WEATHER CLIMATE WATER
TEMPS CLIMAT EAU

ADVANCES & CHALLENGES IN AIR QUALITY MODELING & FORECASTING

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World Meteorological Organization
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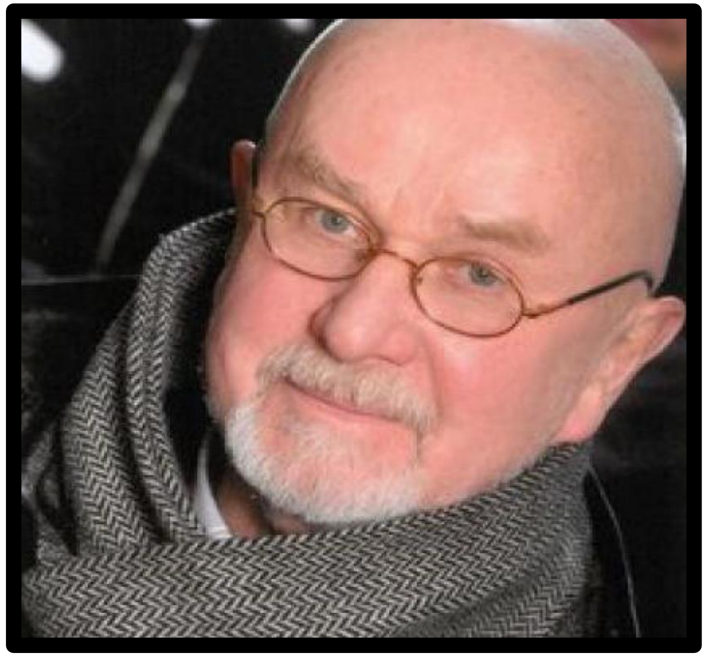
GAW

Tributes and Memories
Professor Sergej Zilitinkevich
Дань памяти профессору Сергею Сергеевичу Зилитинкевичу



13.04.1936 – 15.02.2021

Dedicated to the memory of an outstanding scientist, teacher and closest friend

Памяти выдающегося ученого, учителя и близкого друга посвящается

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Presentation Focus and Key Issues

Summary

- Advance approaches in AQF combine an ensemble of state-of-the-art models, high-resolution emission inventories, space observations and surface measurements of most relevant chemical species to provide hindcasts, analyses and forecasts from global to regional air pollution and downscaling for selected countries and urban areas.

Introduction

- The importance of and interest to research and investigations of atmospheric composition and its modeling for different applications are substantially increased (see e.g. WWOSC, 2015; CCMM, 2016; GAW IP, 2017). Air quality forecast (AQF) and assessment systems help decision makers to improve air quality and public health, mitigate the occurrence of acute air pollution episodes, particularly in urban areas, and reduce the associated impacts on agriculture, ecosystems and climate.

Results

- Based on published reviews (e.g. *Carmichael et al. 2008, Hollingsworth 2008, Zhang 2008, Menut and Bessagnet 2010, Grell and Baklanov 2011, Kukkonen et al. 2012, Zhang et al. 2012a,b, Baklanov et al. 2014, 2017, Ryan 2016, Benedetti et al. 2018, Bai et al. 2018, Kumar et al. 2018, Sokhi et al. 2019, etc.*) and recent analyses, the presentation discusses main gaps, challenges, applications and advances, main trends and research needs in further developments of atmospheric composition and air quality modeling and forecasting.

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Trends in development of modern atmospheric composition modelling & AQF systems:

(i) Seamless prediction of the Earth system approach;

(ii) Online coupling of atmospheric dynamics and chemistry models;

(iii) Multi-scale prediction approach;

(iv) Emission modeling for improved emission data;

(v) Data fusion, machine learning methods & bias correction techniques;

(vi) Multi-platform observations and data assimilation;

(vii) Ensemble approach;

(viii) Subseasonal to seasonal forecast;

(ix) Fit for purpose approach;

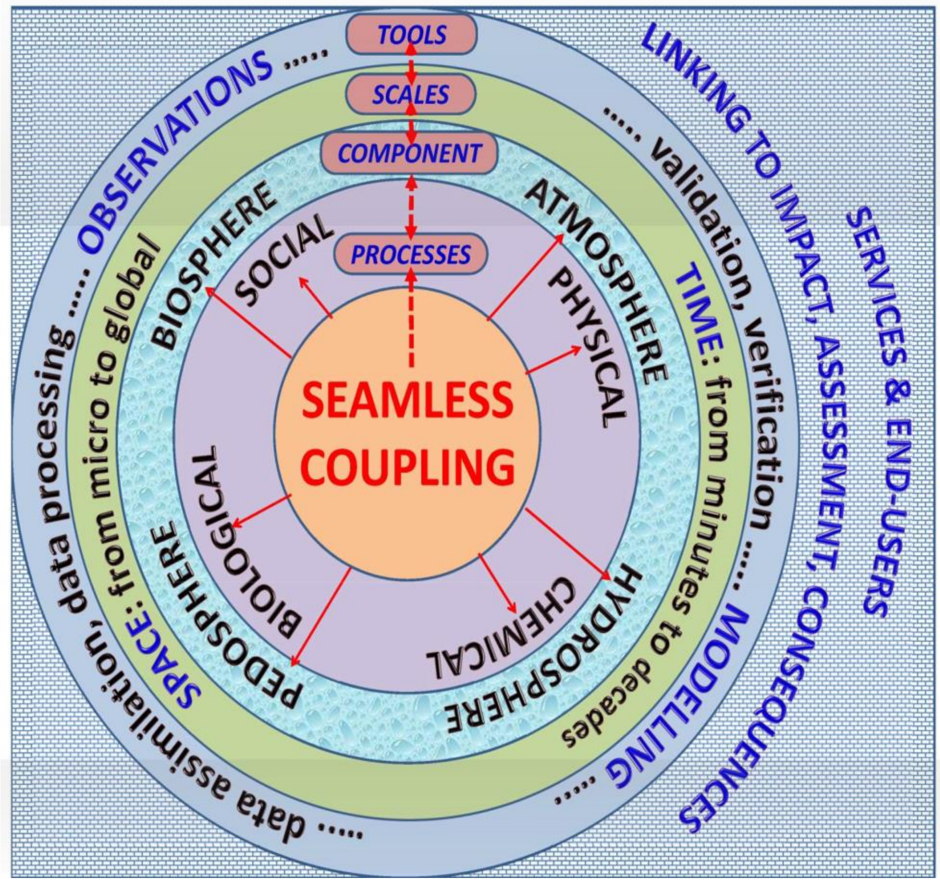
(x) Impact based forecast;

(xi) Capacity building, training and education aspects.

(i) Seamless prediction of the Earth system approach

Several dimensions of the seamless coupling/integration, including:

- Time scales: from seconds and nowcasting to decadal and centennial (climate) time-scale;
- Spatial scales: from street-level to global scale (downscaling and upscaling);
- Processes: physical, chemical, biological, social;
- Earth system components/environments: atmosphere, hydrosphere, lithosphere, pedosphere, ecosystems/biosphere;
- Different types of observations and modelling as tools: observations-model fusion, data processing and assimilation, validation and verification;
- Links with health and social consequences, impact, assessment, and services and end-users.



(Baklanov, Mahura et al., 2017)

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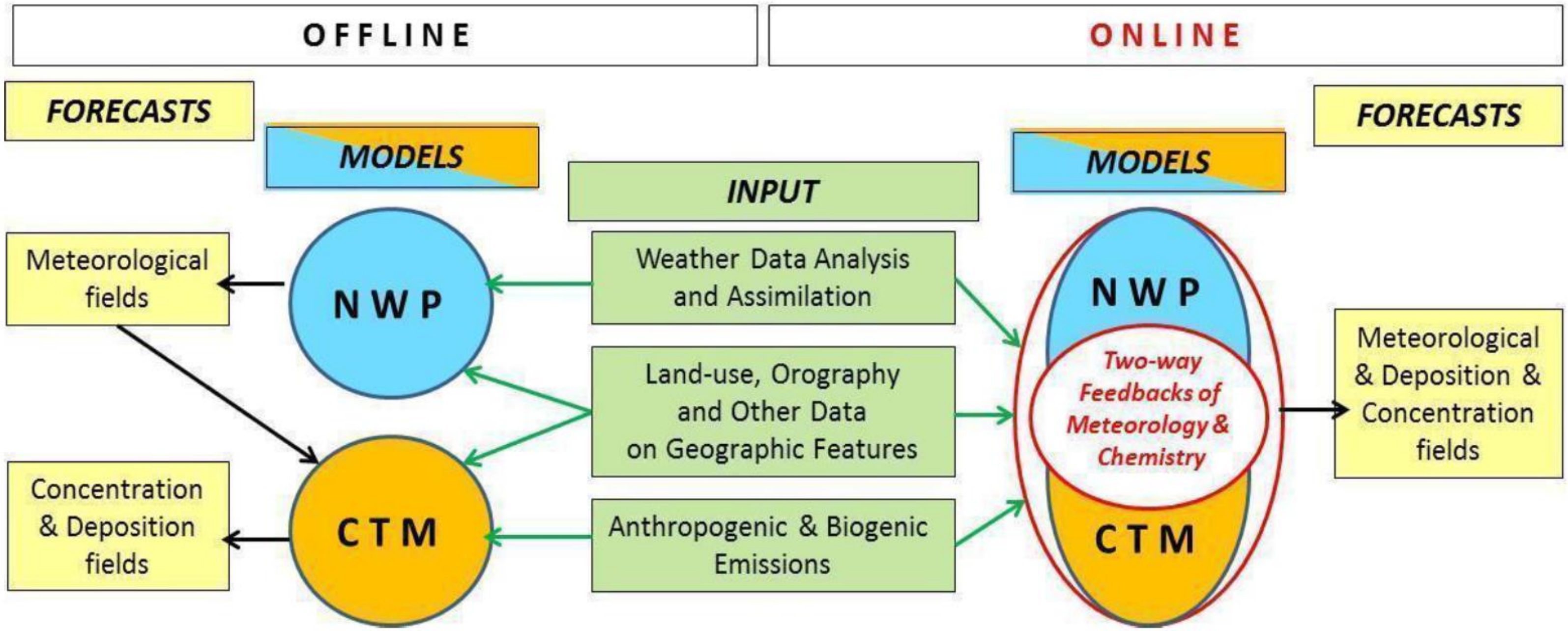
(ii) Online coupling of atmospheric dynamics and chemistry models

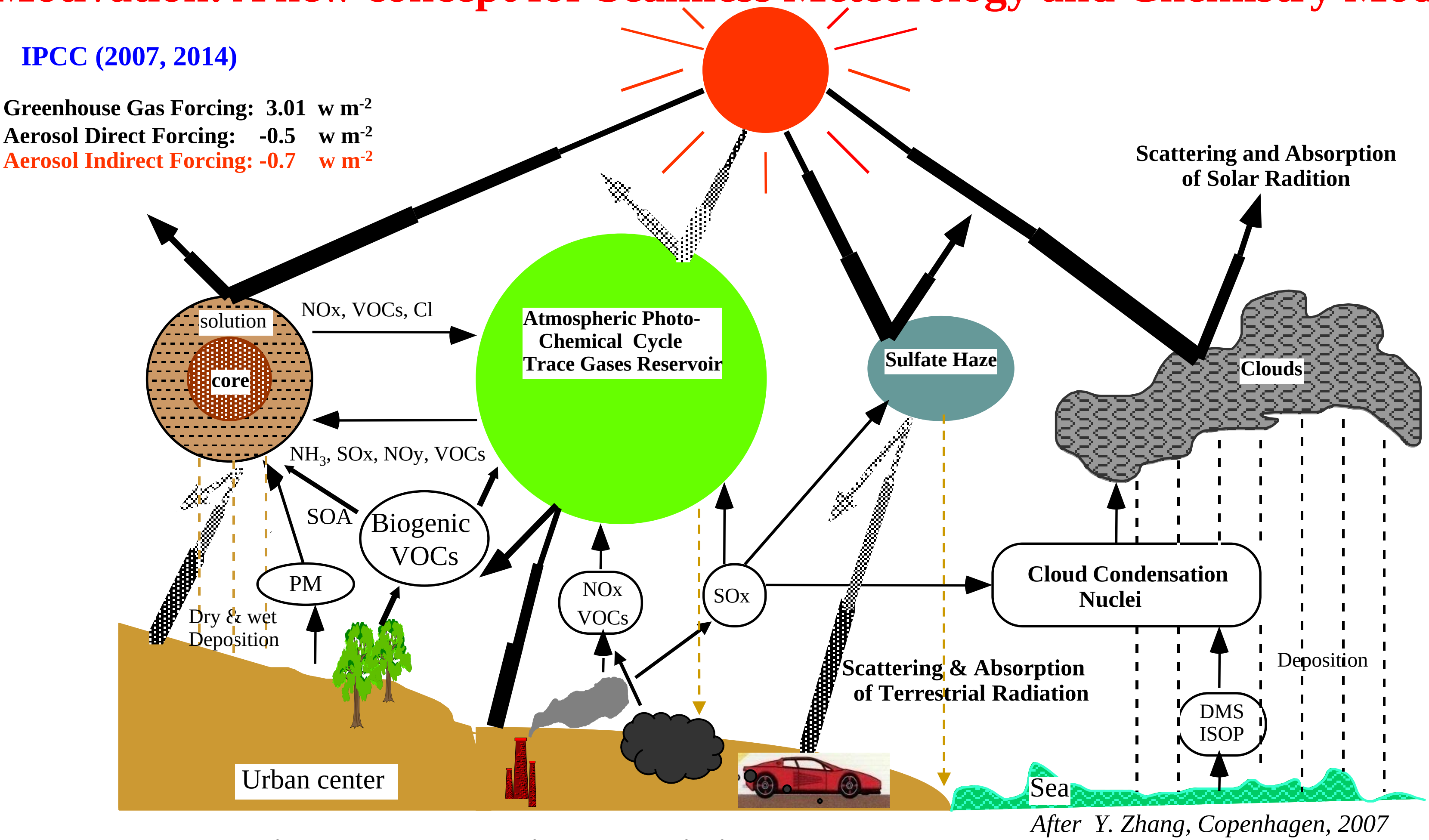
- Physical and Chemical Weather: dependence of meteorological processes (incl. precipitation, thunderstorms, radiation, clouds, fog, visibility and PBL structure) on atmospheric concentrations of chemical components (especially aerosols).
- Meteorological data assimilation (in particular assimilation of radiative properties) also depends on chemical composition.
- Air quality forecasts loose accuracy when CTMs are run offline.
- Climate modeling: large uncertainty of SLCFs, water vapor feedbacks, etc.

=> Need for a new generation of seamless integrated meteorology and chemistry modelling systems for predicting atmospheric composition, meteorology and climate evolution !



Atmosphere Interactions:
Gases, Aerosols, Chemistry, Transport, Radiation, Climate

Motivation: A new concept for Seamless Meteorology and Chemistry Modelling



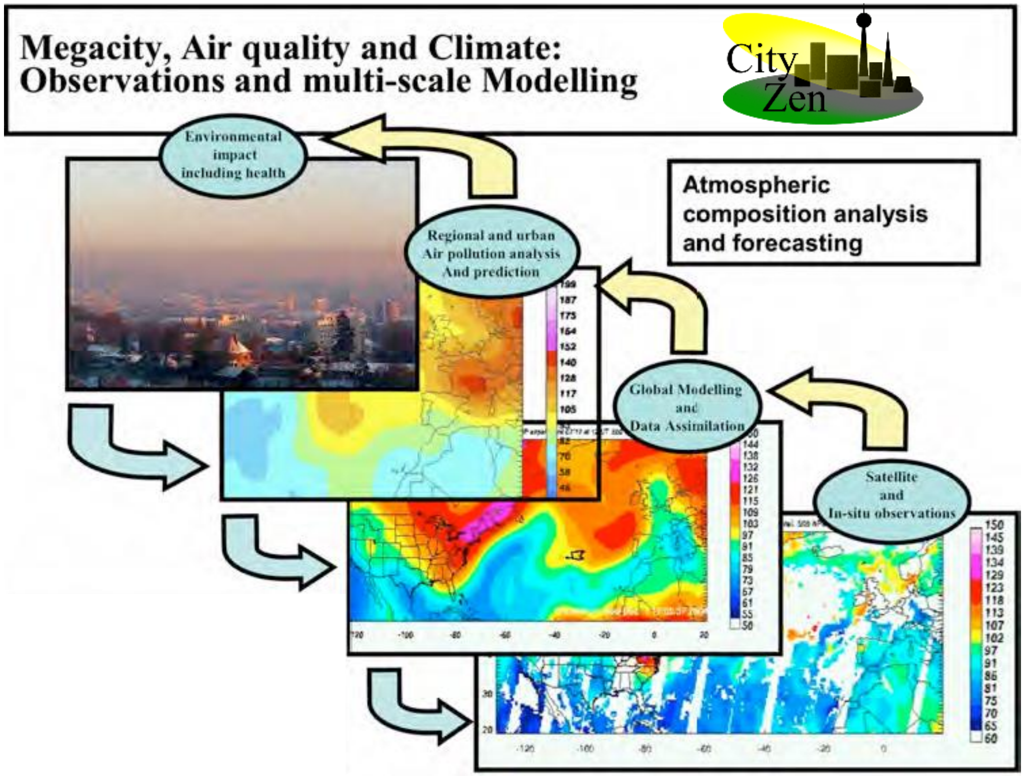
Temperature → chemistry → concentrations → radiative processes → temperature
Aerosol → radiation → photolysis → chemistry
Temperature gradients → turbulence → surface concentrations, boundary layer outflow/inflow
Aerosol → cloud optical depth through influence of droplet number on mean droplet size →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

(iii) Multi-scale prediction approach

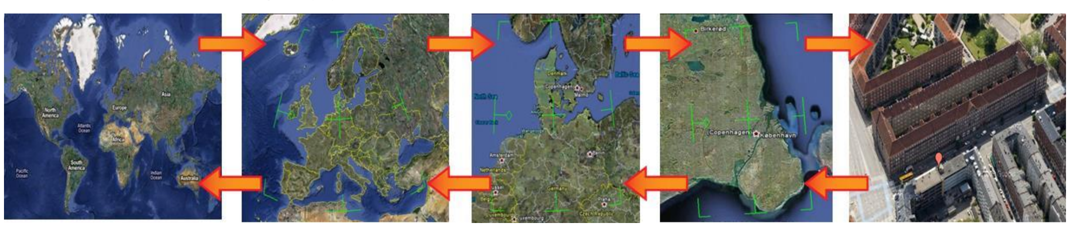
- Monitoring, analysis and forecasting systems should operate at different spatial scale from the global scale to the regional, national, urban and sub-urban scales
- Zooming or special nesting grid techniques (e.g. WRF-Chem, COSMO-Art, EnvHIRLAM
- One-way nesting (sometimes referred to as downscaling), 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
- Street level AQ the downscaling with microscale models (e.g., obstacle-resolved computational fluid dynamics (CFD) type or parameterized).
- Seamless unified modelling system on a single platform across-scales is a substantial advancement in both the science and efficiency (e.g. MPAS-A, MUSICA)
- Major challenges include globalization/ downscaling with consistent model physics and two-way nesting with mass conservation and consistency.
- Unified global-to-urban scale modelling provides a new scientific capability for studying problems that require a consideration of multi-scale feedbacks.

Seamless Methodology and Research Tools

Multi-scale modelling Chain / Framework: from Street to Global



GAW Modelling Application SAG < == > GURME SAG



2-way nesting, Zooming, Nudging, Parameterizations, Urban increment

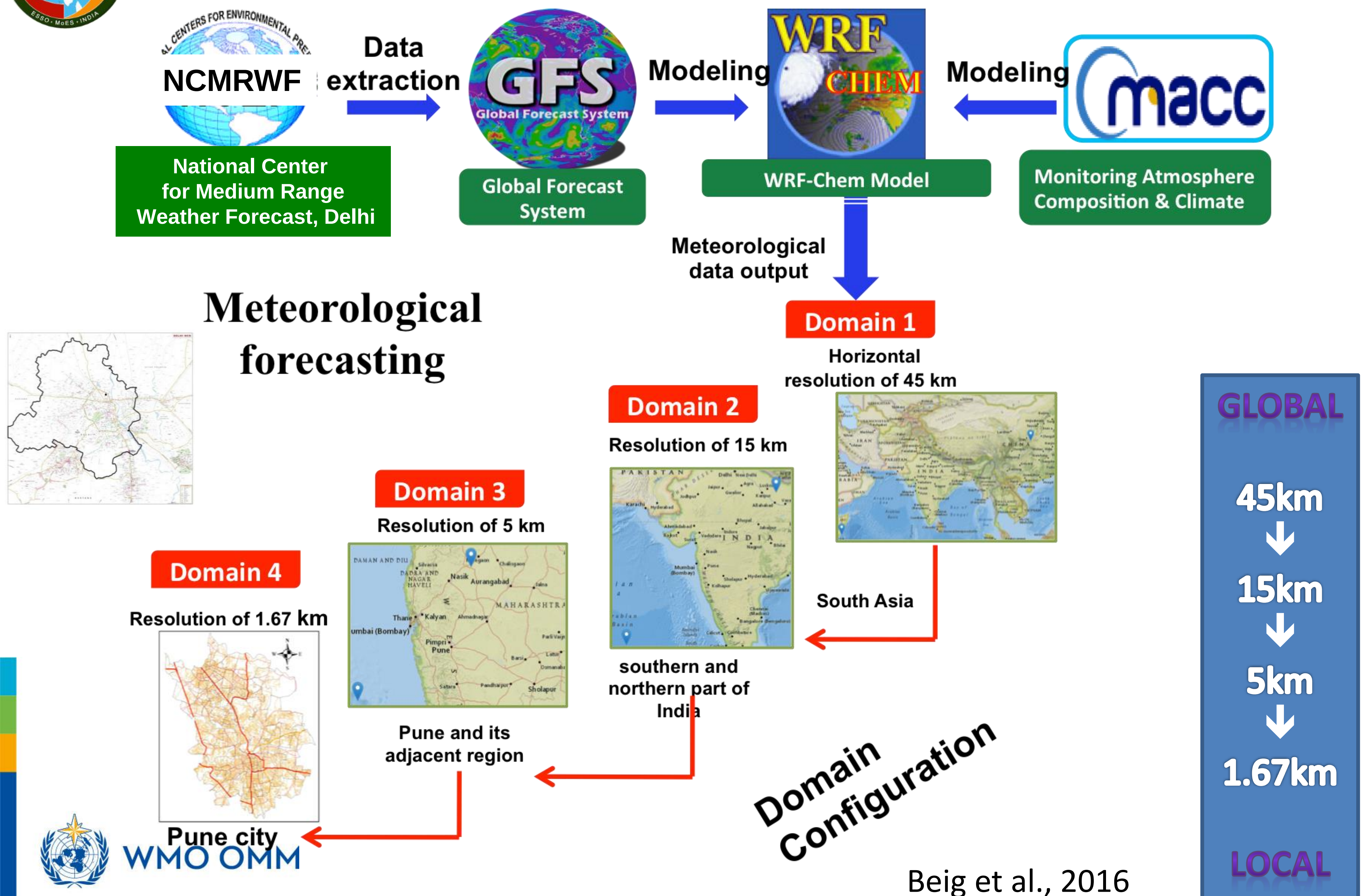
Seamless coupling for:

- Time scales: from nowcasting till decades
- Spatial scales: from street till global
- Processes: physical, chemical, biological, social
- Earth system elements: atmosphere, water, urban soil, ecosystems
- Different types of observations and modelling
- Links with health and social consequences, services and end-users

=> New generation of integrated models

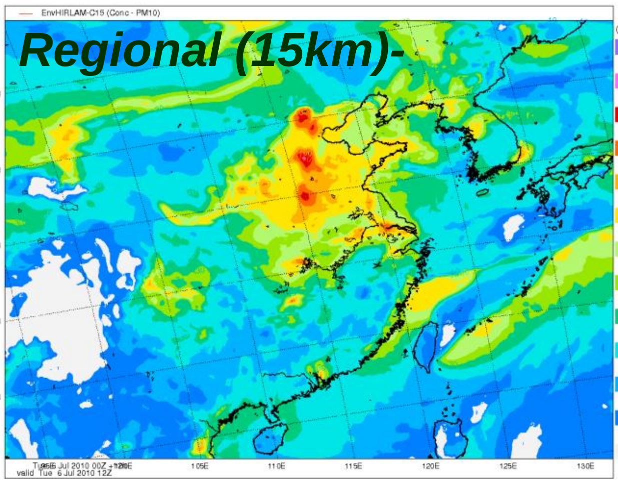
Baklanov, Molina, Gauss, AE, 2016

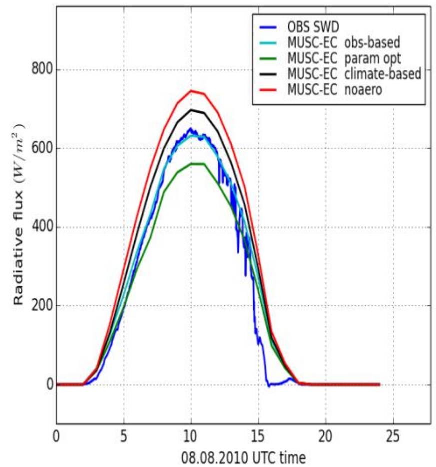
SAFAR Modeling Set-up for City Level AQ Forecast

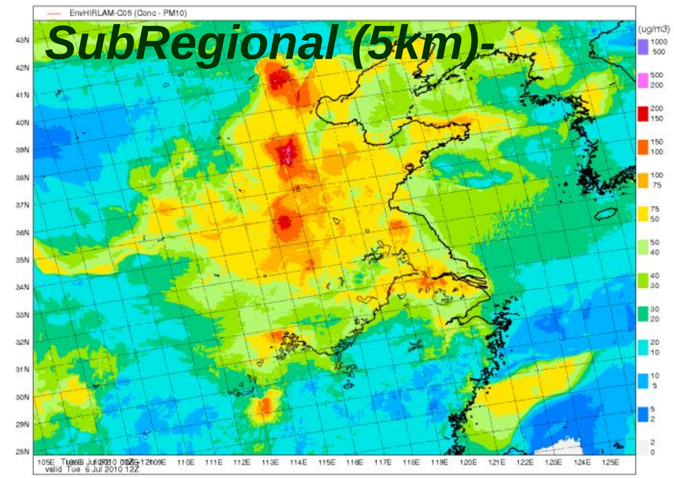


Beig et al., 2016

DMI: Reg-Subreg-Urban Downscaling: Enviro-HIRLAM & HARMONIE Modelling Chain and Aerosols Effects in China





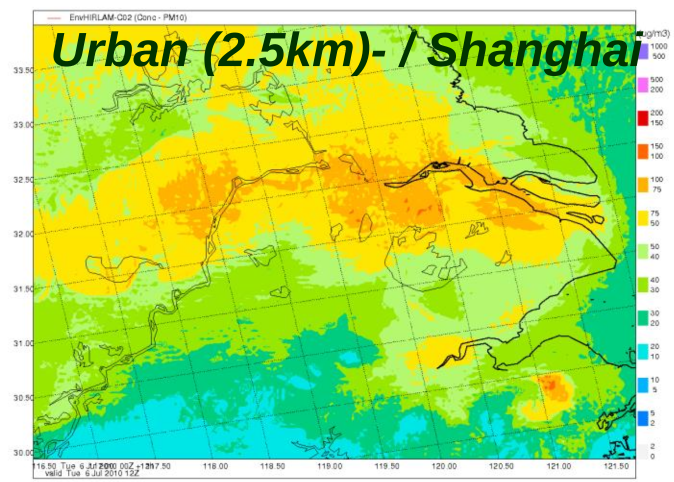


Enviro-HIRLAM model forecasting (preoper. & migration);

- 15-5-2.5 km horiz.resol.; time step - 240,120,60 sec;
- 40 vert. levels; up to 48 h FL;
- output every 1h; PM10, PM2.5, NO2, O3 (required) &+

HARMONIE case studies (Shanghai MA; Jan & Jul 2010), 2.5 km h.res.

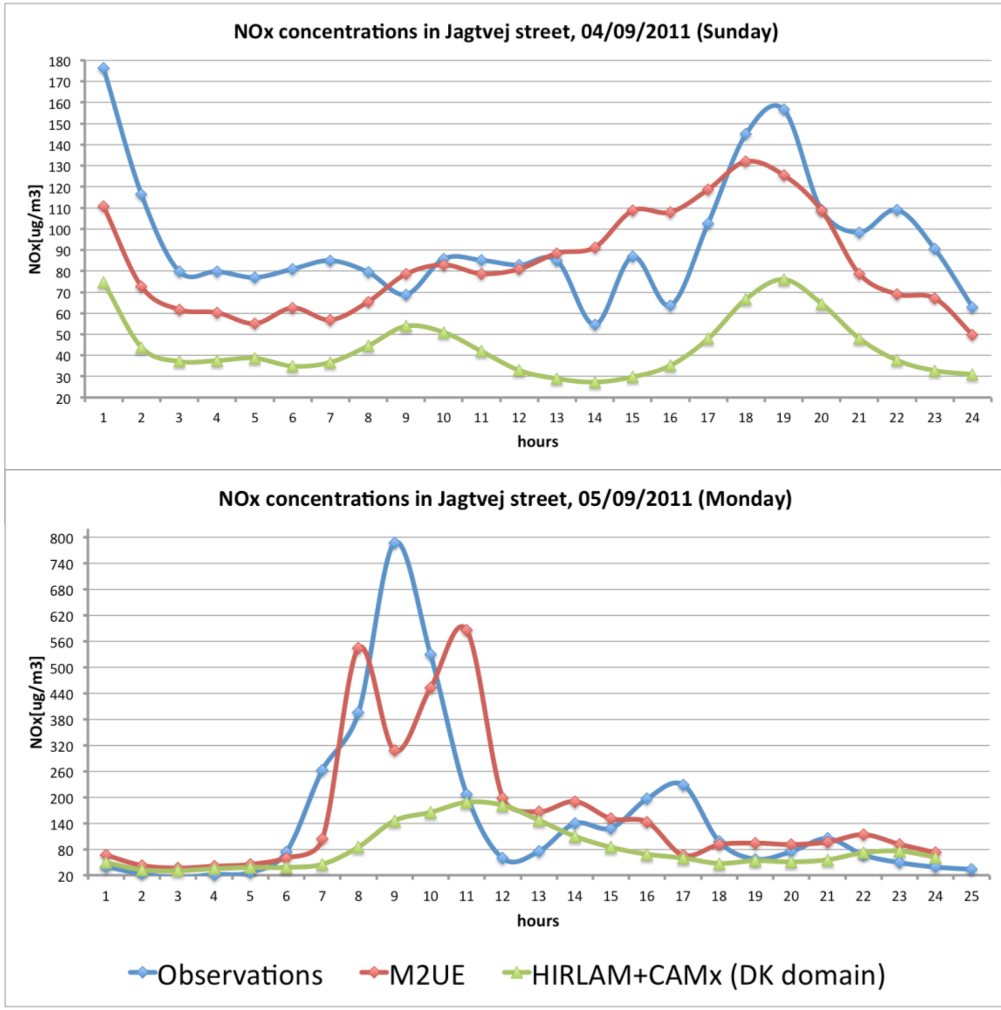
- sensitivity of direct and indirect aerosol effects;
- sensitivity of varying single scattering albedo and asymmetry factor of aerosols.



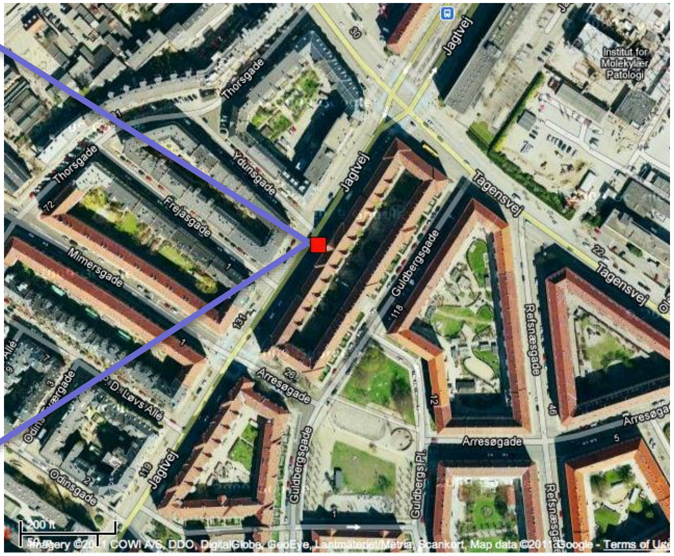
Mahura et al., 2016

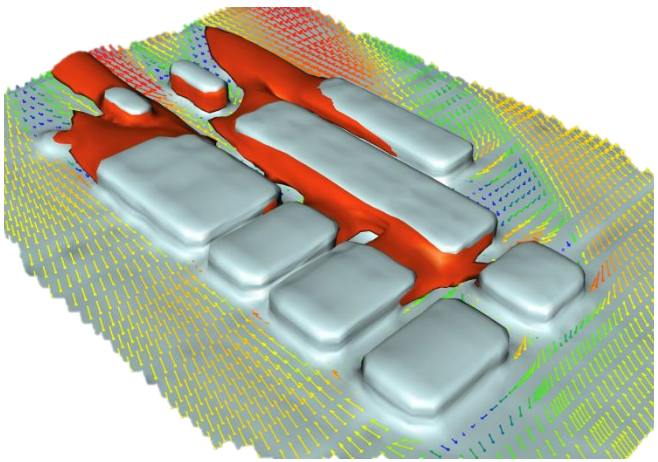
Enviro-HIRLAM output for PM10 conc.

Copenhagen: Downscaling to Street scale



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





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

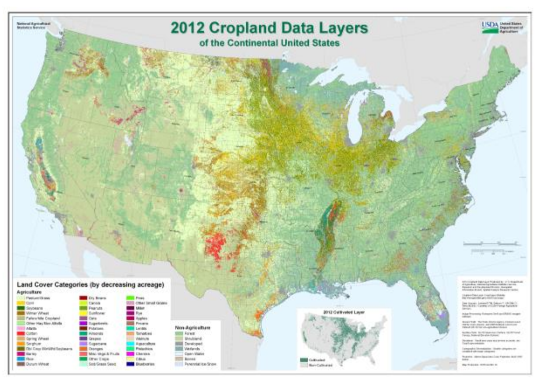
Nuterman et al. (2021)

(iv) Emission modeling for improved emission data

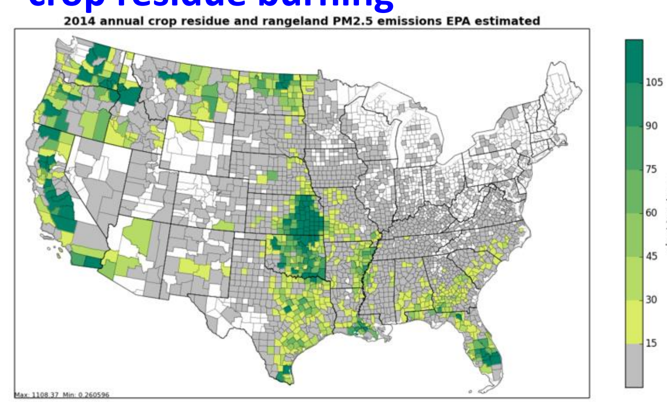
- **Emissions modeling:** using either observed or modeled activity information associated with one or more physical processes and estimating emissions using an algorithm.
- **Examples:** MOVES for mobile sources, MEGAN or BEIS3 for biogenic emissions
- **Emissions modeling is different from emissions processing** (e.g., using SMOKE emission processor, or downscaling coarse resolution to high resolution emissions)
- **Case study: a new method to compute crop residue burning emissions (Pouliot, 2018)**
  - Use Hazard Mapping System (HMS) fire detections
  - For GOES detects, remove "duplicate" detections (same time, locations within 2km)
  - Locate Agriculture Fires using a crop map with specific crop type maps
  - Identify crop type and determine emission factors (EF) and field size
  - Calculate Emissions: E=area burned*combustion completeness*EF*Fuel Loading
  - Separate Grass/Pasture from crop residue emissions using land use

HMS

Cropland Use Data

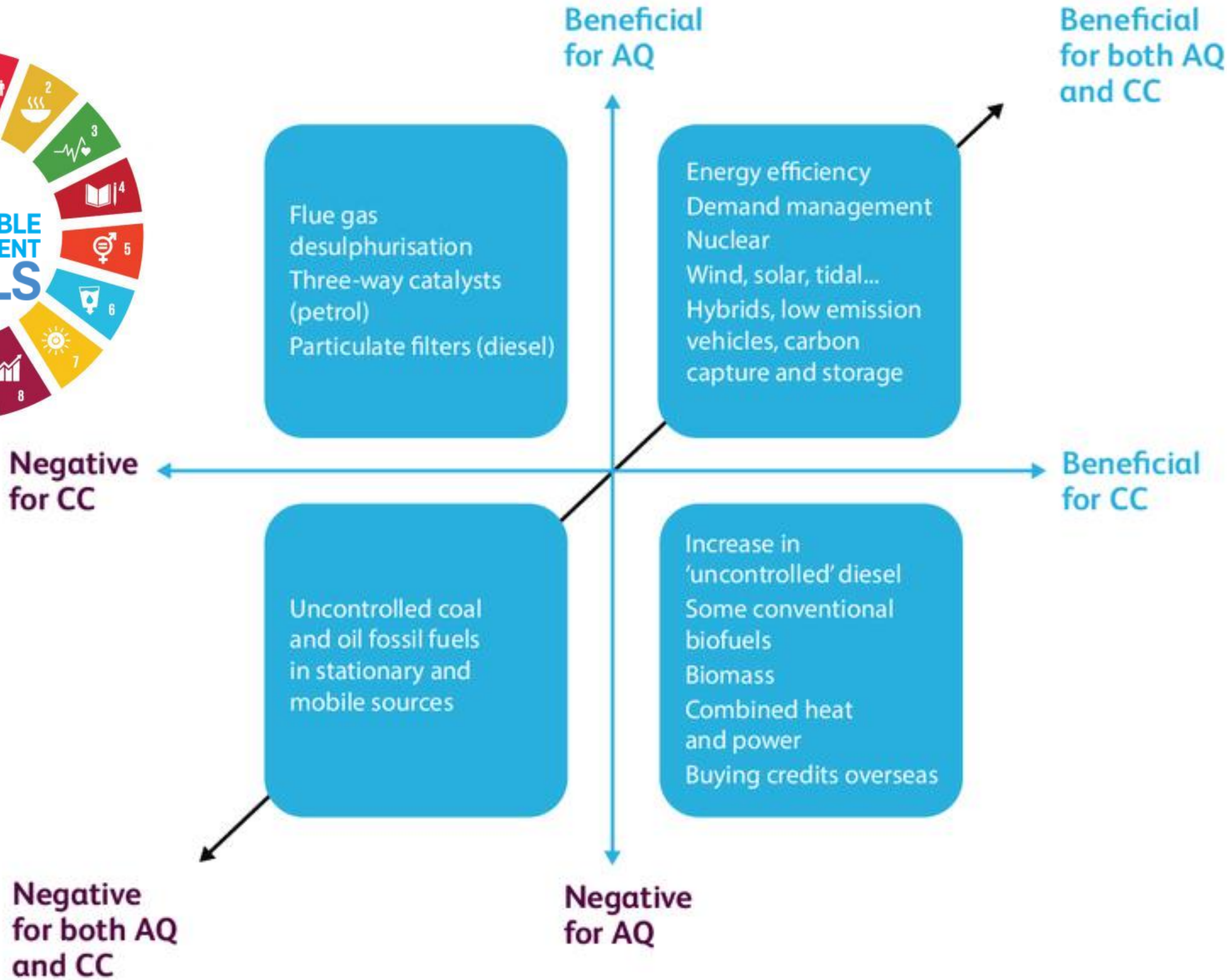


Gridded $PM_{2.5}$ emissions from crop residue burning



Emission Control: Co-benefits for Environment & Climate

SUSTAINABLE DEVELOPMENT GOALS



(v) Data fusion, machine learning methods and bias correction techniques

- Tremendously growing number and different types of observations became available now, require and give a strong impulse for development of new methods for measurement-model fusion to improve AQF
- Other than DA types of data fusion algorithms, such as the statistical methods, optimal interpolation, objective analysis, bias correction, as well as relatively new artificial intelligence, neural network, machine learning and hybrid methods, are actively developing
- Statistical methods are simple, but require a large amount of historical data and highly depend on them. Artificial intelligence, neural network and machine learning methods have better performance, but can be unstable and also depend on data.
- Hybrid or combined methods have a better quality. Such methods can also improve AQF utilising additional observational data.
- More advanced bias correction methods, e.g. the Kalman Filter (KF) and Kolmogorov-Zurbenko (KZ) filter technique.

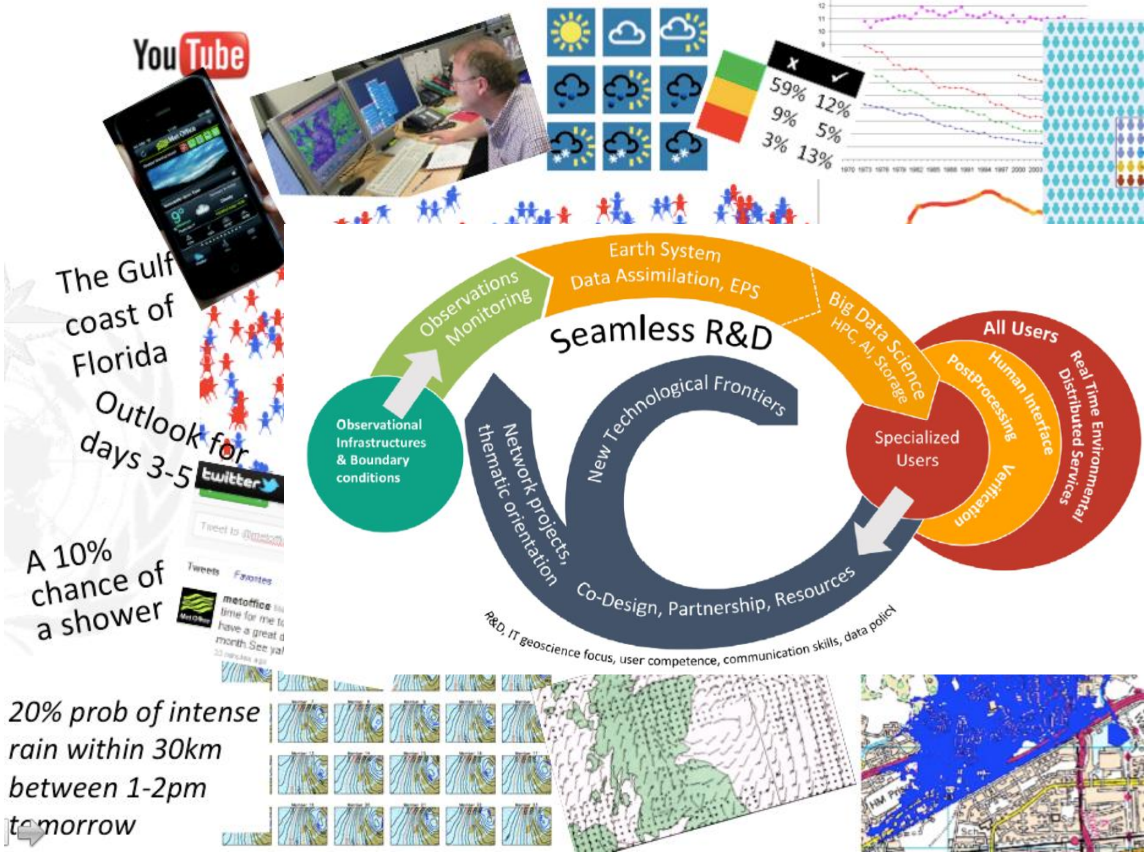
(vi) Multi-platform observations and data assimilation (DA)

- Meteorological and Chemical Concentration Observations
  - Surface networks
  - Upper air measurements (e.g., sounding)
  - Aircraft measurements
  - Satellite-Based Observations
- Data Assimilation Methods
  - Meteorological data assimilation
  - Chemical data assimilation
  - Inverse modeling using data assimilation
  - Multiscale DA, challenges with urban DA
  - Combined chemical DA and ensemble forecasting

Overview by Bocquet et al., ACP, 2015

(vi) Multi-platform observations and DA for IUS

- **Multi-purpose**: forecasts, research, planning, mitigations, service
- **Multi-function**: High impact weather, air quality, floods, urban climate, special end user needs
- **Multi-scale:** macro/mesoscale, urban, neighbourhood, street canyons, buildings
- **Multi-variable:** thermal, dynamic, chemical, hydrological, biometeorological, ecological
- **Multi-tool/platform**: radar, wind profiler, ground-based, airborne, satellite based, in situ observation, sampling, NRT time assess for DA;
- **Multi-linked**: linkages between all platforms, big data solutions



Tan et al., 2015

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Better communications – impacts & risks

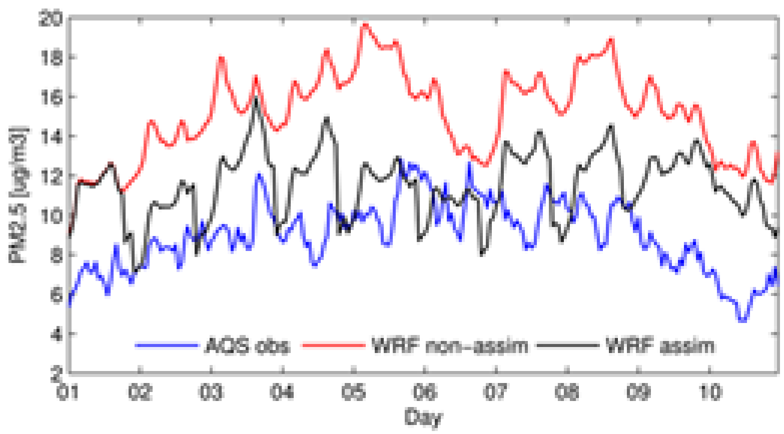
Measurement / instrumentation needs for CCMM

Variables	Measurement/instrumentation needs
Aerosol sizing	Optical particle counters and mobility particle size spectrometers
Aerosol composition	Analysis of filter sample, filterpack, aerosol mass spectrometers, elemental carbon/organic carbon analyzers
Aerosol optical properties	Aethalometer, nephelometer
Aerosol nucleation	Condensation particle counters, size resolved CCN, Zurich Ice Nucleation Chamber, tandem differential mobility analyzers
Radiation	Downward and upward shortwave and longwave radiation, diffuse/direct components
Aerosol remote sensing	AOD, absorption AOD, Angstrom exponent, fine fraction
Cloud properties	Cover, optical depth, liquid/ice water path, droplet/ice number concentration
Radiative fluxes	In the atmosphere and at the surface
Turbulent fluxes	In the atmosphere and at the surface
Information on PBL height/stratification	Time dependent, spatially resolved

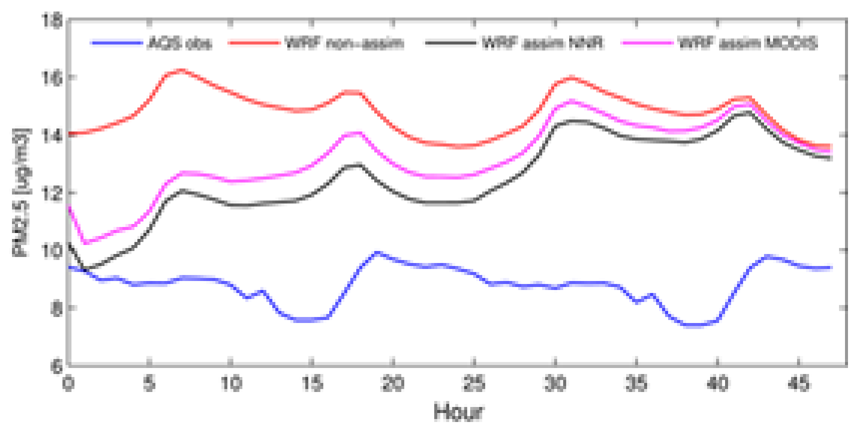
WMO CCMM, 2016

Data assimilation
in coupled chemistry meteorology models

Assimilation of satellite AOD data into WRF-Chem
(Source : P. Saide and G. Carmichael)



Model and observed mean $PM_{2.5}$ over AQS sites in California and Nevada.



Mean $PM_{2.5}$ as a function of forecast hour for the same sites.

Results when assimilating satellite retrieved AOD with 3D-Var over the southwestern U.S. for 1-10 May 2010 (Modified from Saide et al., 2013).

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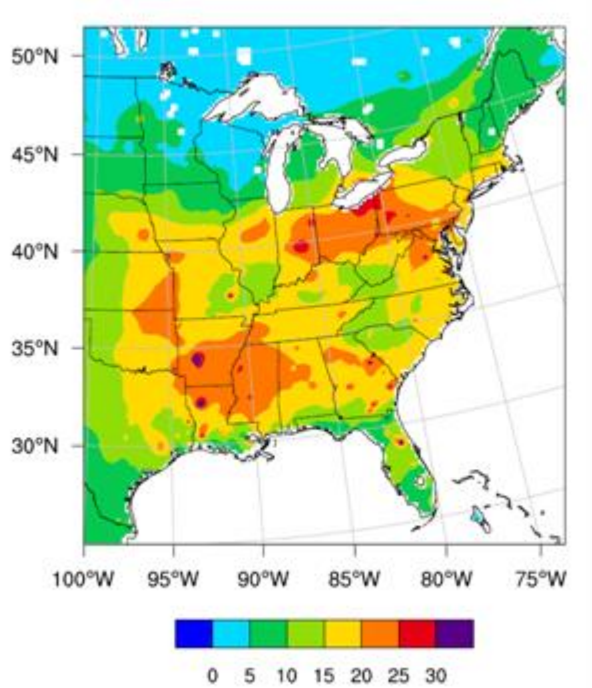
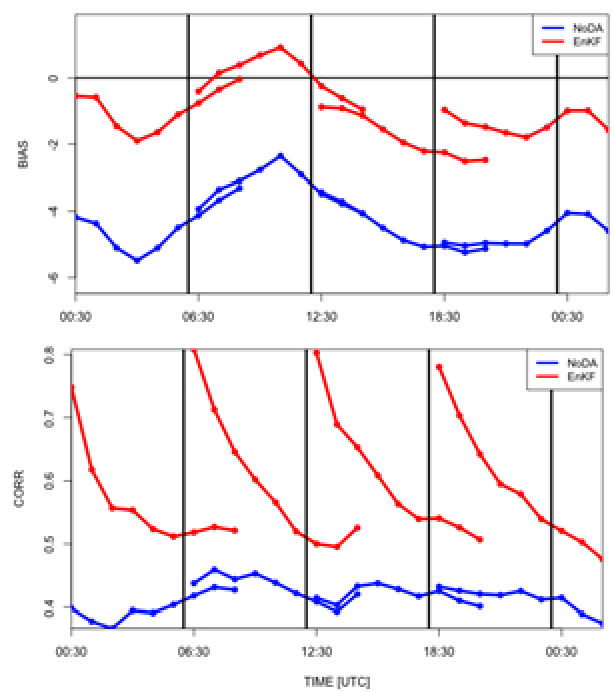
Data assimilation in coupled chemistry meteorology models

Assimilation of surface $PM_{2.5}$ data into WRF-Chem
(Source : M. Pagowski and G. Grell)



$PM_{2.5}$ concentrations simulated on 29 June 2012, over the eastern U.S.



Bias (top) and correlation (bottom) for simulated $PM_{2.5}$ against observations for the 28 June -7 July period without (blue line) and with (red line) EnKF data assimilation

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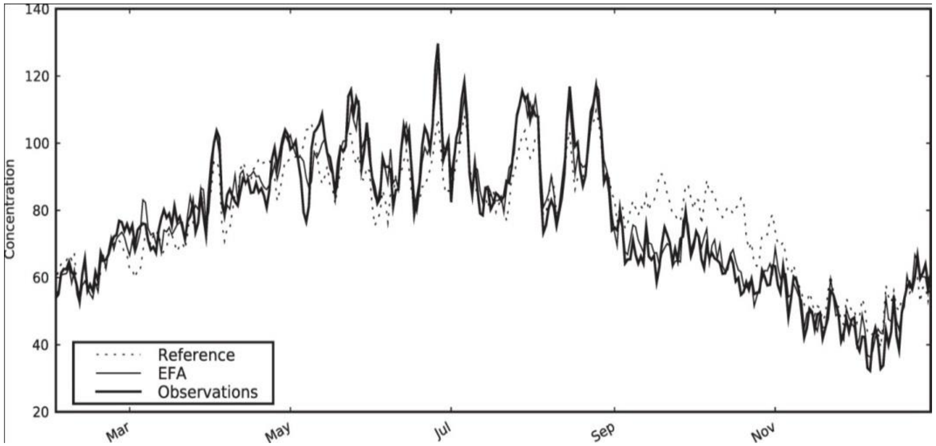
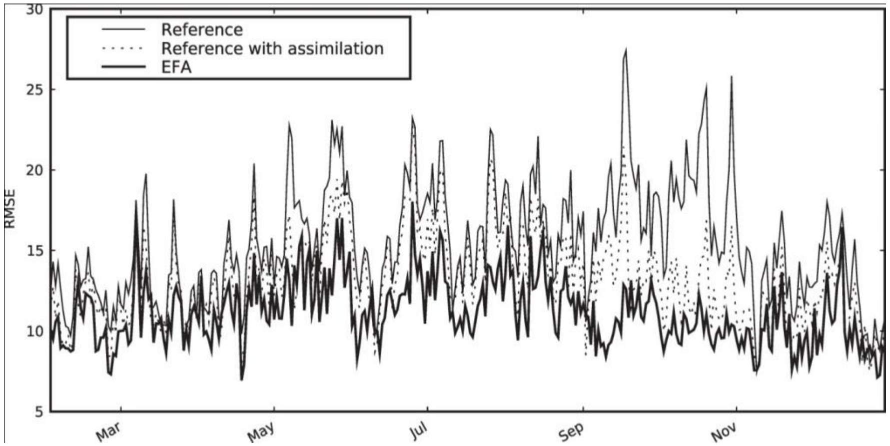
(vii) Ensemble approach

- **Types** (one model but with different inputs or multiple models)
- **Methods** (e.g., Monte Carlo simulations, multimodel ensembles, ensembles calibrated for uncertainty estimation, sequential aggregation, coupled sequential aggregation, classical data assimilation, the Ensemble Forecast of Analyses (EFA))
- **Example:** EFA (Mallet, 2010)
  - Combination of sequential aggregation (SA) and Data Assimilation (DA) to linearly combine multivariate ensemble simulations
  - Overcomes the limitations of sequential aggregation without loss of performance
  - Requires an ensemble and the application of a data assimilation method, which are not available on every operational platform

Surface O_3 Conc. ($\mu g m^{-3}$)



RMSE ($\mu g m^{-3}$)



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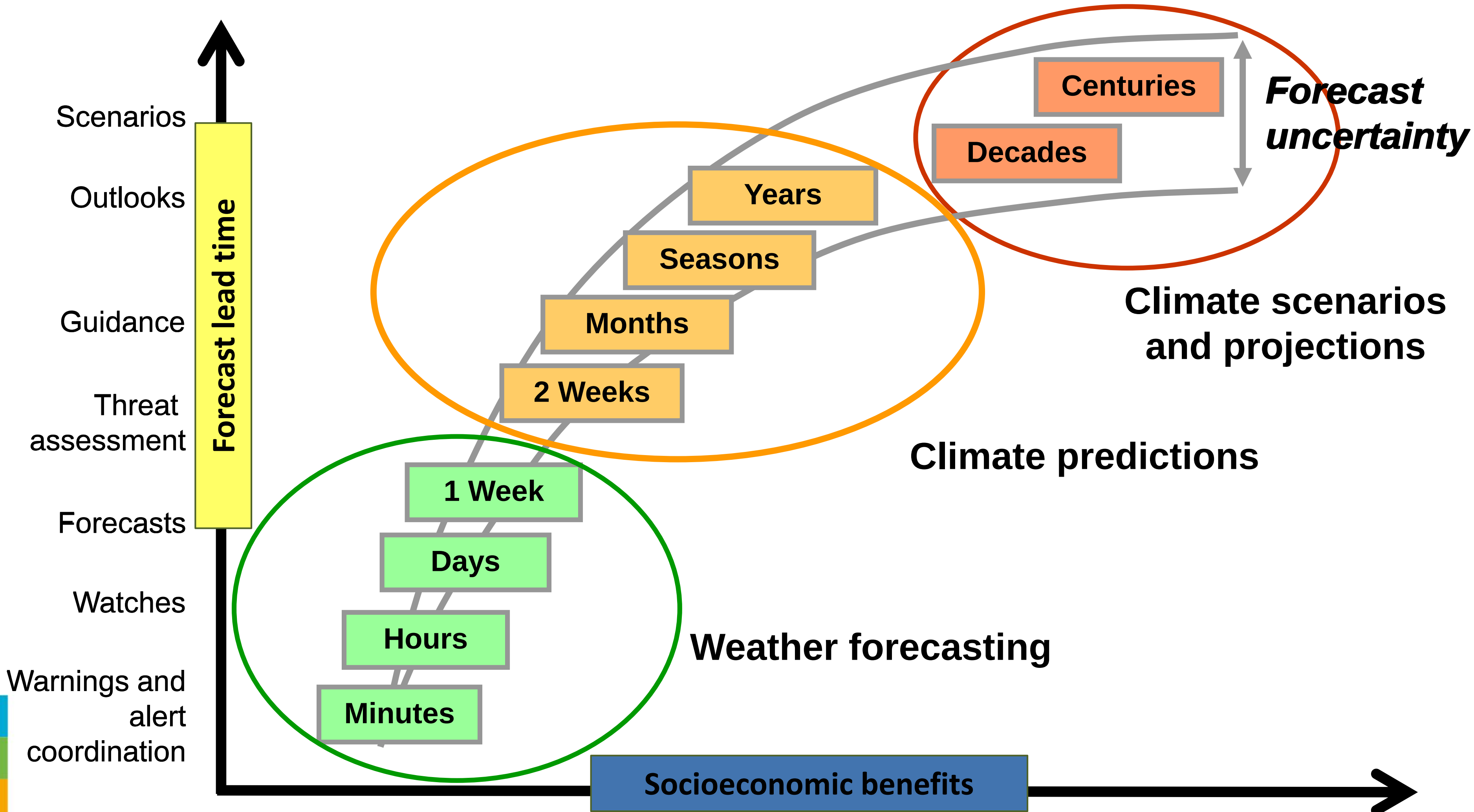
(viii) Subseasonal to seasonal forecast

- Significant progress in recent decades on medium-range weather forecasts and seasonal climate predictions.
- Seasonal and subseasonal forecasts are generated at monthly intervals out to 7 months and weekly intervals out to 5 weeks.
- The subseasonal to seasonal forecast will bridge the gap between weather and climate.
- Subseasonal weather and AQ forecasts is identified as research and operation priorities by WMO (Vitart et al., 2012) and several countries e.g. U.S. (Cortinas, 2017; NASEM, 2018).
- Large societal benefits, as many market behaviors and management decisions in agriculture and food security, water, risk reduction of weather disaster and hazards and health.

Weather-climate: seamless framework



Adapted from NOAA 2011

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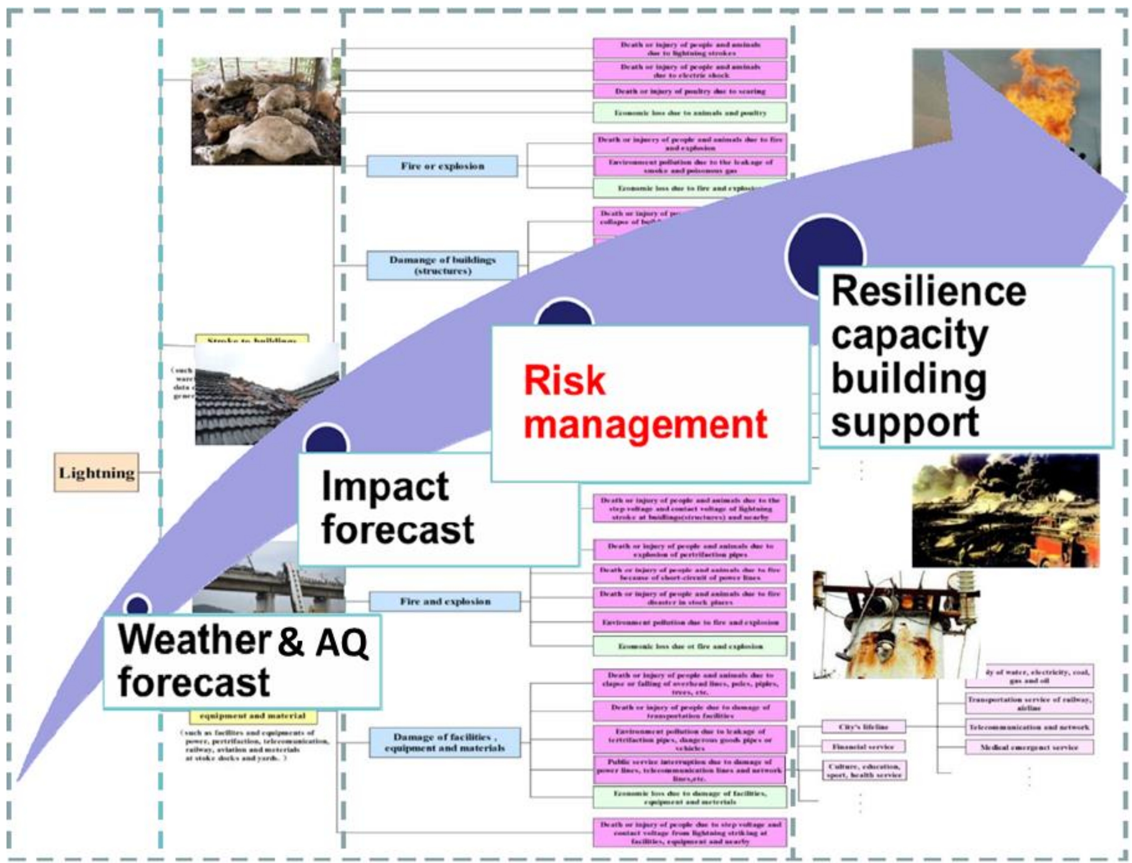
(ix) Fit for purpose approach

- There are also several user communities (e.g., NWP, climate) and specialized applications of AQF system developments for long-term prediction and specific episodes of atmospheric harmful contamination, affecting not only health but many other sectors of economics.



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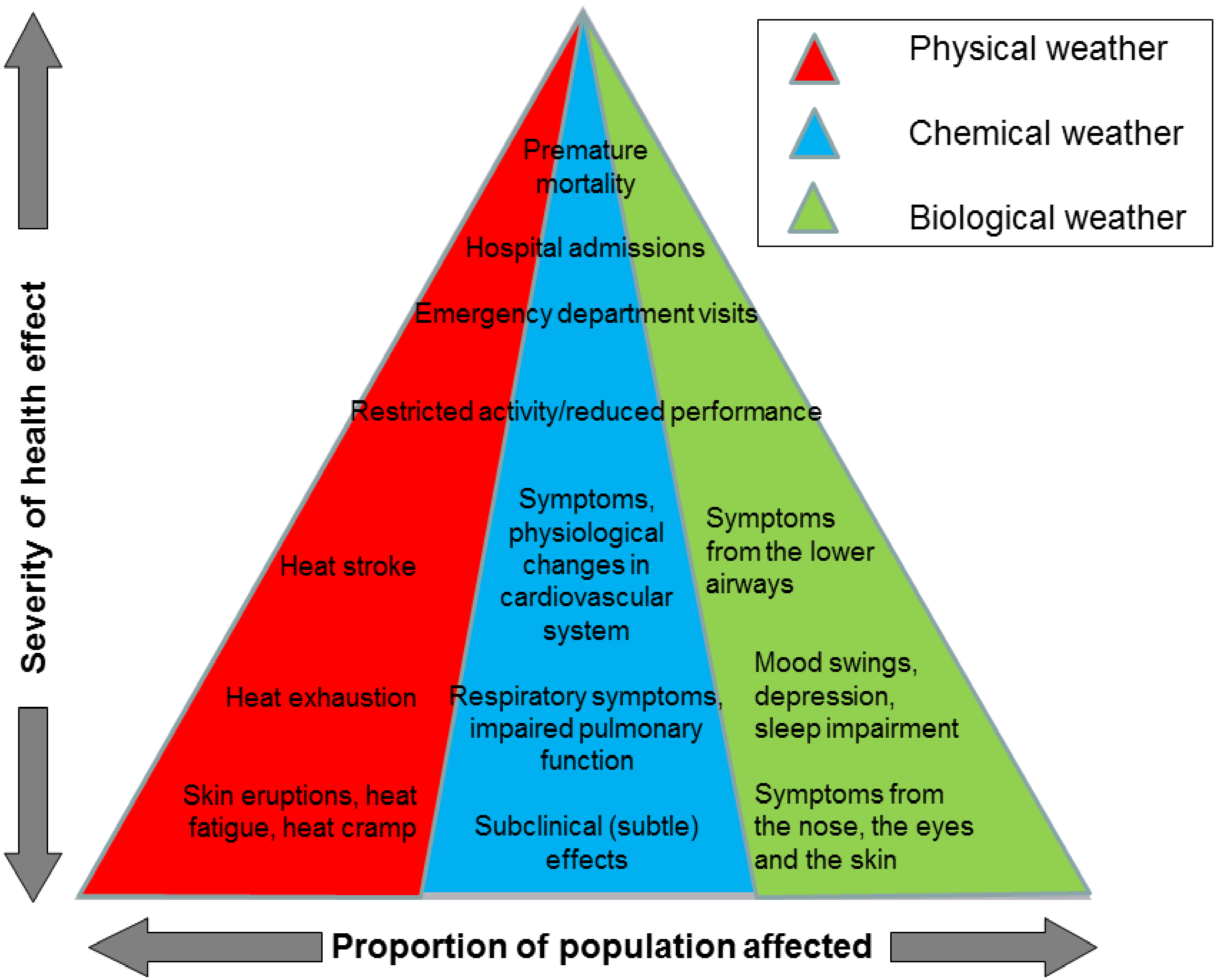
Meteorological, chemical and biological processes relevant for *health effects and meteorological, chemical and biological weather*

- Meteorological processes
  - Impacted by physical atmospheric variables.
- Chemical processes
  - Impacted by chemical variables.
- Biological processes
  - Impacted by bioaerosols (e.g. pollen, fungal spores).

⇒ Interaction of all processes

⇒ Towards Integrated Models



Based on Klein et al. (2012)

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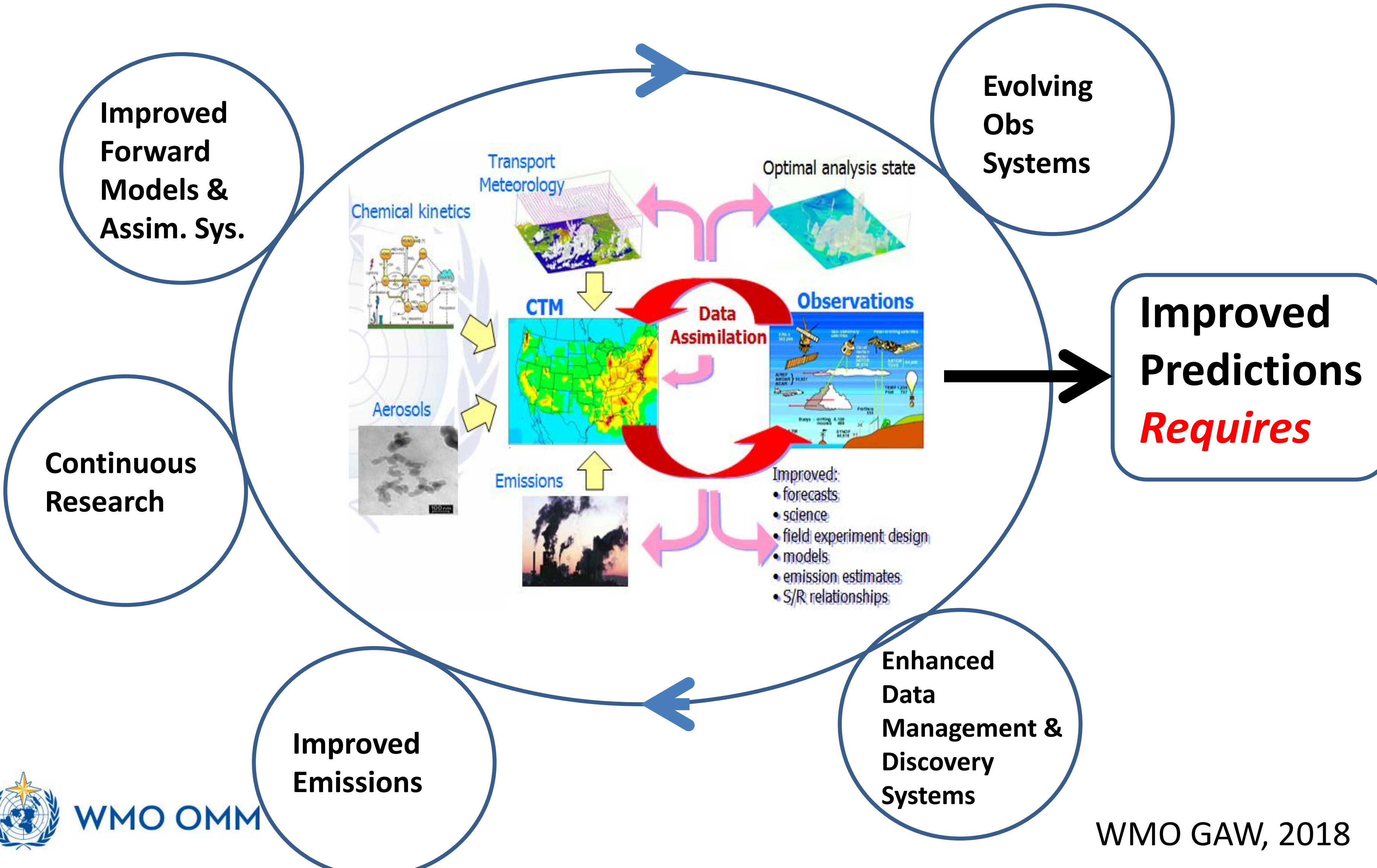
The Growing Interest in Improving Air Quality Predictions/Services and the Role of Atmospheric Composition in Weather and Climate Applications Offer Great Opportunities for Our Community



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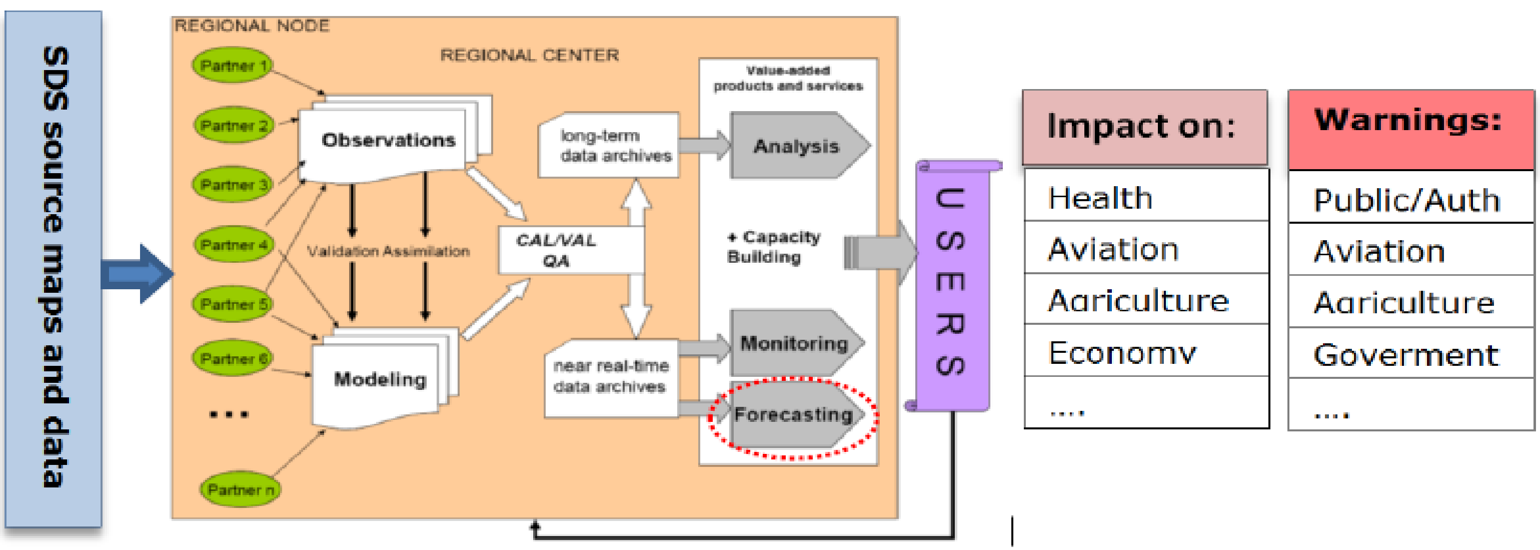
WMO GAW, 2018

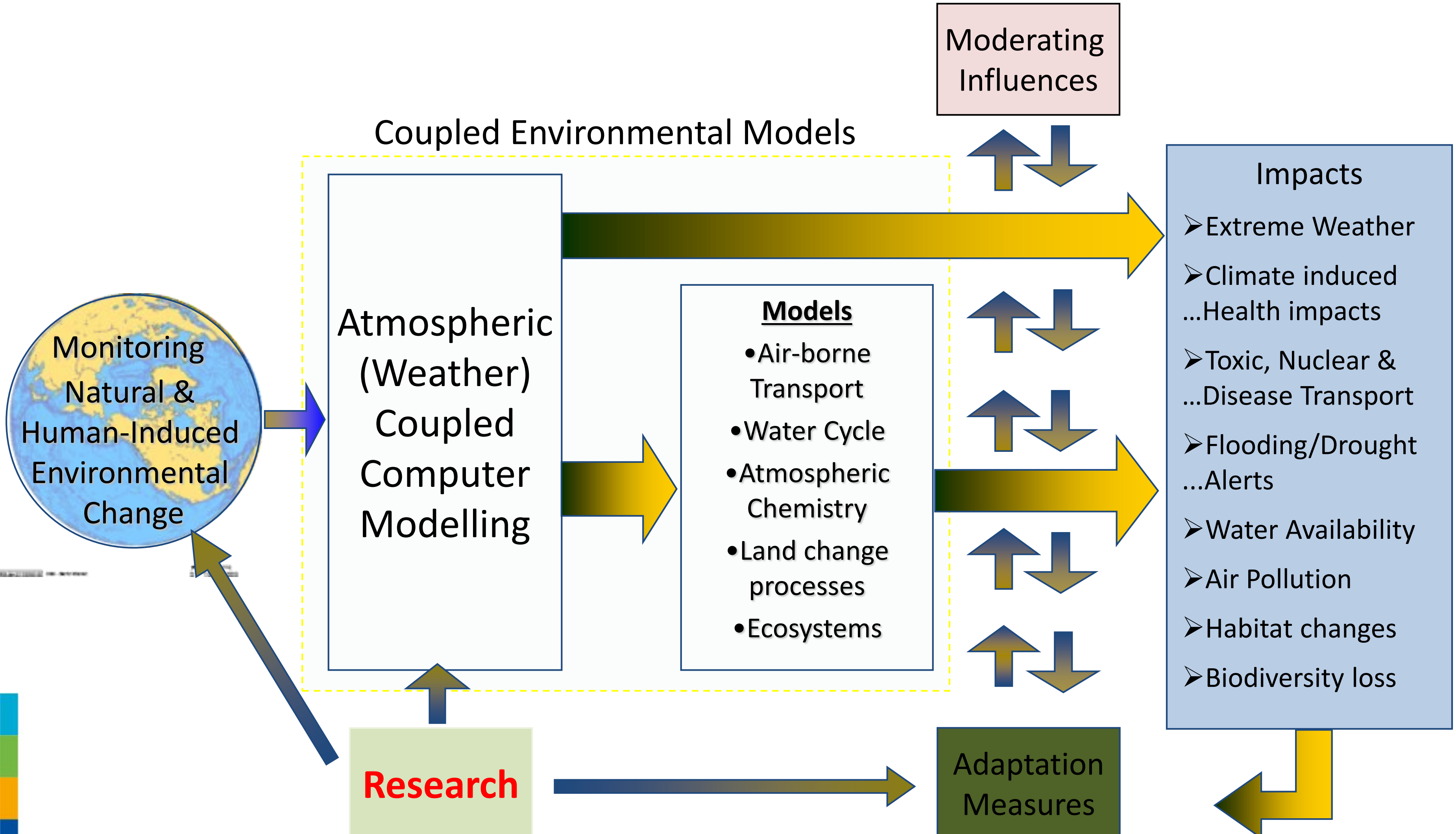
(x) Fit for purpose approach & Impact based forecast

- There are also several user communities (e.g., NWP, climate) and specialized applications of such system developments for long-term prediction and specific episodes of atmospheric harmful contamination, affecting not only health but many other sectors of economics.
- Example of impact-based forecast and assessment systems for the WMO Sand and Dust Storm Warning Advisory and Assessment System (SDS-WAS) (after Nickovic et al., 2015).



- Help stakeholders and responsible agencies to improve AQ and public health, mitigate occurrence of acute harmful AP episodes.

Overarching Research Need: Improve Prediction Capabilities via Incorporating/Integrating Composition, Weather and Climate



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Across Relevant Temporal and Spatial Scales

WMO, 2019

(xi) Capacity building, training and education aspects

- **Develop long-lasting training books:** Training Materials and Best Practices for Chemical Weather /Air Quality Forecasting (CW-AQF), 587 pages, edited by Y. Zhang and A. Baklanov, 2019, sponsored and to be published by WMO
- **Organize annual training workshops in developing countries** (e.g., 2019 October training workshop on RT-AQF in Nairobi, Kenya with > 40 participants from 16 countries)
- **Sponsor training in established research laboratories (e.g., Europe, North America)**

(xi) Capacity building, training & education aspects

Available from: https://library.wmo.int/doc_num.php?explnum_id=10439

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Background

- **Increasing needs for CW-AQF with increasing number of forecasters worldwide, increasing involvements of NMHSs**
- **Increasing complexity of the 3-D numerical models for CW-AQF with recent scientific advancements in numerical weather prediction (NWP) and CW-AQF**
- **Common mistakes leading to unsuccessful implementation and application**

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**

Specific Objectives

- **Help forecasters worldwide, especially those in developing countries on using 3-D CW-AQF models for best practices and operations**
- **Provide practical information about the best CW-AQF practices and standardized procedures for the successful deployment and application**
- **prepare materials that could be adapted for training by NMHSs, WMO training centers, and other users from environmental authorities and academic institutions**

Scientific Advancements to Improve RT-AQF

- **Improvement of Meteorological Forecasts**
  - Representations of episodes that typically have very weak dynamical forcing (PBL schemes under strongly stable conditions and for nocturnal mixing layers)
  - Mesoscale circulations (e.g., land-sea breeze, topographic induced circulations, sea-breeze circulations, and their interactions with synoptic flows)
  - Meteorological forecasts at 1-km or smaller (stable/stagnation conditions, turbulence and vertical mixing, deep convection, low-level jets, land-surface processes, and precipitation)
- **Improvement of Chemical Inputs**
  - Initial and boundary conditions (outputs from a global CTM, assumed climatological profiles, and adaptation of satellite and surface data for chemical profiles)
  - Emissions (offline emissions; online emissions (e.g., mobile, biogenic, pollen, electric power generation, surface coating, wildfires, dust, sea-salt, and re-emissions))
- **Improvement of Physical, Dynamic, and Chemical Treatments**
  - Parameterizations of the urban environment (e.g., heterogeneity of building disposition, rough surface, anthropogenic heat fluxes the streets geometry)
  - Gas-phase chemistry representations (e.g., SAPRC2011/2007, CB05-TU, CB6)
  - Heterogeneous chemistry (e.g., HONO, reactions on sea-salt, photochemistry on soot)
  - Aerosol dynamics and chemistry (e.g., new particle formation and subsequent growth processes, SOA formation, mixing states)

Numerical/Computational Techniques to Improve RT-AQF

- **Improvement in Initial Conditions (ICONs)**
- Simple approaches to improve model ICONs (e.g., the climatology of concentration profiles, satellite data with a broad spatial coverage)
- Advanced approches based on chemical data assimilation (e.g., 3DVAR, 4DVAR)
- Meteorological forecasts at 1-km or smaller (stable/stagnation conditions, turbulence, deep convection, low-level jets, land-surface processes, precipitation)

- **Improvement of Emissions, Boundary Conditions, or Model Parameters**
- Inverse modeling using data assimilation
- Multiscale data assimilation method

- **Ensemble Forecasting**
- Types (one model but with different inputs or multiple models)
- Methods (e.g., Monte Carlo simulations, multimodel ensembles, ensembles calibrated for uncertainty estimation, sequential aggregation, coupled sequential aggregation and classical data assimilation)

- **Other Types of Techniques**
- Simple bias correction methods
- Data fusion methods
- Combination of several bias-correction methods

SUMMARY AND PERSPECTIVES (1)

Air quality forecast and assessment systems help decision makers to improve air quality and public health, mitigate the occurrence of acute air pollution episodes, particularly in urban areas, and reduce the associated impacts on agriculture, ecosystems and climate.

- Future improvements to AQF will follow several directions:

– Online coupling of atmospheric dynamics and chemistry models,

– Better representation of aerosol processes and feedbacks,

– Improved data assimilation,

– Toward seamless Earth system modelling,

– Multi-scale prediction approach,

– Subseasonal to seasonal forecasting,

– Impact based forecast and fit for purposes systems.

SUMMARY AND PERSPECTIVES (2)

- Seamless modelling is a prospective way for future single-atmosphere modelling systems with advantages for applications at all space- and timescales for multi applications not only for AQ, but also for NWP, climate, etc.
- The advance approach combines an ensemble of state-of-the-art models, high-resolution emission inventories, space observations and surface measurements of most relevant chemical species to provide hindcasts, analyses and forecasts of from global to regional AP and downscaling for selected countries and urban areas.
- Improved DA, both in terms of techniques and choice of aerosol variables to be assimilated. Key questions are whether there is a benefit to move from assimilating AOD to assimilating clear-sky radiances in the SW spectrum and how to make the use of vertical profiles from lidar observations.

Thank you!

WEATHER CLIMATE WATER
TEMPS CLIMAT EAU

WMO OMM

World Meteorological Organization
Organisation météorologique mondiale

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