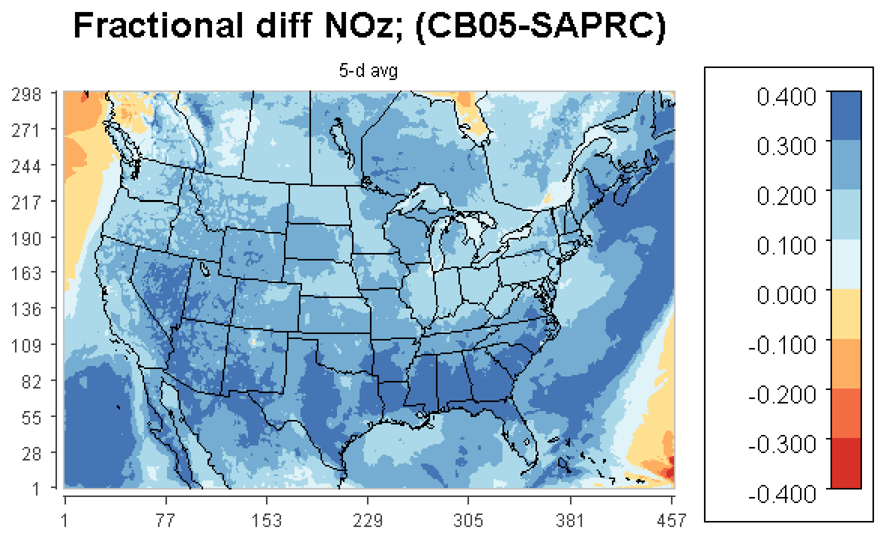
Challenges for chemical mechanisms in NGAQM

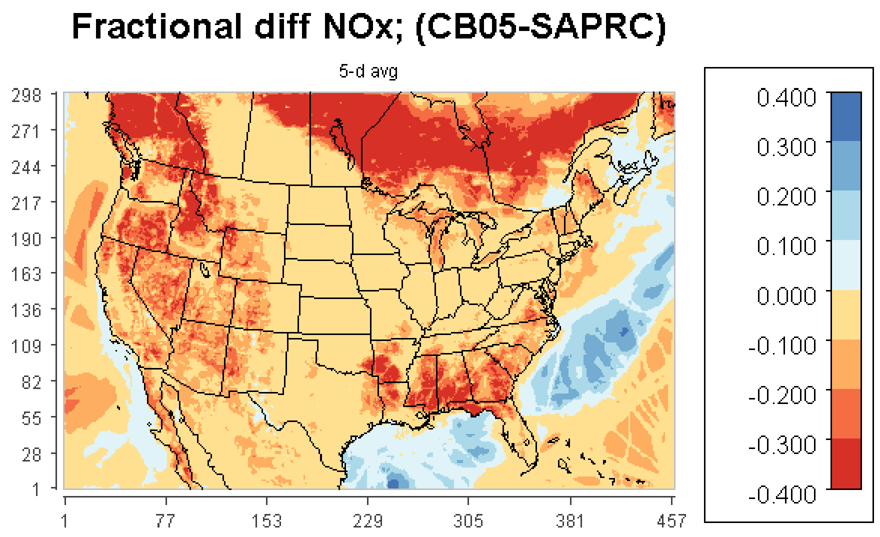
- Derive mechanisms from a robust, well-documented archive so that different versions of mechanisms are consistent; i.e. they all "start from the same place."
  - Reconcile the large differences in intermediates
  - Improve comparisons between simulations using different mechanisms
  - Strive for better consistency from global to regional to urban scales
- Semi-automate the mechanism derivation, condensation, and evaluation process
  - Increase the ability of the mechanisms to respond quickly to "new" pollutants from new energy sources, new technologies, changing state of the atmosphere, new toxics
  - Decrease the time between when new scientific information becomes available and when it is reflected in atmospheric chemistry (i.e. no more 8-year update cycles!).
- Better characterize the direct precursors to SOA formation (research in identifying, MCM to help us create them) and gas-aerosol-aqueous feedbacks (CAPRAM-type mechs?)
  - Increase confidence on the magnitude/direction of PM2.5 due to emission reductions

Courtesy of Deborah Luecken

Example: Ozone predictions by CB05 and SAPRC





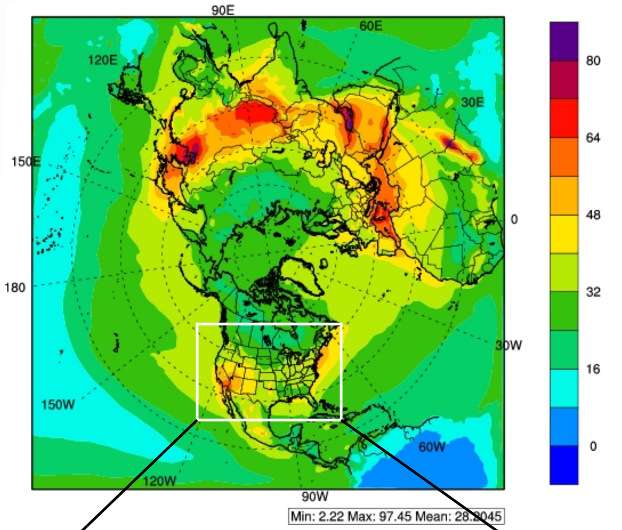


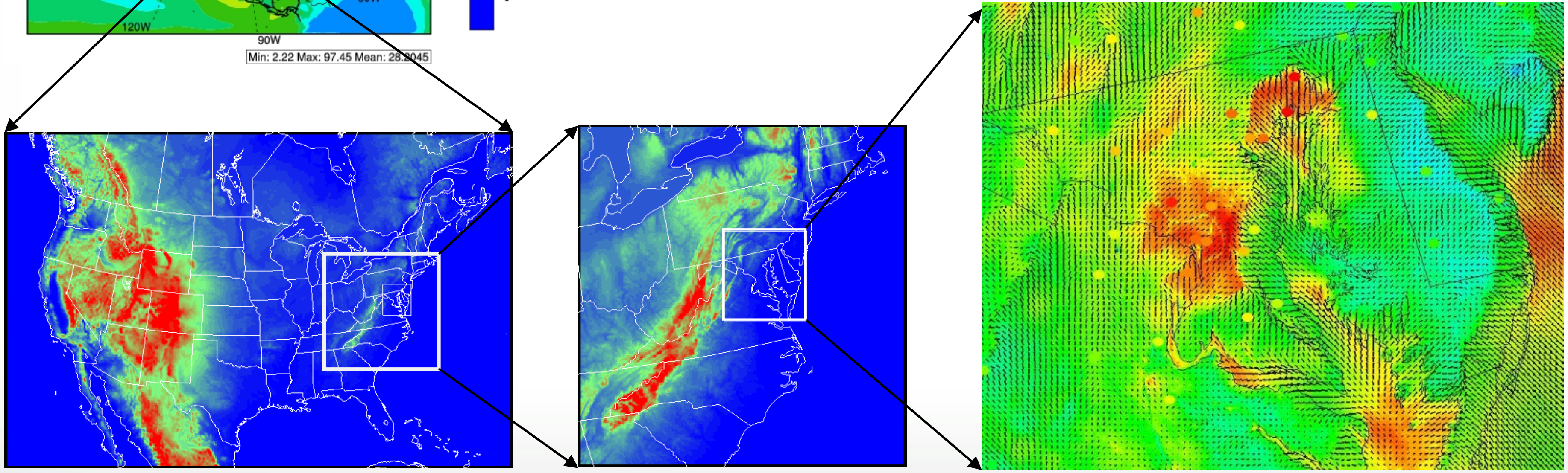
Similar ozone but large differences in intermediate species

Courtesy of Deborah Luecken

Current Multi-scale Modeling System

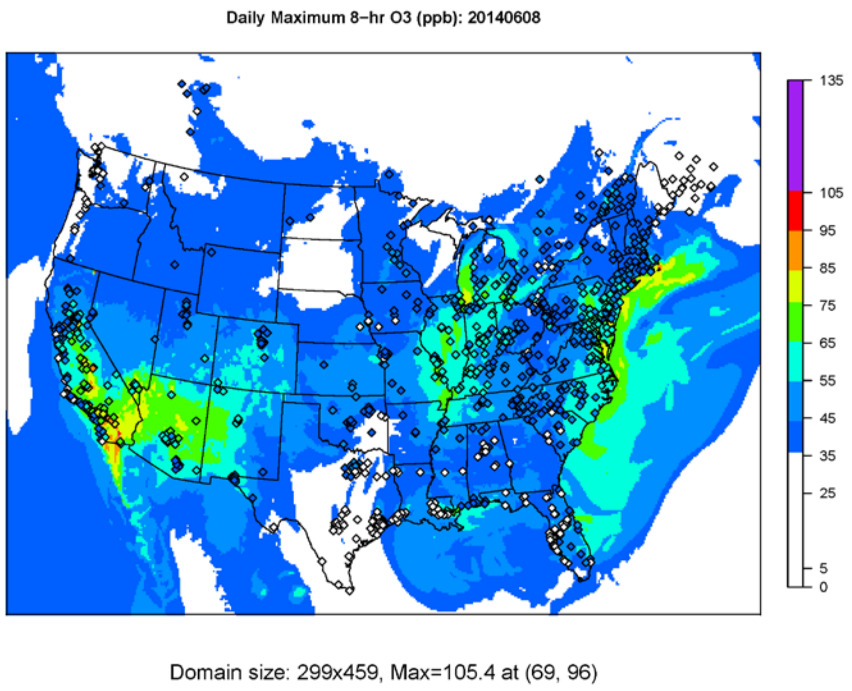
- Hemispheric model at 108 km provides LBCs for 12 km CONUS with nests to 4 km and 1 km
  - Multi-step process
  - Many opportunities for user mistakes
  - Interpolation errors on boundaries
  - Resolution discontinuities
  - No upscale feedback



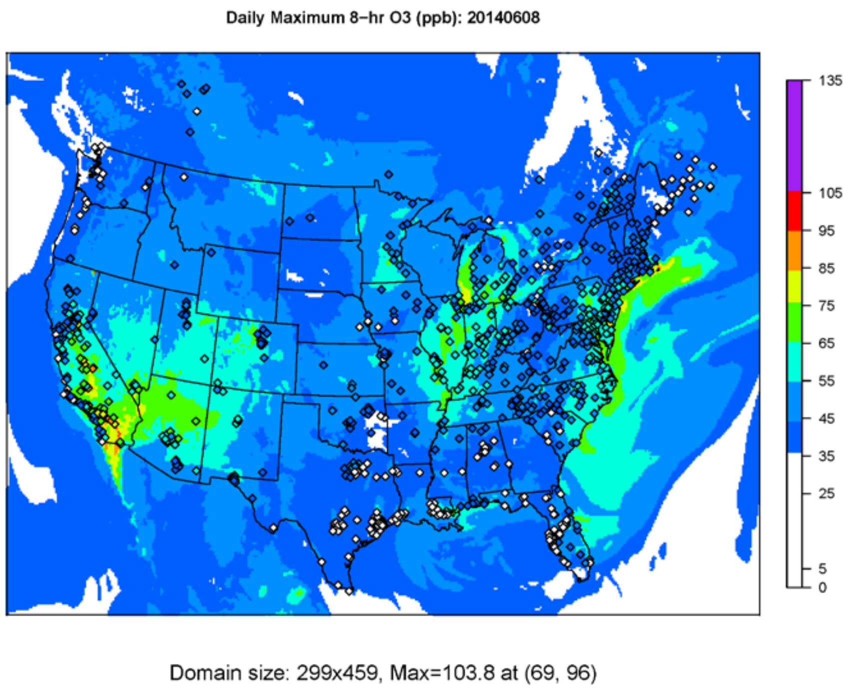


Hemi as LBC for CONUS 12 km

WRF-CMAQ max 8-hr average ozone on June 8, 2014



Hourly LBCs from WRF-CMAQ Hemispheric run

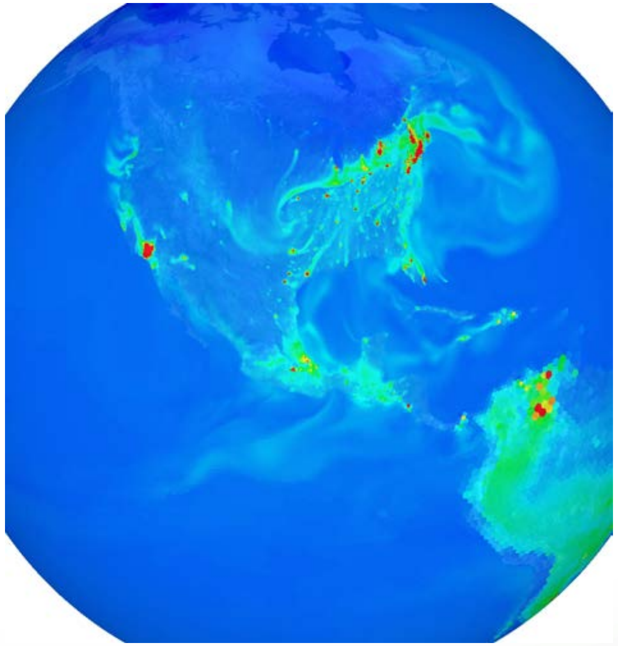


Monthly average LBCs from GEOS-Chem

Using 108 km hemispheric WRF-CMAQ improves ozone simulation especially in Texas and Canada compared to monthly average static LBCs derived from global model (GEOS-Chem)

Global Multiscale model

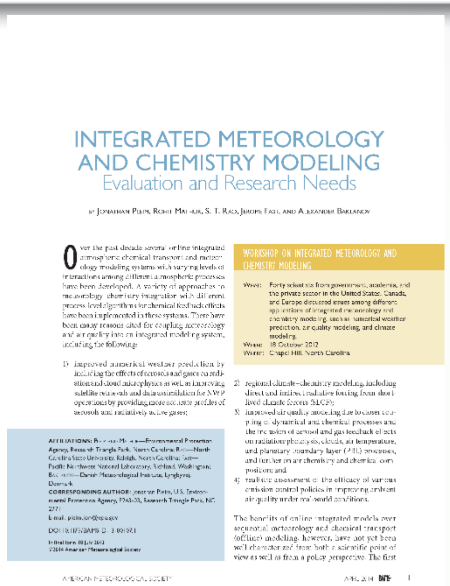
- Need AQ modeling at Global to Continental to Regional to Urban scales
  - Seamless multi-scale grid refinement (e.g OLAM, MPAS)
    - Minimize interpolation errors in transition from coarse to fine resolution
- Tighter AQ standards require global modeling:
  - Inter-continental transport (Ozone and PM)
  - Stratospheric ozone
  - Marine chemistry
- Earth system Linkages
  - Greenhouse gases
  - Nitrogen, carbon cycling
  - AQ – Climate interactions
  - Eco, hydro linkages



OLAM-Chem

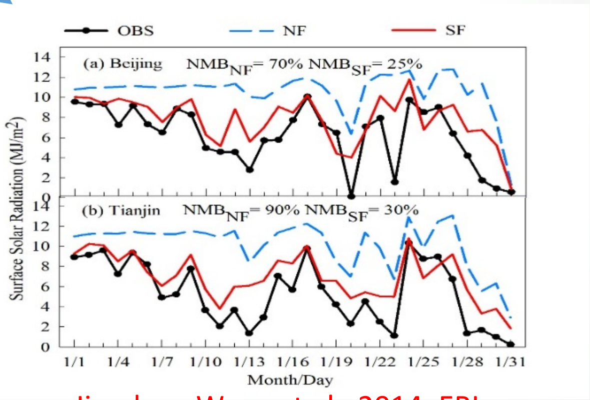
Need for online Met-Chem model

- Growing trend toward integrated Met-Chem modeling
  - Improve NWP – radiative feedbacks and satellite data assimilation
  - Regional climate-chemistry modeling including SLCF
  - Improve AQ modeling
- Chem affects Met which affects AQ
  - Aerosol direct effects
    - Reduced SW ground → reduces PBL → greater concentrations
  - Aerosol indirect effects
    - Effects cloud cover, COD, radiative forcing, precipitation
    - Effects propagate through AQ
  - Gaseous direct effects on LW
    - Ozone, methane, N_2O, etc
  - AQ effects on land surface
    - Ozone damages stomatal function which affects:
      - Transpiration, CO_2 uptake, dry deposition
    - CO_2 changes, including regulatory controls, affect stomatal conductance


INTEGRATED METEOROLOGY AND CHEMISTRY MODELING
Evaluation and Research Needs

WORKSHOP ON INTEGRATED METEOROLOGY AND CHEMISTRY MODELING

BAMS 2014



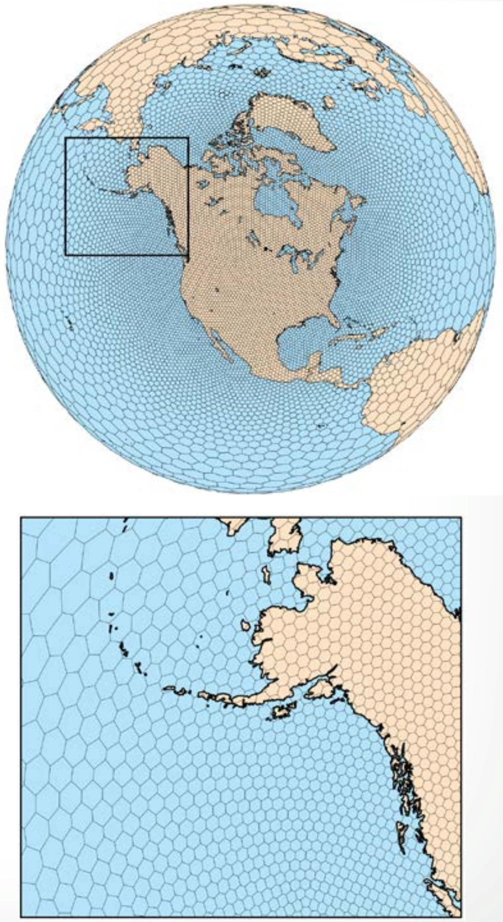
Jiandong Wang et al., 2014, ERL

Integrated Met-Chem modeling

- High temporal coupling (data exchange frequency > once per hour)
  - Better resolve high-frequency meteorological dynamics
    - WS, WD changes, PBL height variations, cloud formation, rainfall
  - Affects chemical transport, transformation, and removal at high spatial resolution
- More consistent dynamical, physical, and numerical modeling
  - More constant cloud convective transport of chemistry and met
  - Closer integration of cloud microphysics and aqueous chemistry
  - More consistent advection and diffusion
- On-line chemistry necessary for global models with non-uniform, refining grid meshes (e.g. OLAM, MPAS)
  - Advection and horizontal diffusion must be integrated in dynamics solver

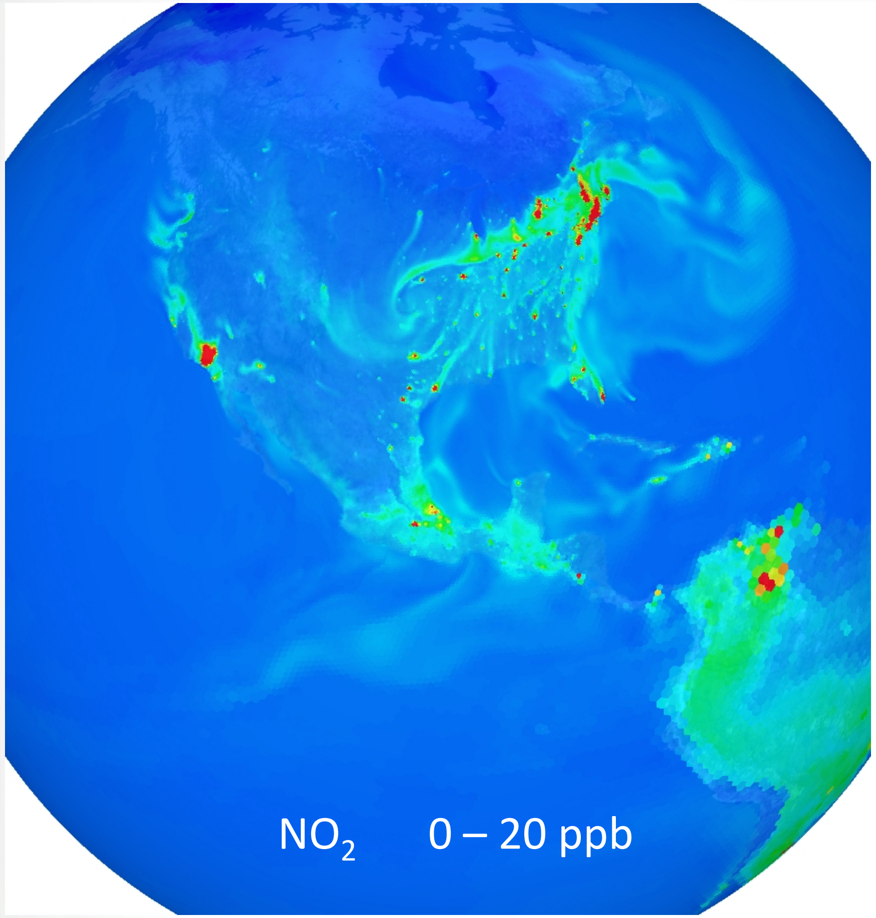
Vision for Next Generation Model

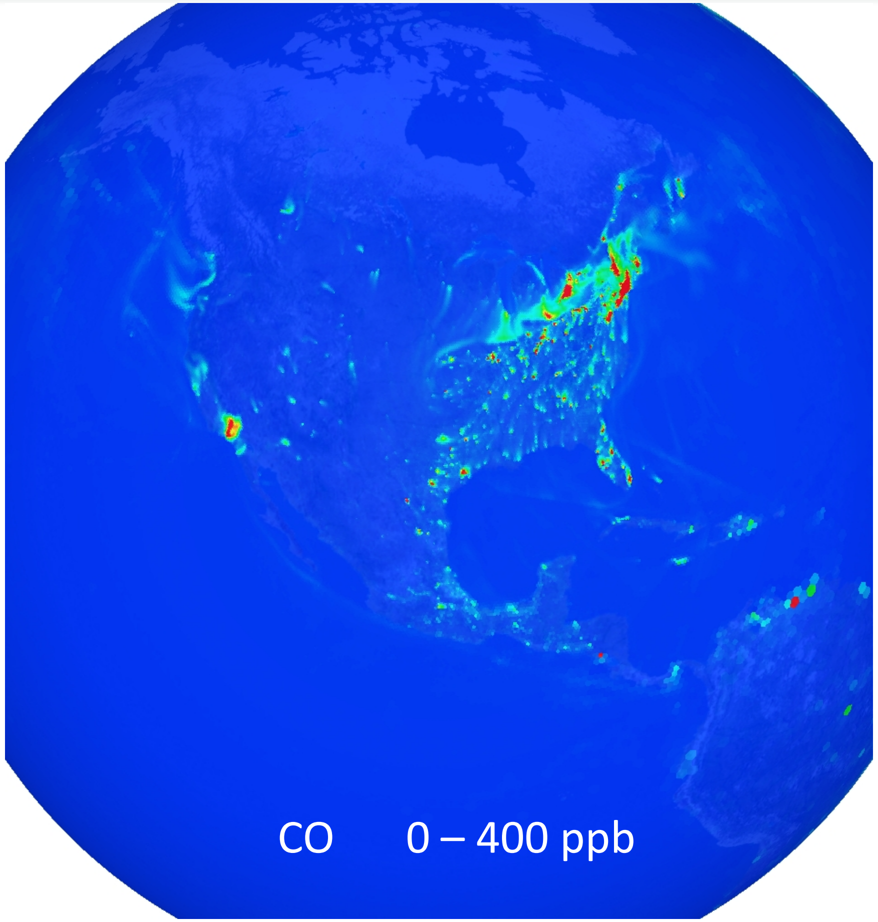
- Extend to global scales
  - Single global mesh with seamless refinement to local scales
  - Integrated chemistry, dynamics, physics
- Three configurations of flexible systems:
  - On-line global variable grid (e.g. MPAS, OLAM)
  - Online regional (WRF-AQ or limited area MPAS)
  - Offline regional (redesigned CMAQ)
- Interoperability of as much model code as possible
  - 1-D AQ component coupled to met model
  - Gas, aerosol, aqueous in modular box
  - Modules for biogenic emissions, dry dep/bidi, wind-blown dust, photolysis, etc
- Transport in met models for online systems (adv, diffusion)
  - Ensure mass conservation
  - Consistency with met parameters
  - Minimize numerical diffusion and dispersion

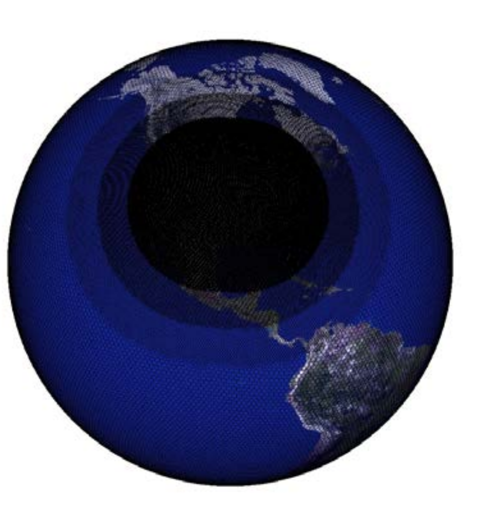


MPAS

Example of OLAM-Chem







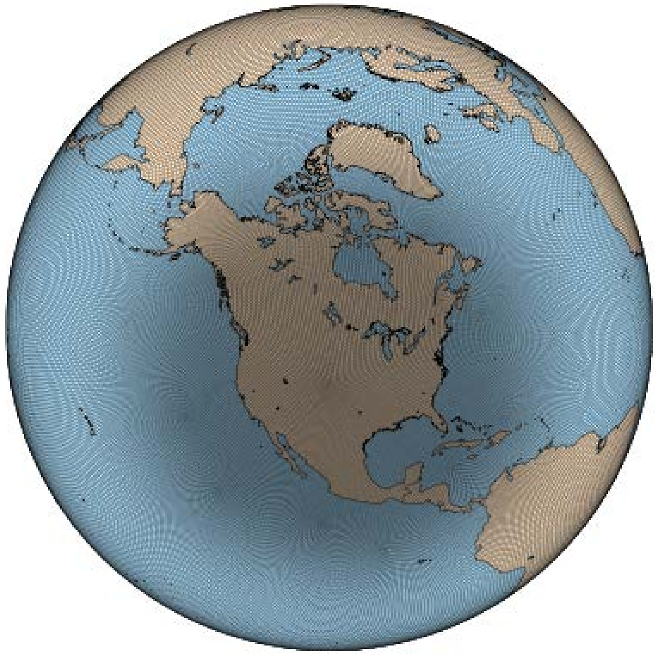
- Note the coarse resolution in South America and much finer resolution in North America

Courtesy of Martin Otte

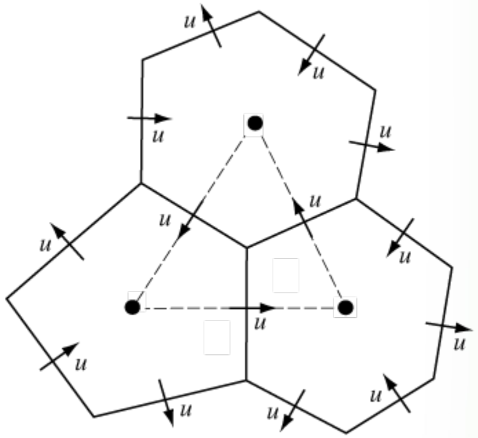
MPAS
Model for Prediction Across Scales

- Fully-compressible, non-hydrostatic dynamics
- Finite volume discretization on centroidal Voronoi (nominally hexagonal) grids
- Single global mesh with seamless refinement to local scales
- Latest version: MPAS 4.0 (released May 22, 2015)

MPAS uniform mesh (240 km)



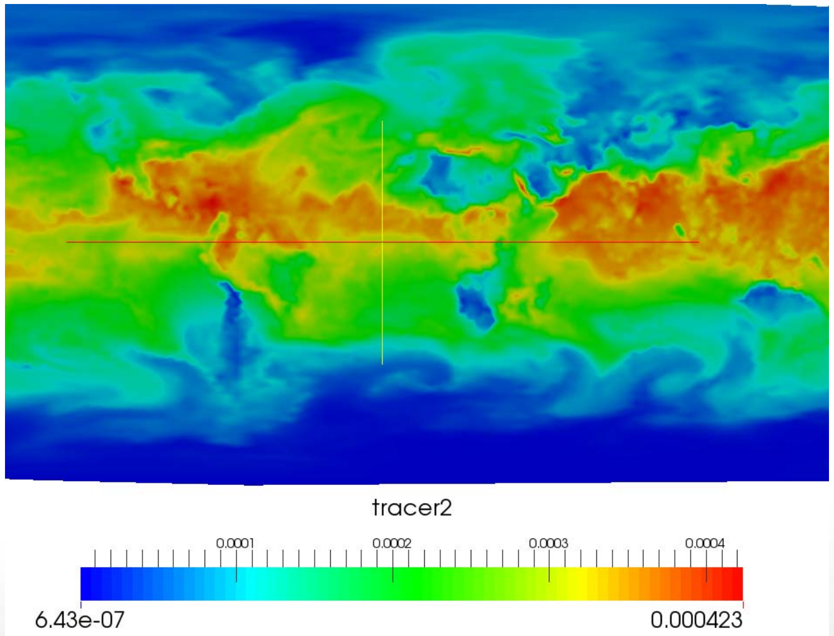
MPAS non-uniform mesh (92km – 25km)
Refinement over CONUS



Evaluation of the transport in MPAS

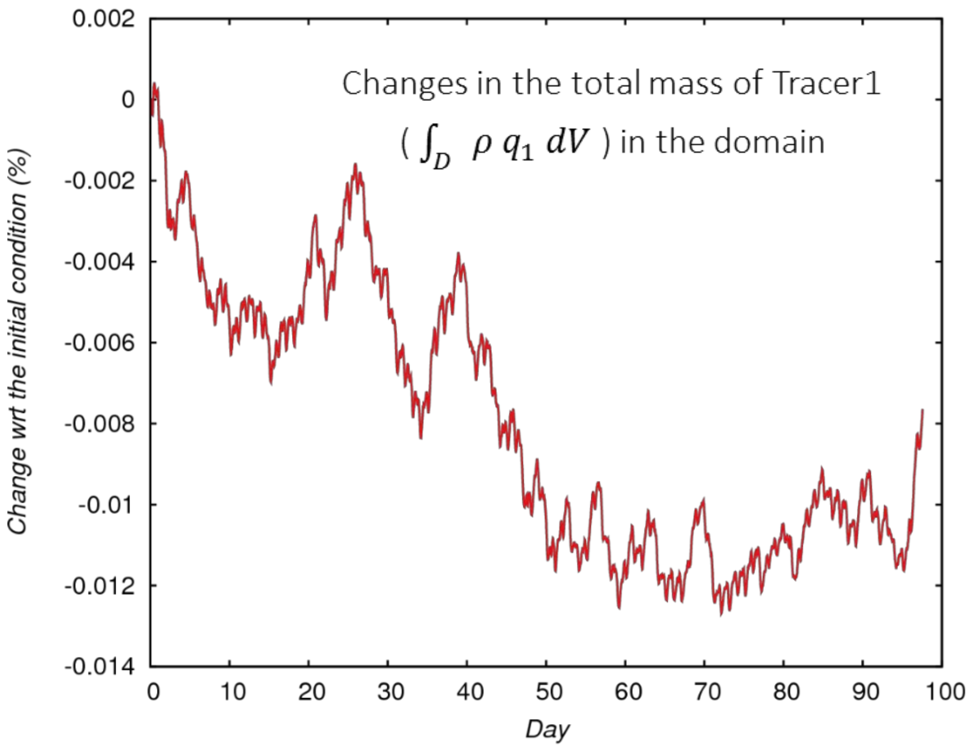
- Implementation of several passive tracers in MPAS - *Hosein Foroutan*
- Testing for global conservation of mass and tracers
- Test case:
  - Simulations starting on September 17, 2013
  - Uniform mesh (240 km)
  - 41 vertical layers
  - YSU PBL
  - Noah LSM
  - RRTMG radiation
  - Kain-Fritsch convective clouds

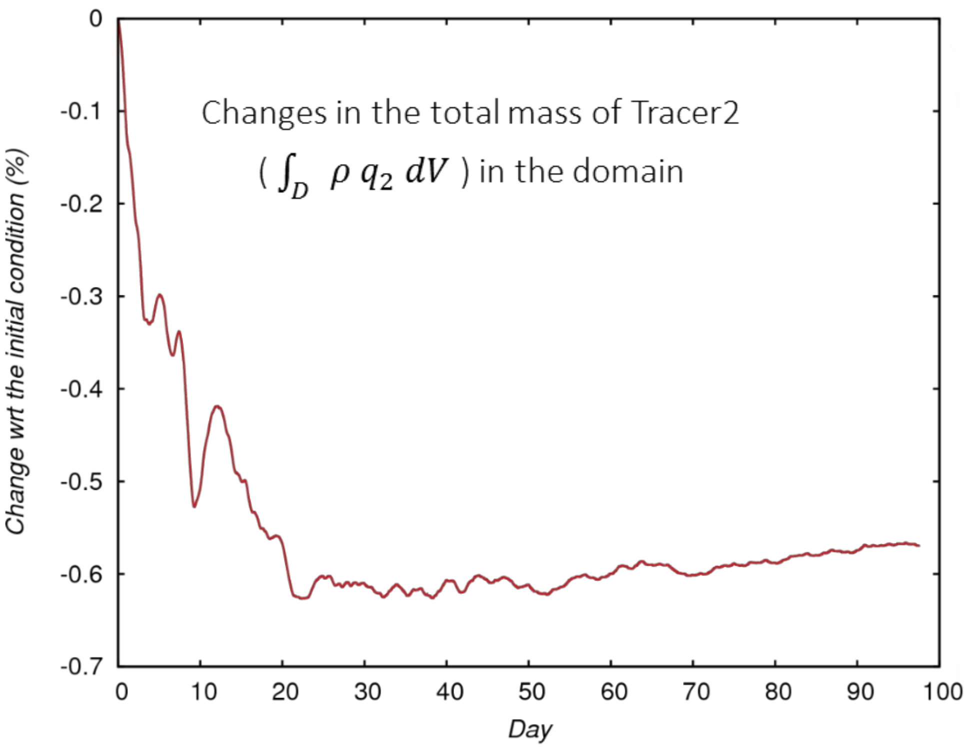
  - Tracer1 : uniform initial distribution
  - Tracer2 : 2% of water vapor as an initial distribution



Initial distribution (mixing ratio) of Tracer2

Evaluation of the transport in MPAS





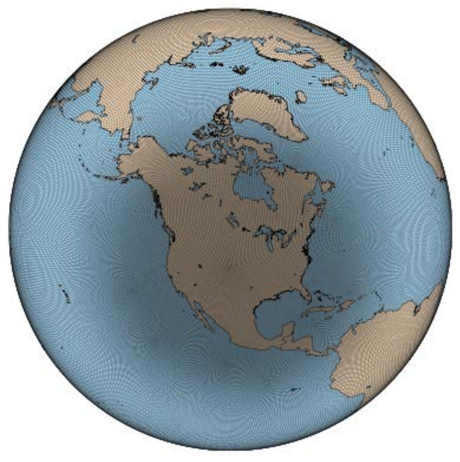
- Change in tracer 1 is identical to total mass of dry air
- Consistency between transport of the dry air and tracers
- Acceptable conservation of mass of the dry air and tracers

(Implemented different schemes for horizontal transport but no improvement was seen)

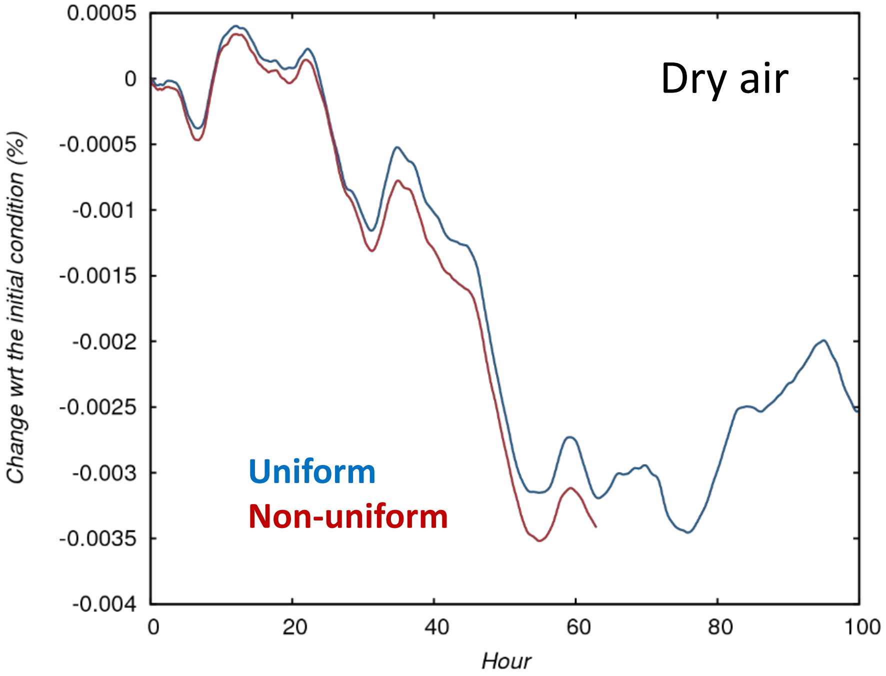
Evaluation of the transport in MPAS

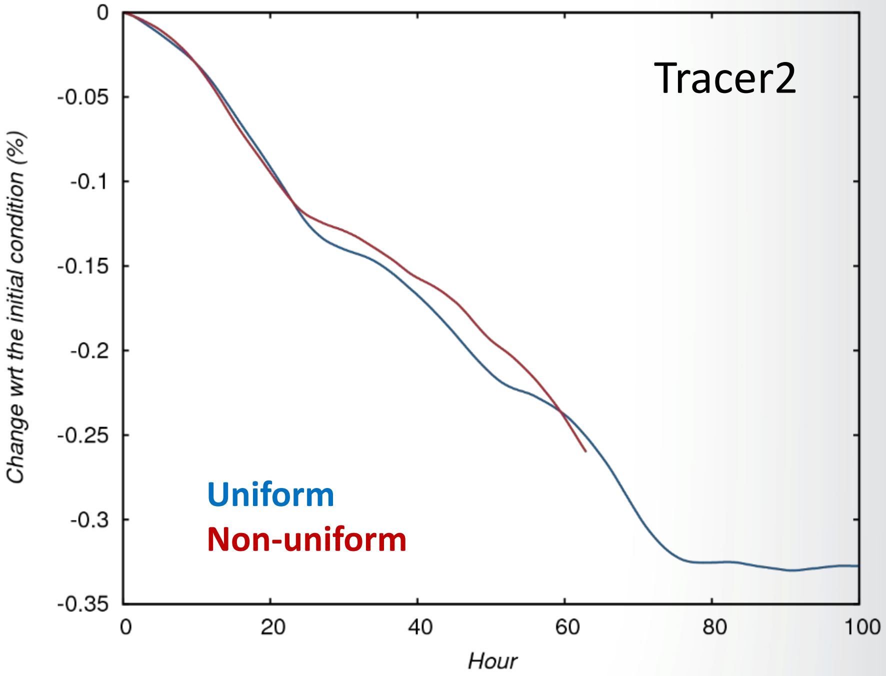
- Similar test case with non-uniform mesh

Uniform mesh (240 km)

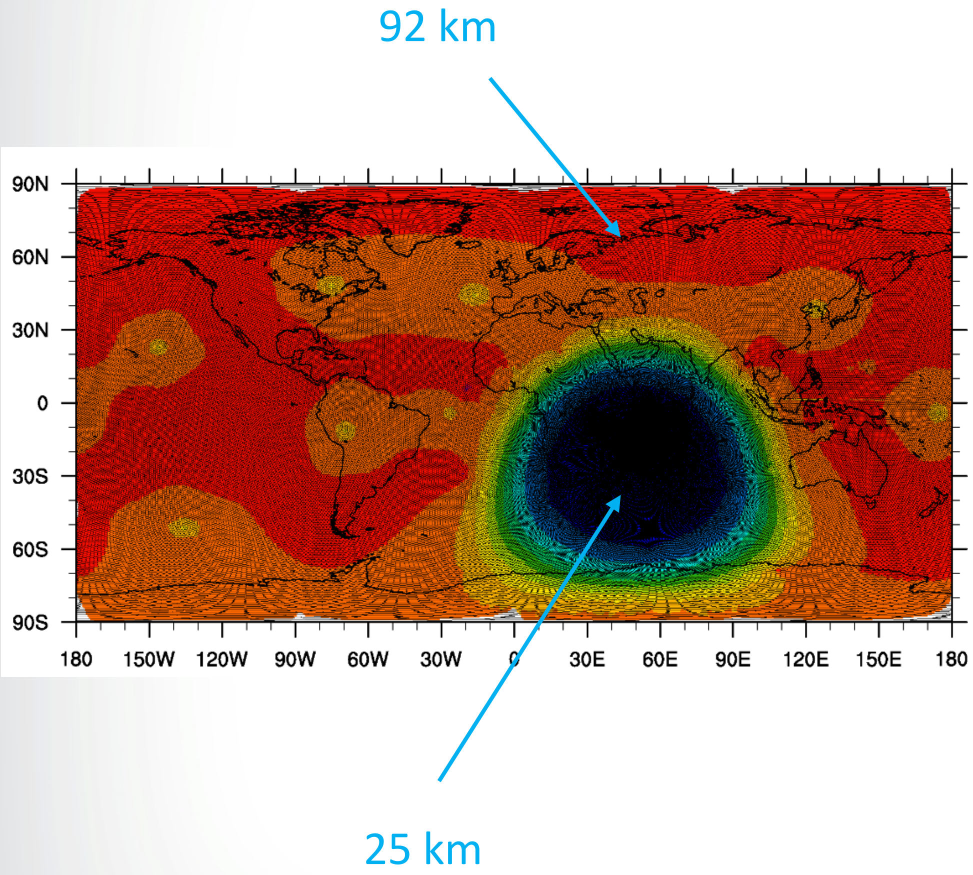


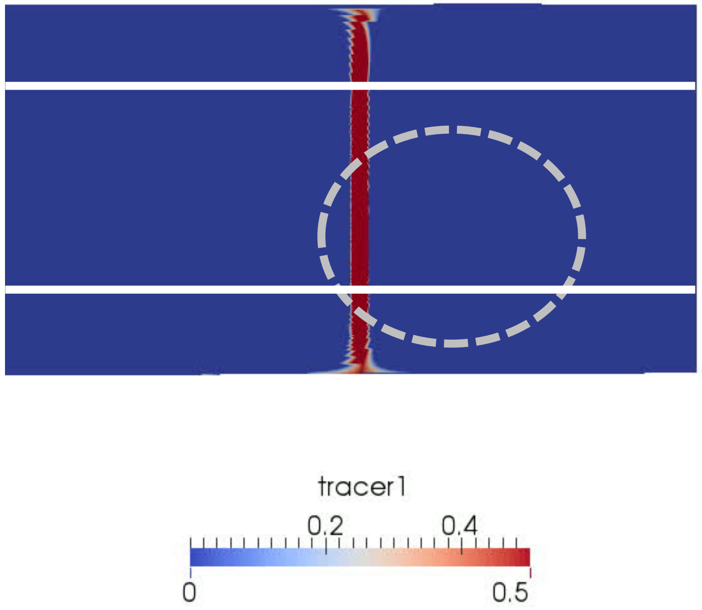
Non-uniform mesh (92 km – 25 km)

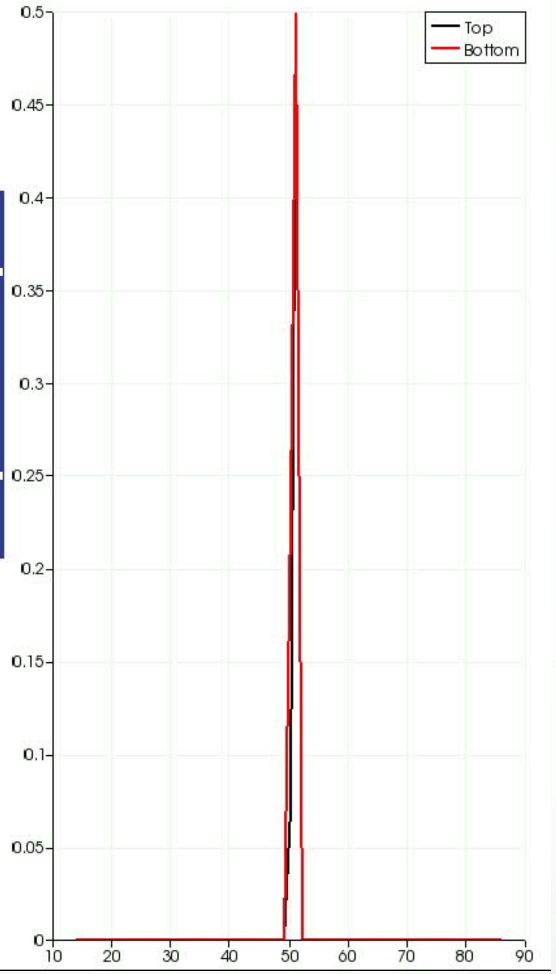




Evaluation of the transport in MPAS







Summary

- The Next Generation model will be a 1-D AQ component coupled to meteorology models
  - Chemical tracers to be transported in meteorology model
  - Meteorology models will include global model with grid refinement and limited area model
  - Development need for integrated physics
  - Off-line AQ model probably also needed
- Development of model science and algorithms will continue
  - Master Chemical Mechanism
  - Organic aerosols
  - Emission process modeling – (dust, biogenic, bidirectional flux)
- Continue support and updates to CMAQ until NGAQM in ready