Fundamentals of Air Quality Modeling and Forecasting- Connecting Regional and Urban Scales

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World Meteorological Organization's

"Training course on Seamless Prediction of Air Pollution in Africa"

Online webinars, 12-25 September 2024

Outline

- **Fundamentals of Atmospheric Models**
  - Importance and Overview
  - Fundamentals of Numerical Air Quality Modeling
  - Methods and Examples for Air Quality Prediction Improvement
- **Multiscale Modeling**
  - Examples of Global, Regional, and Multiscale Models
  - Multiscale Predictions: Needs and Approaches
  - Examples of Multi-scale Air Quality Modeling
- **Summary**

Major sources: Carmichael (2019); Zhang (2024), Zhang et al. (2012), Zhang and Baklanov (2020)

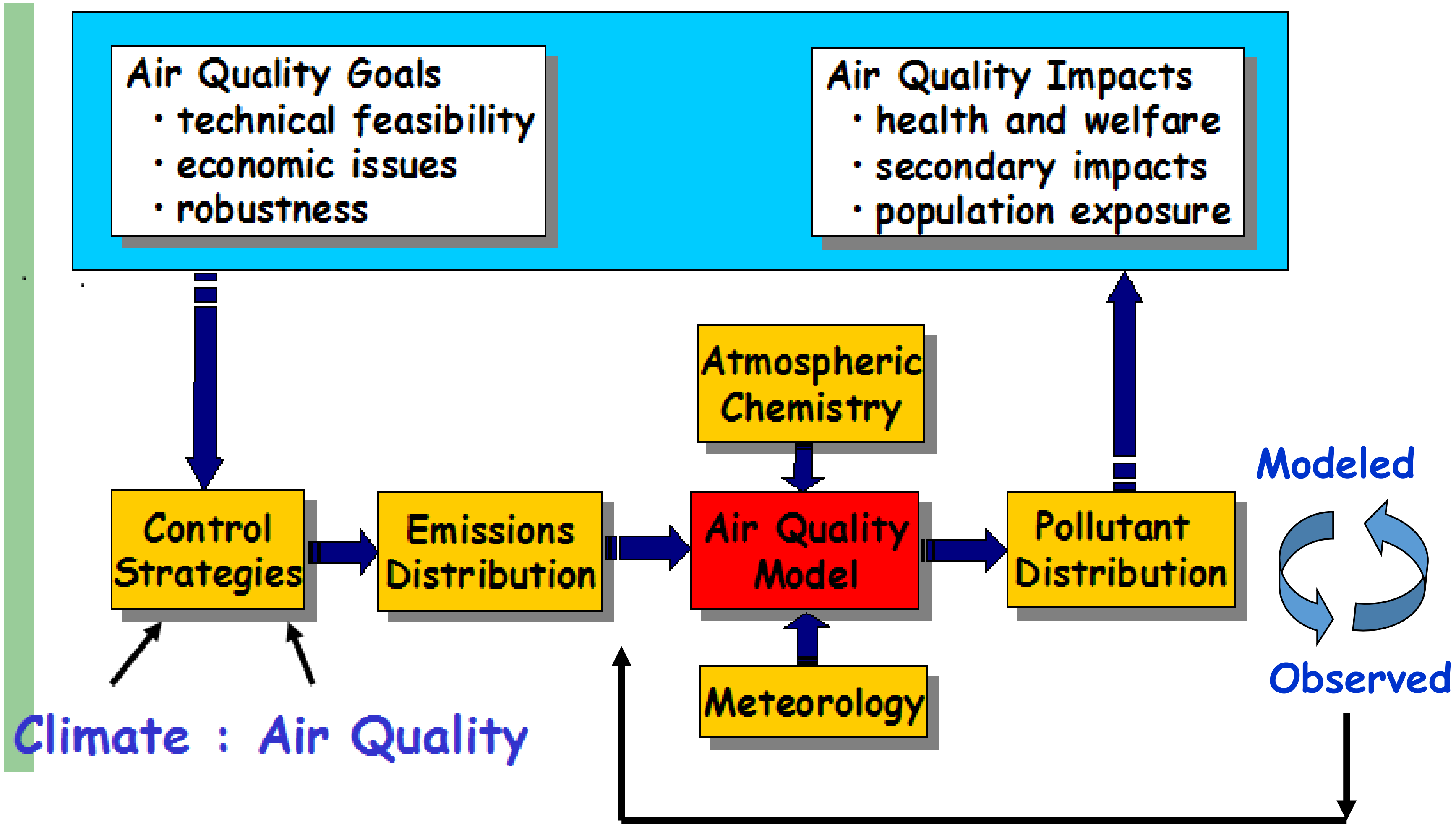
Models are an Integral Part of Air Quality Studies

(Carmichael, 2019)

- Field experiment planning
- Measurement site selection
- Provide 4-Dimensional context of the observations
- Facilitate the integration of the different measurement platforms
- Evaluate processes (e.g., role of biomass burning, heterogeneous chemistry….)
- Evaluate emission estimates (bottom-up as well as top-down)
- Emission control strategies testing
- Air quality forecasting
- Earth system modeling

Models Play a Critical Role in Linking Emissions to Aerosol and Trace Gas Distributions and Subsequent Effects

(Carmichael, 2019)



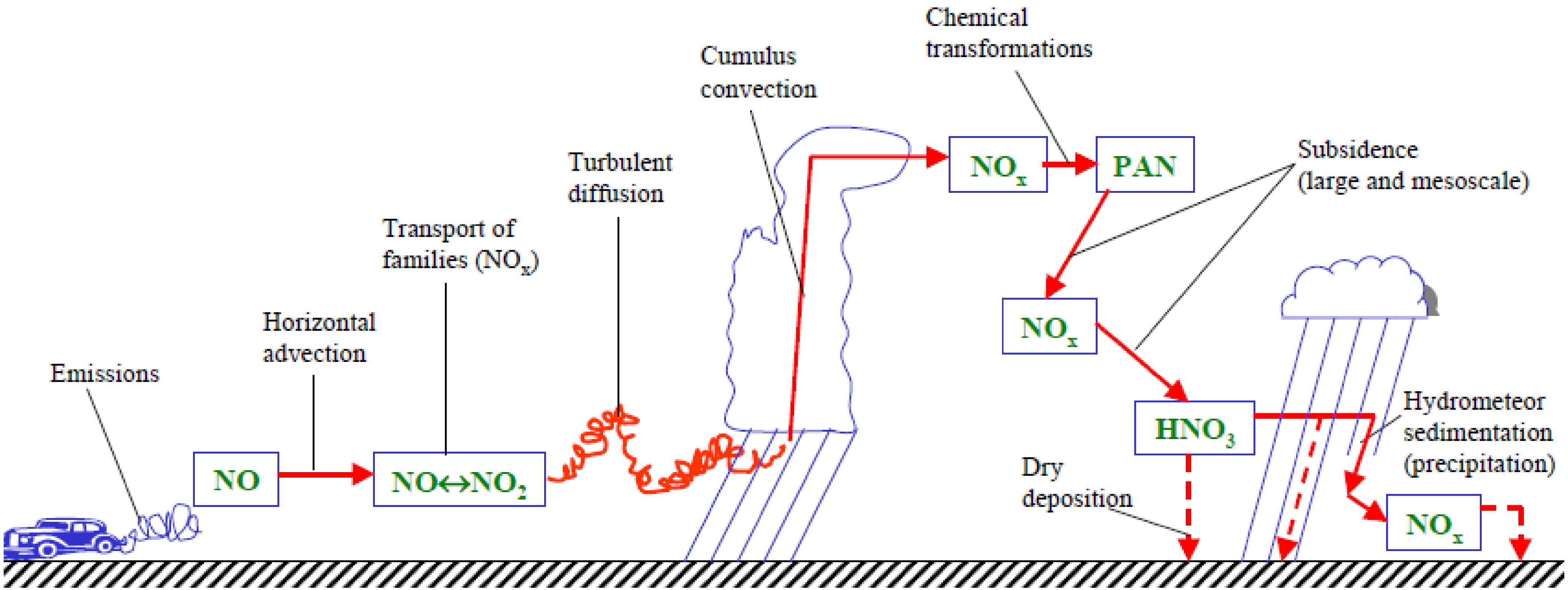
Air Quality Goals
- technical feasibility
- economic issues
- robustness

Air Quality Impacts
- health and welfare
- secondary impacts
- population exposure

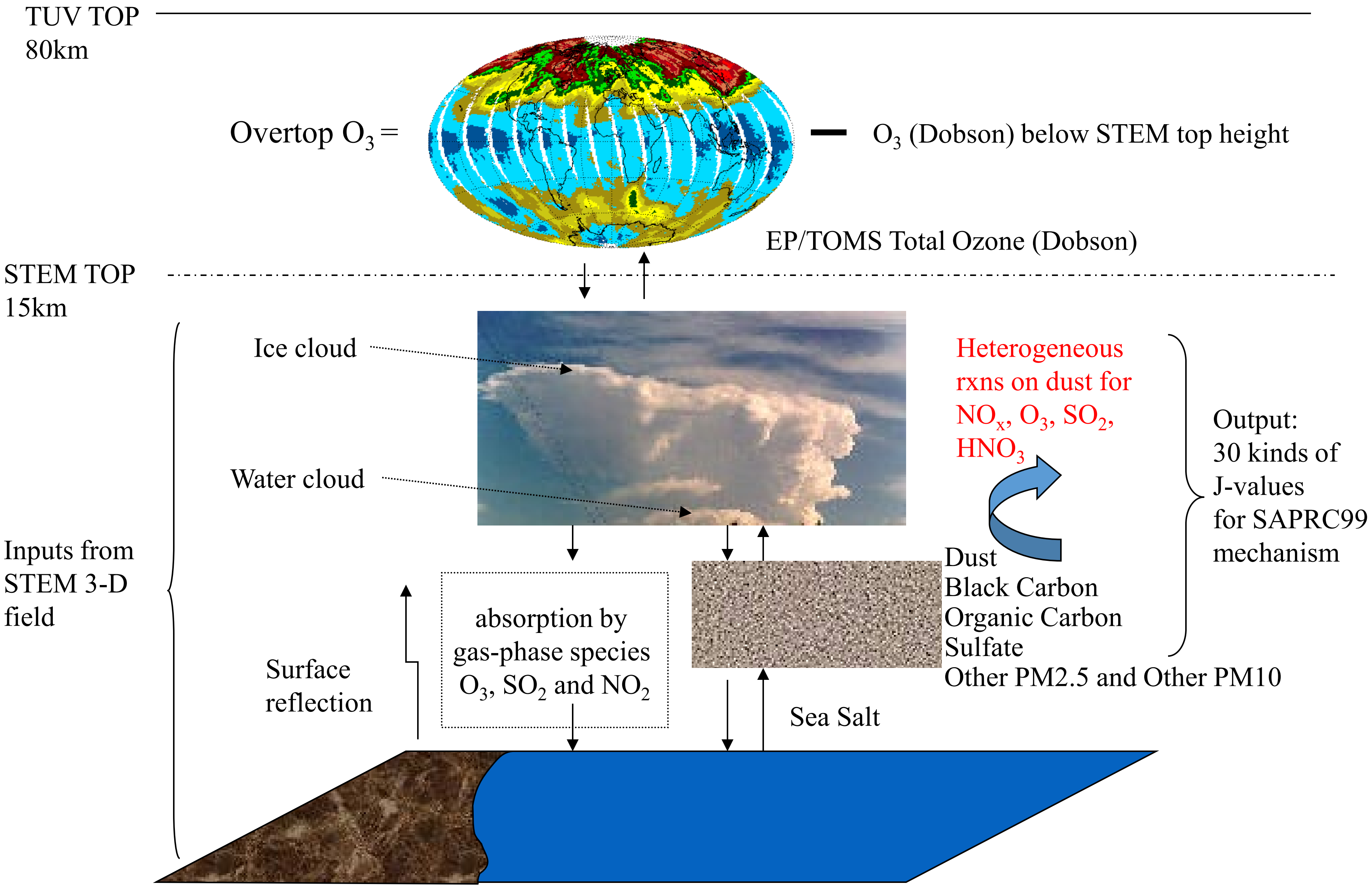
Factors Controlling Tracer Distributions

(Carmichael, 2019)

Example: Reactive Nitrogen



Aerosols Are a Key Component in Urban Environments: Impacting Chemistry and Physics (Carmichael, 2019)



TUV TOP
80km

Overtop O_3 = − O_3 (Dobson) below STEM top height

EP/TOMS Total Ozone (Dobson)

STEM TOP
15km

Ice cloud

Water cloud

Heterogeneous rxns on dust for NO_x, O_3, SO_2, HNO_3

Output:
30 kinds of J-values
for SAPRC99 mechanism

Inputs from STEM 3-D field

Surface reflection

absorption by gas-phase species O_3, SO_2 and NO_2

Dust
Black Carbon
Organic Carbon
Sulfate
Other PM2.5 and Other PM10

Sea Salt

Atmosphere Interactions:

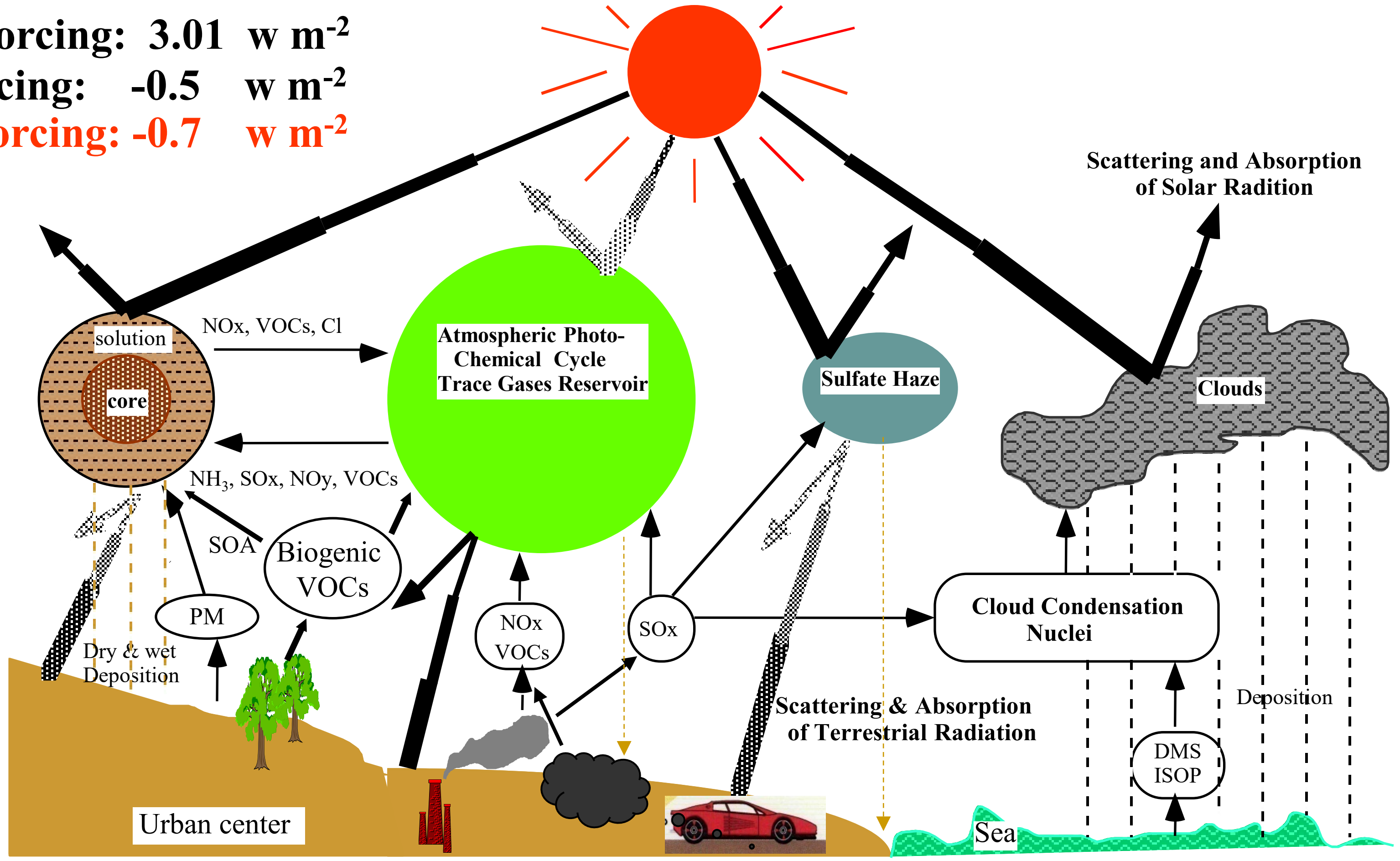
Gases, Aerosols, Chemistry, Transport, Radiation, Climate (Zhang, 1994, 2007)

IPCC (2007, 2014)

Greenhouse Gas Forcing: 3.01 w m^{-2}

Aerosol Direct Forcing: -0.5 w m^{-2}

Aerosol Indirect Forcing: -0.7 w m^{-2}



Temperature → chemistry → concentrations → radiative processes → temperature
Aerosol → radiation → photolysis → chemistry
Temperature gradients → turbulence → surface concentrations, boundary layer outflow/inflow
Aerosol → cloud optical depth through influence of droplet number on mean droplet size → initiation of precipitation
Aerosol absorption of sunlight → cloud liquid water → cloud optical depth

Chemical Transport Model

(Carmichael, 2019)

- The continuity equation from a 3D atmospheric transport-chemistry model (STEM-III)

$$\frac{\partial c_i}{\partial t} = -u \cdot \nabla c_i + \frac{1}{\rho} \nabla \cdot (\rho K \nabla c_i) + f_i(c) + E_i$$

where chemical reactions are modeled by nonlinear stiff terms

$$f_i(c) = P_i(c) - D_i(c) c_i$$

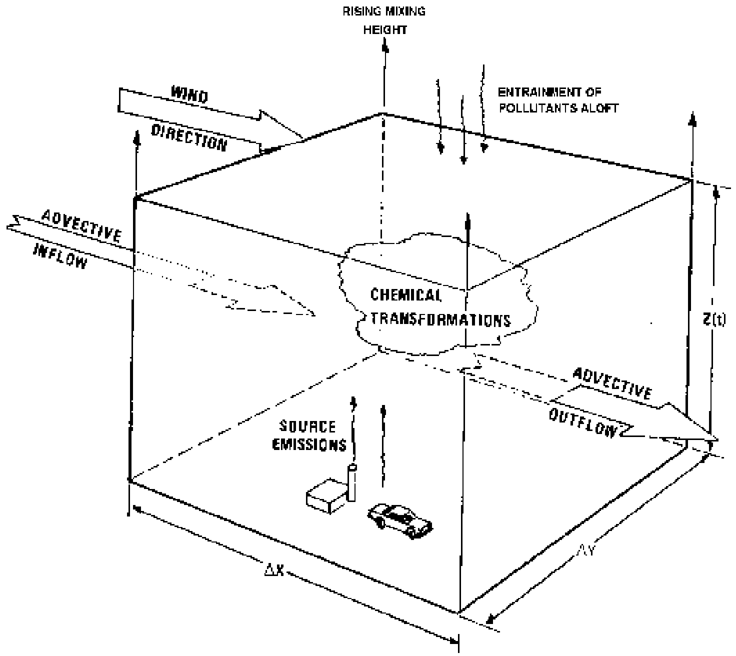
- Use operator splitting to solve CTM

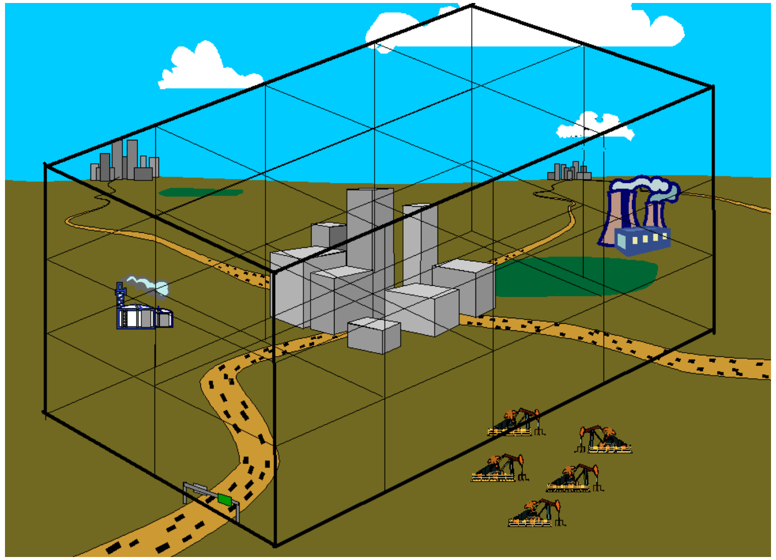
$$\mathrm{M}_{[t,t+\Delta t]} = T_X^{\Delta t/2} \cdot T_Y^{\Delta t/2} \cdot T_Z^{\Delta t/2} \cdot C^{\Delta t} \cdot T_Z^{\Delta t/2} \cdot T_Y^{\Delta t/2} \cdot T_X^{\Delta t/2}$$

Numerical Air Quality Modeling

(Carmichael, 2019; Zhang, 2024)

- **Mathematically represents the important processes that affect pollution**
- **Requires a system of models to simulate the emission, transport, diffusion, transformation, and removal of air pollutants**
  - Meteorological models
  - Emissions models
  - Chemical transport models (CTM)
- **Model approach**
  - Eulerian (e.g., STEM-III, Models-3/CMAQ)
  - Lagrangian (e.g., the ANL ASTRAP)
- **Model dimensionality**
  - Box model (0-D) (e.g., PNNL MaTChem)
  - Column model (1-D) (e.g., PNNL SC-MIRAGE)
  - 2-D (AER’s 2-D global model)
  - 3-D (STEM-III, CMAQ, CAMx)





Meteorological Modeling

(https://www.tceq.texas.gov/airquality/airmod/overview/am_met.html; Zhang, 2024)

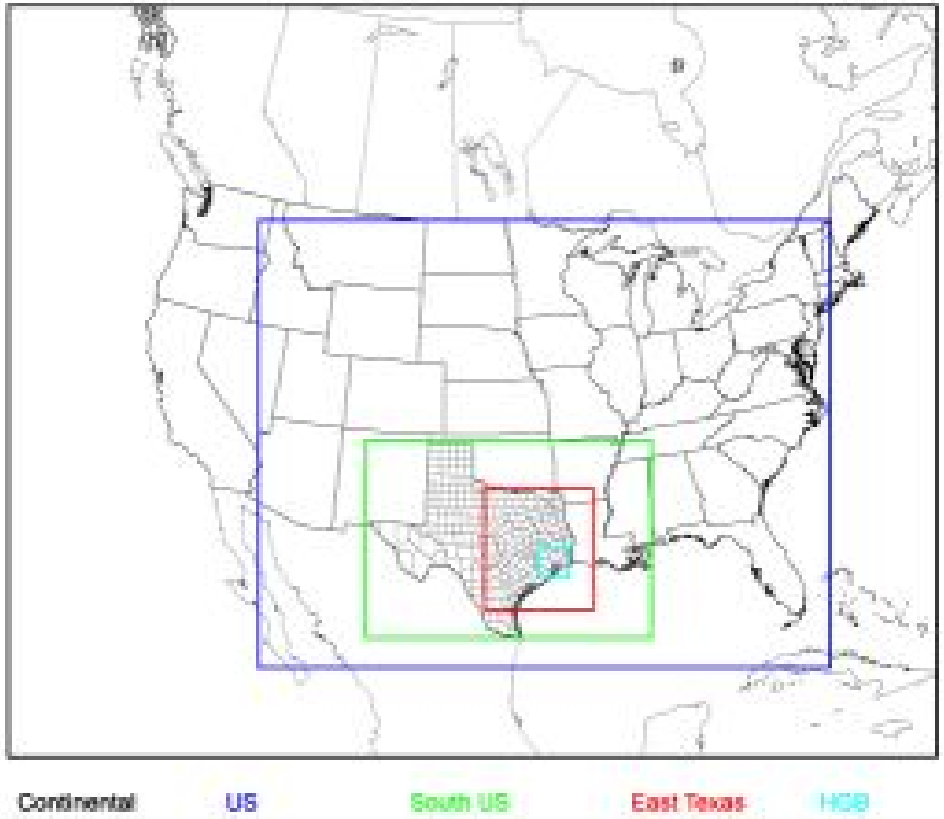
Main features

- Simulate meteorological conditions (e.g., wind, solar radiation, humidity, air temperature) and processes (horizontal and vertical transport, sea-breezes) that affect air pollutant concentrations.
- Use universal laws of atmospheric physics and empirical relationships to predict meteorological parameters in 3-D grid boxes
- Need forcing from large weather patterns to properly simulate conditions at the local scale by running the model on multiple nested domains
- Use Four-Dimensional Data Assimilation (FDDA) or nudging to produce meteorological parameters that are valid according to atmospheric physics laws yet closely matching with observations

Example models

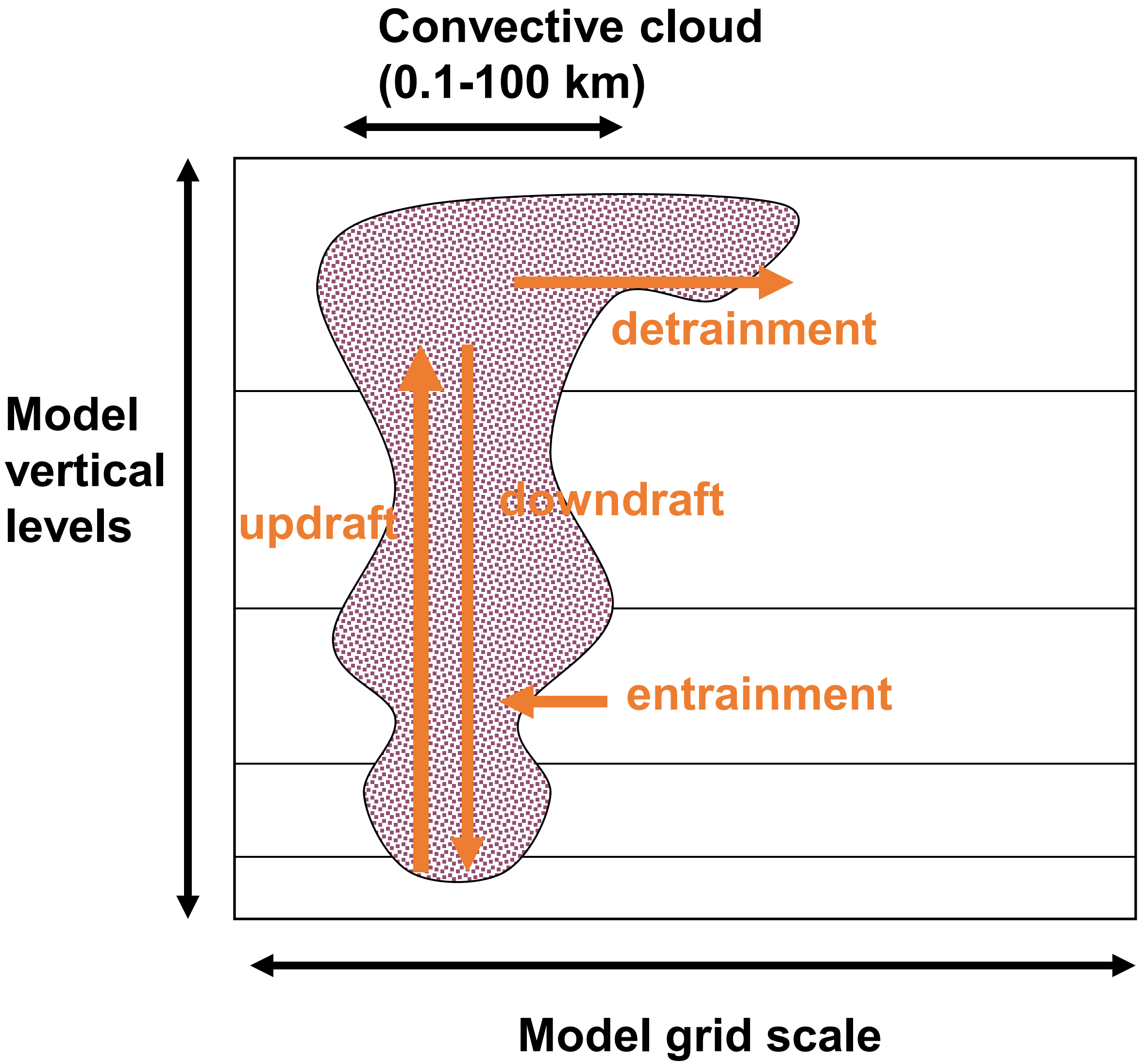
  - Global: The Unified Forecast System (UFS)
  - Regional-urban: The Weather Research and Forecasting (WRF)
  - Urban (3-km): the Rapid Refresh Forecast System (RRFS)

TCEQ nested modeling domain



Vertical Turbulent Transport (Buoyancy) (Carmichael, 2019)

- Generally dominates over mean vertical advection
- K-diffusion OK for dry convection in boundary layer (small eddies)
- Deeper (wet) convection requires non-local convective parameterization



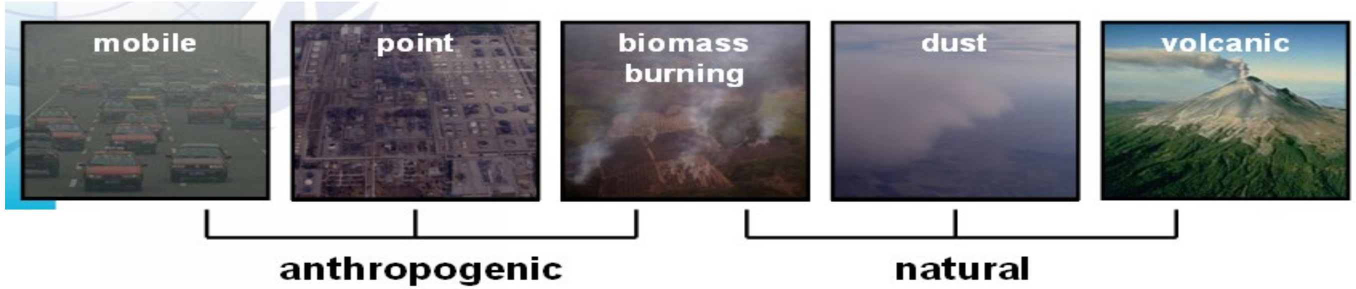
Wet convection is subgrid scale in global models and must be treated as a vertical mass exchange separate from transport by grid-scale winds.

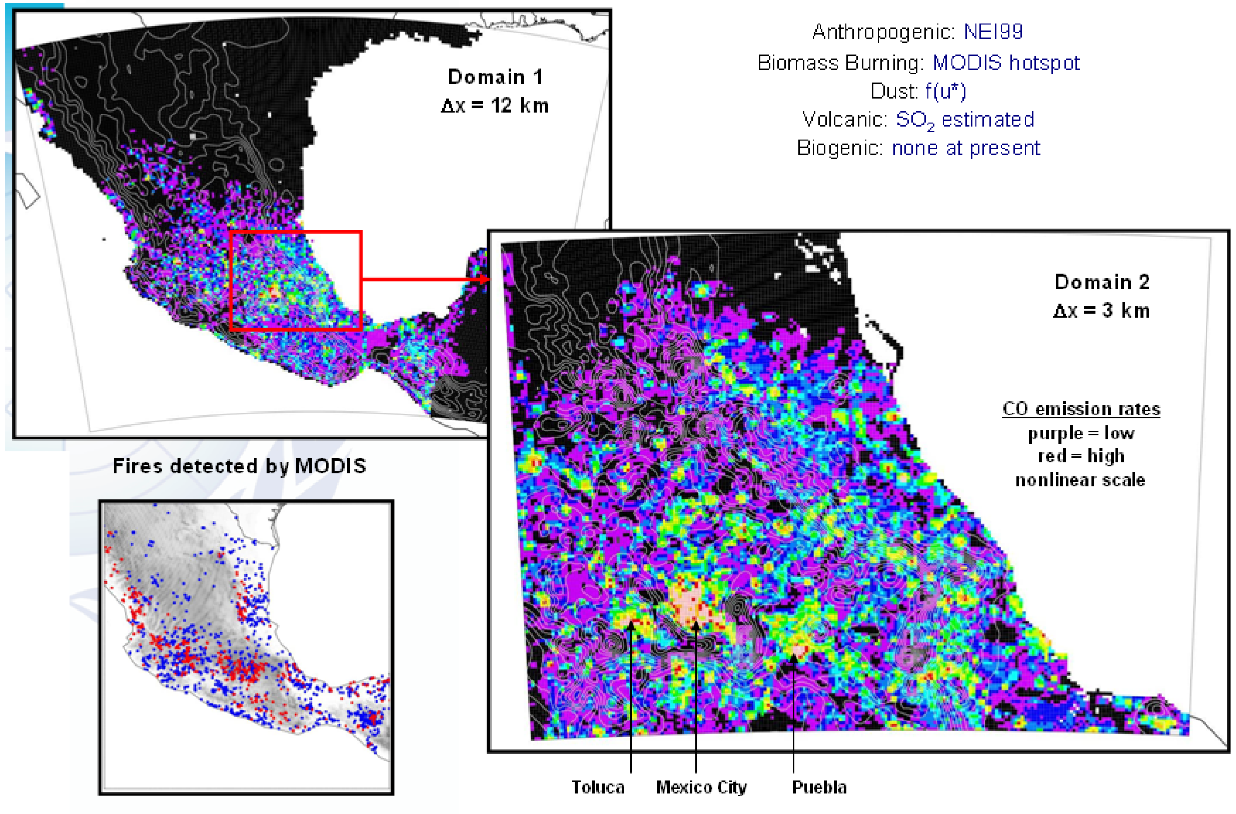
Need info on convective mass fluxes from the model meteorological driver.

Emission Processing and Modeling

- **Types of Emission Sources**
  - Stationary area sources
  - Non-road mobile sources
  - On-road mobile sources
  - Point sources
  - Natural Sources
- **Emission Inventory:** global and regional
- **Emission processing**
  - Convert emission inventory data to the resolution and chemical species needed
  - Distribute into space and time
  - **Process at appropriate Scales**
- **Emission modeling**
  - Using either observed or modeled activity information associated with one or more physical processes and estimating emissions using an algorithm
  - Improve existing emissions
- **Example models:**
  - SMOKE for anthropogenic emissions
  - MEGAN2 for biogenic emisions

(Pouliot, 2021; Carmichael, 2019; Zhang, 2024)

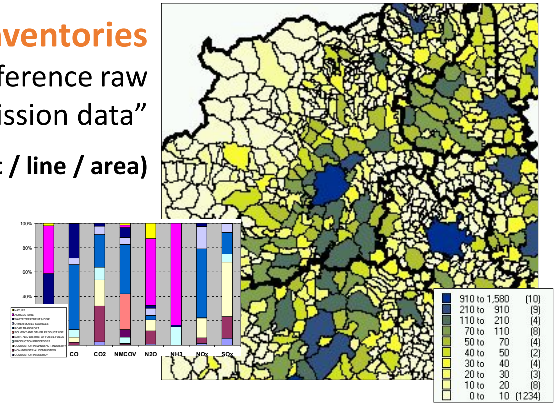




Emissions Processing for AQM

(Carmichael, 2019)

Inventories
"reference raw emission data"
(point / line / area)

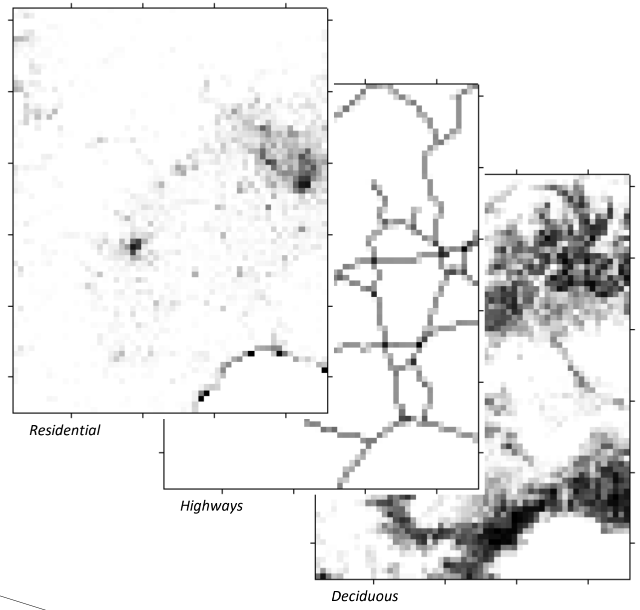


SPACE DISAGGREGATION

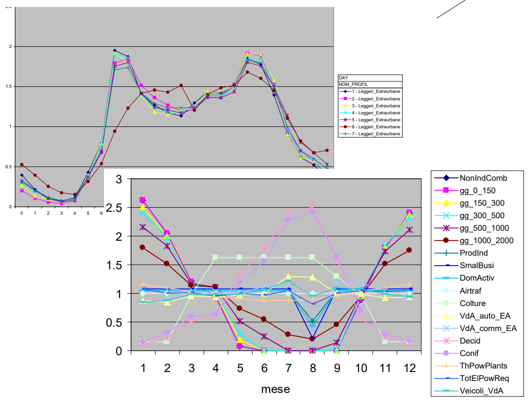
TIME MODULATION

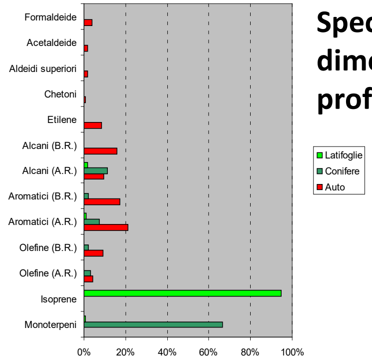
NMVOC & PM SPECIATION & SIZE

Thematic data



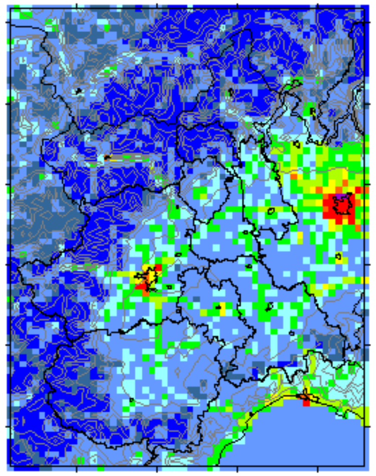
Modulation profiles
(hourly, daily, monthly)





Speciation & dimensional profiles

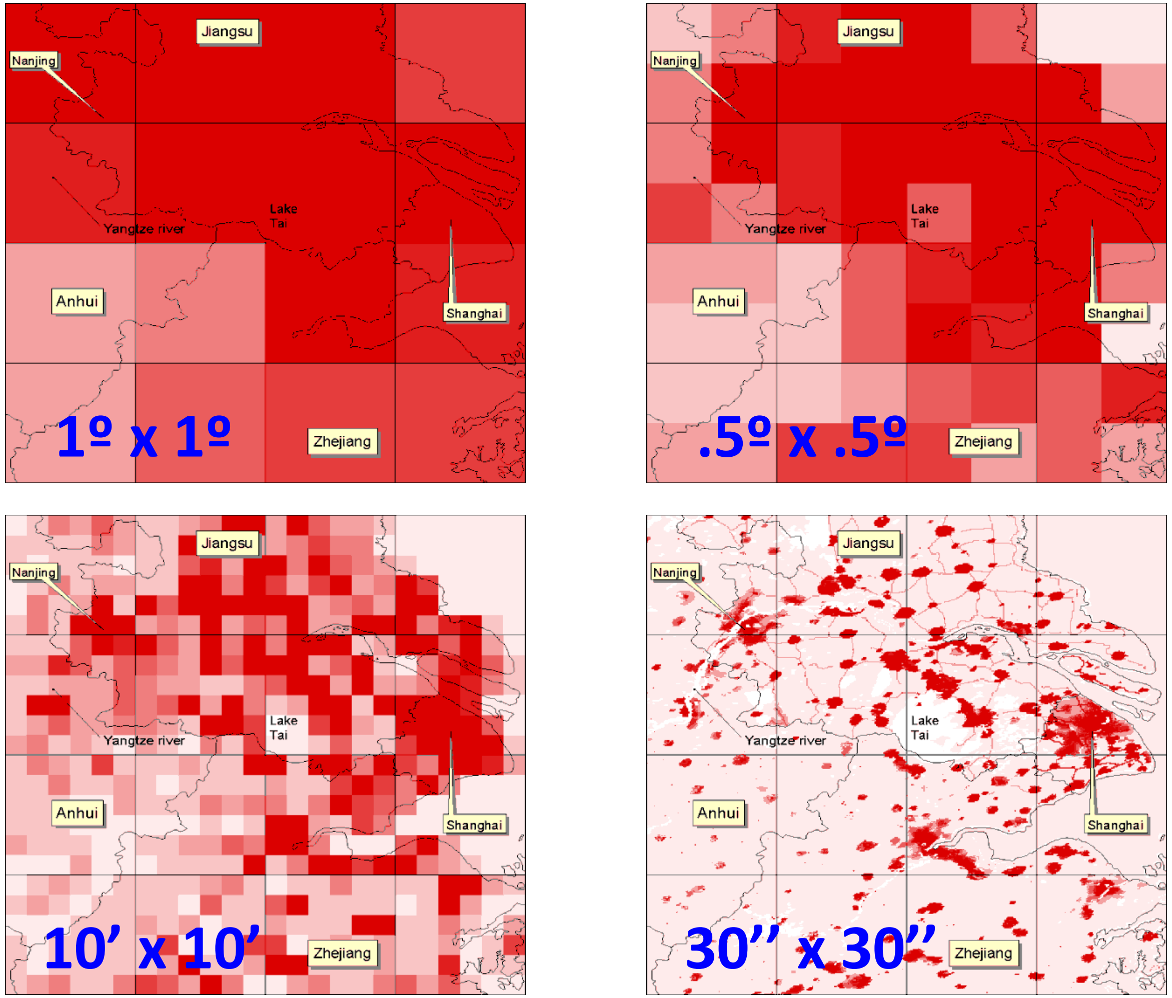
Model-ready input
(hourly, gridded, speciated emissions)



Detail: A Matter of Scale

(Carmichael, 2019)

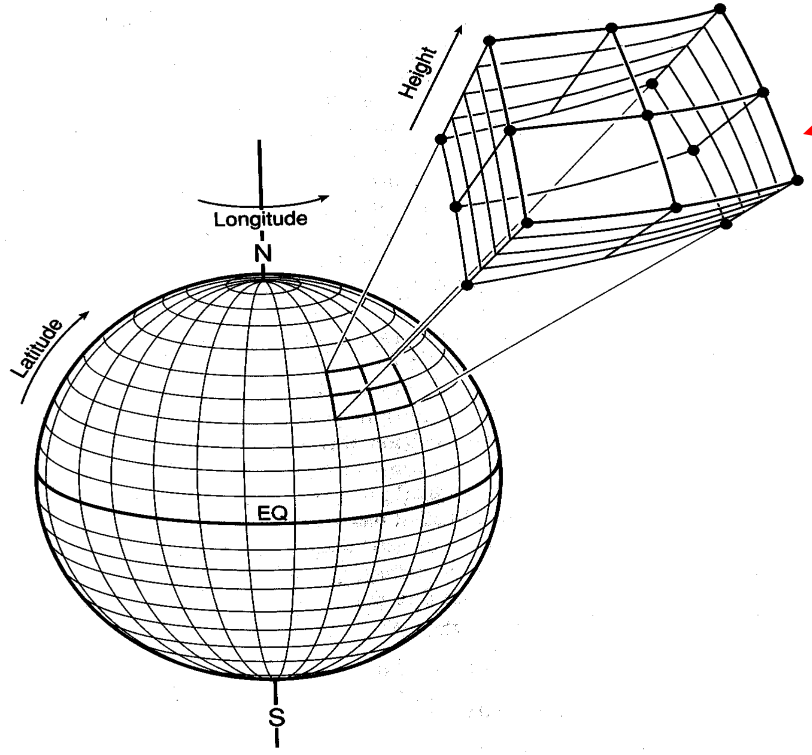
SO_2 emissions in the vicinity of Shanghai, China



Eulerian Models Partition Atmospheric Domain Into Gridboxes

(Jacob, 1999)

This discretizes the continuity equation in space



Solve continuity equation for individual gridboxes

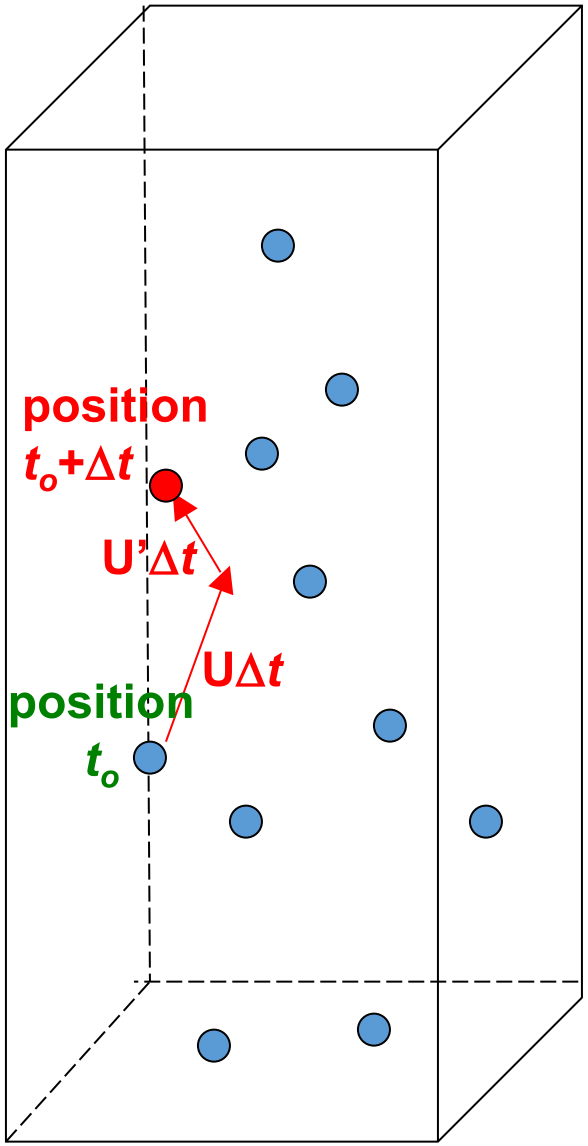
- **Detailed chemical/aerosol models can presently afford -10^6 gridboxes**

- **In global models, this implies a horizontal resolution of ~ 0.5-1^o (~50 to 100 km) in horizontal and ~ 0.5-1 km in vertical**

- **Chemical Transport Models (CTMs) use external meteorological data as input (or run on-line)**
- **General Circulation Models (GCMs) compute their own meteorological fields**

Lagrangian Approach: Track Transport of Points In Model Domain (No Grid)

(Jacob, 1999)



- Transport large number of points with trajectories from input meteorological data base (U) + random turbulent component (U') over time steps Δt
- Points have mass but no volume
- Determine local concentrations as the number of points within a given volume
- Nonlinear chemistry requires Eulerian mapping at every time step (semi-Lagrangian)

PROS over Eulerian models:

- no Courant number restrictions
- no numerical diffusion/dispersion
- easily track air parcel histories
- invertible with respect to time

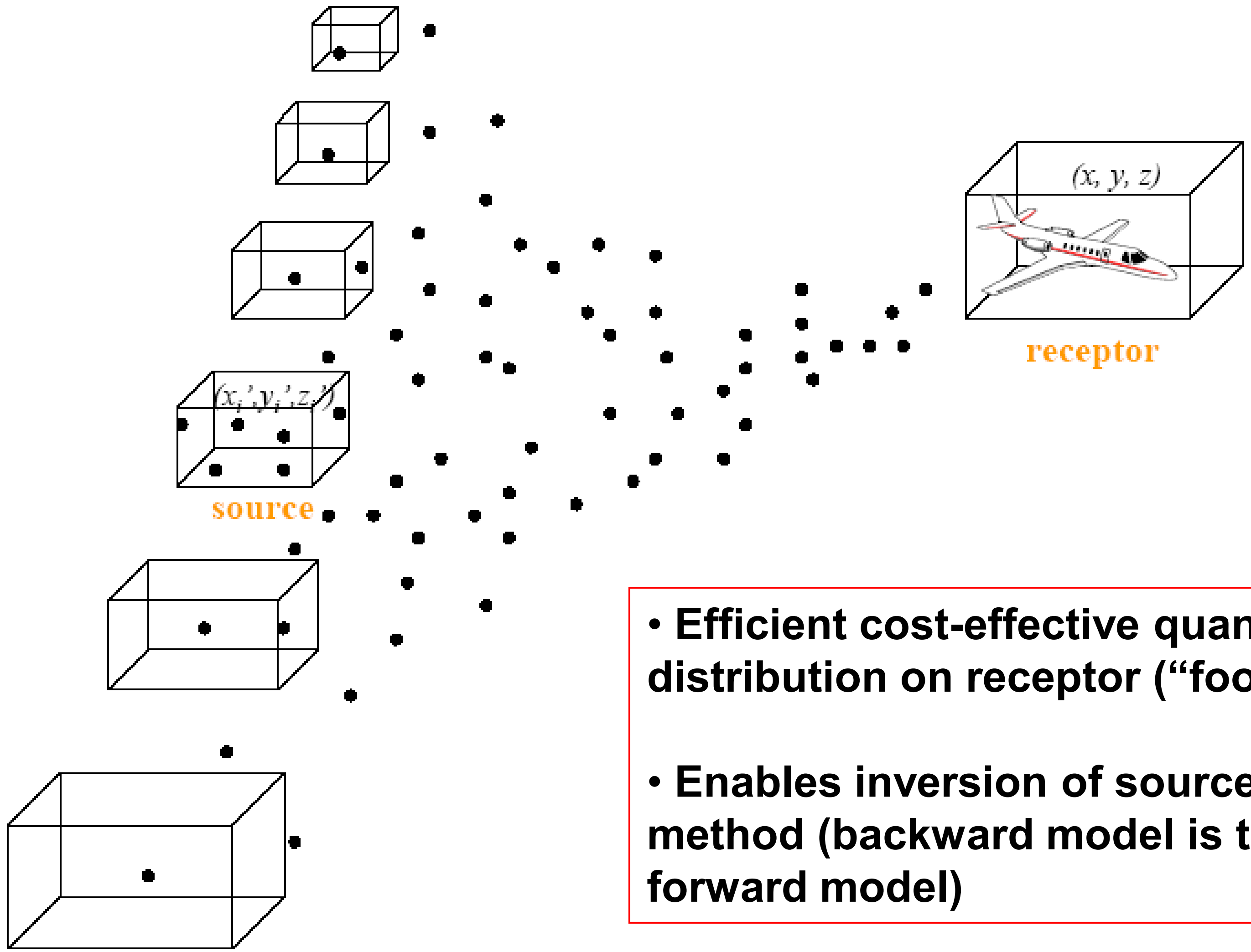
CONS:

- need very large # points for statistics
- inhomogeneous representation of domain
- convection is poorly represented
- nonlinear chemistry is problematic

Lagrangian Receptor-oriented Modeling

(Jacob, 1999)

Run Lagrangian model backward from receptor location, with points released at receptor location only



- **Efficient cost-effective quantification of source influence distribution on receptor ("footprint")**

- **Enables inversion of source influences by the adjoint method (backward model is the adjoint of the Lagrangian forward model)**

0-3 Dimensional Models

(Seinfeld and Pandis, 2016)

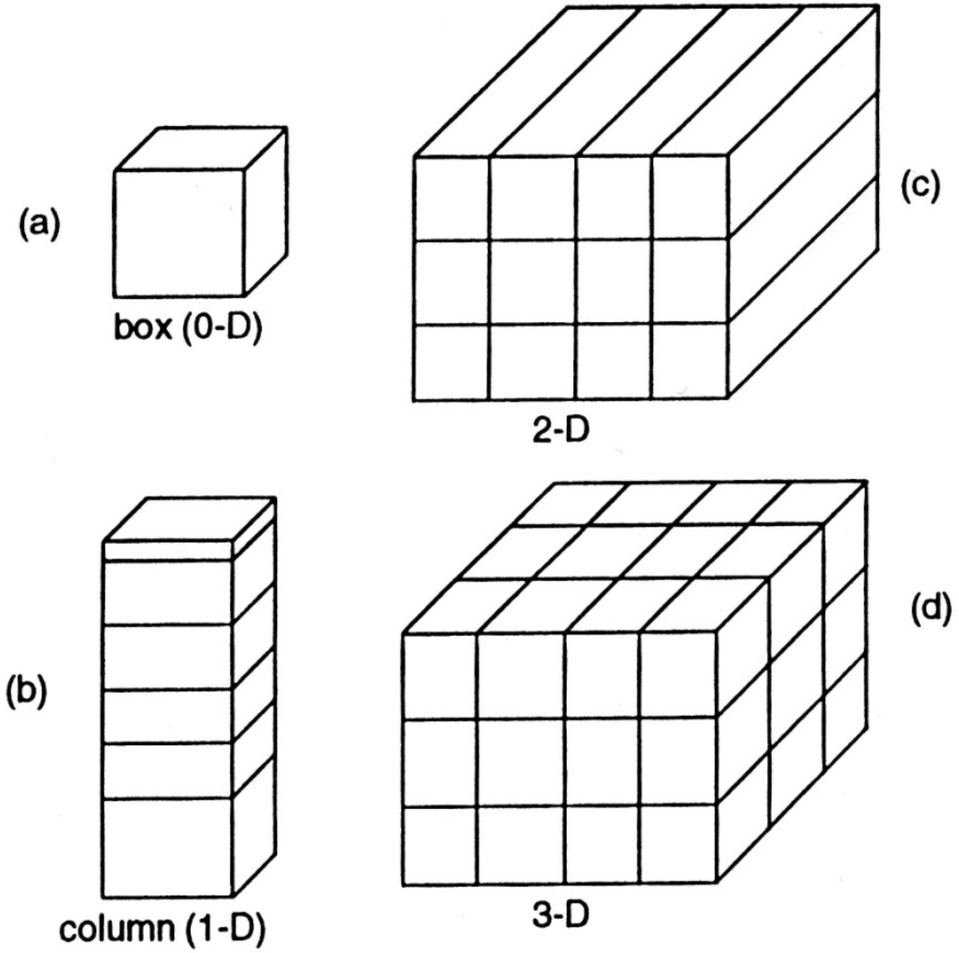


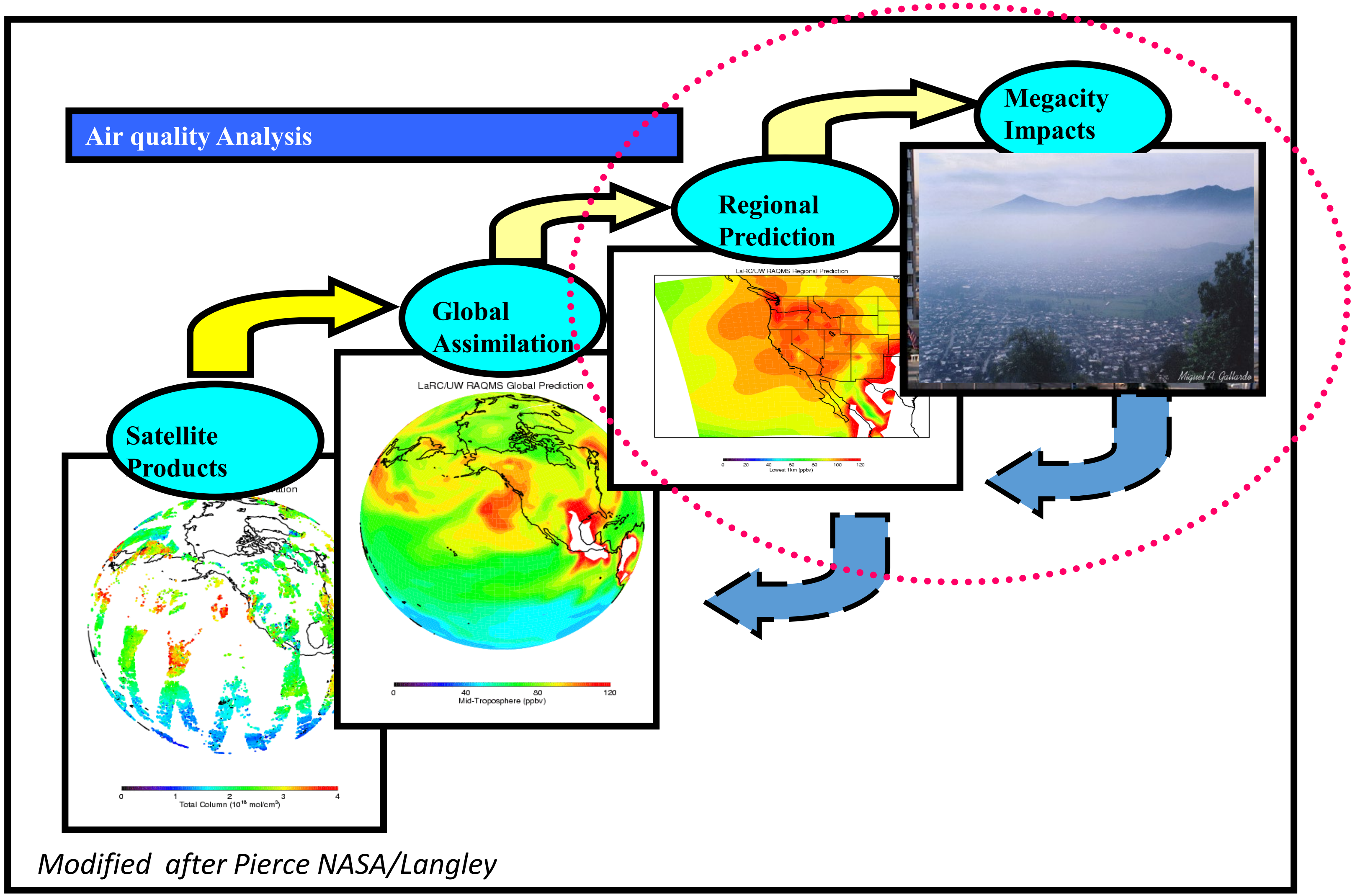
FIGURE 23.3 Schematic depiction of (a) a box model (zero-dimensional), (b) a column model (one-dimensional), (c) a two-dimensional model, and (d) a three-dimensional model.

0-D: C(t)
1-D: C(z, t)
2-D: C(x, z, t) or C(y, z, t)
3-D: C(x, y, z, t)

Air Quality Prediction: A Challenge of Scales and Integration

(Carmichael, 2019)

- **Model spatial scales**
  - Global
  - Hemispheric
  - Regional
  - Urban
  - Hyperlocal
- **Multiscale models**
  - One atmosphere
  - Inter-scale connections
  - Across-scale formulations



Air quality Analysis

Satellite Products

Global Assimilation

Regional Prediction

Megacity Impacts

Modified after Pierce NASA/Langley

Types of Coordinate Systems used in CTMs

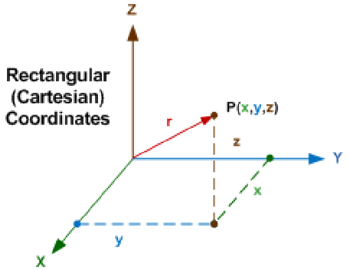
(Jacobson, 2005; Zhang 2024)

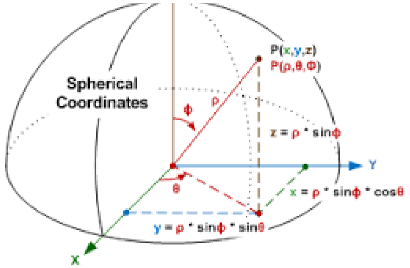
Horizontal Coordinates

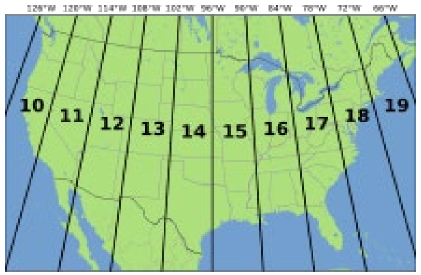
- Cartesian (Rectangular) Coordinate
  - » Based on x, y
  - » Used when the earth's curvature is small (e.g., small grid resolution)
- Spherical Coordinates
  - » Based on longitude, latitude (λ, ϕ)
  - » Accounts for the effect of the earth's curvature
- Universal Transverse Mercator (UTM) Coordinate
  - » The region of the earth is divided into a group of rectangles
  - » Separate rectangular meshes are superposed over the globe
  - » UTM coordinate locations are mapped back to spherical coordinate locations using the UTM-to-spherical conversion equation
- Cubed-Sphere Coordinates
  - » A cube onto the surface of a sphere represented as six adjoining grid faces which seamlessly cover the whole globe
  - » avoid the numerical difficulties of the spherical poles, suited for adaptive grid

Vertical Coordinates

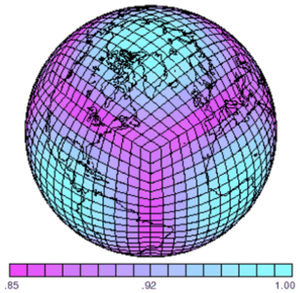
- Height-Based Coordinates
  - » Based on z, z', or ζ
- Pressure-Based Coordinates
  - » Based on p, or σ-p, or σ-z







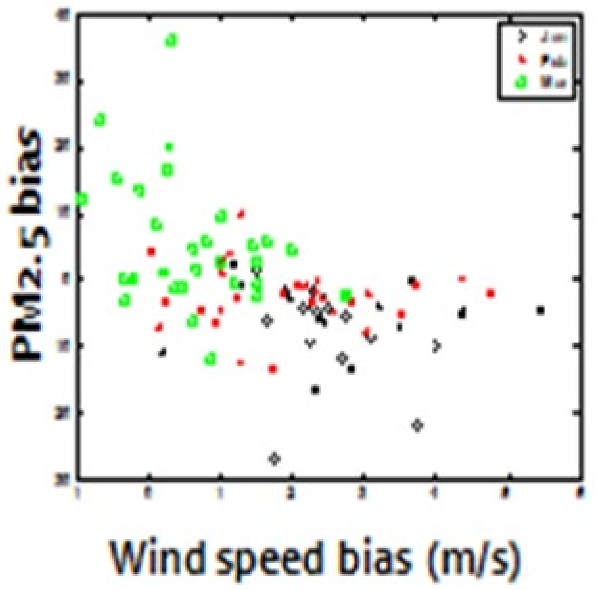
UTM for US

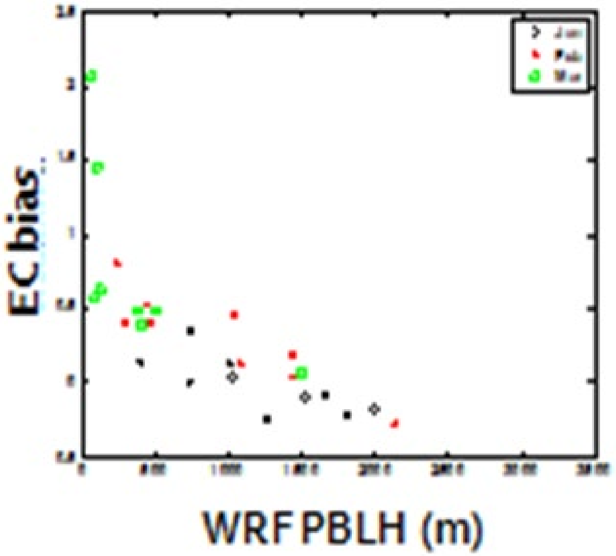


Major Sources of Errors and Uncertainties

(Carmichael, 2019; Zhang, 2024)

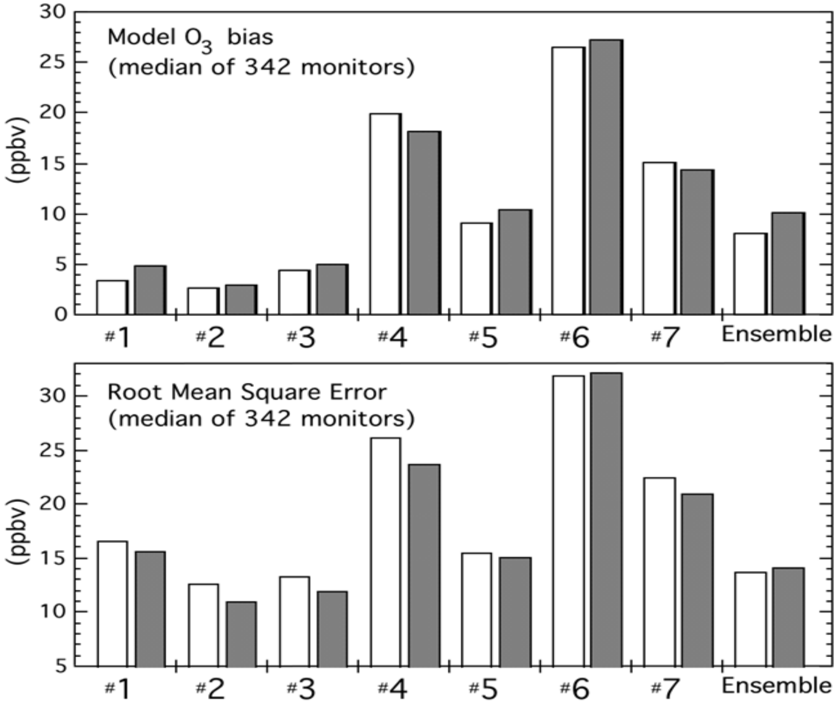
- Emissions
- Boundary conditions
- Key meteorological aspects (e.g., PBL, clouds, temperature, water vapor, precipitation)
- Other key model inputs (e.g., land use, surface roughness, anthropogenic heat flux)
- Chemical processes (e.g., secondary organic and inorganic Aerosol, nighttime chemistry)
- Model configurations (e.g., grid resolution, nesting, physics and chemistry options)





Methods to Improve Air Quality Prediction (Carmichael, 2019)

- **Bias correction**
- **Ensemble modeling**
- **Data assimilation**
- **Data fusion and ML/AI**

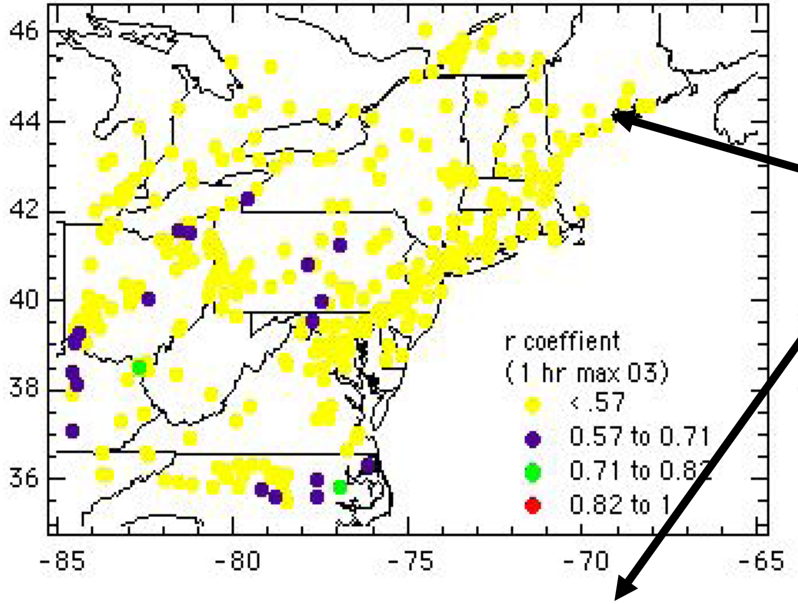


White bar: max 1-hr O_3 bias

Shaded bar: max 8-hr O_3 bias

(McKeen et al., 2005)

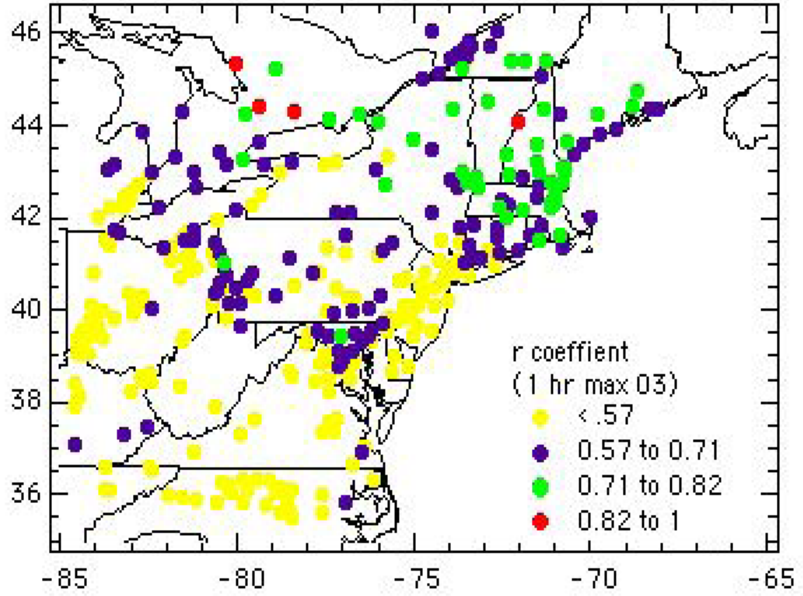
Forecasting Air Quality an Important Activity in Air Quality Management

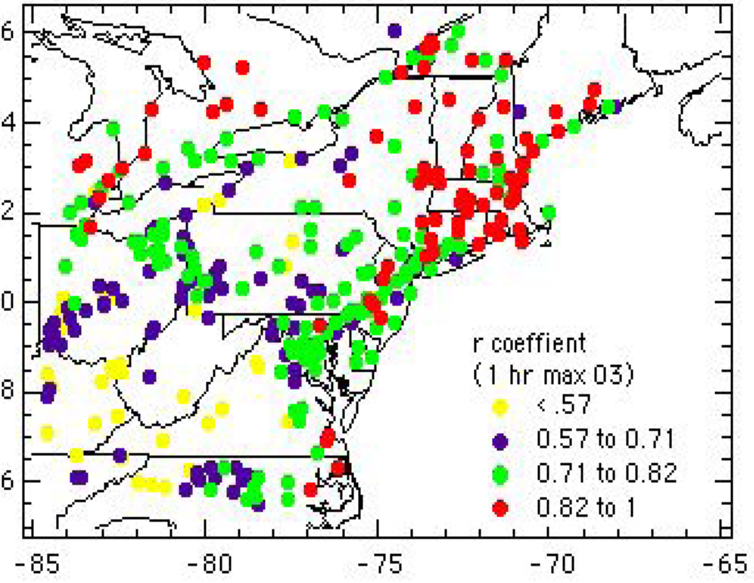


*** Persistence**

*** Single Forward Model w/o assimilation**

*** Ensemble forecast (8 models) w/o assimilation** ***(further improvements with bias corrections based on obs)***





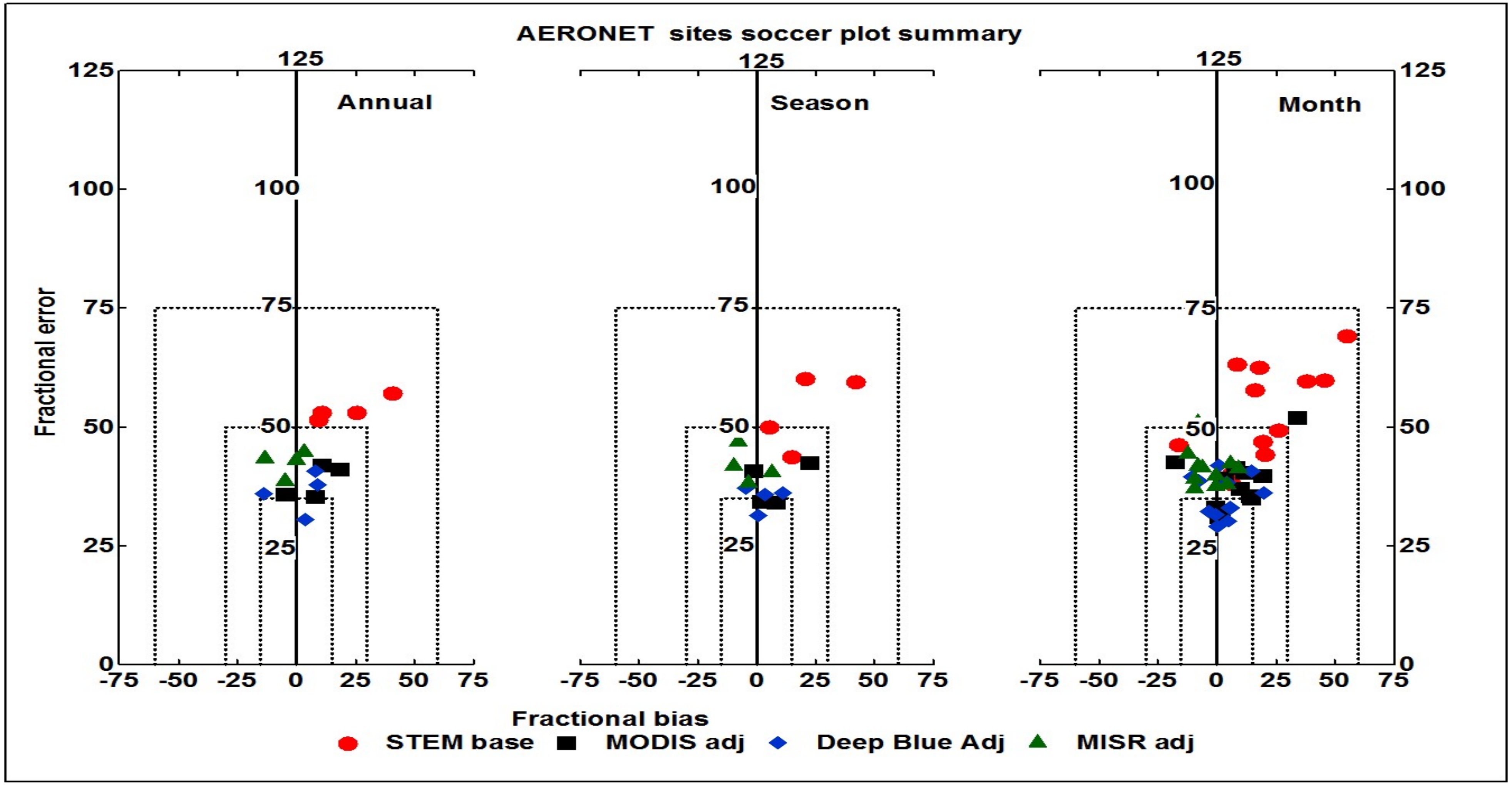
Data Assimilation Methods and Challenges

(Bocquet et al., 2015; Carmichael, 2019)

- **“Simple” data assimilation methods**
  - Optimal Interpolation (OI)
  - 3-Dimensional Variational data assimilation (3D-Var)
  - Kriging
- **Advanced data assimilation methods**
  - 4-Dimensional Variational data assimilation (4D-Var)
  - Kalman Filter (KF) - Many variations, e.g. Ensemble Kalman Filter (EnFK)
  - Hybrid Methods
- **Challenges in chemical data assimilation**
  - A large amount of variables (~300 concentrations at each grid points)
  - > 200 chemical reactions coupled together (lifetimes of species vary from seconds to months)-stiff differential equations
  - Chemical observations are very limited, compared to meteorological data

Total AOD - Assimilation Reduces Annual/Seasonal and Monthly Bias and Error

(Carmichael, 2019)



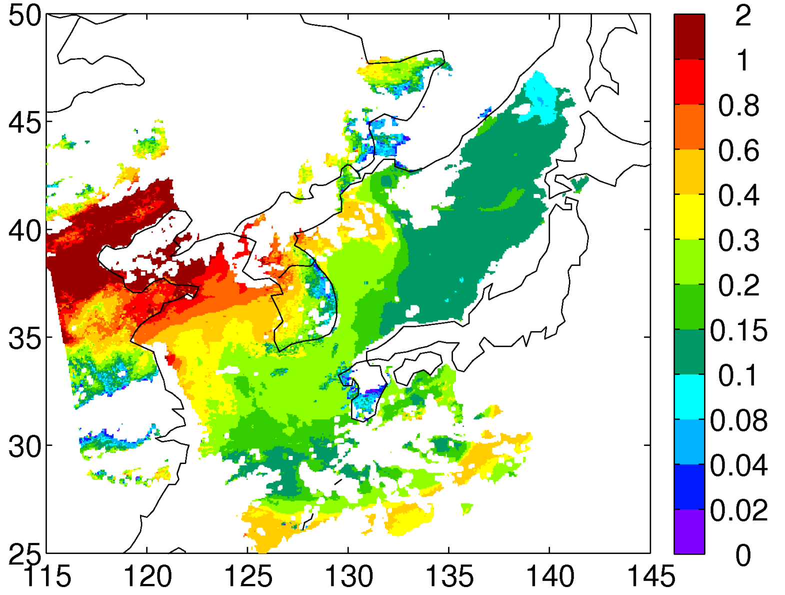
Annual/Seasonal/Monthly Soccer Plots across the domain (Best configuration case)

Impacts of Geostationary AOD Assimilation *(Are we "ready " to see an impact?)*

(Saide et al., 2014)

- **Objectives:** Assess performance of assimilating Geostationary GOCI AOD into a system already assimilating MODIS AOD
- **System:** WRF-Chem - GSI for MOSAIC sectional aerosol model (Saide et al., ACP 2013) allows assimilation of multiple data
- **Experiments:** GSI AOD assimilation every 3 hours, MODIS only, MODIS+GOCI. (Only over-sea AOD used)

GOCI AOD



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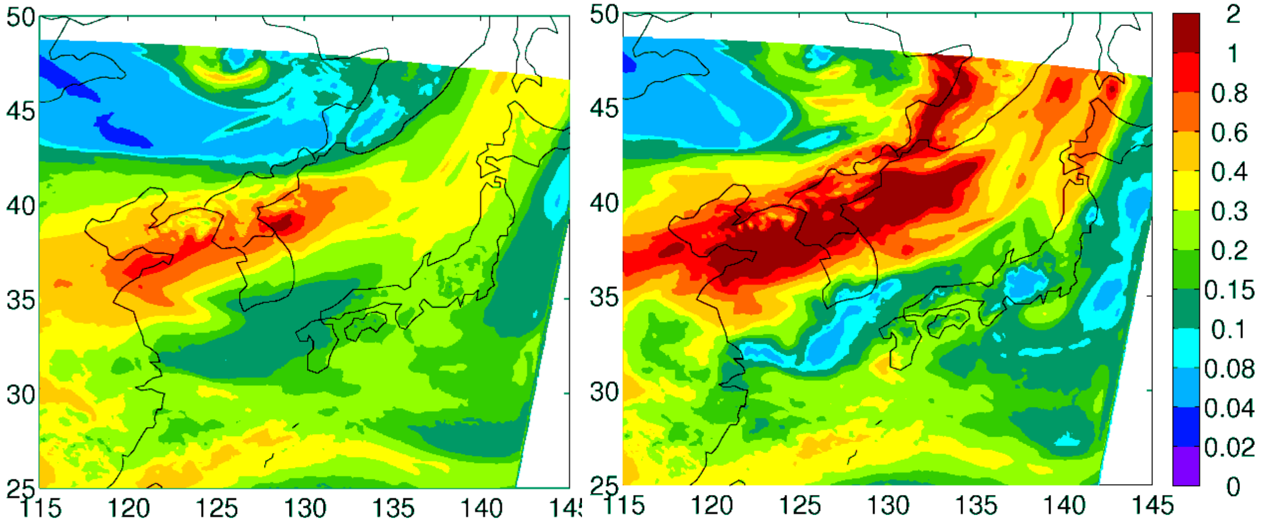
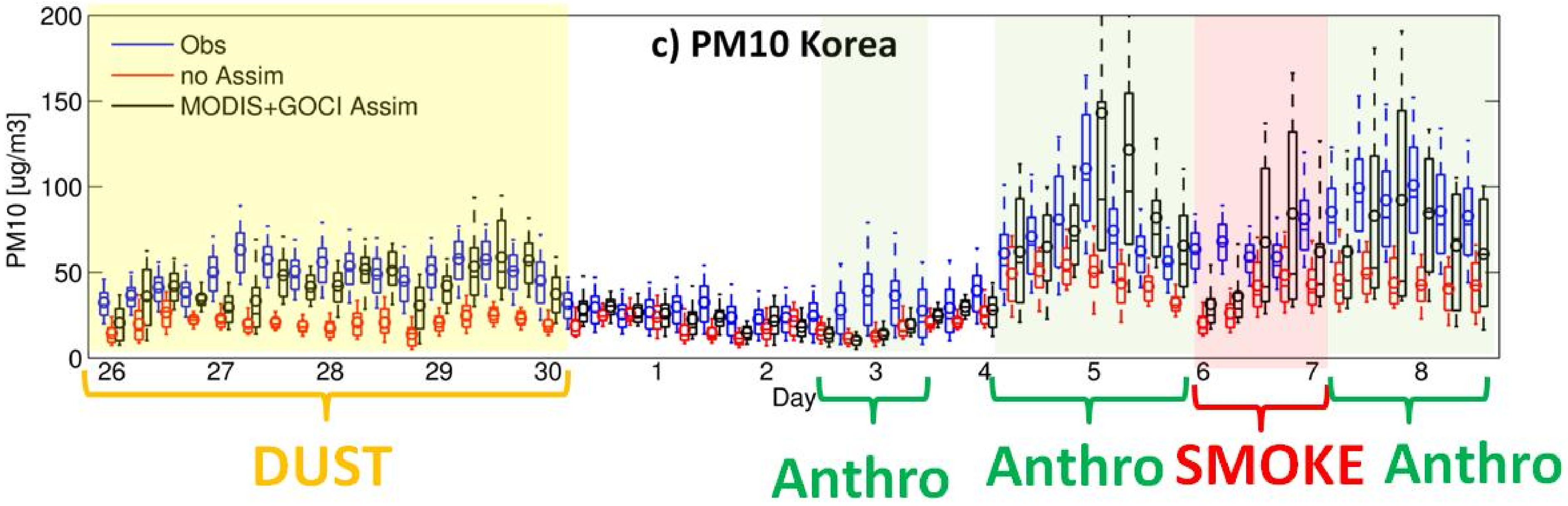


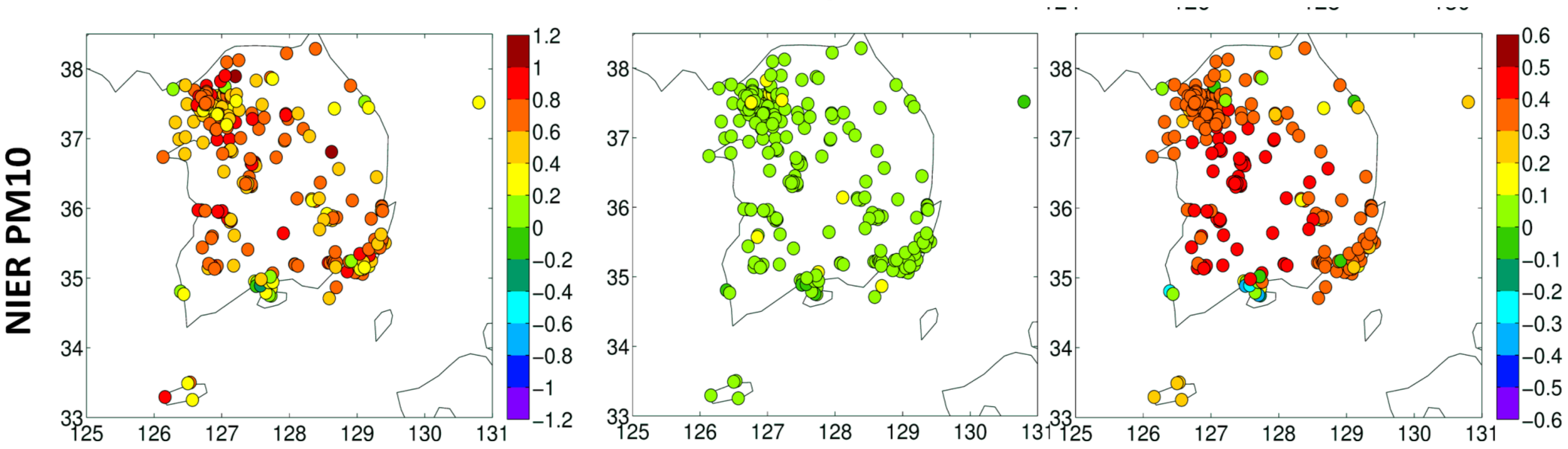
WRF-Chem NO Assimilation

WRF-Chem MODIS+GOCI Assimilation

Impact of GOCI on PM_{10} Prediction

(Saide et al., 2014)





Fractional Bias reduction

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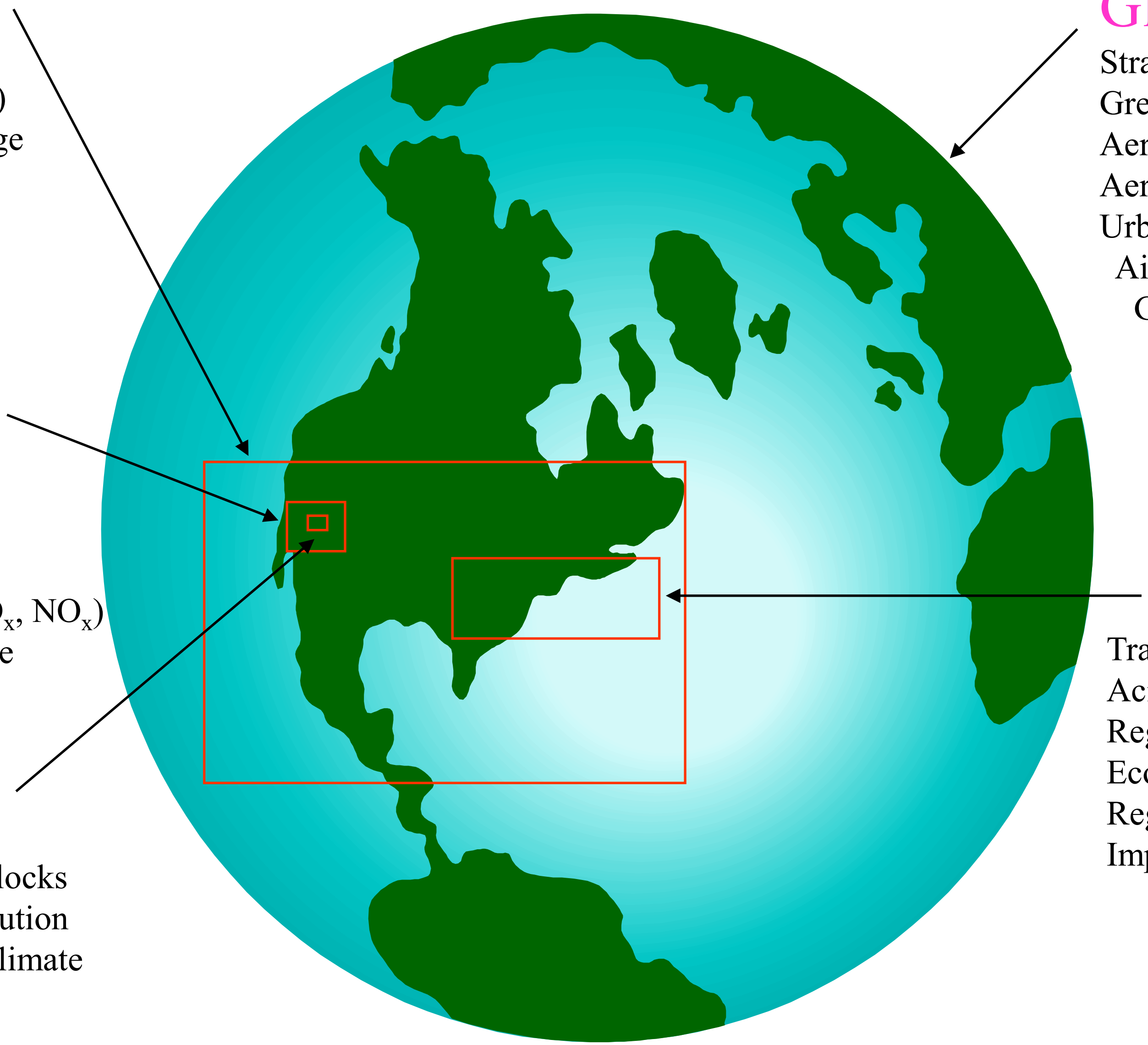
- **Summary**

Major sources: Carmichael (2019); Zhang (2024), Zhang et al. (2012), Zhang and Baklanov (2020)

One Atmosphere: Multiscale Multi-Pollutant Air Quality Modeling

(Zhang, 2024)



Hemispheric

Intercontinental
transport (SO$_x$,NO$_x$,O$_3$)
Regional climate change
Urban/regional impact
Air toxics(e.g., Hg)

Global

Stratospheric O$_3$ hole
Greenhouse effect (CO$_2$/CH$_4$/O$_3$)
Aerosol direct forcing
Aerosol indirect forcing
Urban/regional impact
Air toxics (e.g., Hg)
Global climate change

Urban

Smog:O$_3$, VOCs, SOA
Visibility reduction
Health effect of PM$_{2.5}$
Air toxics (Hg, As)
Power plant plume (SO$_x$, NO$_x$)
Impact of global change

Regional

Transport of SO$_x$/NO$_x$/O$_3$)
Acid deposition (SO$_x$/NO$_x$)
Regional haze (SO$_4^{2-}$)
Ecosystem damage (Hg)
Regional climate change
Impact of global change

Hyperlocal

PM$_{2.}$ hot spots in city blocks
Street-scale traffic pollution
Impact of microscale climate
Environmental justice

WMO Training Materials and Best Practices for Chemical Weather /Air Quality Forecasting

WORLD
METEOROLOGICAL
ORGANIZATION

WEATHER CLIMATE WATER

Training Materials and Best Practices for Chemical Weather/Air Quality Forecasting

Scientific Editors:
Yang Zhang and Alexander Baklanov

Overarching goals

- Provide best existing experience from NMHSs and academic community to build scientific capacity of researchers and operational meteorologists in developing countries through bridging sciences into operations
- Make sustained contributions towards the implementation of relevant policy and decision support aimed at improving quality of life through enhancing the science-policy interface

Content

- 12 Chapters, 573 pages, 49 tables, 111 figures
- 51 authors from 15 countries
- 17 Global and 51 regional CW-AQF models
- 24 demonstration cases over Global (3), Europe (4), North America (3), Asia (5), South America (2), Oceania (3), and Africa (4)

https://elioscloud.wmo.int/share/s/WB9UoQ5kQK-dmgERjSAqIA

17 Global CW-AQF Models (Zhang and Baklanov, 2020)

Country/ Organization	Model System	Meteorological Model (MetM)	Air Quality Model (AQM)	Microscale Models	Scale	MetM -AQM coupling
Canada/EC	GEM-MACH	GEM	GEM-MACH15	None	Global/ Regional	Unified Online
Canada/ York Univ.	GEM-AQ	GEM	AQ	None	Global/ Regional	Unified Online
China/MCA and CAMS	GRAPES - CUACE	GRAPES	CUACE	None	Global/ Regional	Unified Online
Finland/FMI	SILAM	ECMWF/IFS; WRF; HIRLAM; AROME; COSMO HARMONIE	SILAM	None	Global/ Regional	Offline
France/LMD	LMDzt -INCA	ECMWF/IFS; LMDzt v4.0 with nudged with NCEP	INCA v3	None	Global	Separate Online
France/MF-CNRM	MOCAGE	ARPEGE (global) ALADIN (regional) ECWMF	MOCAGE	None	Global/ Regional	offline
Germany/MPIM	ECHAM5	ECHAM5	ECHAM5	None	Global	Unified Online
Norway NIAR/ FLEXPART	FLEXPART	ECMWF NCEP	FLEXPART	None	Global	offline
Japan-FRCGC	GR-RT-AQF	CCSR/NIES/FRCGC atmospheric GCM (global) WRF (regional)	CHASER (global) WRF/Chem (regional)	None	Global/ Regional	Offline for global/regional Unified online for regional
Japan/JMA	MASINGAR	AGCM	MASINGAR	None	Global	Online
Spain, BSC-CNS	NMMB/BSC-CTM	NMMB	BSC-CTM (dust module)	None	Global/ regional	Separate Online
UK/ECMWF, MACC	ECMWF-IFS CTMs; ECMWF/CAMS	IFS	MOZART-3, TM5, or MOCAGE; C-IFS	None	Global/ Regional	Separate online
UK/Met Office	MetUM	MetUM	Dust module	None	Global/ Regional	Unified Online
US/FNMOC/NRL	NAAPS	NOGAPS	NAAPS	None	Global	Offline
US/NASA	GEOS-5 ESM	GEOS DAS	GEOS-Chem GOCART	None	Global	Unified Online
US/NCAR, Germany/MPIC	MATCH-NCAR	NCEP/NCAR	MATCH-NCAR	None	Global	offline
US/NOAA-NCEP	NEMS GFS-NGAC	NEMS GFS	NGAC (dust only)	None	Global	Unified Online

51 Regional/Urban CW-AQF Models (Zhang and Baklanov, 2020)

Country/ Organization	Model System	Meteorological Model (MetM)	Air Quality Model (AQM)	Microscale Models	Scale	MetM -AQM coupling
Australia/CSIRO	AAQFS Or AQFx	LAPS, UM, CCAM; ACCESS	CSIRO's CTM, C-CTM	None	Regional	offline
Austria/ZAMG	ALADIN- CAMx	ALADIN-Austria	CAMx	None	Regional	offline
Brazil/CPTEC	CCATT-BRAMS	BRAMS	CCATT	None	Regional	Unified Online
Canada/EC	GEM-AURAMS	regional GEM	AURAMS	None	Regional	offline
Canada/EC	GEM-CHRONOS	regional GEM	CHRONOS	None	Regional	offline
Canada/EC	GEM-MACH15	GEM	chemistry from AURAMS	None	Regional	Unified Online
China/IAP-CAS	EMS-Beijing	MM5	NAQPMS, CMAQ, CAMx	None	Regional	offline
China/Zhejiang Univ.	Two-way coupled WRF-CMAQ	WRF (ARW)	CMAQ	None	Regional	Separate Online
Denmark/DMU-ATMI	THOR	The US NCEP, Eta	DEOM DEHM (UPM, OSPM)	BUM OSPM DREAM	Regional	offline
Denmark/DMI	DACFOS	HIRLAM	MOON, CAMx, Enviro-HIRLAM	M2UE	Hemispheric/ Continental/ regional	offline/ Separate Online
Denmark, Finland, Norway, Spain, Italy/FUMAPEX UAQIFS[3]	1. UAQIFS-Norway 2. UAQIFS-Finland 3. UAQIFS-Spain 4. UAQIFS-Italy1 5. UAQIFS-Italy2 6. UAQIFS-Denmark	1. HIRLAM 2. HIRLAM 3. RAMS 4. RAMS 5. LAMI 6. HIRLAM	1. AirQUIS (dispersion) 2. CAR-FMI (dispersion) 3. CAMx (O_3 only) 4. FARM 5. NINFA-OPPIO/ADAM 6. DERMA-ARGOS	Some include population exposure models, some include urban dispersion/statistical models	Regional /local	offline
Egypt/EMA; South Africa/SAWS	RegCM-CHEM	RegCM4.6	RegCM-CHEM4.6	None	Regional	Unified Online

51 Regional/Urban CW-AQF Models (Zhang and Baklanov, 2020)

Country/ Organization	Model System	Meteorological Model (MetM)	Air Quality Model (AQM)	Microscale Models	Scale	MetM -AQM coupling
France/AIRPARIF[2]	ESMERALDA	MM5	CHIMERE	None	Regional	offline
France/INERIS	Prev'air	MM5, WRF, ECWMF/IFS	CHIMERE, MOCAGE, Polair3D	None	Regional	offline
France/CEREA	POLYPHEMUS	ECMWF, MM5, WRF	Polair3D	MUNICH	Regional/urban	offline
France/CNRS, Météo-France	Meso-NH-C	Meso-NH-C	Meso-NH-C	None	Continental/ regional/urban/local	Unified online
Germany/FRIUUK, RIU, Cologne	EURAD-RIU	MM5	EURAD-IM	None	Regional	offline
Germany/FU-Berlin, Institute for Meteorology	RCG	GME	REM- CALGRID	None	Regional	offline
Germany/KIT	COSMO- ART	COSMO	ART	None	Continental/regional	Unified Online
Germany/LITR	COSMO-MUSCAT	COSMO	MUSCAT	None	Continental/regional	Separate Online
Germany/Uni. of Hamburg	M-SYS	METRAS	MECTM	MITRAS-MICTM	Regional/urban/local	Unified Online
Germany/IMK-IFU	MCCM (MM5-Chem)	MM5	Chem	None	Continental/regional/urban	Unified Online
Greece/Aristotle University	MEMO/MARS	MEMO	MARS-aero	None	Regional/urban	Separate Online
Greece/ NKUA	CAMx- AMWFG	SKIRON/Dust	CAMx	None	Regional	offline
Greece/NKUA, AUT	MM5-CAMx	MM5	CAMx	None	Regional	offline
Greece/UA	SKIRON/TAPM	SKIRON/dust;Eta	CAMx v4.31	None	Regional	Offline
Italy/CETEMPS	ForeChem	MM5	CHIMERE	None	Regional	offline
Italy/ARIANET s.r.l.	FARM	RAMS	FARM	None	Regional	offline
Italy/CNR-ISAC	BOLCHEM	BOLAM	CHEMistry modules	None	Continental/regional	Separate Online
Italy/ITCP	RegCM-Chem	RegCM4	RegCM-Chem4	None	Continental/regional	Unified Online
Japan/Kyushu University	CFORS	RAMS	Parameterized chemical tracers in RAMS	None	Regional	Unified Online
Morocco/Maroc Météo	ADMS URBAN 3.1	ALADIN	GRS Chemical Model	Urban canopy	Regional/local	Separate online?
Netherlands/KNMI, TNO, RIVM, PBL/KN	LOTOS-EUROS	Archived analyses, ECMWF, RACMO2	LOTOS-EUROS	None	Regional	Offline/ Separate Online

51 Regional/Urban CW-AQF Models (Zhang and Baklanov, 2020)

Country/ Organization	Model System	Meteorological Model (MetM)	Air Quality Model (AQM)	Microscale Models	Scale	MetM -AQM coupling
Norway/ MET-NO	EMEP-Unified	ECMWF/IFS	Unified EMEP-CWF	None	Regional	offline
Singapore/MSS	ATLAS-NAME	UM	NAME	None	Regional	Offline
Spain/BSC-CNS	CALIOPE	WRF, MM5	CMAQ, DREAM, CHIMERE,	None	Regional	offline
Spain/TUM, LHTEE, AUT, NCAR/Pen	OPANA v4.0	MM5 MEMO	CMAQ	MICROSYS	Regional /local	offline
Sweden/SMHI	MATCH	ECMWF/IFS HIRLAM	MATCH	None	Regional	offline
UK/Uni. Of Hertfordshire	WRF-CMAQ	WRF(ARW)	CMAQ v5.02	None	Regional/ national	Offline
UK/AEA	WRF/CMAQ	WRF	CMAQ	None	Regional	offline
UK Met Office	AQUM	MetUM	UKCA	None	Sub-regional/ national	Unified Online
UK/Met Office	NAME-III	ECMWF, Met Office Unified Model	NAME-III	None	Regional /local	offline
US/BAMS	MAQSIP-RT CMAQ	BAMS-MM5, WRF	MAQSIP CMAQ	None	Regional	offline
US/WSU	AIRPACT3	MM5	CALGRID, CMAQ	None	Regional	offline
US/SUNY-Albany	AQFMS	SKIRON/Eta; WRF (NMM and ARW)	CAMx, CMAQ	None	Regional	offline
US/UI	STEM-2K3	MM5, WRF	STEM	None	Regional	offline
US/NOAA, ARL	NAQFC (NAM-CMAQ)	Eta, WRF (NMM), NAM	CMAQ	None	Regional/ national	Offline
US/NCAR, Greece	MM5-CHIMERE	MM5	CHIMERE	None	Regional	offline
US, Greece	RAMS/ICLAMS	RAMS	ICLAMS	None	Continental/ urban	Separate Online
US/NOAA, EMSL	WRF/Chem	WRF (ARW)	WRF/Chem	None	Regional/urban	Unified Online
US/NCSU and NU	WRF/Chem-MADRID	WRF (ARW)	WRF/Chem	None	Regional/urban	Unified Online

Multi-scale Prediction: Needs and Approaches

(Baklanov and Zhang, 2020; Zhang, 2024)

The needs

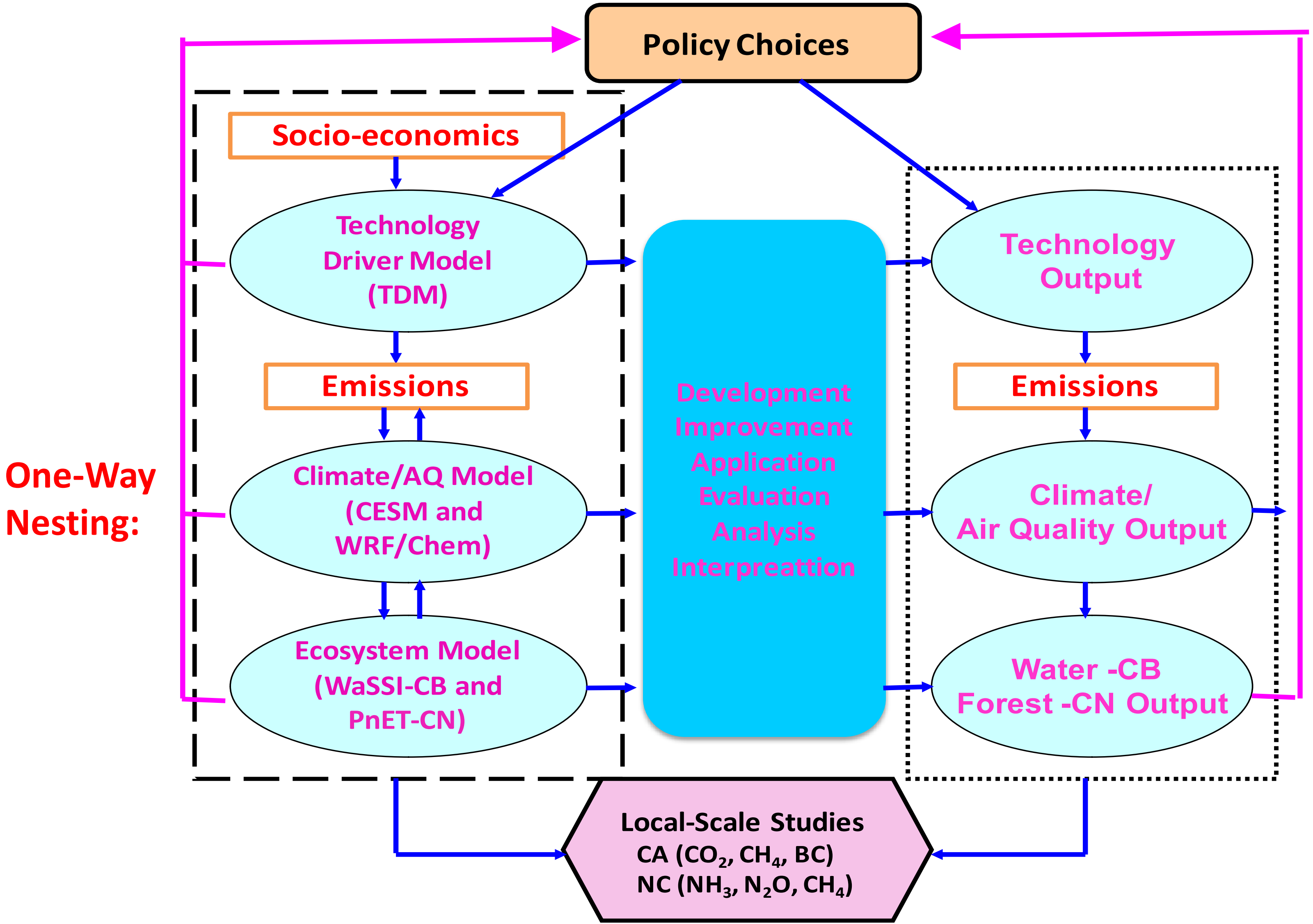
- Ability to represent multiscale feedbacks and inter-scale connections in one atmosphere
- The use of consistent model physics with across-scale formulations and parameterizations

Approaches

- **Nesting grid techniques (e.g. WRF-Chem, COSMO-Art, EnvHIRLAM)**
  - One-way nesting (aka downscaling), when values of the modelled variables at a coarse resolution are used as boundary conditions for finer (subscale) resolution runs.
  - Two-way nesting, when information from the higher resolution scale is in addition transmitted across the boundaries to the coarser resolution
- **Coupling of two or more models**
  - One-way coupling, when the outputs from a regional model are used to drive a hyperlocal model, e.g., WRF-Chem-MUNICH
  - Two-way coupling: when a regional model and a hyperlocal model exchange information every time step, e.g., Street-in-Grid (SinG)
- **Seamless unified modeling system on a single platform across scales** (e.g. MPAS-A, MUSICA)

Integrated Technology-Driven Earth System Model (ITDEaSM) Overview (Zhang, 2017)

- Address model deficiencies in representing the feedbacks among climate change, air quality, water resource, and ecosystem, and improve model representations of those feedbacks;
- Perform decadal simulations from global through urban scales to quantify the impacts/ uncertainties and identify technology choices for co-benefits of climate/Earth system mitigation



Policy Choices

Socio-economics

Technology Driver Model (TDM)

Emissions

Climate/AQ Model (CESM and WRF/Chem)

Ecosystem Model (WaSSI-CB and PnET-CN)

Development
Improvement
Application
Evaluation
Analysis
Interpreattion

Technology Output

Emissions

Climate/ Air Quality Output

Water -CB Forest -CN Output

One-Way Nesting:

Local-Scale Studies
CA (CO_2, CH_4, BC)
NC (NH_3, N_2O, CH_4)

Scientific Questions

- How will technology policy choices affect anthro. emissions that in turn affect future Earth System?
- What are the choices for co-benefits of climate change mitigation, and air/water quality, and ecosystem management at all scales?

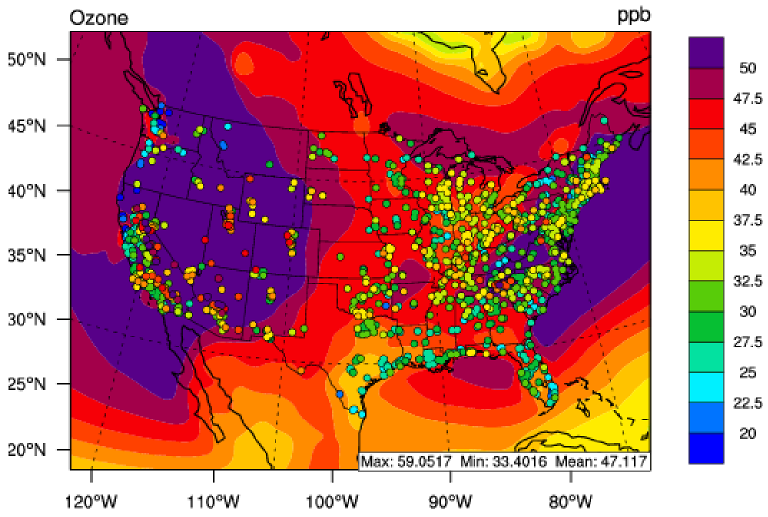
TDM-Technology Driver Model;
CESM-Community Earth System Model;
WRF/Chem-Weather Research and Forecasting Model with Chemistry;
WaSSI-CB-Water Supply Stress Index model with Carbon and Biodiversity;
PnET-CN- Photosynthesis-Evapotranspiration for Carbon and Nitrogen model

One-Way Nesting: Benefit of Downscaling: CESM vs. WRF/Chem (RCP 4.5)

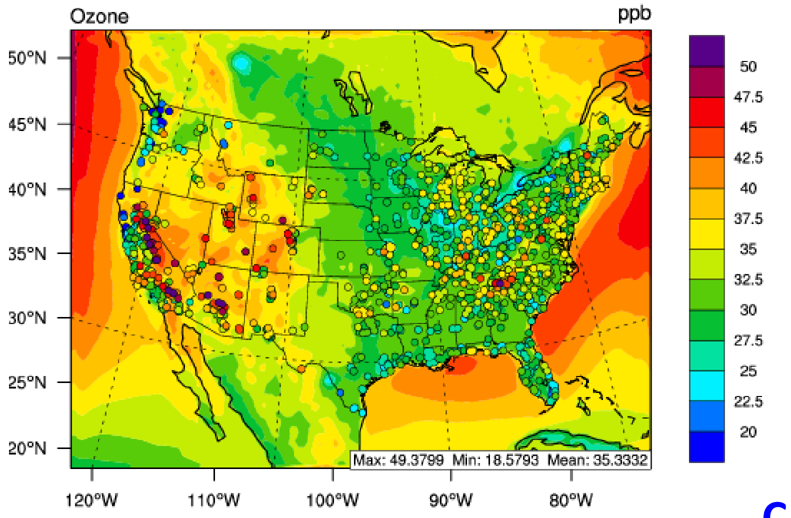
(Zhang, 2017
Glotfelty et al., 2017a,b;
Yahya et al., 2017a,b)

CESM/CAM5 **WRF/Chem**

O_3



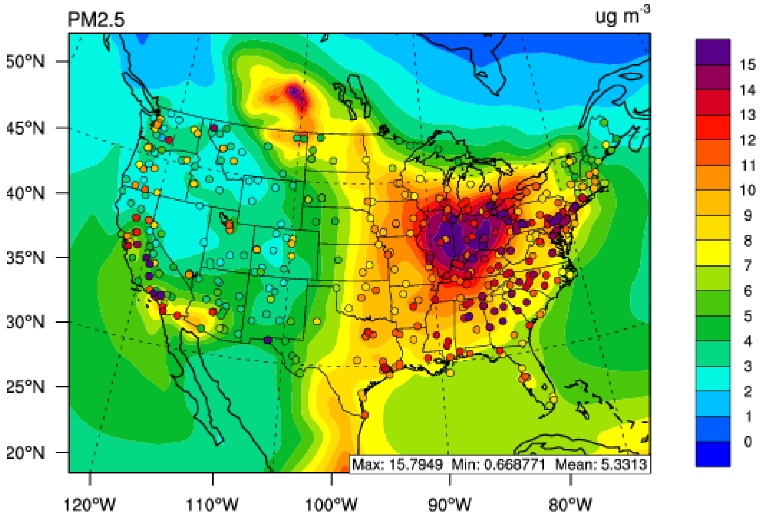
NMB =40.6%, 59.2%



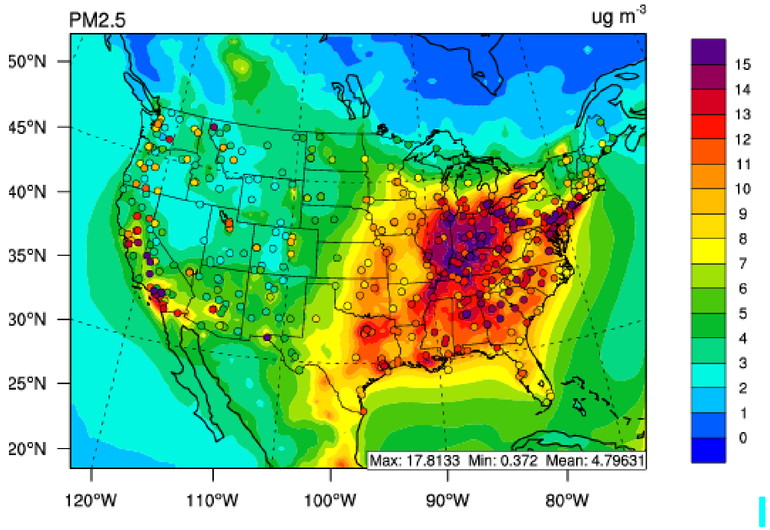
NMB = -6.1%, 9.3%

CASTNET
AQS

$PM_{2.5}$



NMB =4.6%, -25.3%



NMB =5.6%, -13.2%

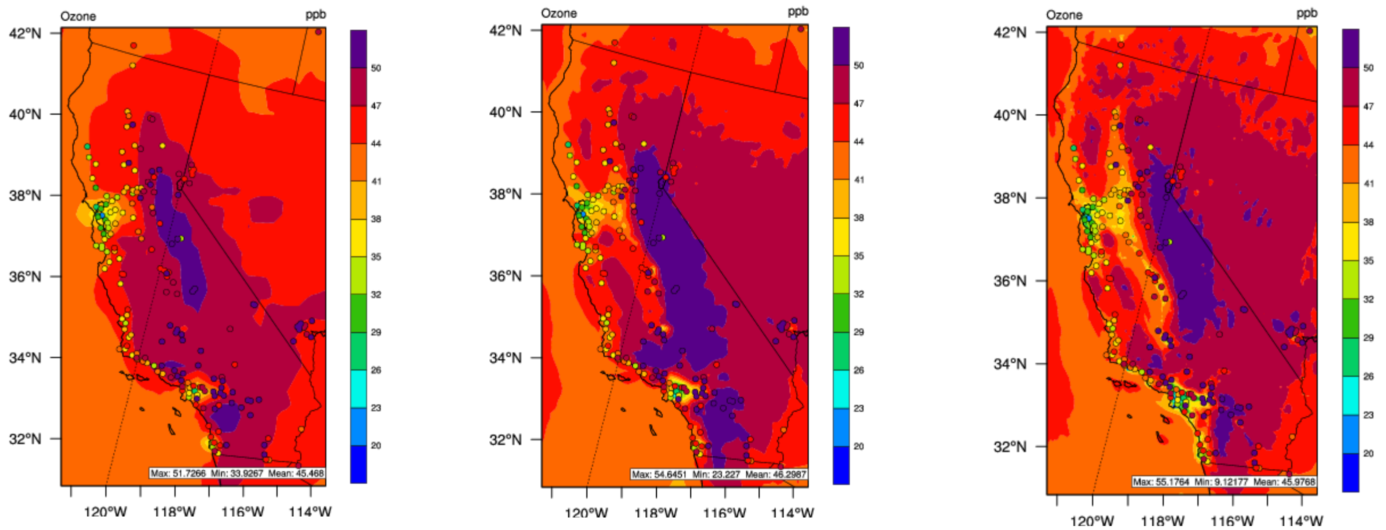
IMPROVE
STN

WRF/Chem outperforms CESM for most meteorological and chemical variables

One-Way Nesting: Annual Mean Performance of WRF/Chem over California in 2005 (Zhang, 2017)

36-km 12-km 4-km

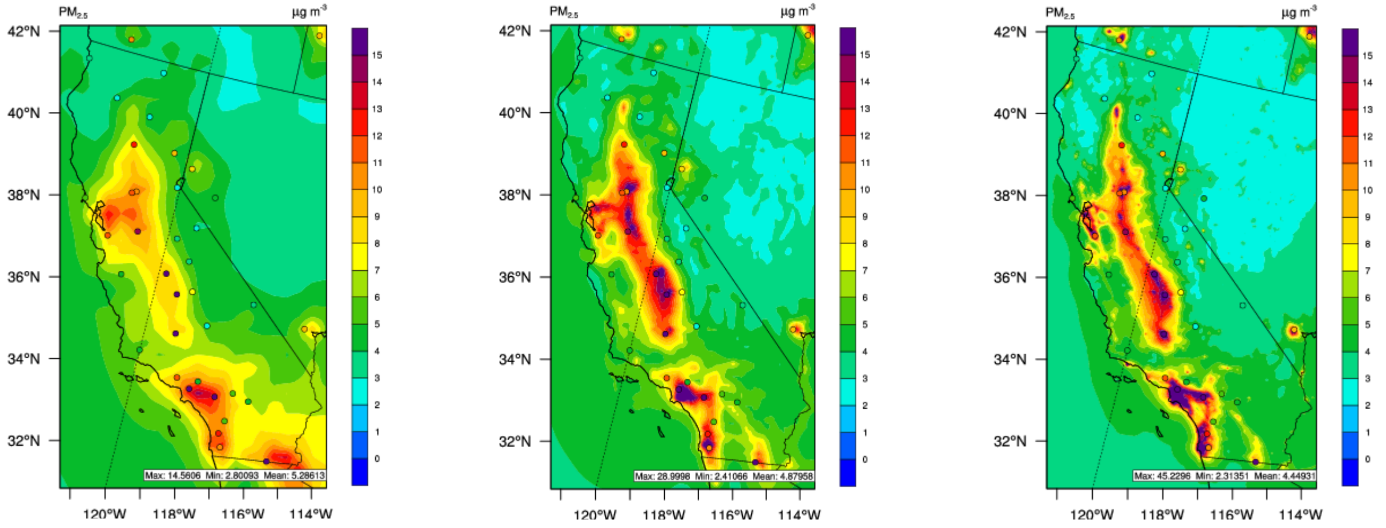
O_3



NMB: -16.8%, 7.8% **-13.5%, 3.8%** **-14.6%, 1.3%**

CASTNET
AQS

$PM_{2.5}$

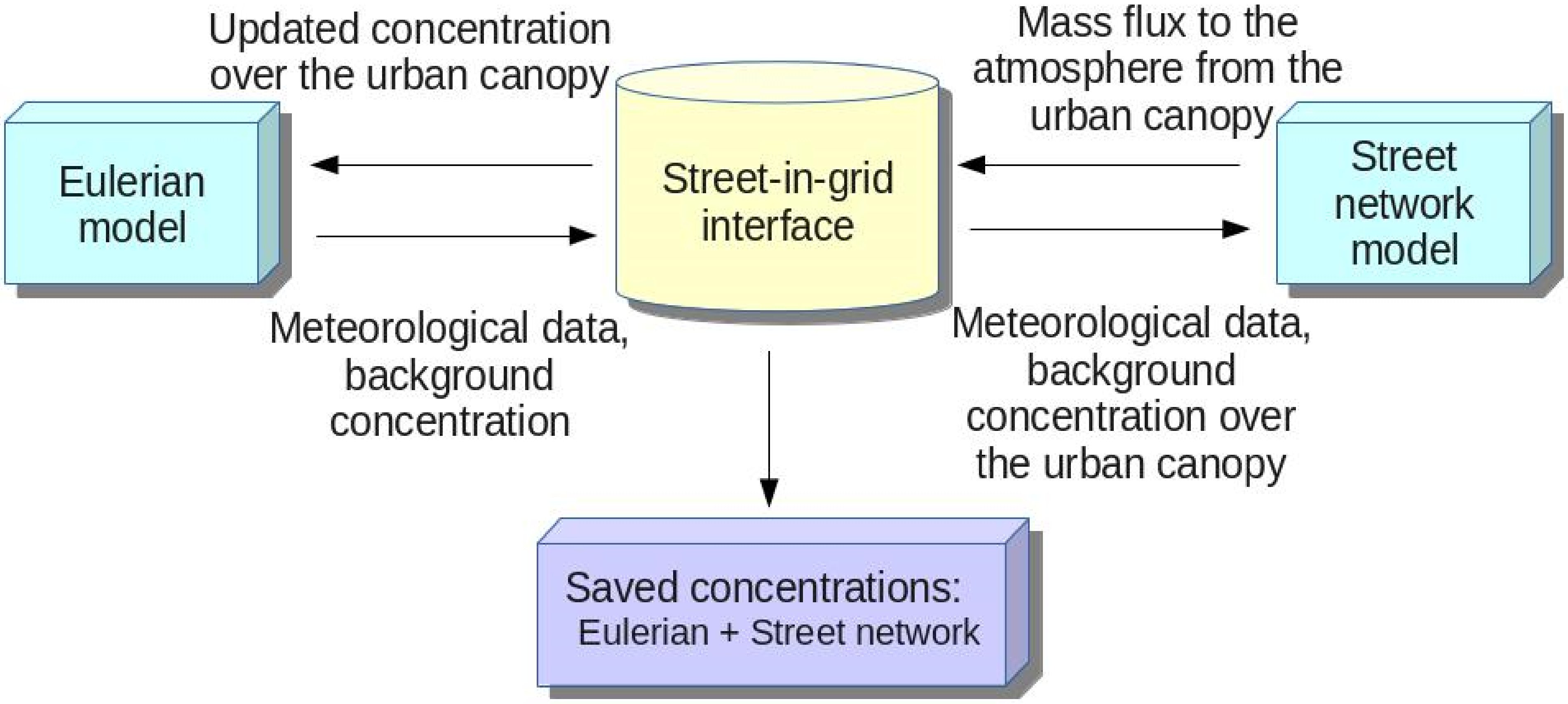


NMB: 39.5%, -33.2% **17.3%, -0.5%** **1.3%, -18.8%**

IMPROVE
STN

WRF/Chem outperforms at finer grid resolutions

Two-way coupling: a Street-in-Grid (SinG) Model (Kim et al., 2018)


Updated concentration over the urban canopy

Mass flux to the atmosphere from the urban canopy

Eulerian model

Street-in-grid interface

Street network model

Meteorological data, background concentration

Meteorological data, background concentration over the urban canopy

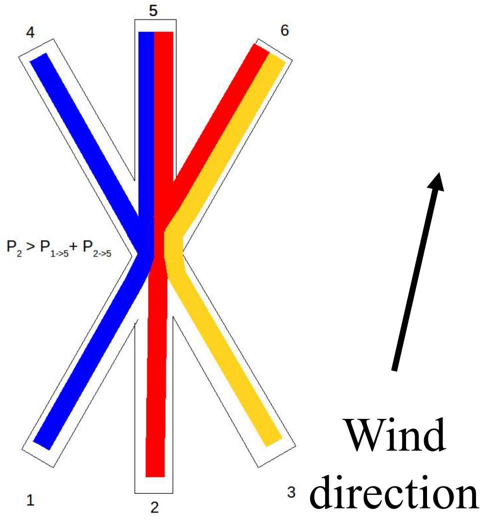
Saved concentrations: Eulerian + Street network

- Simultaneous simulation of the urban background pollution (spatial scale > 1 km) and the traffic pollution (spatial scale ~ 10 to 100 m)
- A 3-D CTM provides urban background pollution; a street network model combining traffic, emissions, and dispersion simulates pollution near traffic

Model of Urban Network of Intersecting Canyons and Highways" (MUNICH)

(Soulhac et al., 2008; Kim et al., 2018, 2022)

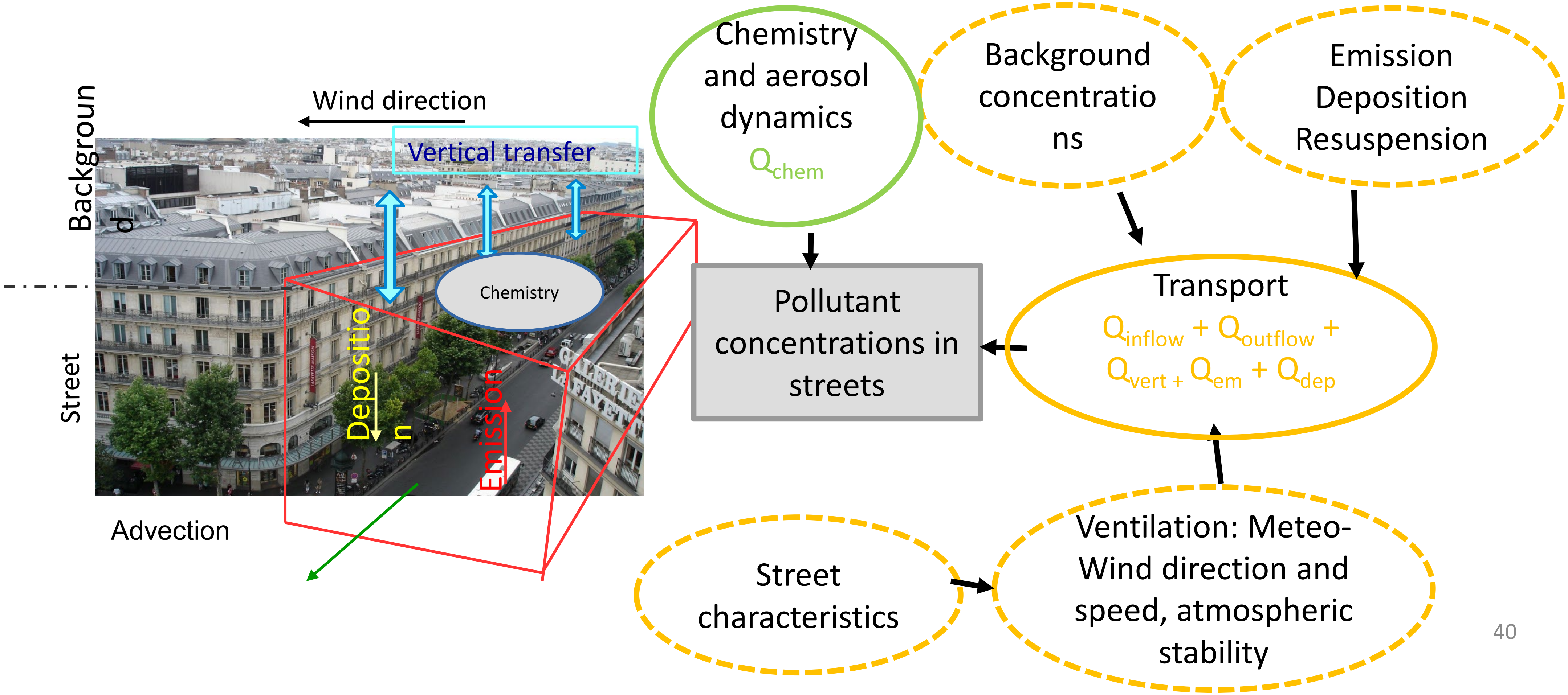
- **Street-canyon component**
  - Concentrations are uniform in each segment of the street-canyon
  - Building heights and street widths are uniform in the street-canyon
  - Wind direction follows the direction of the street and the average wind speed is calculated using an exponential vertical profile
  - Mass flux occur at intersections and at roof level
- **Street-intersection component**
  - Flow lines do not intersect
  - Account for fluctuations in wind direction
  - Mass balance is calculated across the intersection
- **Calculation of concentrations**
  - The CB05 chemical kinetic mechanism
  - Assumption of the steady state for each street network in a mesh



Model Process Représentations in MUNICH

(Sartelet et al., 2024)

$$dQ/dt = Q_{em} + Q_{dep} + Q_{inflow} + Q_{outflow} + Q_{vert} + Q_{chem}$$



Chemistry and aerosol dynamics Q_{chem}

Background concentrations

Emission Deposition Resuspension

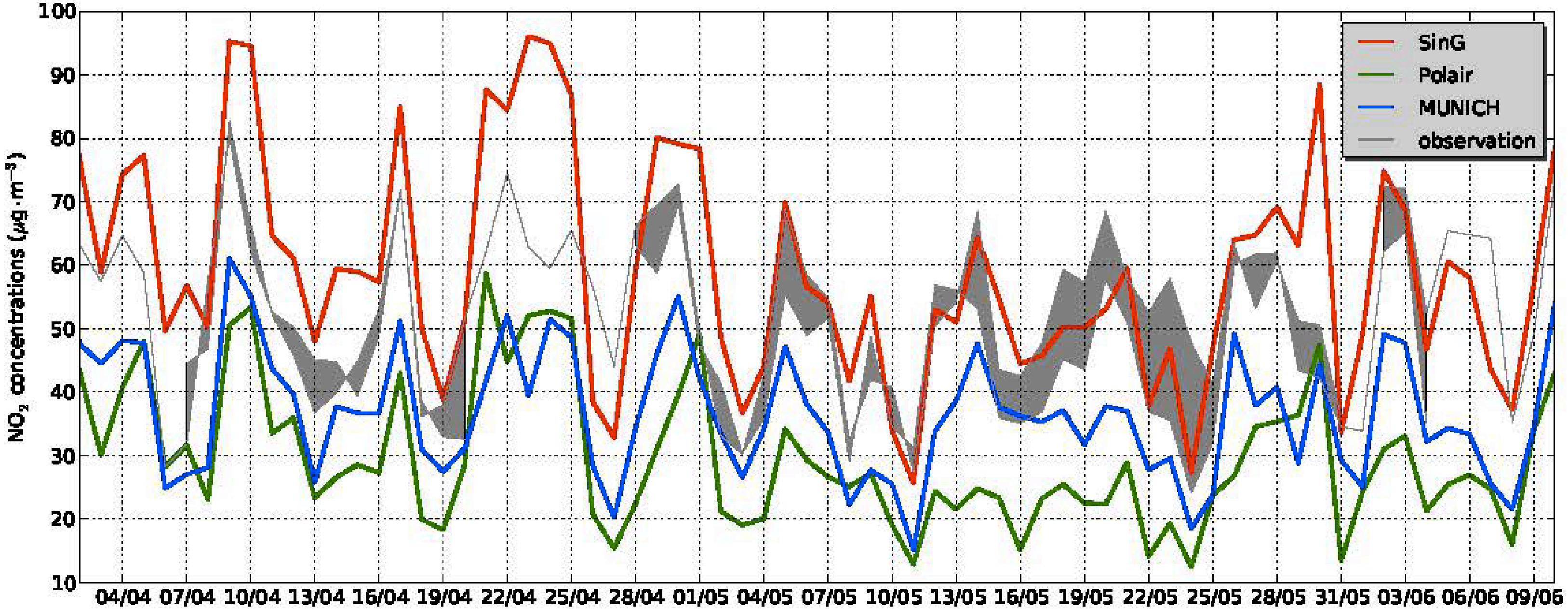
Pollutant concentrations in streets

Transport $Q_{inflow} + Q_{outflow} + Q_{vert} + Q_{em} + Q_{dep}$

Street characteristics

Ventilation: Meteo- Wind direction and speed, atmospheric stability

Temporal Evolution of NO_2 Daily-Averaged Concentrations Nearby Traffic
(Kim et al., 2018)

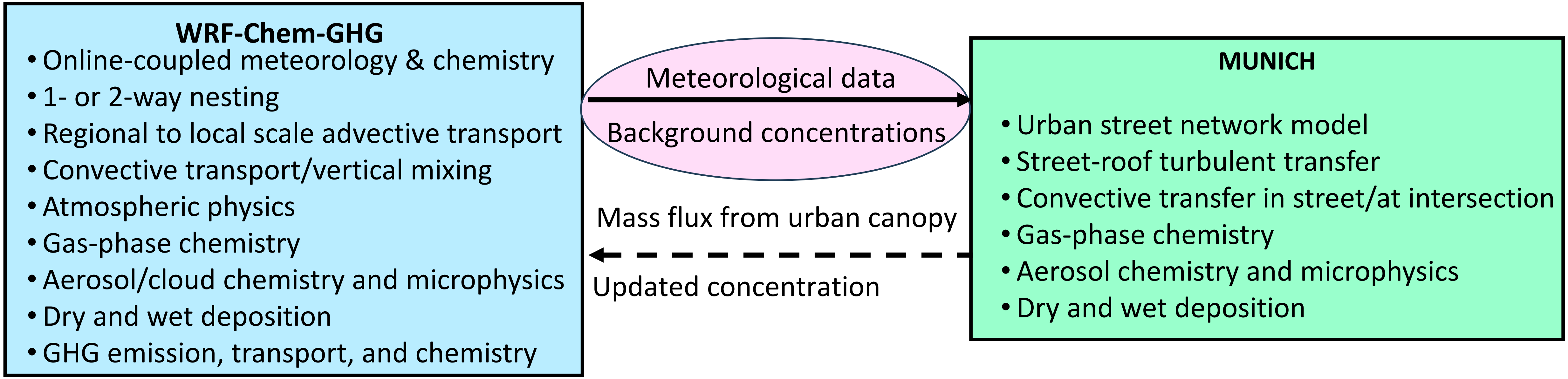


NO2	Polair	MUNICH	SinG
FB	-0.52	-0.32	0.13
R	0.51	0.67	0.64

NOx	Polair	MUNICH	SinG
FB	-1.19	-0.99	-0.64
R	0.54	0.64	0.64

- MUNICH outperforms Polair3D; SinG performs the best in terms of both FB and R
- All models underpredict NO_x, due in part to uncertainties in NOx emissions or an overestimation of NOx transport at roof top

Coupling of Two or More Models: WRF-Chem-GHG-MUNICH (Zhang et al., 2023, 2024)



Regional to Neighborhood Scales

Street-Scale

WRF-Chem-GHG

- Online-coupled meteorology & chemistry
- 1- or 2-way nesting
- Regional to local scale advective transport
- Convective transport/vertical mixing
- Atmospheric physics
- Gas-phase chemistry
- Aerosol/cloud chemistry and microphysics
- Dry and wet deposition
- GHG emission, transport, and chemistry

Meteorological data

Background concentrations

Mass flux from urban canopy

Updated concentration

MUNICH

- Urban street network model
- Street-roof turbulent transfer
- Convective transfer in street/at intersection
- Gas-phase chemistry
- Aerosol chemistry and microphysics
- Dry and wet deposition

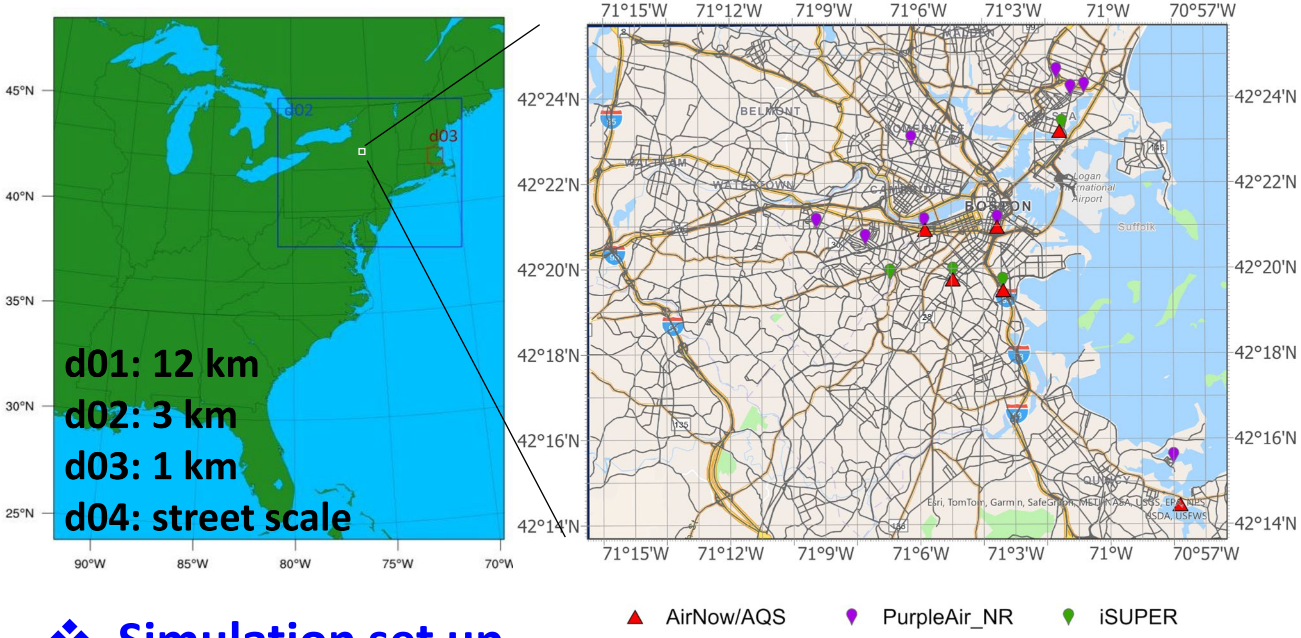
- **WRF-Chem-GHG:** WRF-Chem v3.9 coupled with greenhouse gases
- **MUNICH-SSH:** MUNICH with SCRAM-SOAP-H^2O aerosol model
- **Objectives**
  - **Impact of urban canopy parameters (UCPs) on air quality at local/hyperlocal scales**

WRF-Chem: **W**eather **R**esearch and **F**orecasting model coupled to **Chem**istry **MUNICH:** **M**odel of **U**rban **N**etwork of **I**ntersecting **C**anyons and **H**ighways

SCRAM: Size-Composition Resolved Aerosol Model; **SOAP:** Secondary Organic Aerosol Processor; **H^2O:** Hydrophilic/Hydrophobic Organics

WRF-Chem-GHG-MUNICH Model Setup (Zhang et al., 2024)

❖ Quadruple-Nested Domains



❖ Simulation set up

- Greater Boston (28×21 km^2, ~14,000 segments)
- July 1-31, 2023

❖ Urban Morphological Data:

NUDAPT, WUDAPT, and DSC

❖ Evaluation

1. AirNow/AQS (5 sites)
2. Near-road PurpleAir sensors (within < 50 m, 10 sensors)
3. Northeastern University iSUPER sensor data (4 sensors)

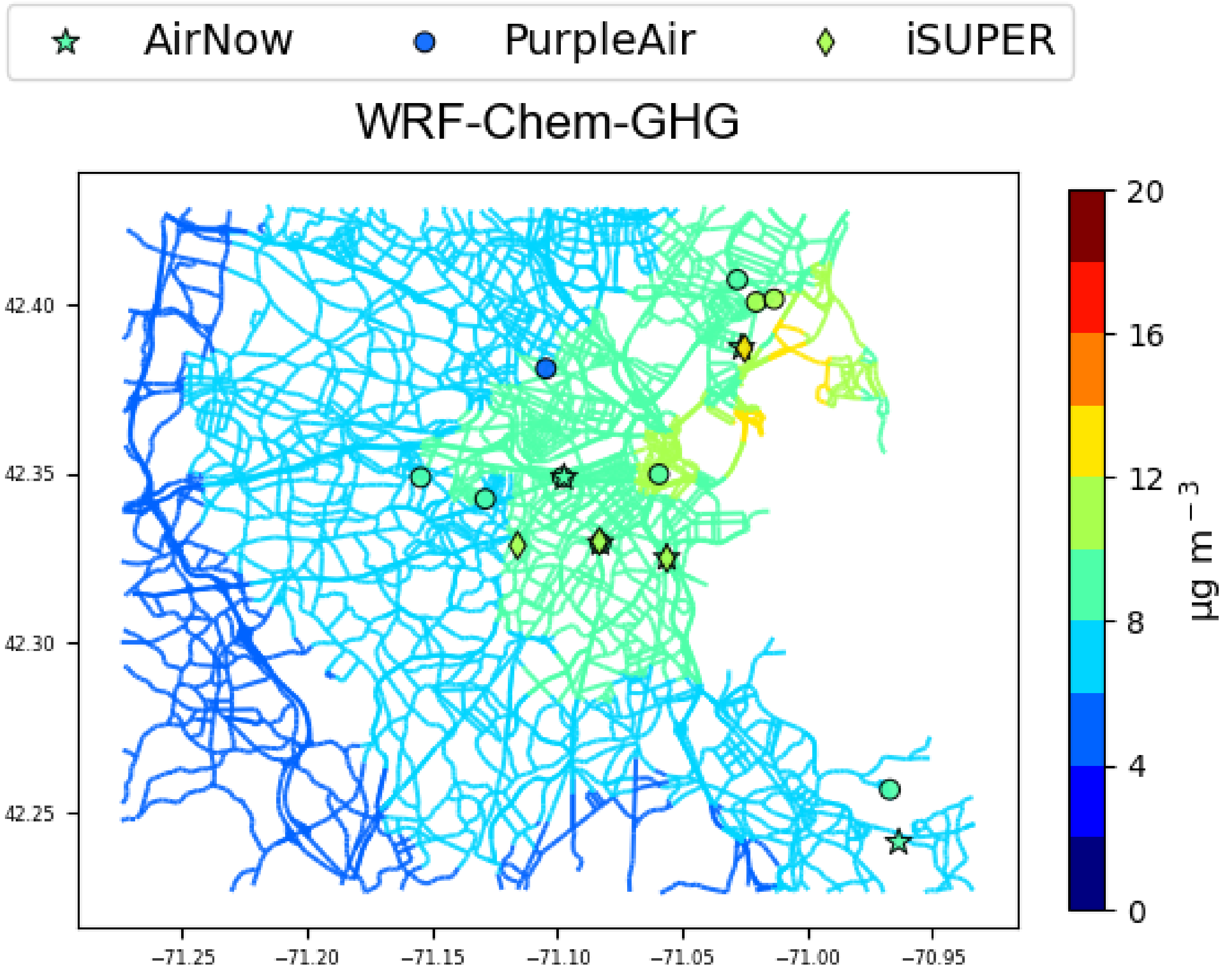
❖ Configuration

Input	Source
Background concentration	WRF-Chem-GHG 1-km results
Meteorological condition	WRF-Chem-GHG 1-km results
Street-level emissions	VEIN estimations
Street geometry	Road Inventory from MassDOT
Street/building height	NUDAPT (baseline), WUDAPT, and DSC

Configuration	Option
Aerosol size distribution	6 bins from 0.01 µm to 10 µm
Gas-phase chemistry	CB05 (Yarwood et al., 2005)
Turbulent transfer	Schulte et al. (2015)
Wind speed	Soulhac et al. (2011)

CB05: Carbon Bond version 5
MassDOT: Massachusetts Department of Transportation
VEIN: Vehicular Emissions Inventory

Spatial and Statistical Evaluation of PM$_{2.5}$ Predictions (Zhang et al., 2024)

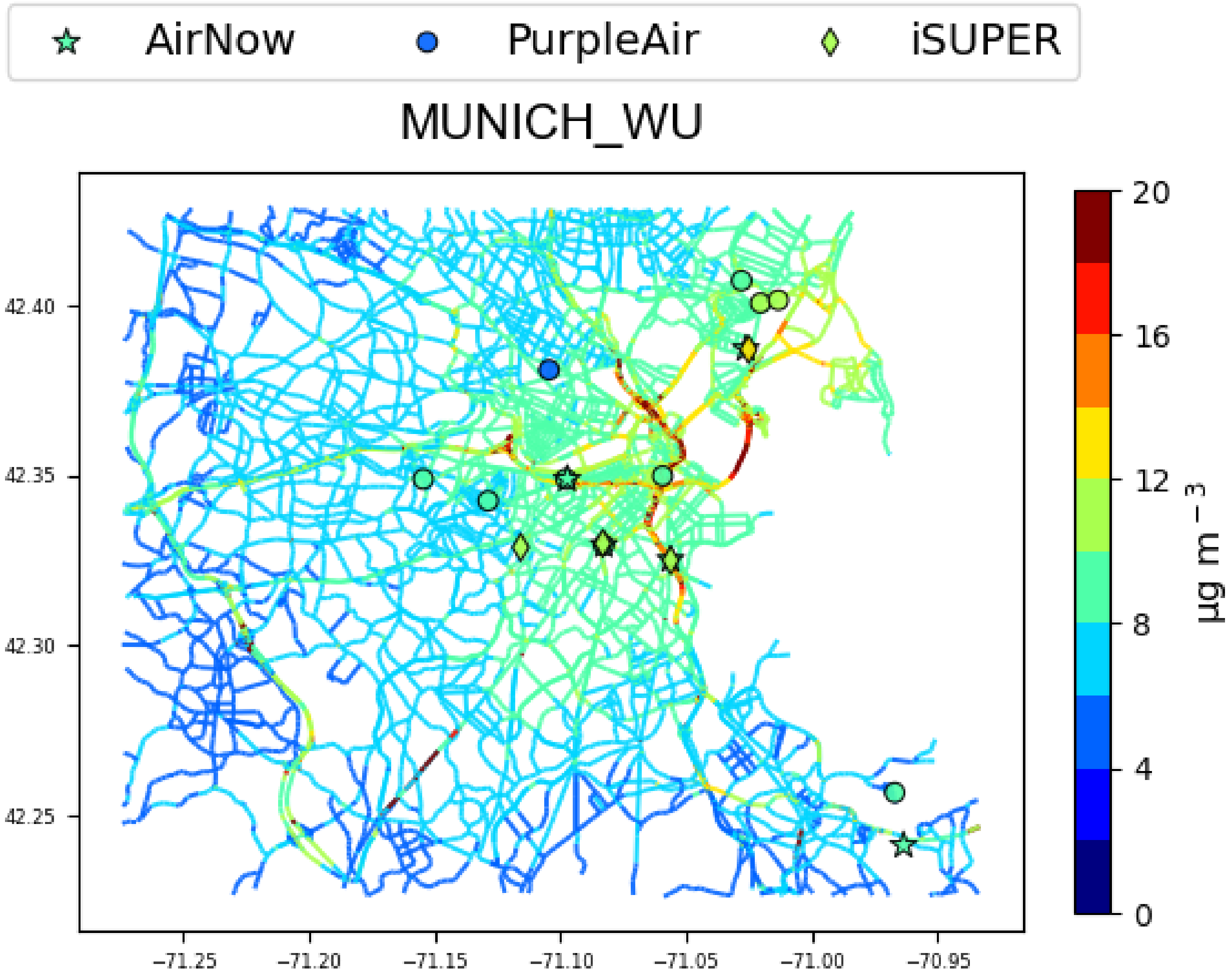


WRF-Chem-GHG

AirNow/AQS: NMB=-5.7%, NME=23.9%

PurpleAir: NMB=-3.4%, NME=34.8%

NU iSUPER: NMB=-19.3%, NME=33.5%



MUNICH_WU

AirNow/AQS: NMB=3.0%, NME=26.1%

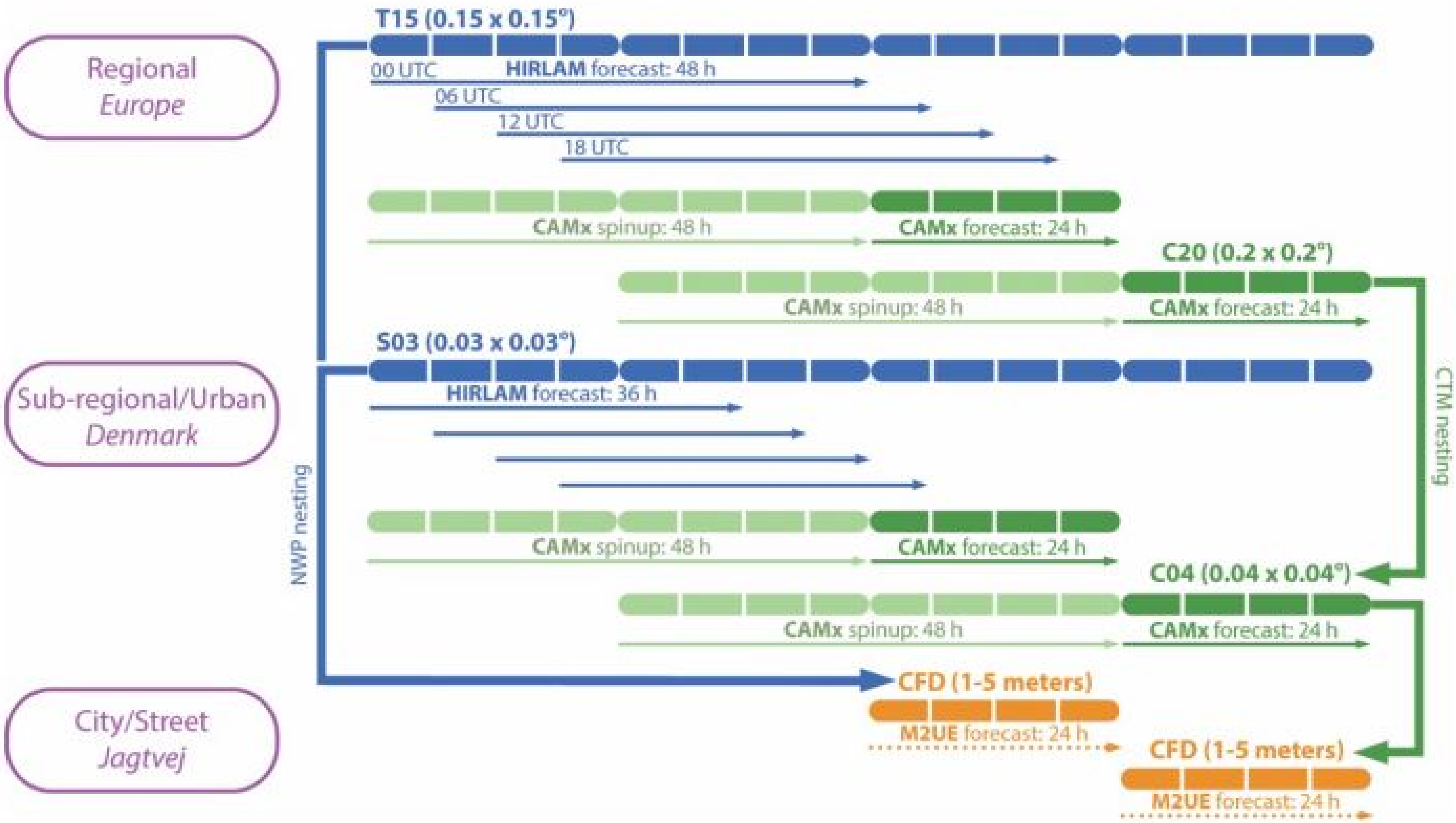
PurpleAir: NMB=0.1%, NME=38.8%

NU iSUPER: NMB=-0.9%, NME=39.6%

- MUNICH shows higher PM$_{2.5}$ in the city and outperforms WRF-Chem-GHG, which underpredicts PM$_{2.5}$ over city center

Copenhagen: Downscaling to Street Scale Using Multi-Models

(Nuterman et al.. 2021)



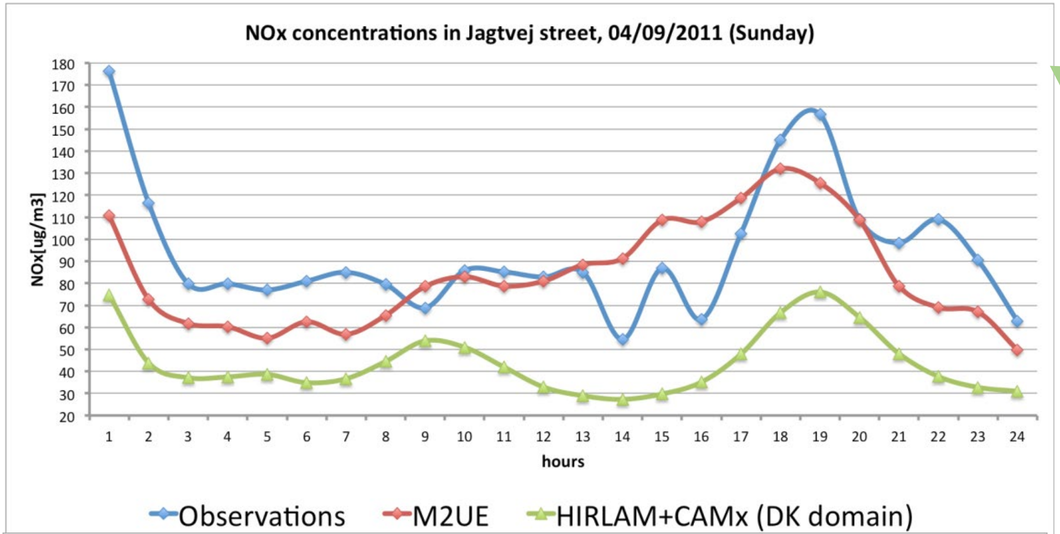
HIRLAM-T15
+CAMx-C20

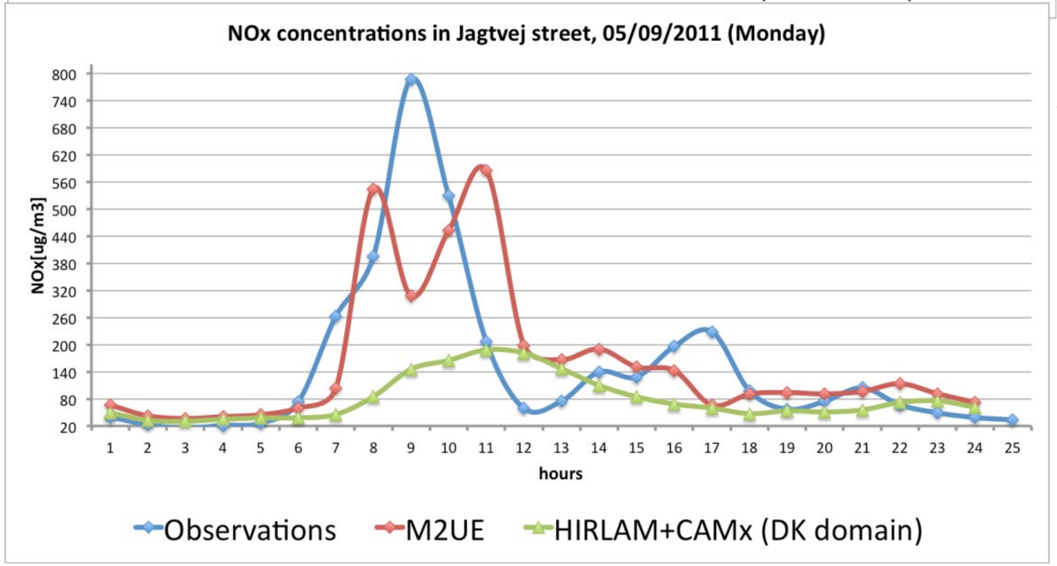
HIRLAM-T03
+CAMx-C04

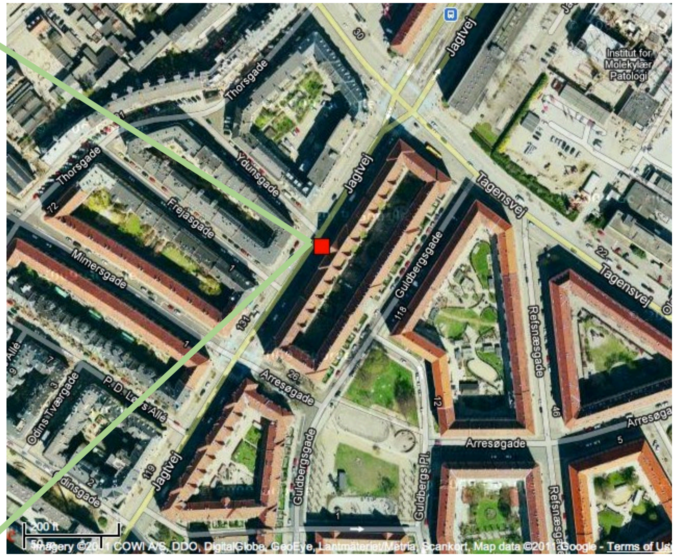
CFD M2UE
1-5 m

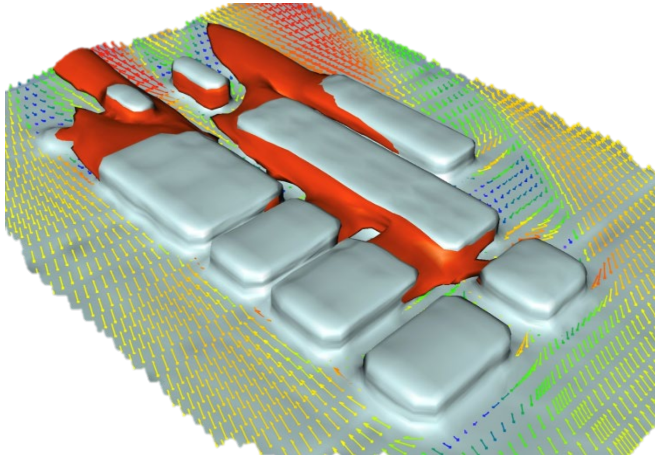
Figure 2: Downscaling modelling system: from the European regional-scale forecast (HIRLAM-T15+CAMx-C20) to the sub-regional/urban Denmark (HIRLAM-T03+CAMx-C04) and city/street scale for Copenhagen (CFD M2UE); the blue, green and orange horizontal bars indicate NWP HIRLAM, CTM CAMx and CFD M2UE forecasts, respectively; horizontal and vertical arrows indicate the forecasts' cycles and downscaling (dataflow), correspondingly.

Copenhagen: Downscaling to Street scale (Nuterman et al., 2021)


NOx concentrations in Jagtvej street, 04/09/2011 (Sunday)


NOx concentrations in Jagtvej street, 05/09/2011 (Monday)





(observations from http://www2.dmu.dk/atmosphericenvironment/byer/forside.htm)

NOx concentration in the street canyon on 5 Sep 2011, 15:00 LST

GMD/ACP Special Issue on Air Quality Research at Street-Level

Editors: Y. Zhang, K. Sartelet, S. Gong, and Q. Zhang

Initiated in Aug 2018, published 19 papers during 2018-2022 (Phase I), 8 papers since 2023, 2023-2025 (Phase II) , https://acp.copernicus.org/articles/special_issue1232.html)

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Air quality research at street level (ACP/GMD inter-journal SI)

Editor(s): Y. Zhang, K. Sartelet, S. Gong, and Q. Zhang

Special issue jointly organized between Atmospheric Chemistry and Physics and Geoscientific Model Development

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24 May 2024

To what extent is the description of streets important in estimating local air-quality? A case study over Paris

Alexis Squarcioni, Yelva Roustan, Myrto Valari, Youngseob Kim, Karine Sartelet, Lya Lugon, Fabrice Dugay, and Robin Voitot

EGUsphere, https://doi.org/10.5194/egusphere-2024-1043, 2024

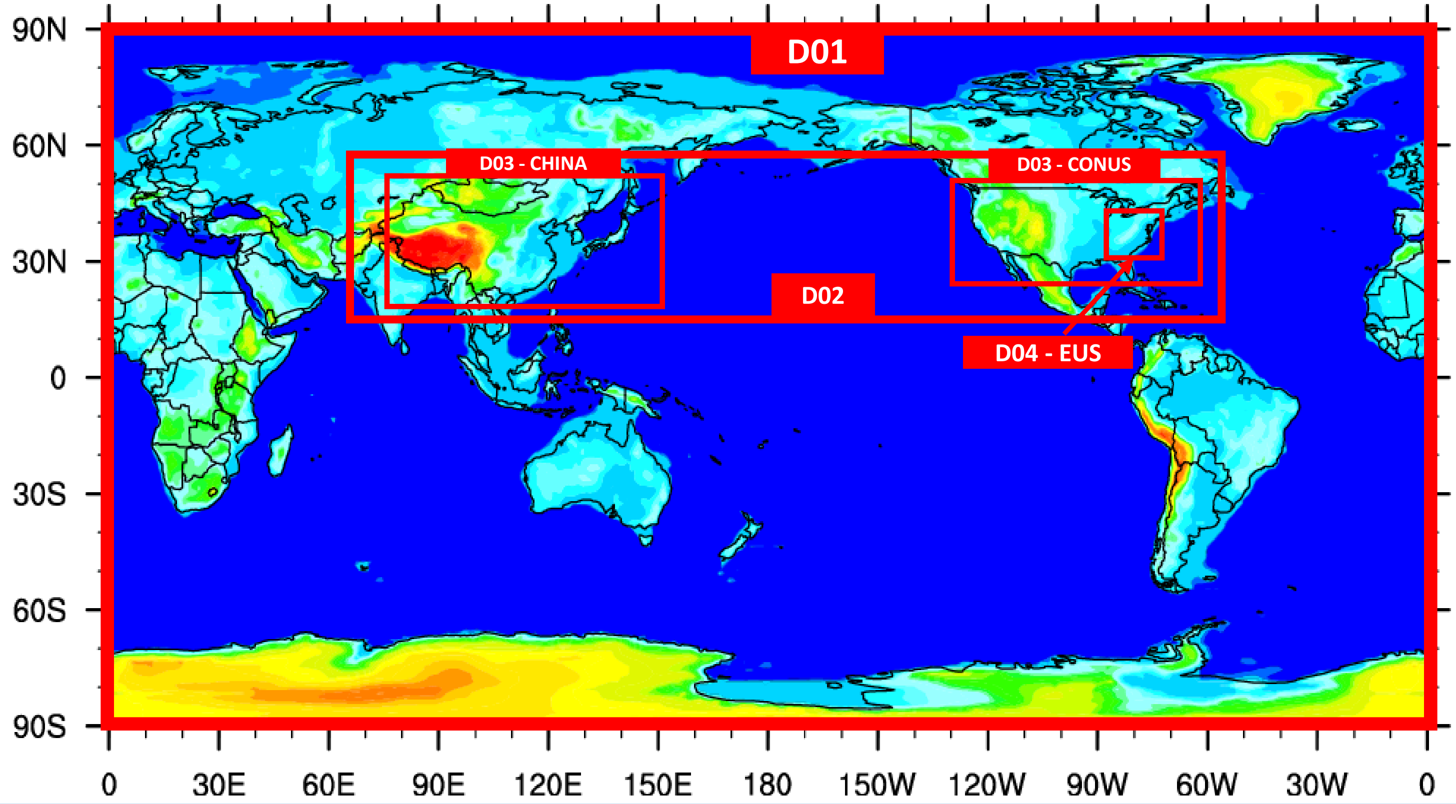
Revised manuscript accepted for ACP (discussion: final response, 3 comments)

▸ Short summary

Seamless Unified Modeling System: GU-WRF/Chem (Zhang et al., 2012)

- **Period:** **Met only:** 2001/2050, at 4° × 5° & 1° × 1°,
  w different physics options
  Gas and PM:
  1. 2001 Jan/Jul over D01-D04, w and w/o PM
  2. 2001, 2010, 2020, 2030, 2040, 2050 over D01

- **Domain:** **D01:** 4° × 5°, 45 (lat.) × 72 (long.) (Global)
  D02: 1.0° × 1.25°, 44 × 192 (Trans-Pacific)
  D03-CONUS: 0.33° × 0.42°, 84× 168 (CONUS)
  D03-China: 0.33° × 0.42°, 99× 177 (China)
  D04: 0.08° × 0.10°, 136× 144 (E. US)



D01: Global D02: Trans-Pacific D03: CONUS and China D04: E. US

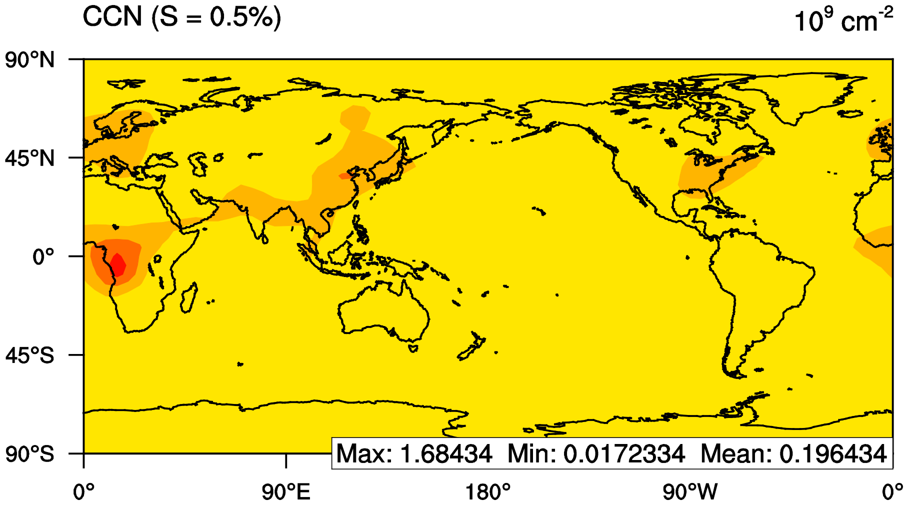
Evaluation of Chemical and Meteorological Predictions in July 2001 (Zhang et al., 2012)

Performance Statistics (NMB,%)

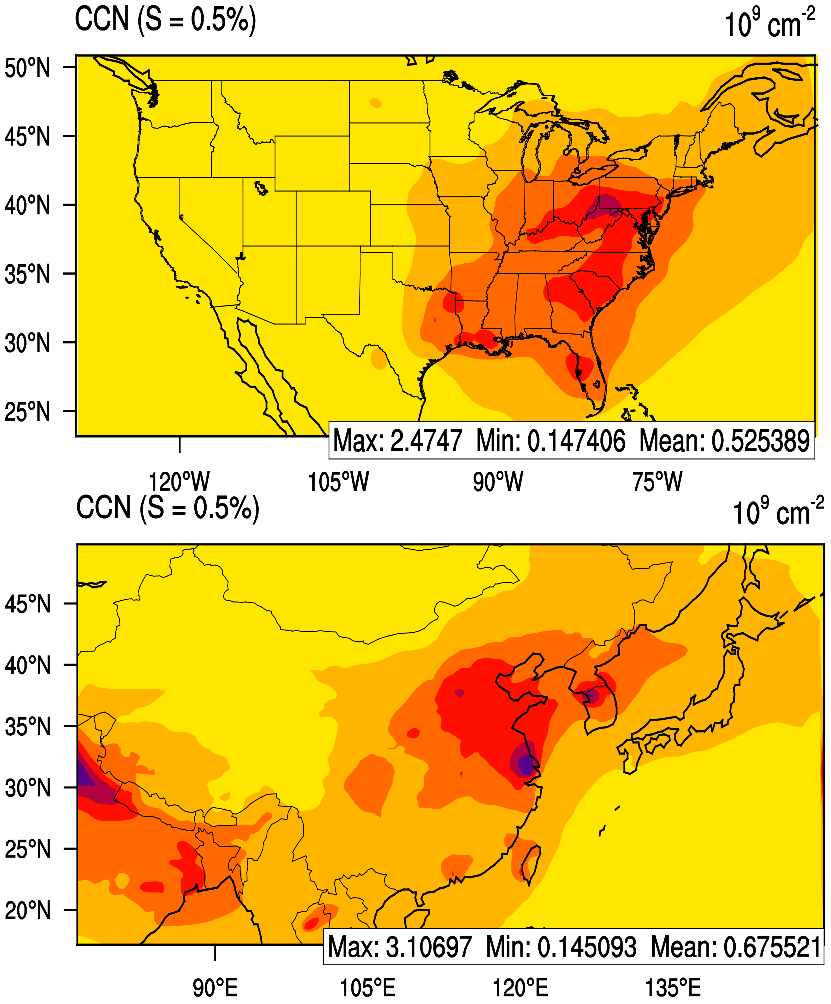
		Global (D01)	Trans Pacific (D02)		CONUS (D03)		
		GU-WRF/Chem	GU-WRF/Chem	MM5/CMAQ	GU-WRF/Chem	Meso-WRF/Chem	MM5/CMAQ
2-m Temperature	CASTNET	3.8	3.8	-0.9	1.9	0.3	----
	STN	-5.0	-4.7	-10.0	-3.9	-6.1	----
	SEARCH	-2.4	-1.9	-9.9	0.0	1.5	----
Precip		5.7	14.5	38	44.8	32.2	41
Max 1-hr O_3	CASTNET	-16.8	-17.5	-12.1	-16.3	9.7	-8.7
	AIRS-AQS	-17.8	-16.7	-0.7	-10.5	12.8	-3.6
	SEARCH	-14.3	-14.1	4.3	-7.7	21.8	10.2
Max 8-hr O_3	CASTNET	-10.3	-11.8	-4.2	-12.4	14.5	-0.2
	AIRS-AQS	-8.9	-8.2	6.2	-4.3	18.1	6.9
	SEARCH	-3.5	-3.8	19.0	0.4	30.5	15.9
24-hr avg. $PM_{2.5}$	IMPROVE	44.6	27.7	27.0	18.2	8.5	-30.2
	STN	13.8	7.4	21.7	7.9	21.5	-18.3
	SEARCH	8.7	10.3	32.9	8.5	33.1	41.0
Column CO		20.1	31.1	----	32.5	34.4	
Column NO_2		-22.2	-23.7	-28.3	30.6	47.1	13.4
Column O_3		-23.4	-46.9	-51.9	-53.2	4.5	-17.5
AOD		97.9	51.9	-47.5	56.5	3.7	-61.3
Cloud Fraction		-10.3	-18.5	----	-32.6	----	----
CCN (Ocean)		-8.7	20.1	----	58.0	----	----
CDNC		-41.2	-53.0	----	-68.8	----	----

First Indirect Effects of PM$_{2.5}$ via Column CCN (S=0.5%) (Zhang et al., 2012)

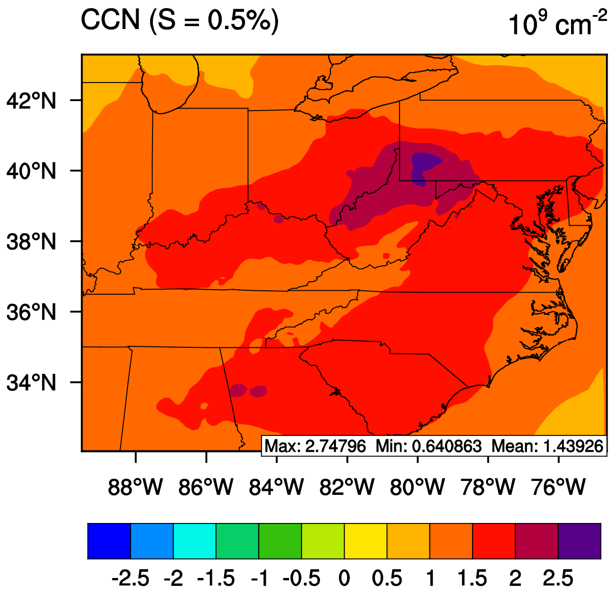
D01



D03



D04



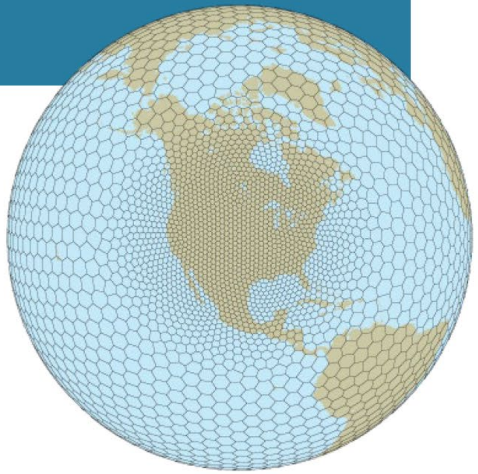
PM$_{2.5}$ enhances CCN at S=0.5% domainwide by up to a factor of 33 (global mean: a factor of 5)

NCAR's MPAS Model (Lawrence and Barth, 2024)

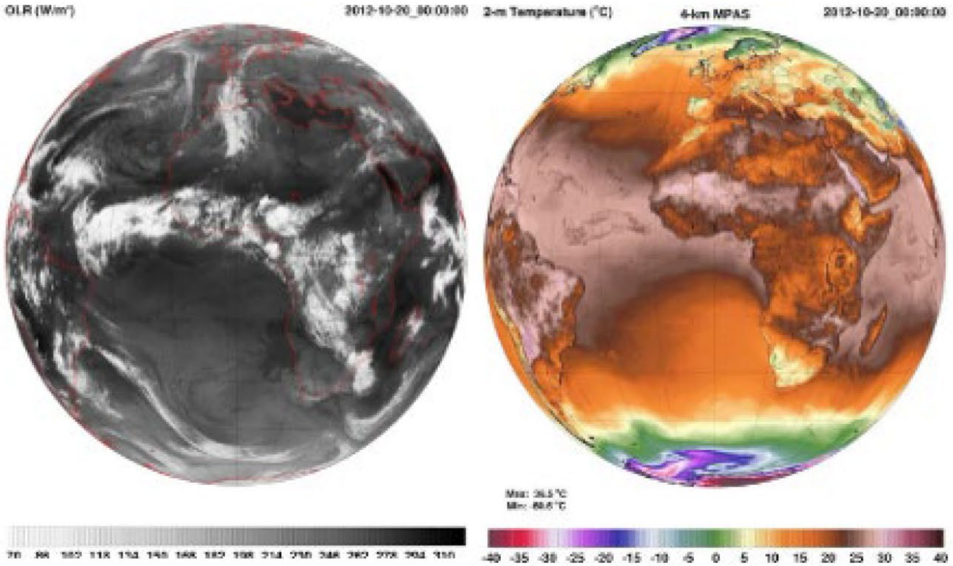
Investigating weather from global to local scales

Global weather modeling with Model for Prediction Across Scales (MPAS)

- Non-hydrostatic capability for local to global atmospheric phenomena
- MPAS includes a limited-area capability
- GPU-accelerated version for MPAS V6.3



Outgoing Longwave Radiation (OLR)



Surface Temperature

Courtesy of Falko Judt (MMM)

NCAR's MUSICA Model (Pfister et al., 2020; NCAR MPAS Tutorial 2021)

MUSICA
Multiscale Infrastructure for
Chemistry and Aerosols

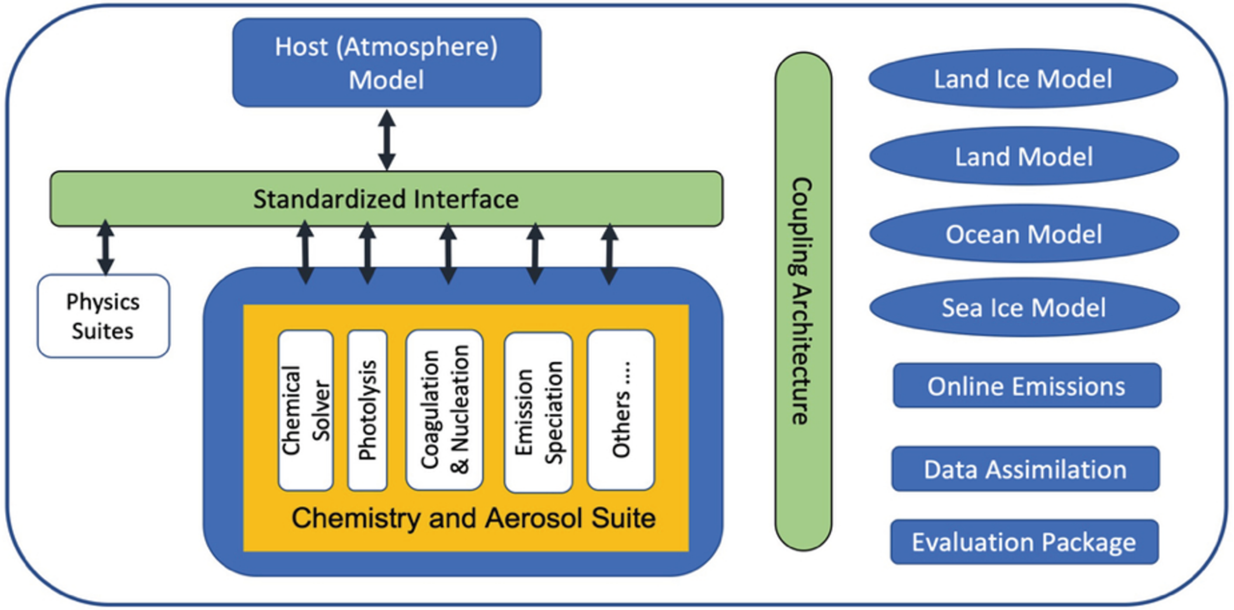
MUSICA: MUlti-Scale Infrastructure for Chemistry & Aerosols

A new model-independent infrastructure, which will enable chemistry and aerosols to be simulated at different resolutions in a coherent fashion

Will **facilitate use of a variety** of chemistry schemes, physics parameterizations and atmospheric models

Coupled to other **earth system** component models (land, ocean, sea ice, etc.)

Whole atmosphere framework: troposphere to thermosphere



https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica

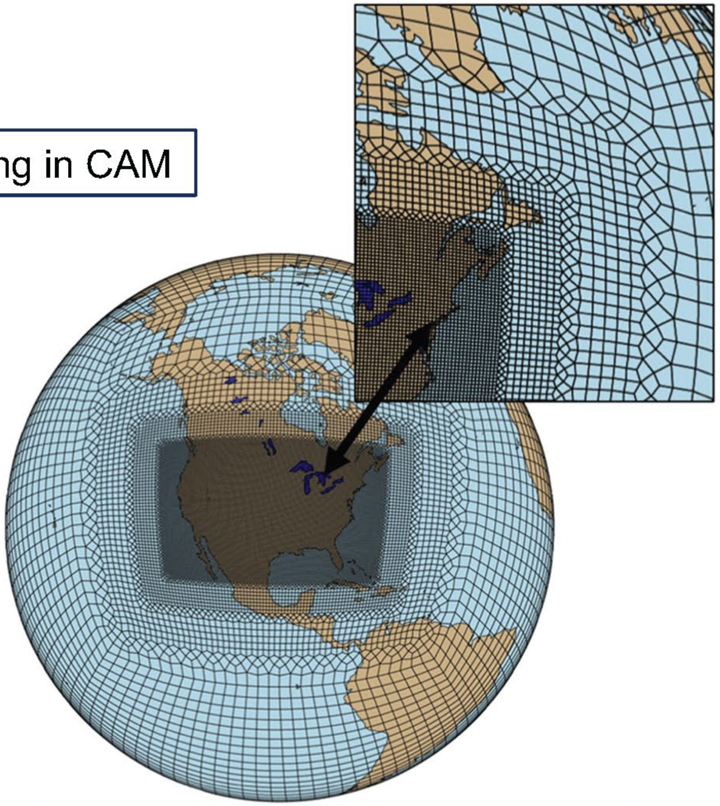
MUSICA Vision paper published in BAMS (Pfister et al., 2020: https://doi.org/10.1175/BAMS-D-19-0331.1)

MUSICA SE and MPAS Dynamical Cores (Pfister et al., 2020)

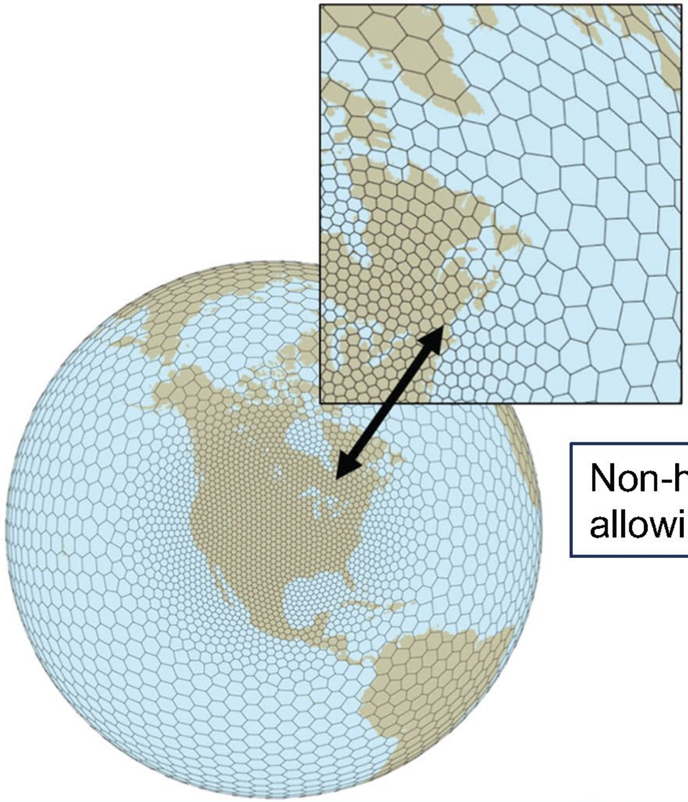
Choices for variable resolution atmosphere models

Spectral Element
(SE - cubed sphere)

Currently running in CAM



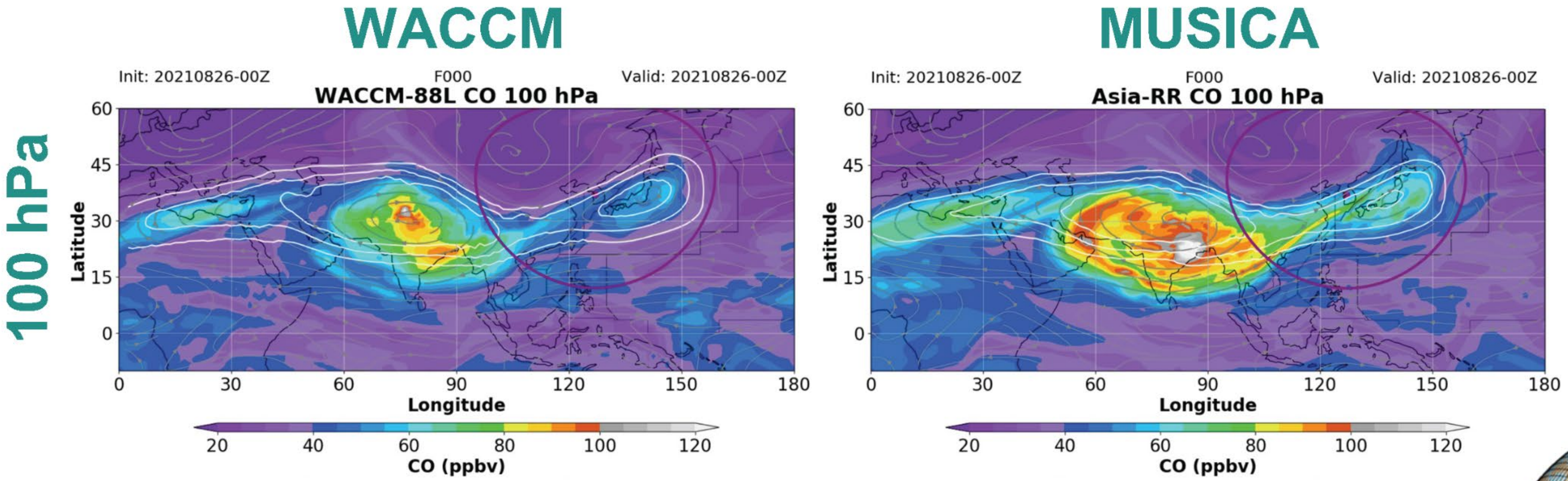
Model for Prediction Across Scales
(MPAS - hexagonal mesh)



Non-hydrostatic
allowing for finer scales

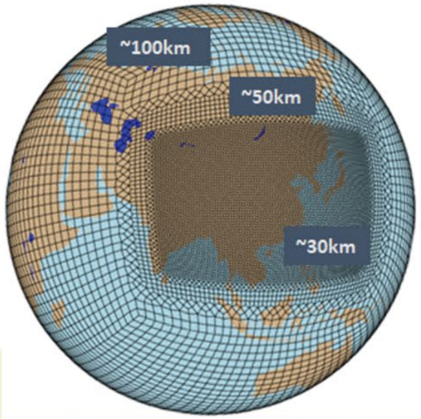
NCAR’s MUSICA Model (NCAR MPAS Tutorial 2021)

Simulations in support of ACCLIP
Asian Summer Monsoon Chemical and Climate Impact Project



The regionally-refined MUSICAv0 Asia grid enhances the convective transport of pollutants by the Asian monsoon into the UTLS when compared to WACCM

Sampling these air masses is a key objective of the ACCLIP field phase in summer 2022



Ren Smith, NCAR/ACOM

Summary

- Numerical air quality models play a critical role in simulating the fate and transport of air pollutants, and their interactions with meteorology and climate at various scales.
- Air quality modeling requires a system of models to simulate the emission, transport, diffusion, transformation, and removal of air pollutants, including meteorological models, emissions models, and chemical transport models.
- Eulerian and Lagrangian frameworks are two major approaches for air quality models, which can be classified into 0 to 3-D and global to hyperlocal spatial scales.
- Model errors may be caused by inaccuracies and uncertainties in model inputs, process representations, and model configurations. These errors can be reduced using bias correction, ensemble modeling, data assimilation, data fusion, and ML/AI.
- Multiscale modeling allows the representations of multiscale feedbacks and inter-scale connections, and ensures the use of consistent model physics with across-scale formulations and parameterizations. Major approaches include nesting grid techniques, coupling of two ore more models, and seamless across-scale unified modeling system.

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