Cover

Numerical modeling for air quality at regional scale: the aerosol challenge.

by
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Outline of the presentation

- Particulate matter: what and why; the synergy between regulations and science.
- Simulations should answer the relevant questions: what are such questions?
- Domains and numerical models: how to use the proper tool.
- Necessary inputs for particulate matter simulations at regional scale.
- Prognostic and diagnostic simulations: same tools, but different work flows.
- New computational approaches: GRID computing

Particulate matter for regional air quality simulations

The focus of air quality simulations at regional scale for aerosols is on **Particulate Matter.**

EEA definition (EEA Glossary http://www.eea.europa.eu)

Aerosol: *"A collective name for fine solid or liquid particles added to the atmosphere by processes at the earth's surface."*

Particulate Matter (PM): *"Particulate matter includes dust, smoke, soot, pollen and soil particles."*

EPA definition (EPA Glossary http://www.epa.gov/climatechange/glossary.html)

Aerosol: *"A collection of airborne solid or liquid particles, with a typical size between 0.01 and 10 micrometers (μm) and residing in the atmosphere for at least several hours."*

Particulate Matter (PM): *"Very small pieces of solid or liquid matter such as particles of soot, dust, fumes, mists or aerosols."*

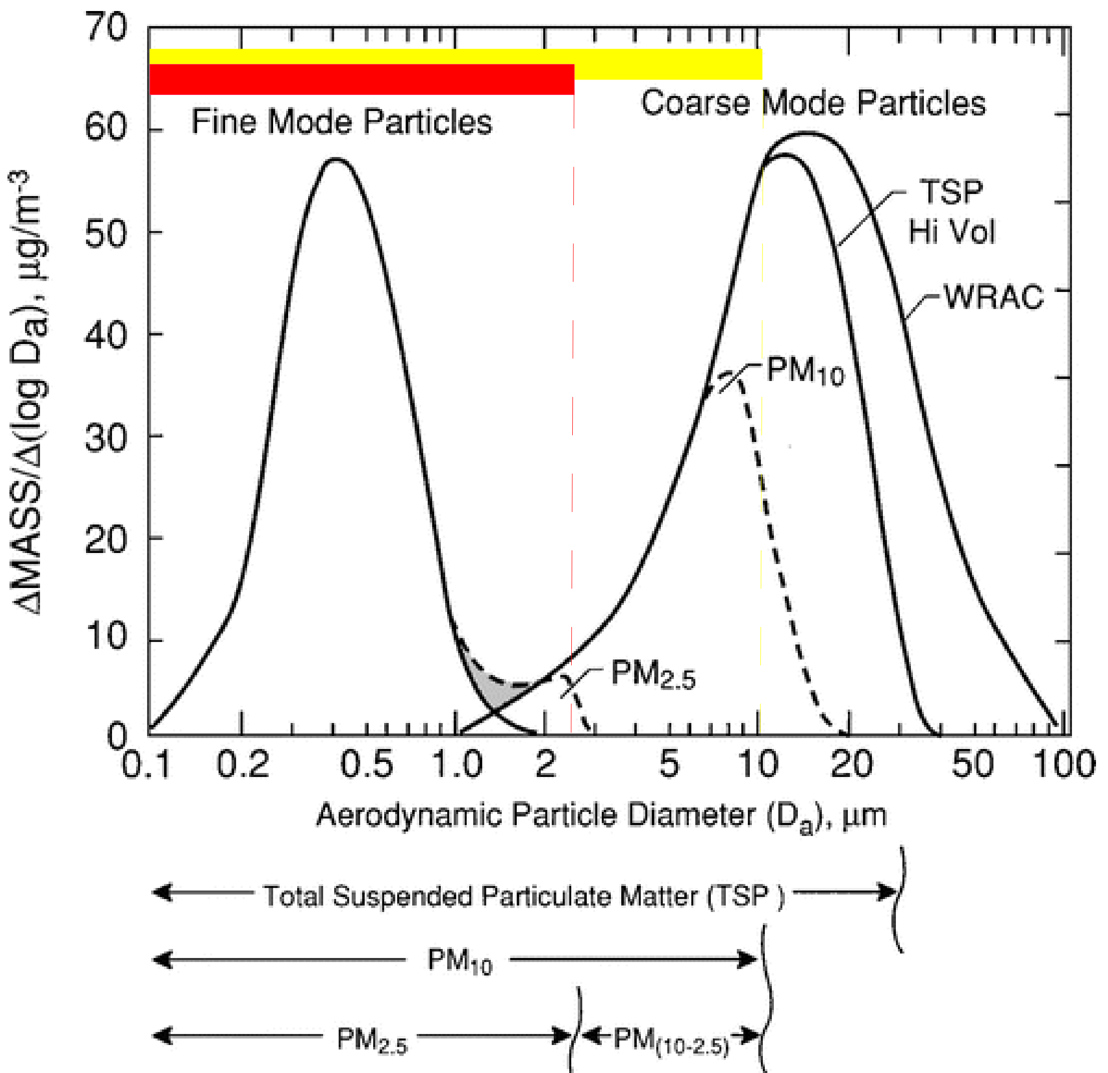
Particulate matter and the aerosol size spectra

The focus is on: **PM10** and **PM2.5**
EC directive 50/2008 (article 2) gives the definitions:

PM10 shall mean particulate matter which passes through a size-selective inlet as defined in the reference method for the sampling and measurement of PM10, EN 12341, with a 50 % efficiency **cut-off at 10 μm** aerodynamic diameter.

PM2.5 shall mean particulate matter which passes through a size-selective inlet as defined in the reference method for the sampling and measurement of PM2.5, EN 14907, with a 50 % efficiency **cut-off at 2.5 μm** aerodynamic diameter.

[2008/50/EC is a directive of the European Parliament and of the Council of the European Union]



(From R. Zellner 1999)

Why the focus on PM10 and PM2.5

The EC and national laws recognize **PM10** and **PM2.5** have impacts on human health. This comes from scientific evidences.

EC " … *establishes the need to reduce pollution to levels which minimise* ***harmful effects on human health****, paying particular attention to sensitive populations, and* ***the environment as a whole****, to* ***improve the monitoring and assessment*** *of air quality including the deposition of pollutants and to provide information to the public.*" [1]

The EC directive 50/2008 confirms the need to limit **PM10** concentration and it highlights the **PM2.5** impacts on human health:

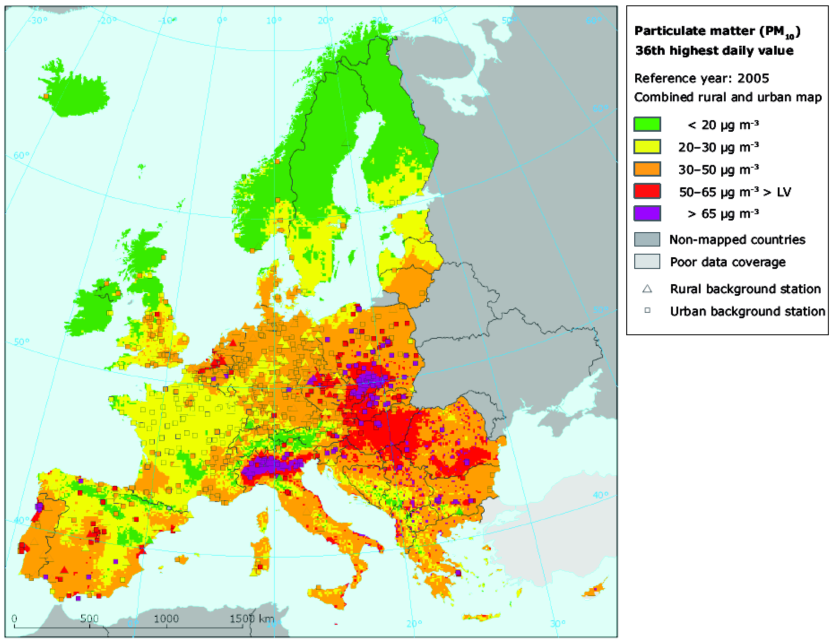
"*Fine particulate matter (PM2.5) is responsible for significant negative impacts on human health. Further, there is as yet no identifiable threshold below which PM2.5 would not pose a risk. As such, this pollutant should not be regulated in the same way as other air pollutants.*" [1]

HUMAN HEALTH	Limit or target (t) value					Assessment threshold values	
Pollutant	Averaging period	Value	Maximum number of	Margin of tolerance	Date applicable	Upper	Lower
PM_{10}	Day Year	50 μgm^{-3} 40 μgm^{-3}	35 0	50% 20%	2010 2010	35 μgm^{-3} 28 μgm^{-3}	25 μgm^{-3} 20 μgm^{-3}
$PM_{2.5}$	Year	25 μgm^{-3} 25 μgm^{-3} (t)	0 0	20% in 2008 to 0% in 2015	2015 2010	17 μgm^{-3}	12 μgm^{-3}

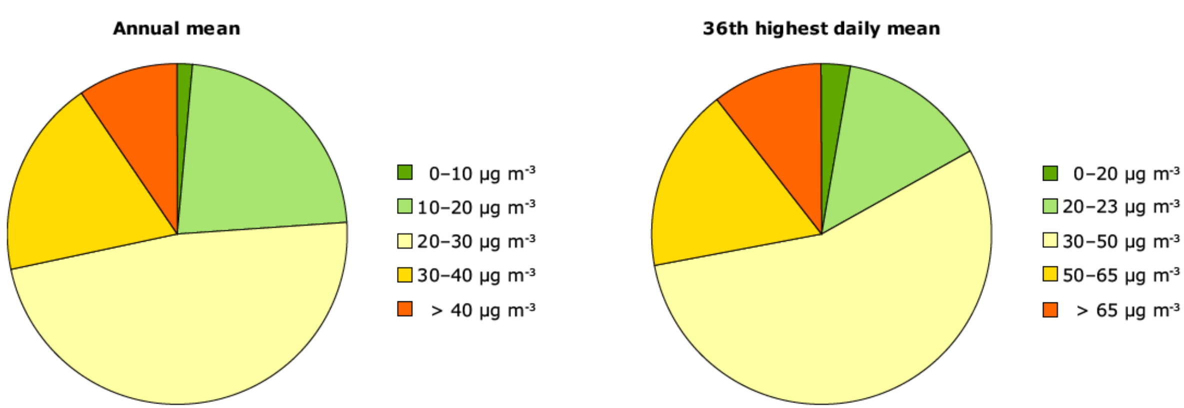
[1] Incipit of the 2008/50/EC which is a directive of the European Parliament and of the Council of the European Union

The scientific evidences of PM10 and PM2.5 impacts on human health.

PM_{10} — 36th maximum daily average value in µg m⁻³, 2005 — the limit value for the protection of human health is 50 µg m⁻³

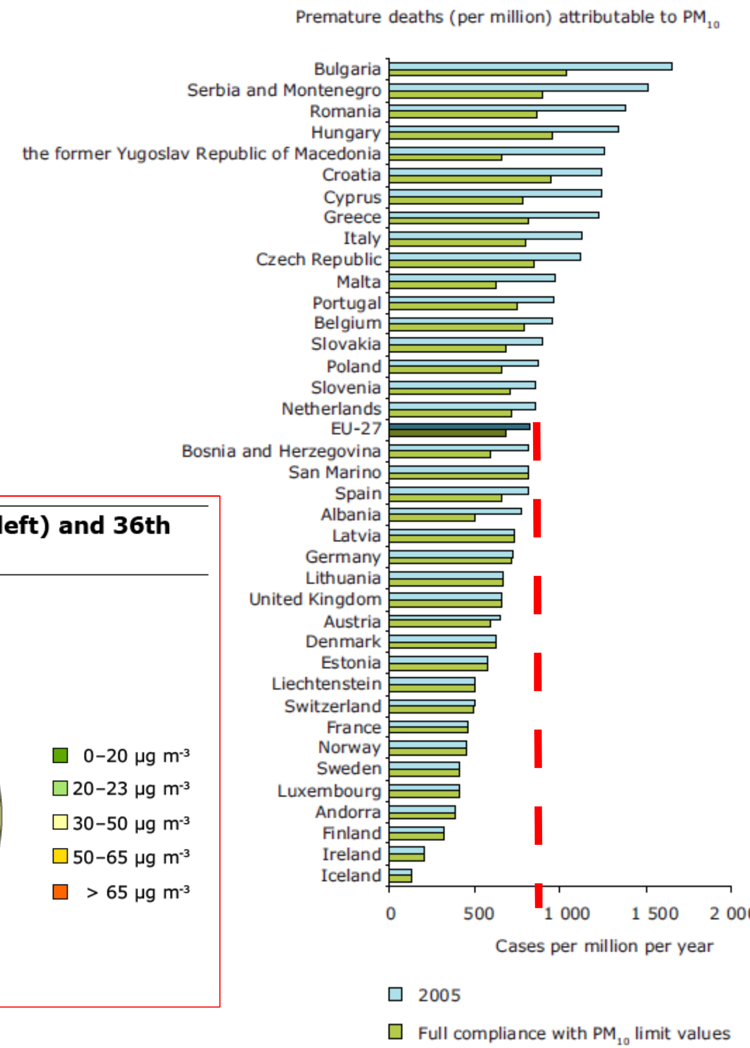


Exposure of the European population to PM_{10} concentrations, annual average (left) and 36th highest daily average (right), 2005

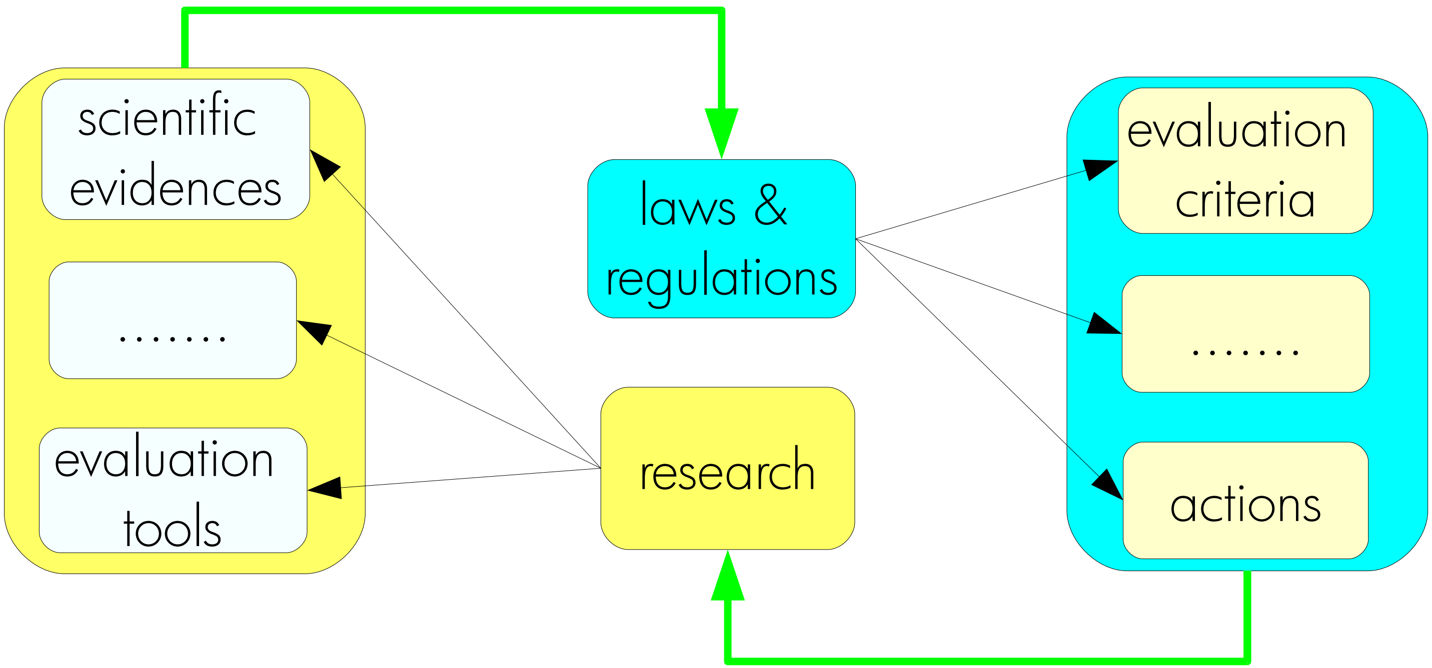


From: Spatial assessment of **PM10** and ozone concentrations in Europe (2005) [EEA technical Report No 1/2009]

Figure 3.4 Number of premature deaths per million inhabitants attributable to PM_{10} exposure in the reference year 2005



The synergy between regulations and science



Nowadays model simulations are considered reliable evaluation tools as measurements.

"Where possible modelling techniques should be applied to enable point data to be interpreted in terms of geographical distribution of concentration. This could serve as a basis for calculating the collective exposure of the population living in the area." [1]

"The results of modelling and/or indicative measurement shall be taken into account for the assessment of air quality with respect to the limit values." [1]

[1] In the 2008/50/EC which is a directive of the European Parliament and of the Council of the European Union

The proper simulations for particulate questions at regional scale

It is necessary to project and execute numerical simulations suitable to answer the given questions, keeping in mind the limits of the models and the inputs.

How to chose the right tool?

FAIRMODE (http://fairmode.ew.eea.europa.eu/) is an initiative involving a lot of research and environmental institutions allover Europe and it is a very good reference source of information to learn how to chose the right tool (**numerical model**).

FAIRMODE aims:

- to provide guidance for the use of air quality modeling in regard to the European Air Quality Directives: interpretation, reference and summary information for both authorities and researchers.
- to promote good practice in air quality modeling and assessment,
- to provide a central reference point and develop a harmonized understanding of model requirements in regard to the European Air Quality Directive.

Basic steps to project a suitable simulation for particulate matter at regional scale

There are four main aspects to be considered to project a useful simulation

purposes
- research
- forecast
- scenarios
- legislation assessments
- education
- impact & risk evaluations

models
- availability
- space domain & resolution
- time interval & resolution
- physics
- chemistry
- Pre-processing & post-processing

inputs
- meteorology
- land use
- orography
- immersed bodies
- Initial & boundary conditions
- emission inventories

resources
- human & knowledge
- computation
- storage
- time (deadlines)

Main aspect of the purposes class

There is an essential distinction among all the purposes for an air quality simulation:

research → Full freedom according the research objectives

- forecast
- scenarios
- legislation assessments
- education
- impact & risk evaluations

→

There are constrains given by current legislation.
The simulations shall allow the computation of the quantities the laws define and it has to match the quality requirements identified by laws.

Examples:
- Yearly and daily averages for PM10 and PM2.5.
- Quantities required to fill the questionnaire of EC directive.
- Quantities necessary for mitigation actions application.

(There more complex indexes that impose constrains in time and space resolution making the simulation complicated or expensive)

Models: availability, pre-processing and post-processing

availability → the code is: open source, available in the frame of a project, a commercial one, etc.

space domain & resolution

time interval & resolution

physics

chemistry

Pre-processing & post-processing → The model has (not) accessory codes suitable to pre-process my inputs.
The model has (not) accessory codes to post-process the outputs computing the quantities I need.

Models: phys & chem

availability

space domain & resolution

time interval & resolution

physics

chemistry

Pre-processing & post-processing

	Area of assessment		
Description	**Local/hotspot (1 – 1000 m)**	**Urban/agglomerate (1 – 300 km)**	**Regional (25 – 10 000 km)**
Model type	Gaussian and non-Gaussian parameterised models Statistical models Obstacle resolving fluid dynamical models Lagrangian particle models	Gaussian and non-Gaussian parameterised models Eulerian chemical transport models Lagrangian particle models	Eulerian chemical transport models Lagrangian chemical models
Meteorology	Local meteorological measurements Obstacle resolving fluid dynamical models Diagnostic wind field models	Mesoscale meteorological models Localised meteorological measurements Diagnostic wind field models	Synoptic/mesoscale meteorological models
Chemistry	Parameterised or none	Ranging from none to comprehensive, depending on application	Comprehensive
Emission modelling	Bottom up traffic emissions Source specific emissions	Bottom up and/or top down emission modelling Emission process models	Top down emission modelling Emission process models
Compound	**Local/hotspot**	**Urban/agglomerate**	**Regional/continental**
PM_{10}	No chemical processes	Deposition Secondary inorganic particle formation	Deposition Primary (combustion) particles Secondary inorganic and organic particle formation Suspended dust Sea salt
$PM_{2.5}$	No chemical processes	Deposition Secondary inorganic particle formation	Deposition Secondary inorganic and organic particle formation

Source: FAIRMODE " Guidance on the use of models for the European Air Quality Directive, ETC/ACC", Bruce Denby, 2010

Models: domains and resolutions for space and time

- availability
- space domain & resolution
- time interval & resolution
- physics
- chemistry
- Pre-processing & post-processing

Resolution: there are constrains given by current legislation. The simulations shall allow the computation of the quantities the laws define.

Examples (from 50/2008/EC)

- Generally, hourly resolution is an accepted standard.
- For industrial areas concentrations should be representative of a 250 x 250 m area.
- For traffic emissions the assessment should be representative for a 100 m street segment.
- Urban background concentrations should be representative of several square kilometres.

Domains: There are constrains given by assessment type

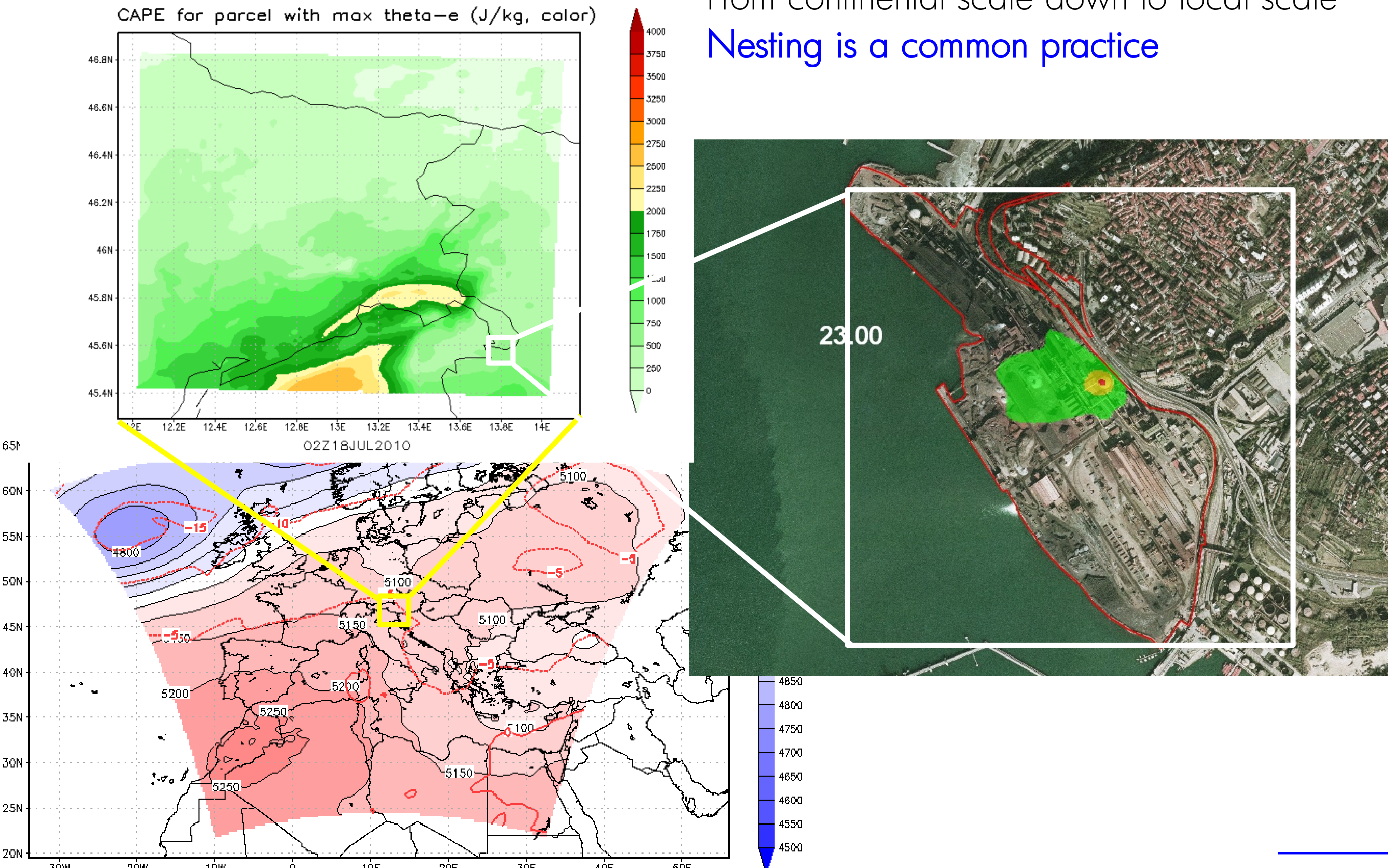
Examples

- Air quality forecasts: from +48H to 96H – specific area
- Mitigation plans: one or more years – administrative area
- New plants impacts: at least one year – potentially affected area

Examples of domains

From continental scale down to local scale

Nesting is a common practice



Available guidance tools for numerical models selections

A comprehensive listing of air quality models used in Europe can be found at:

- EIONET Model Documentation System
  http://air-climate.eionet.europa.eu/databases/MDS/index_html

- COST728
  http://www.mi.uni-hamburg.de/Model-Inventory.6295.0.html?&no_cache=1

Emission modelling tools list and description can be found in:

- EMEP/EEA air pollutant emission inventory guidebook
  http://www.eea.europa.eu/publications/emep-eea-emission-inventory-guidebook-2009

Inputs: meteorology, land use, orography and immersed bodies

The choice has to be made according to:

- models features and sensibilities
- simulation type
- regulation constrains

meteorology →

Assessment	Forecasts	Scenarios
• Measurements+Models • Models	• Models	• Measurements+Models

land use, **orography** →

According to:

- space and time resolution
- availability of local databases

immersed bodies →

According to:

- space resolution
- availability of body details

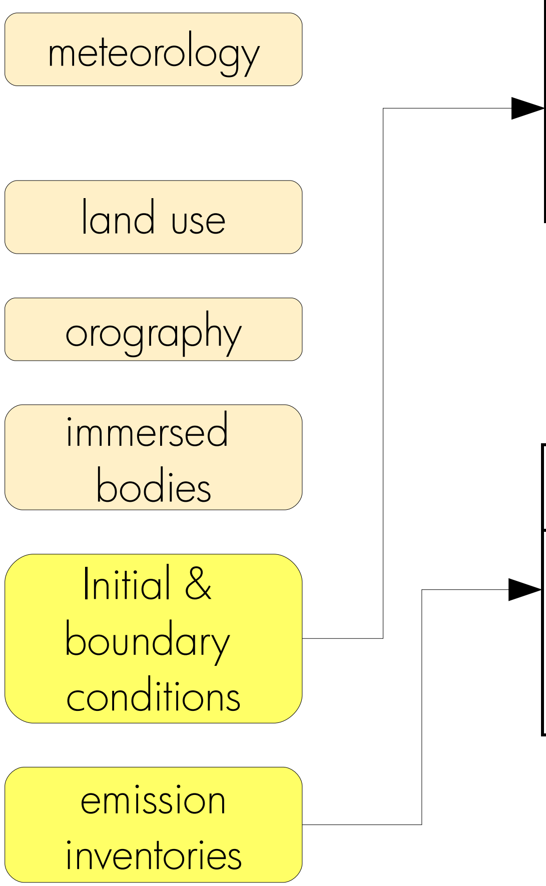
Initial & boundary conditions

emission inventories

Inputs: initial, boundary conditions and emission sources

The choice has to be made according to:

- models features and sensibilities
- simulation type
- regulation constrains

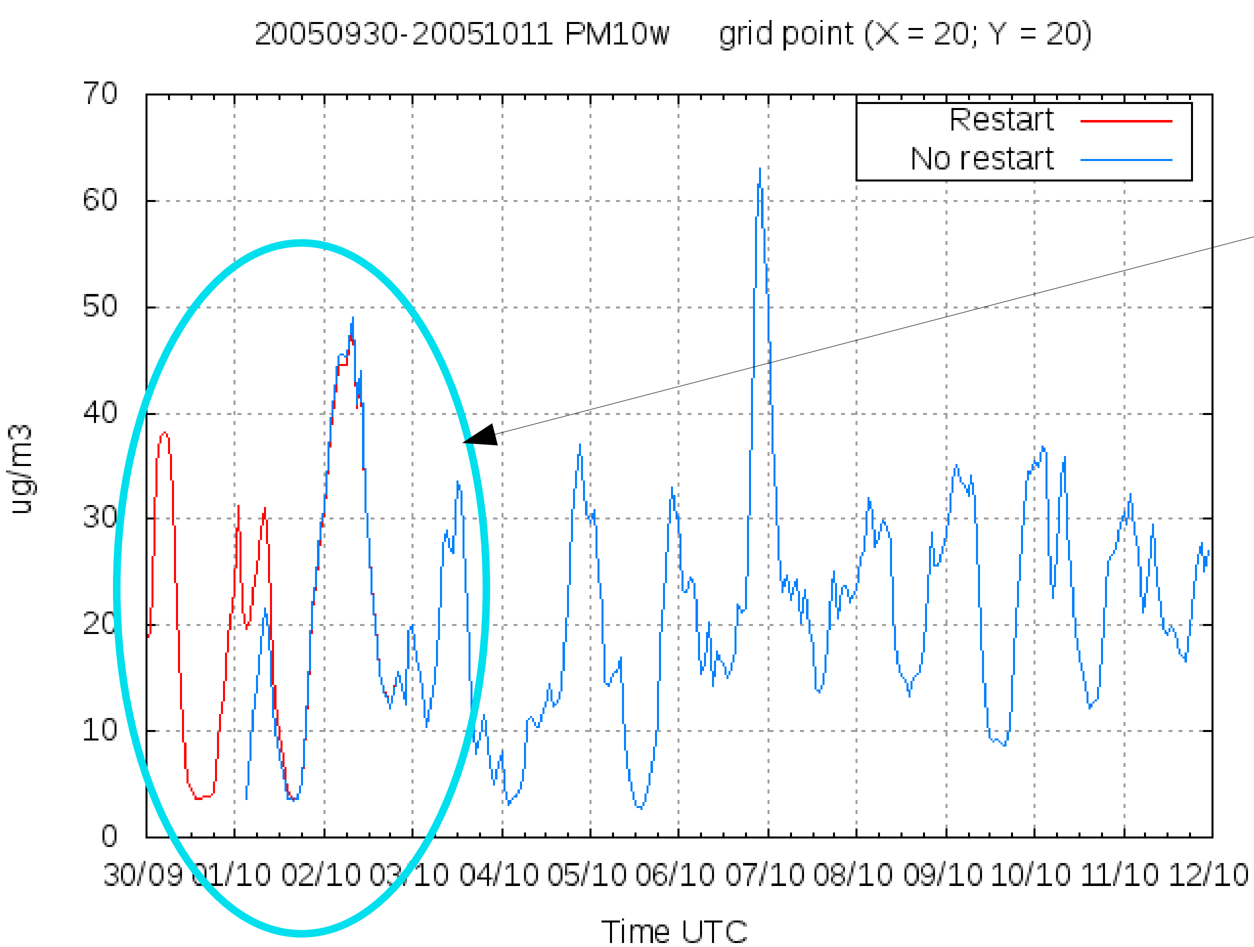


Assessment	Forecasts	Scenarios
• Models • Climatological dataset	• Models	• Models • Climatological dataset

Assessment	Forecasts	Scenarios
• Inventories • Emission process models • Emission monitoring	• Inventories • Emission process models	• Inventories

Example of initial conditions influences on Friuli Venezia Giulia domain

- Eulerian chemical transport model (FARM ®Arianet) – domain 160 km x 160 km – resolution 4 km
- Regional scale emission inventory
- Climatological boundary conditions



One month simulation

The memory of initial conditions disappear in about 12 hours

Assessment mode simulation

Example of boundary conditions influences on Friuli Venezia Giulia domain

Boundary conditions sensitivity experiment

- Eulerian chemical transport model (FARM ®Arianet) – domain 160 km x 160 km – resolution 4 km
- Regional scale emission inventory (INEMAR ARPA FVG) – high space and time resolution
- Simulated boundary condition – continental model (FARM ®Arianet)
- No initial conditions
- Air quality forecasts mode simulation
- Meteorological input WRF (http://www.wrf-model.org)
- Off line mode

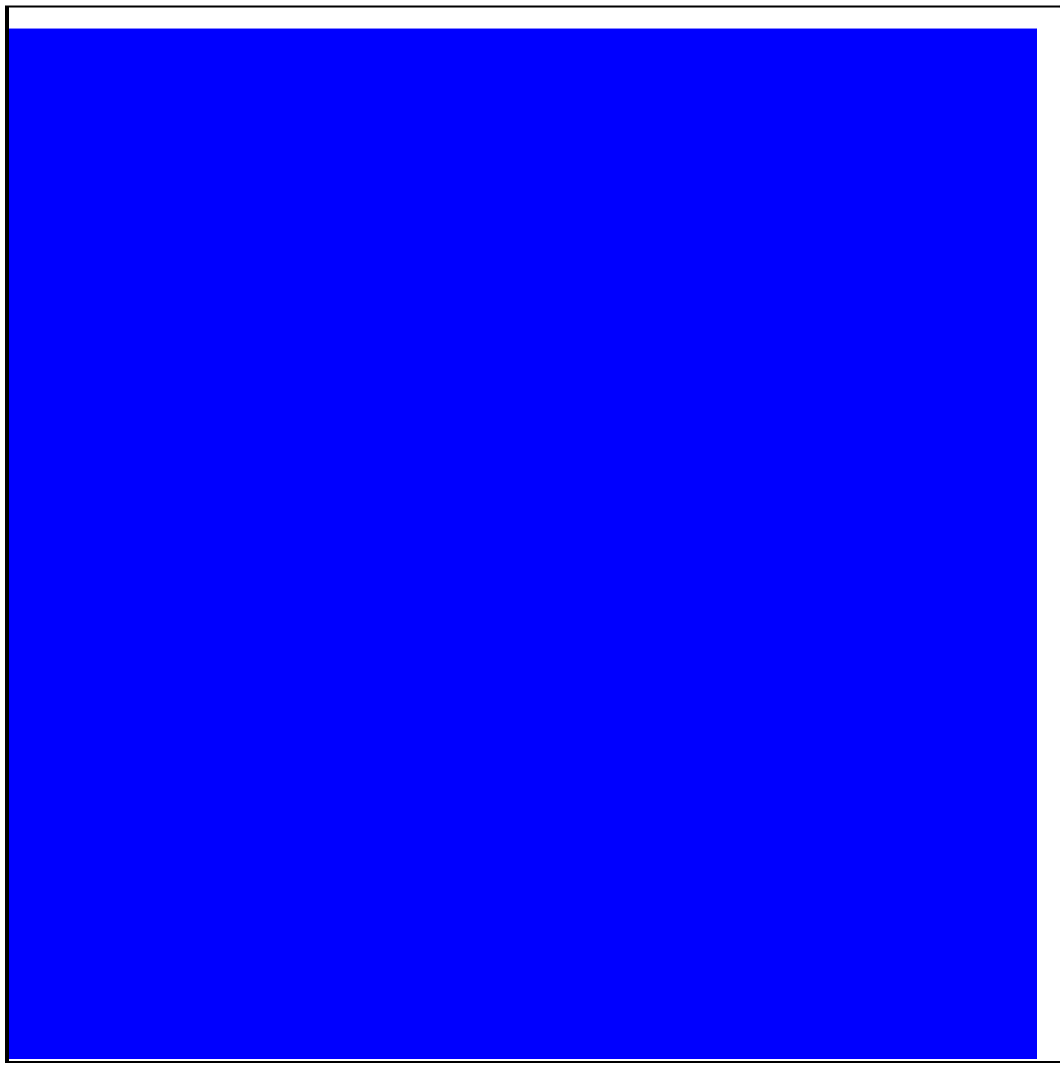
Results

For small domains, boundary conditions are extremely relevant to achieve reliable particulate matter simulations

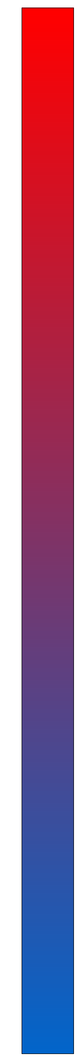
FARM is an Eulerian grid model for dispersion, transformation and deposition of reactive pollutants (photochemistry and aerosols) It is derived from STEM prof. G.R. Carmichael *et al.*, CGRER (Center for Global and Regional Environmental Research), University of Iowa, USA – Available under contract from ARIANET company - Italy

Example of boundary conditions influences: 00UTC Jul 26, 2011 - PM10

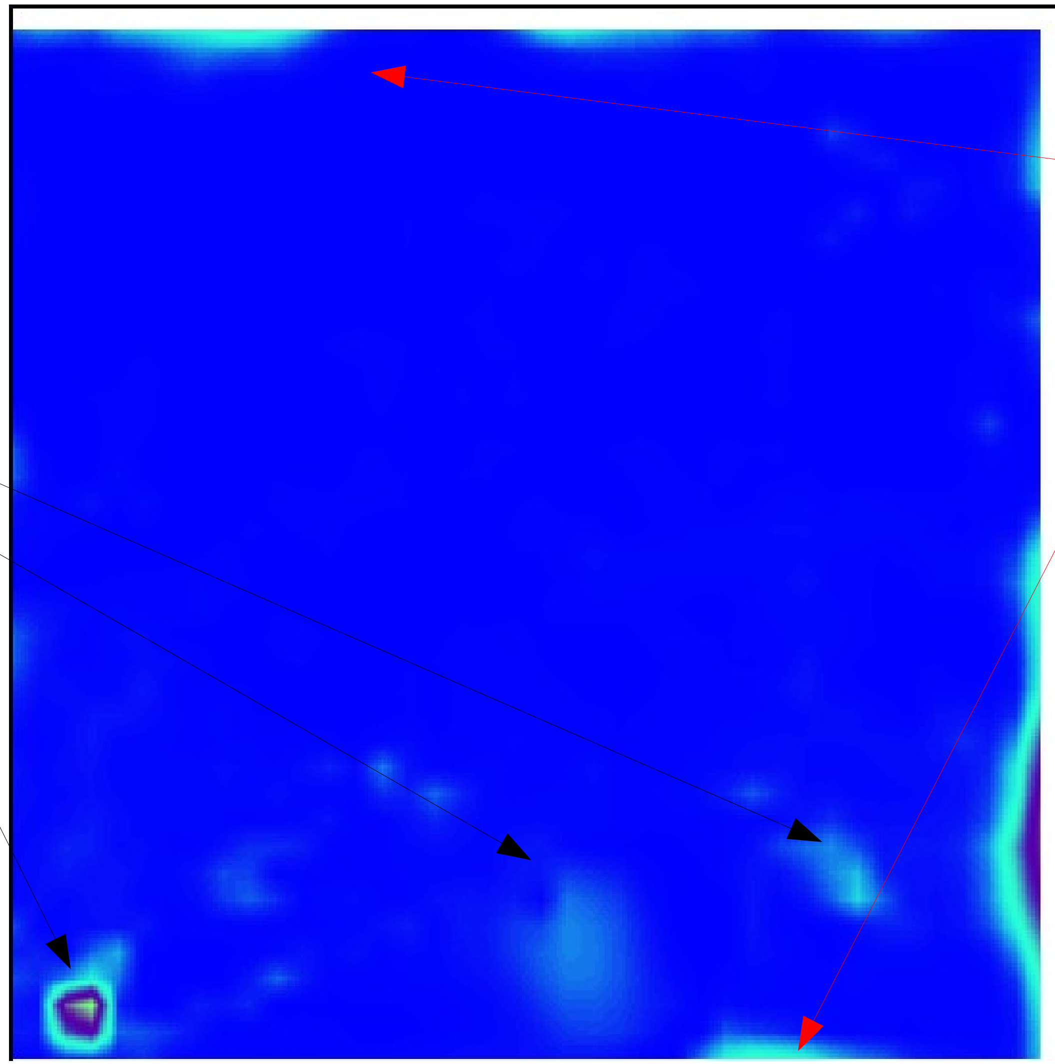
Clean domain



Colors scale



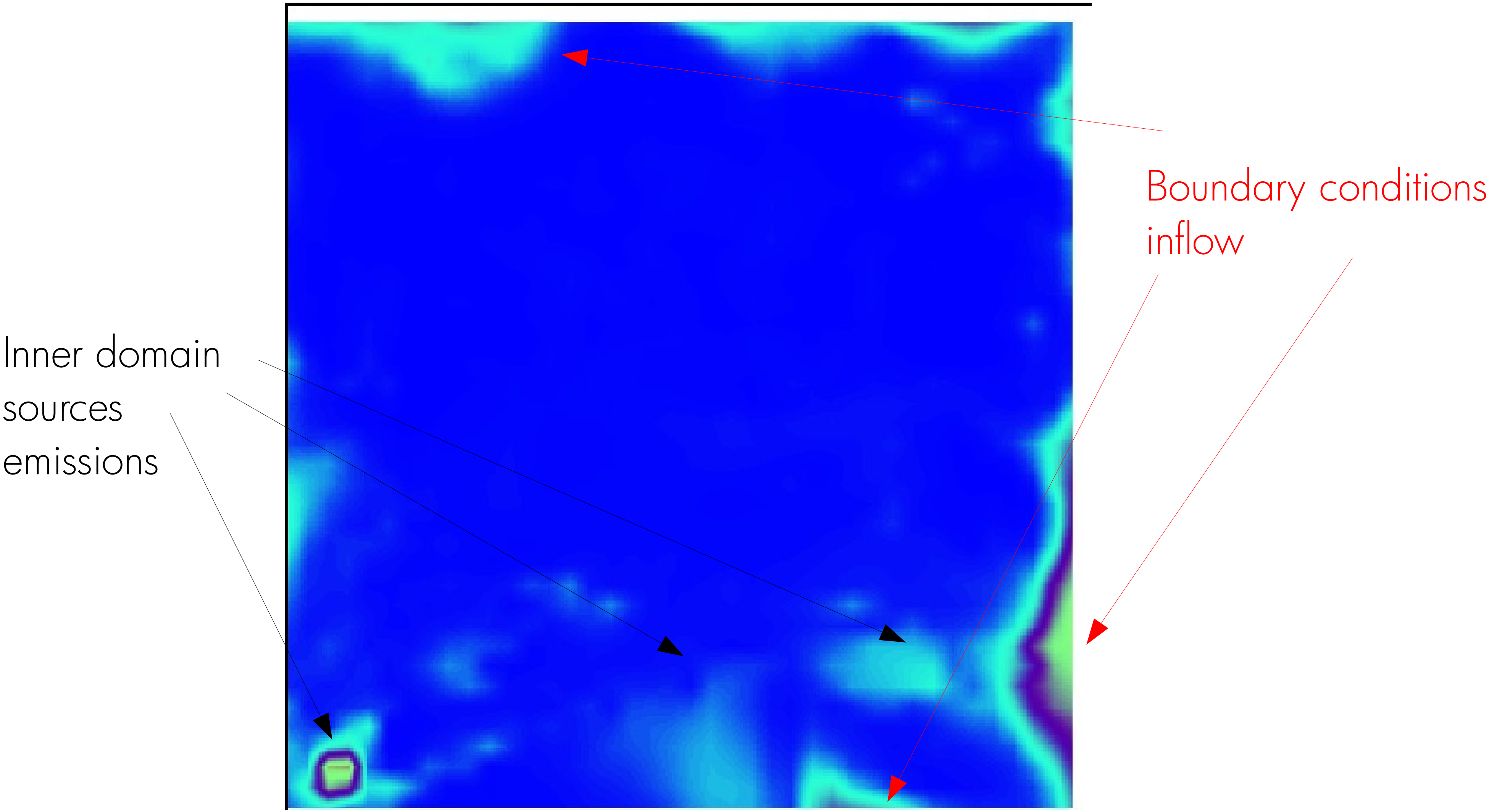
Example of boundary conditions influences: 01UTC Jul 26, 2011 - PM10



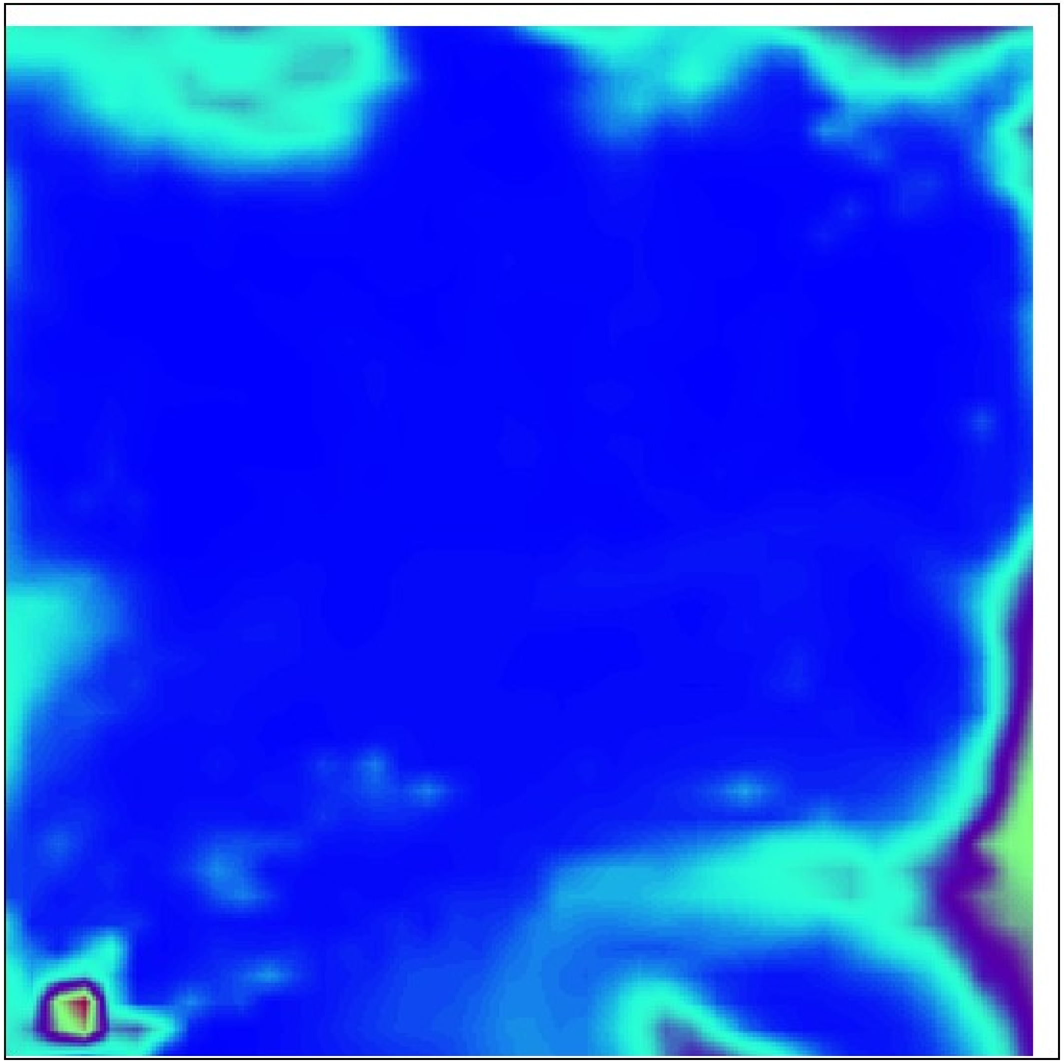
Boundary conditions inflow

Inner domain sources emissions

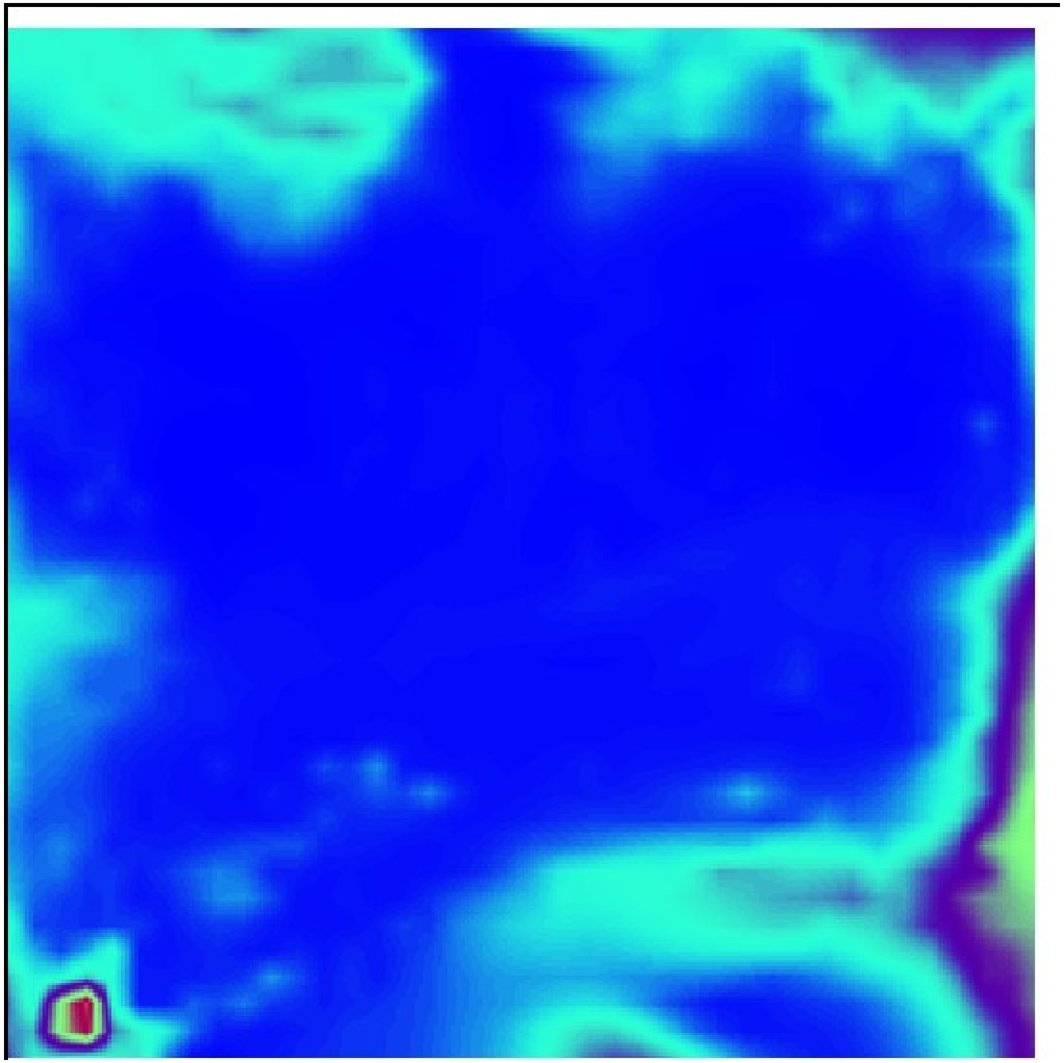
Example of boundary conditions influences: 02UTC Jul 26, 2011 - PM10



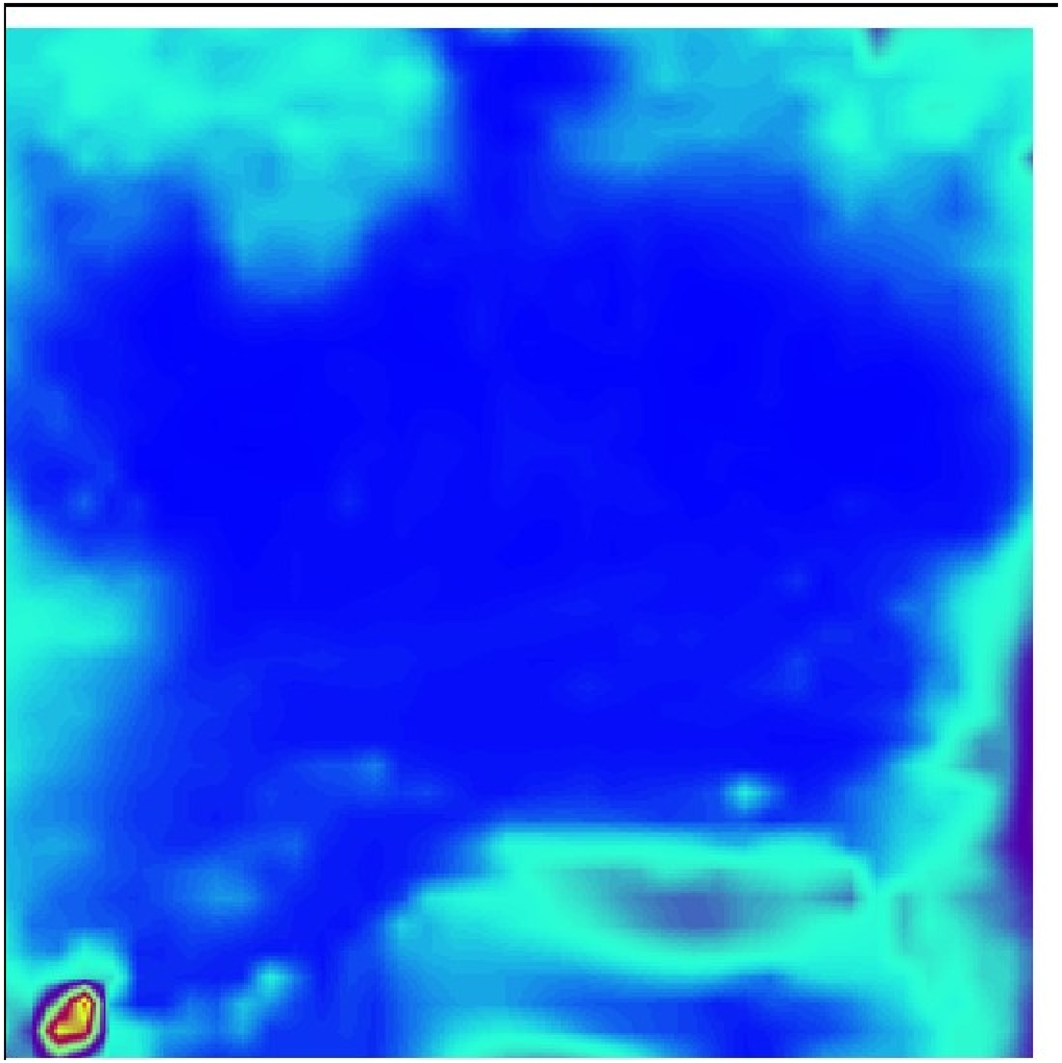
Example of boundary conditions influences: 03UTC Jul 26, 2011 - PM10



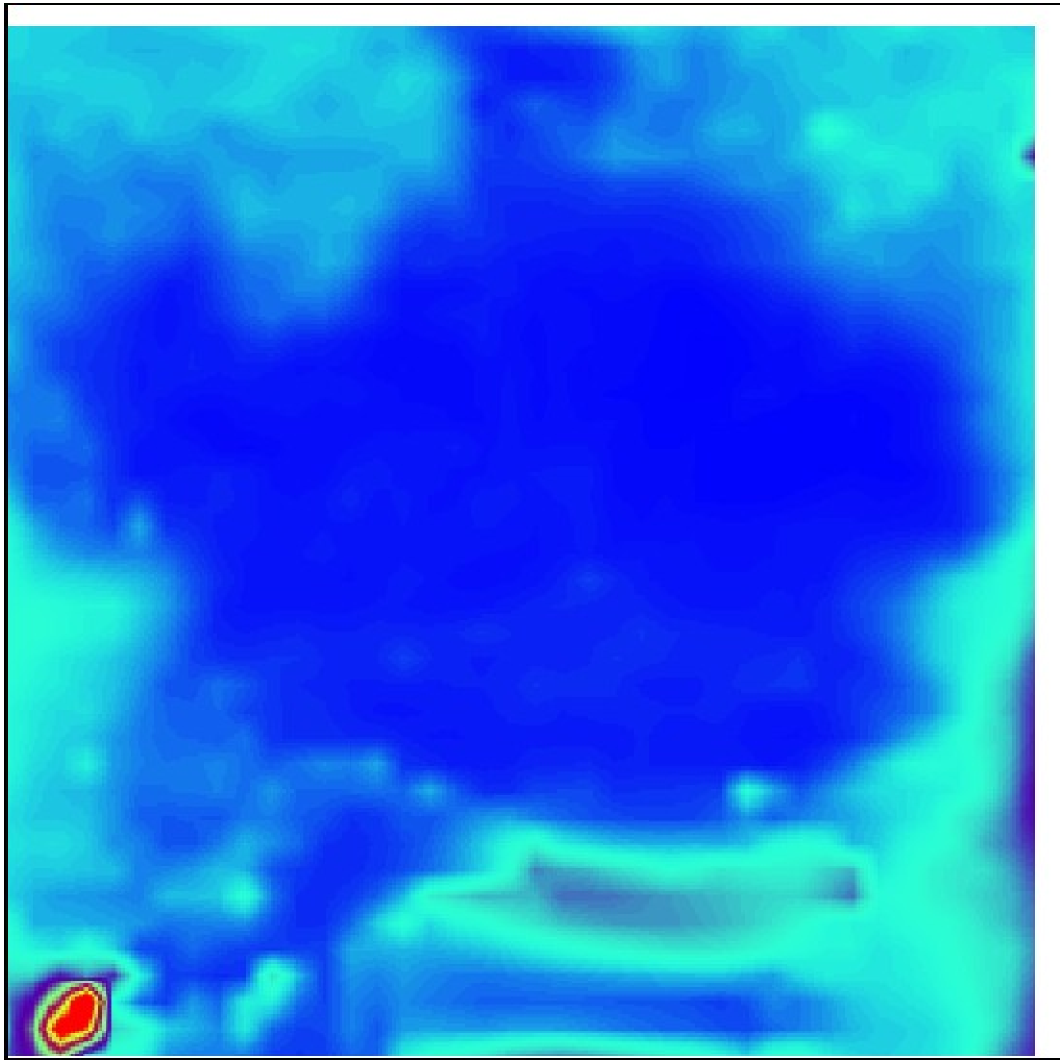
Example of boundary conditions influences: 04UTC Jul 26, 2011 - PM10



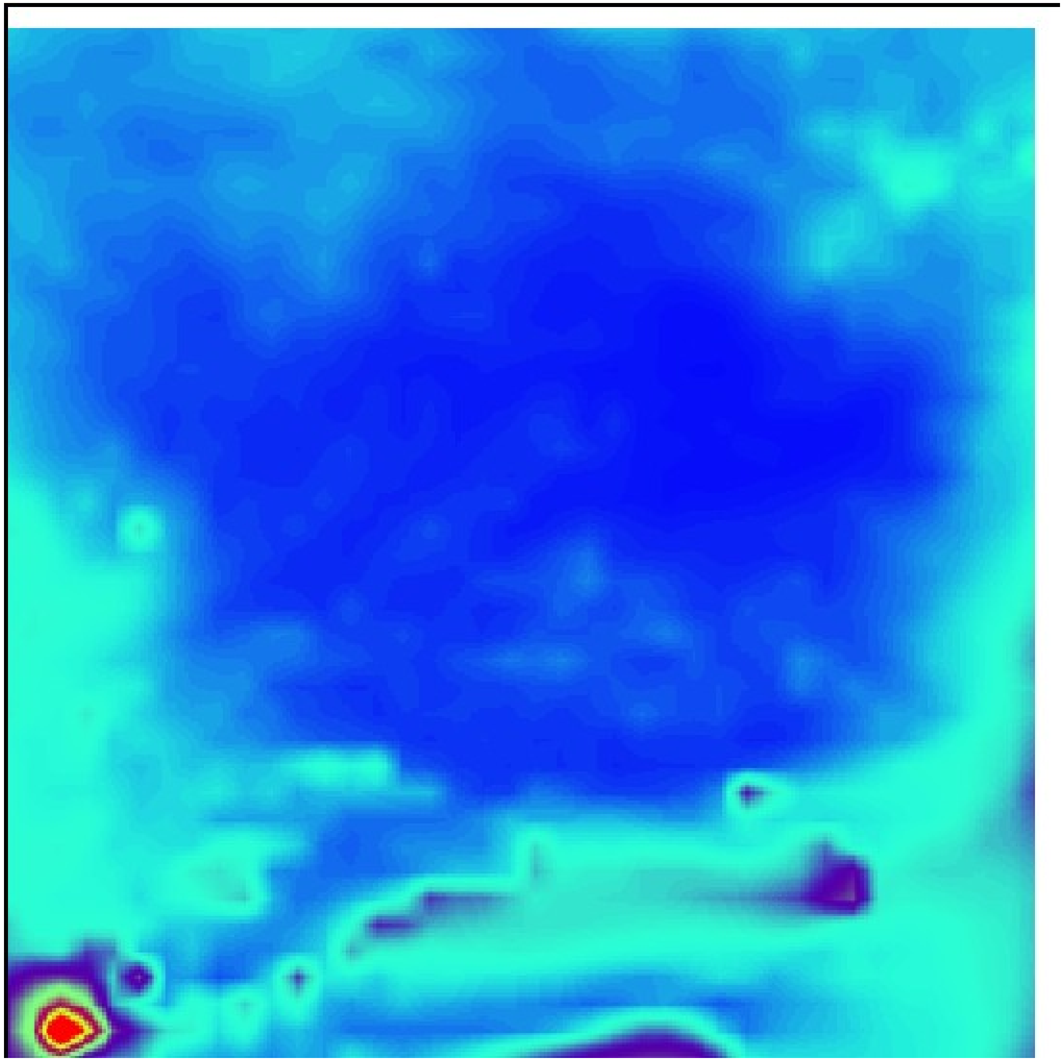
Example of boundary conditions influences: 05UTC Jul 26, 2011 - PM10



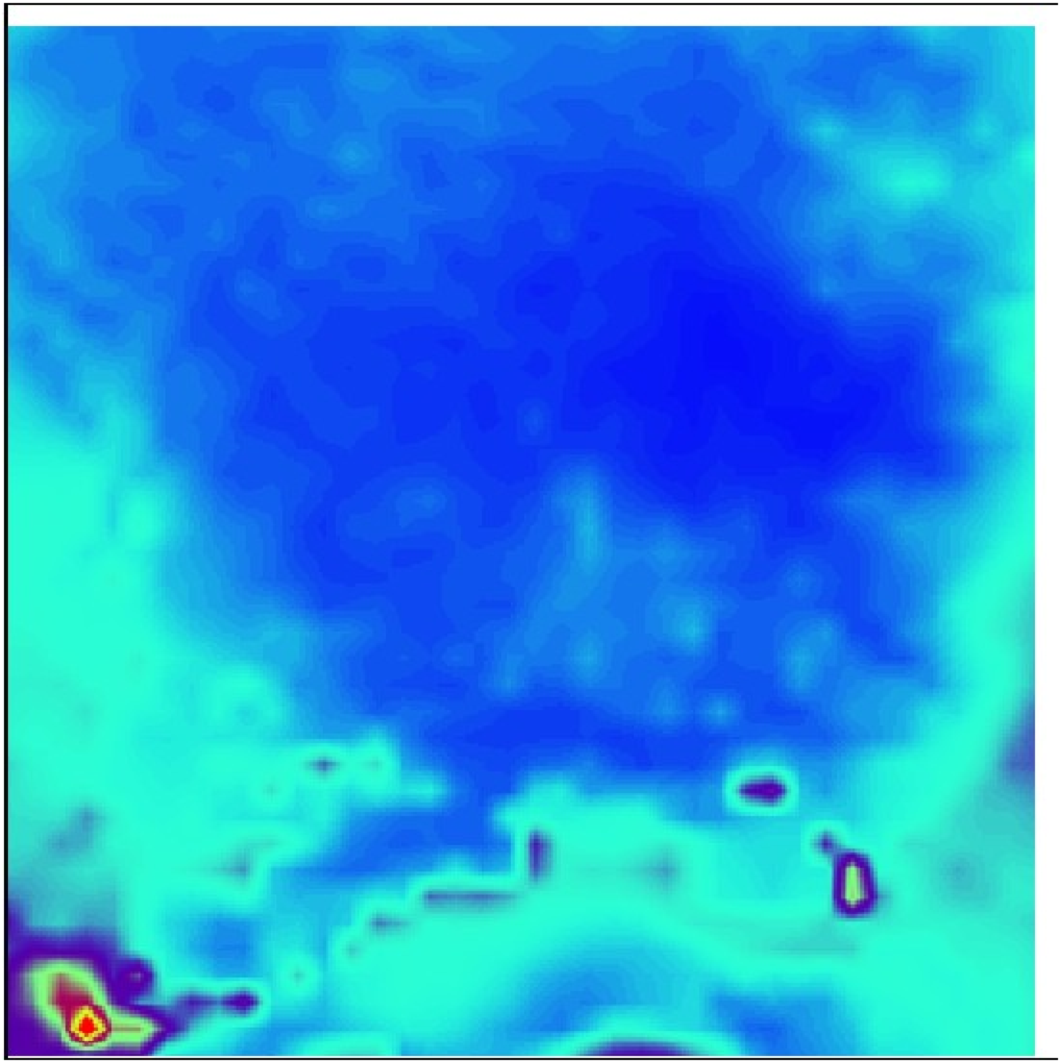
Example of boundary conditions influences: 06UTC Jul 26, 2011 - PM10



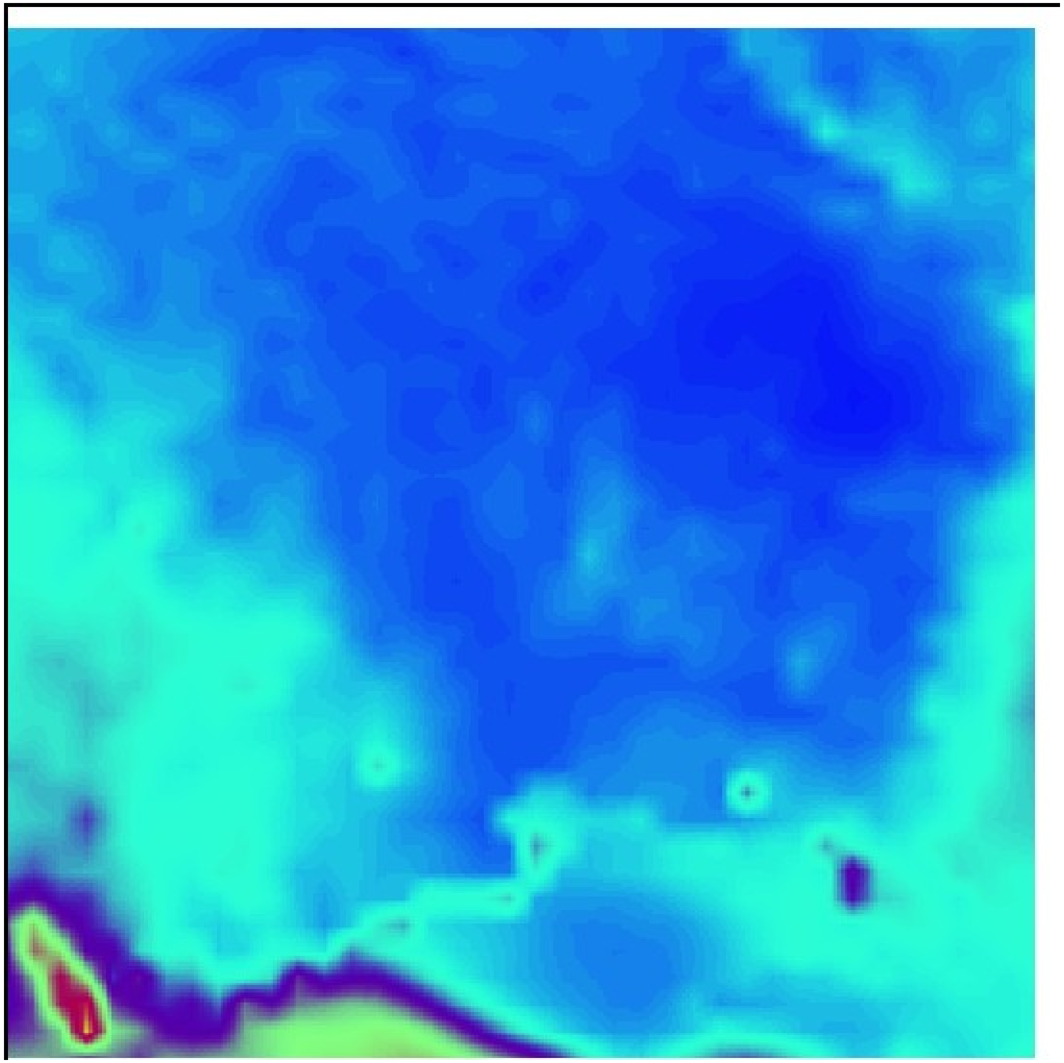
Example of boundary conditions influences: 08UTC Jul 26, 2011 - PM10



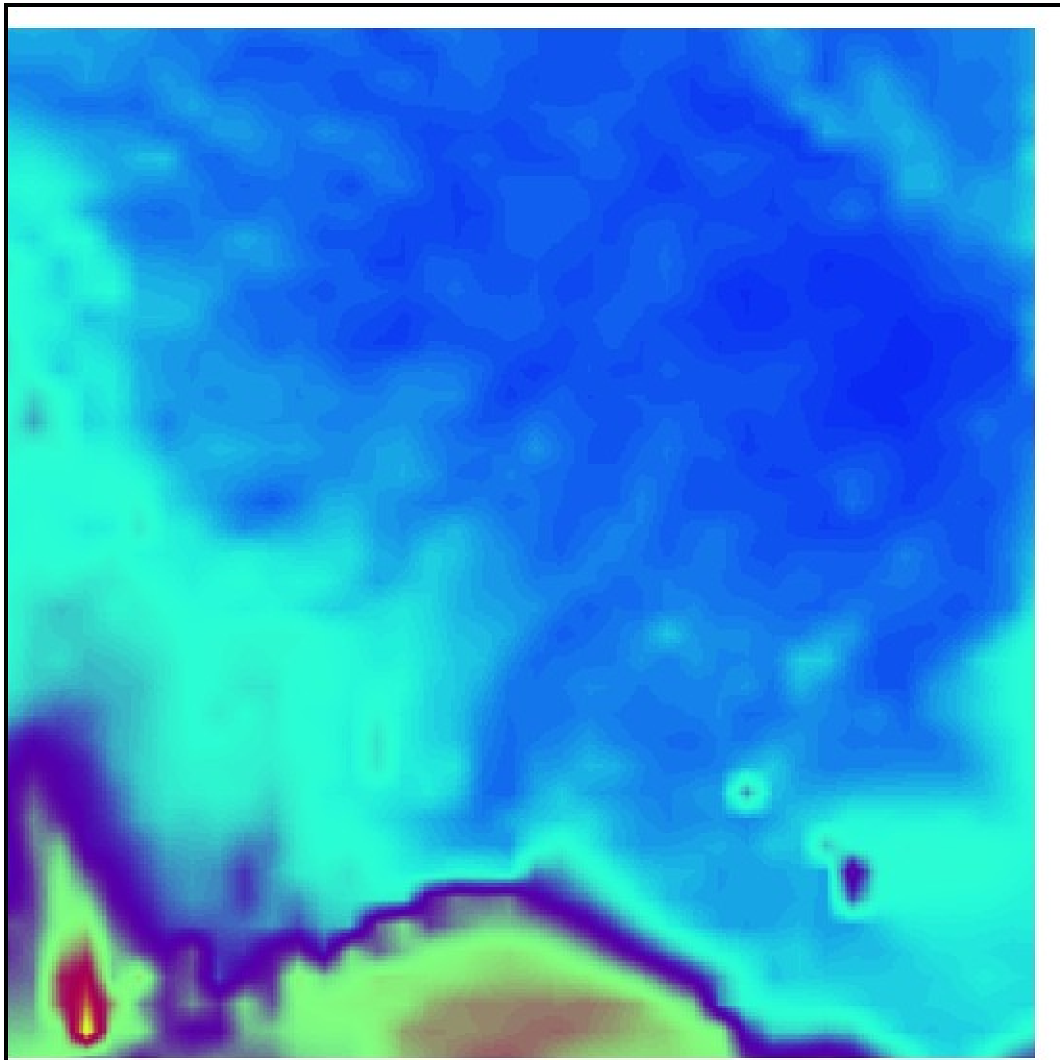
Example of boundary conditions influences: 10UTC Jul 26, 2011 - PM10



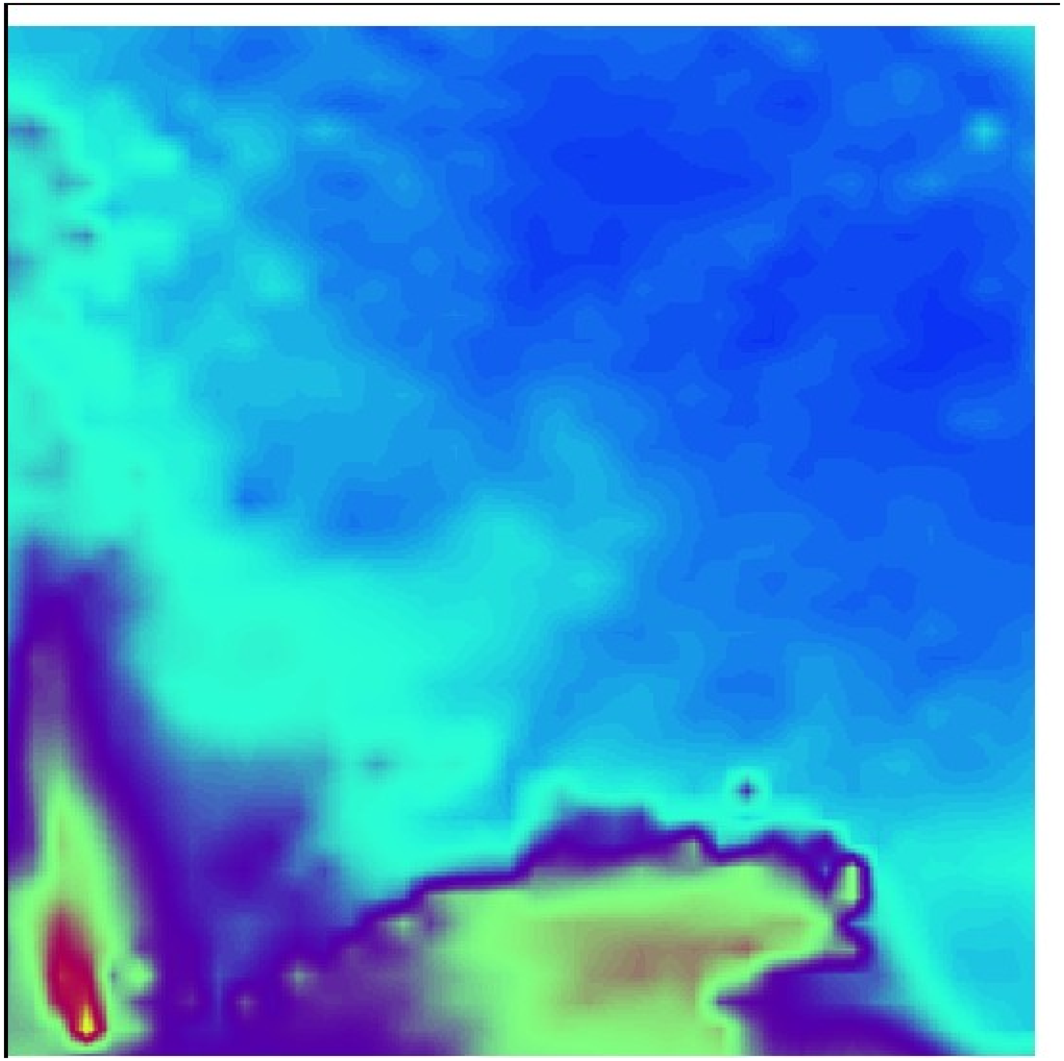
Example of boundary conditions influences: 12UTC Jul 26, 2011 - PM10



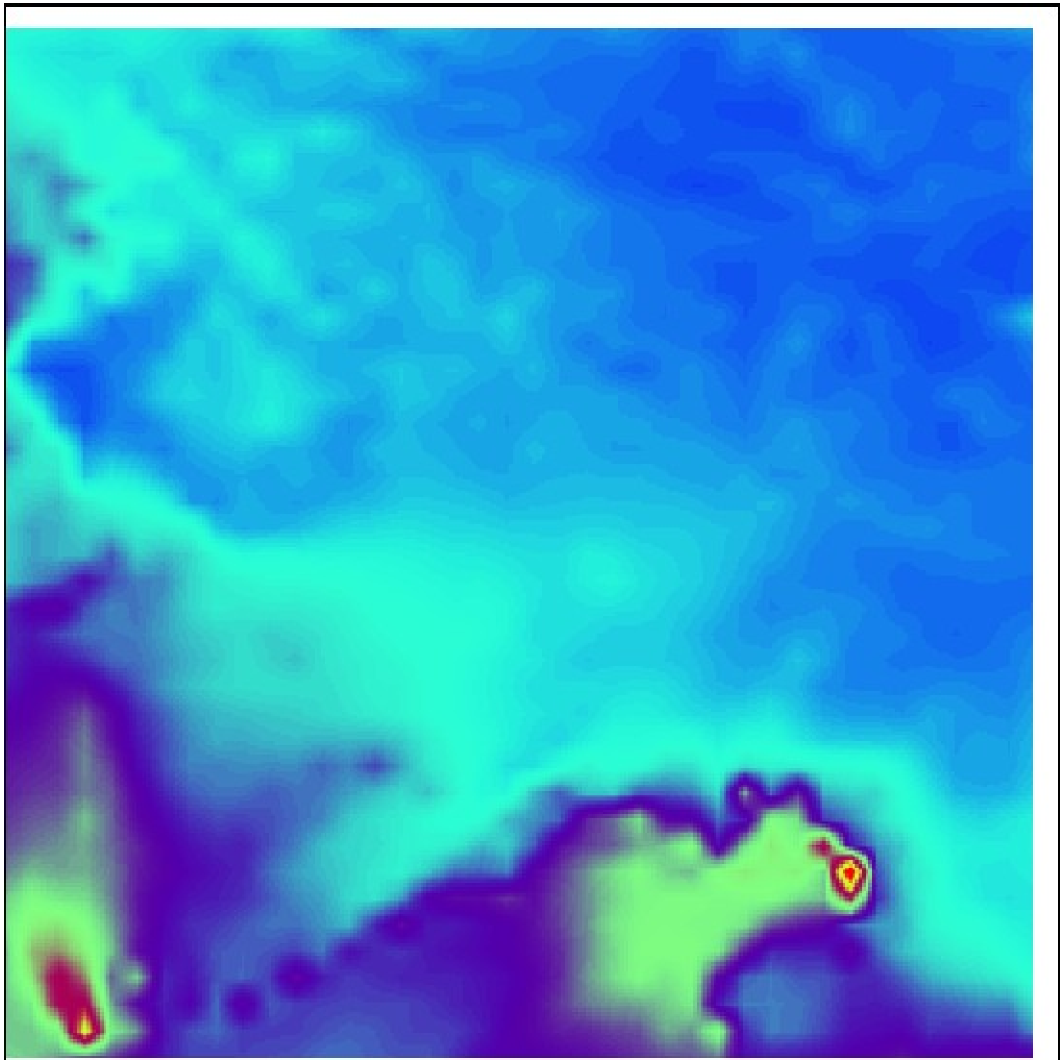
Example of boundary conditions influences: 14UTC Jul 26, 2011 - PM10



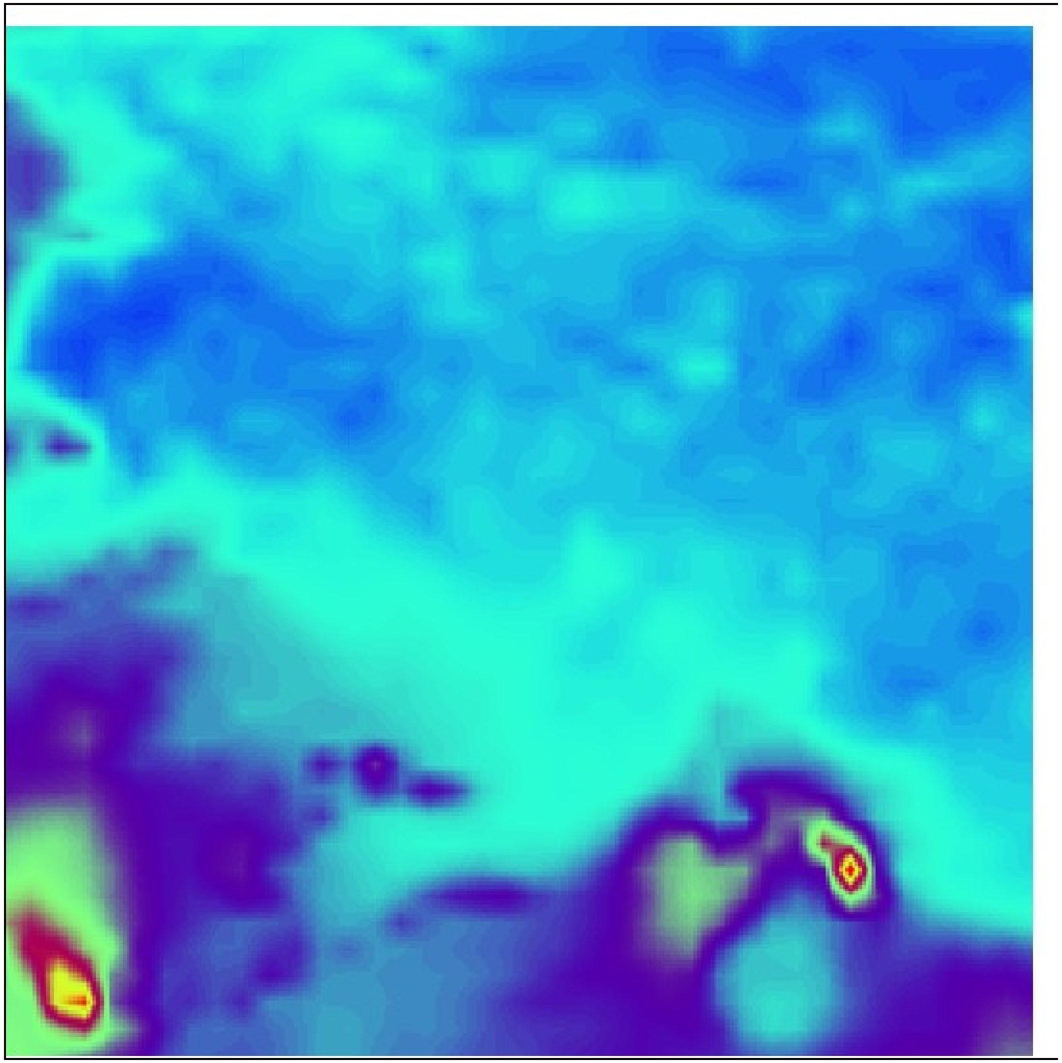
Example of boundary conditions influences: 16UTC Jul 26, 2011 - PM10



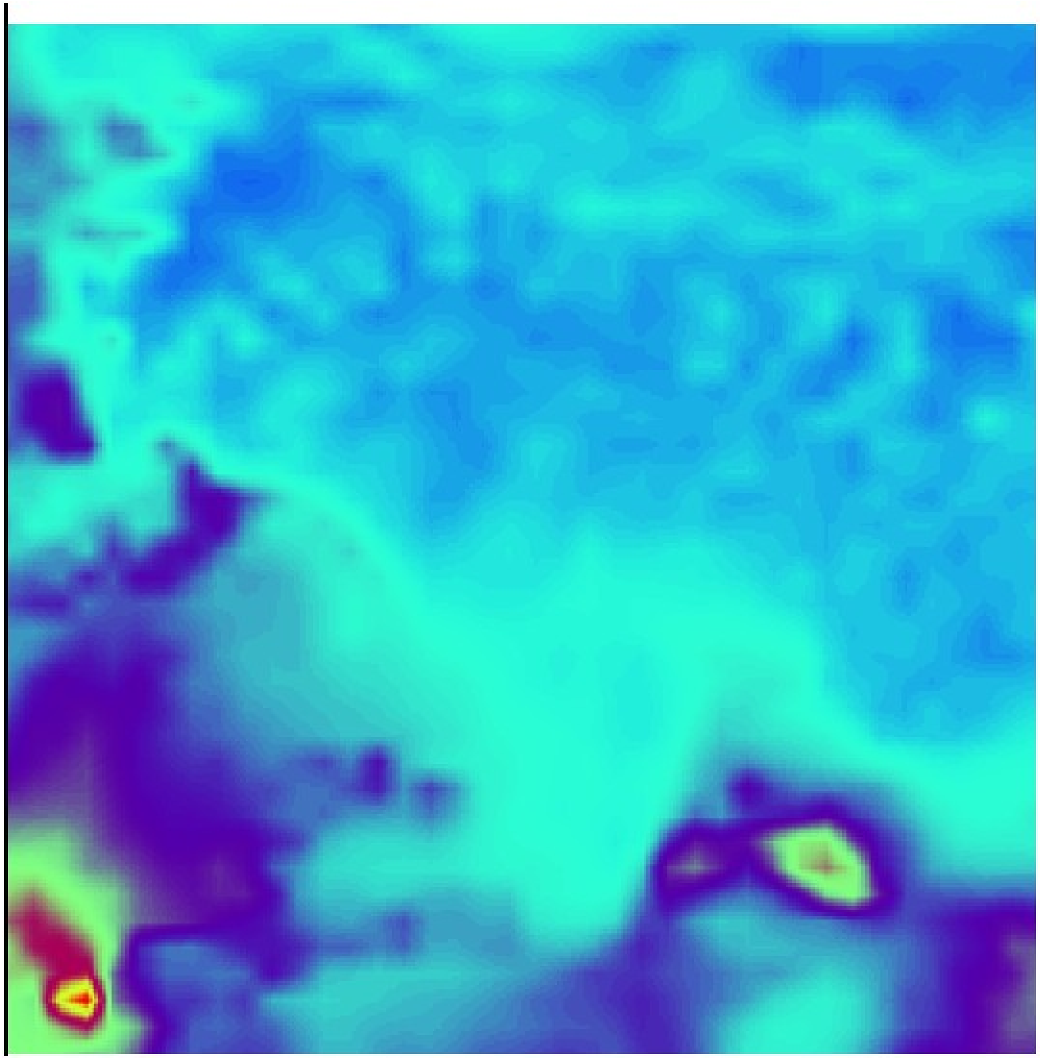
Example of boundary conditions influences: 18UTC Jul 26, 2011 - PM10



Example of boundary conditions influences: 20UTC Jul 26, 2011 - PM10



Example of boundary conditions influences: 22UTC Jul 26, 2011 - PM10



Resources make the choice several time

human & knowledge →

People having skill in: [There is an efficient group]

- the organization of the simulation and its steering;
- the use of the numerical models (in HPC environment);
- the critical evaluation of the inputs and the outputs;
- establishing links between legislation requirements and simulation tools;

computation / **storage** →

- computation power capable to keep simulations below an acceptable threshold [HPC & GRID environments];
- organization of the simulation data archives and efficient information retrieval procedures and utilities;

time (deadlines) →

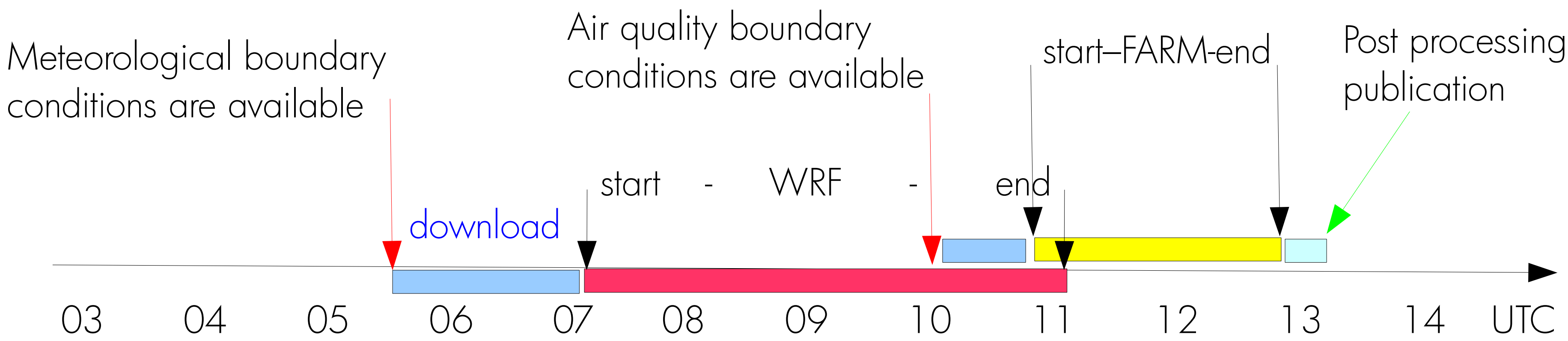
Working time to be considered

- simulation projects and work flow definition;
- work flow implementation;
- computational time;
- outputs validation, data analysis, results presentation;

Example of resources required

<u>Example 1(HPC)</u>

Operational air quality forecasts for Friuli Venezia Giulia +96H (24 cores for WRF)



<u>Example 2 (HTC)</u>

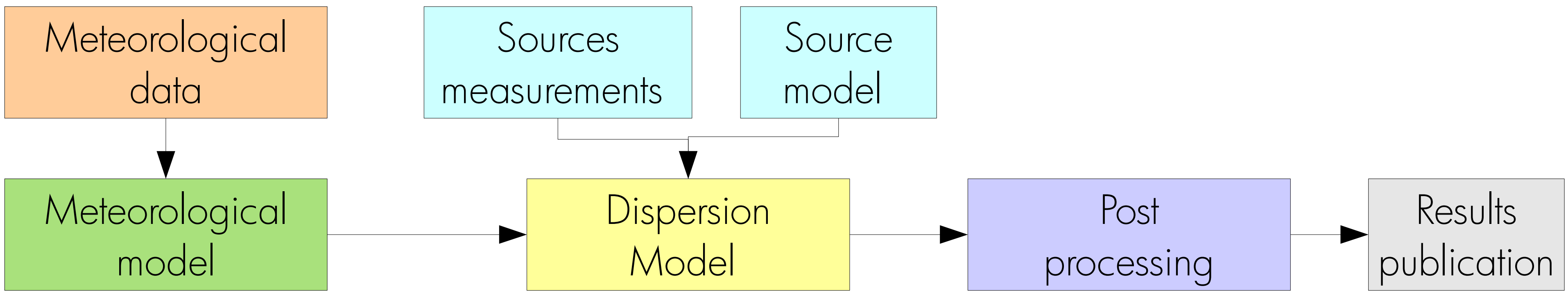
Air quality scenarios Friuli Venezia Giulia (computation only)

- 1/3 hour-core for one simulation day
- 365 days of simulation
- 2 hour-core for one scenario post-proccesing
- 15 scenarios

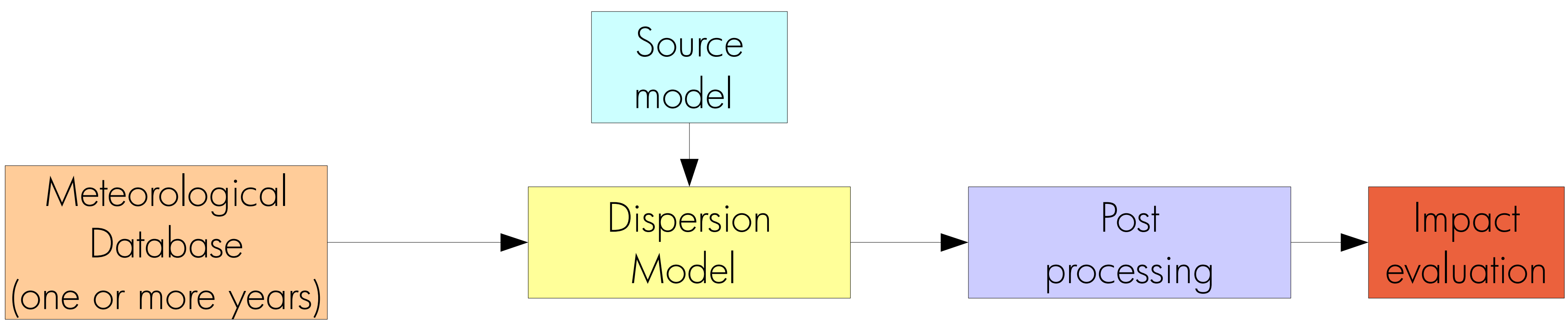
About 1800 hours-core

Diagnostic simulations for PM10: big industrial plants impacts evaluation - workflow

Off-line model simulations are suitable for single or a few sources impacts evaluation

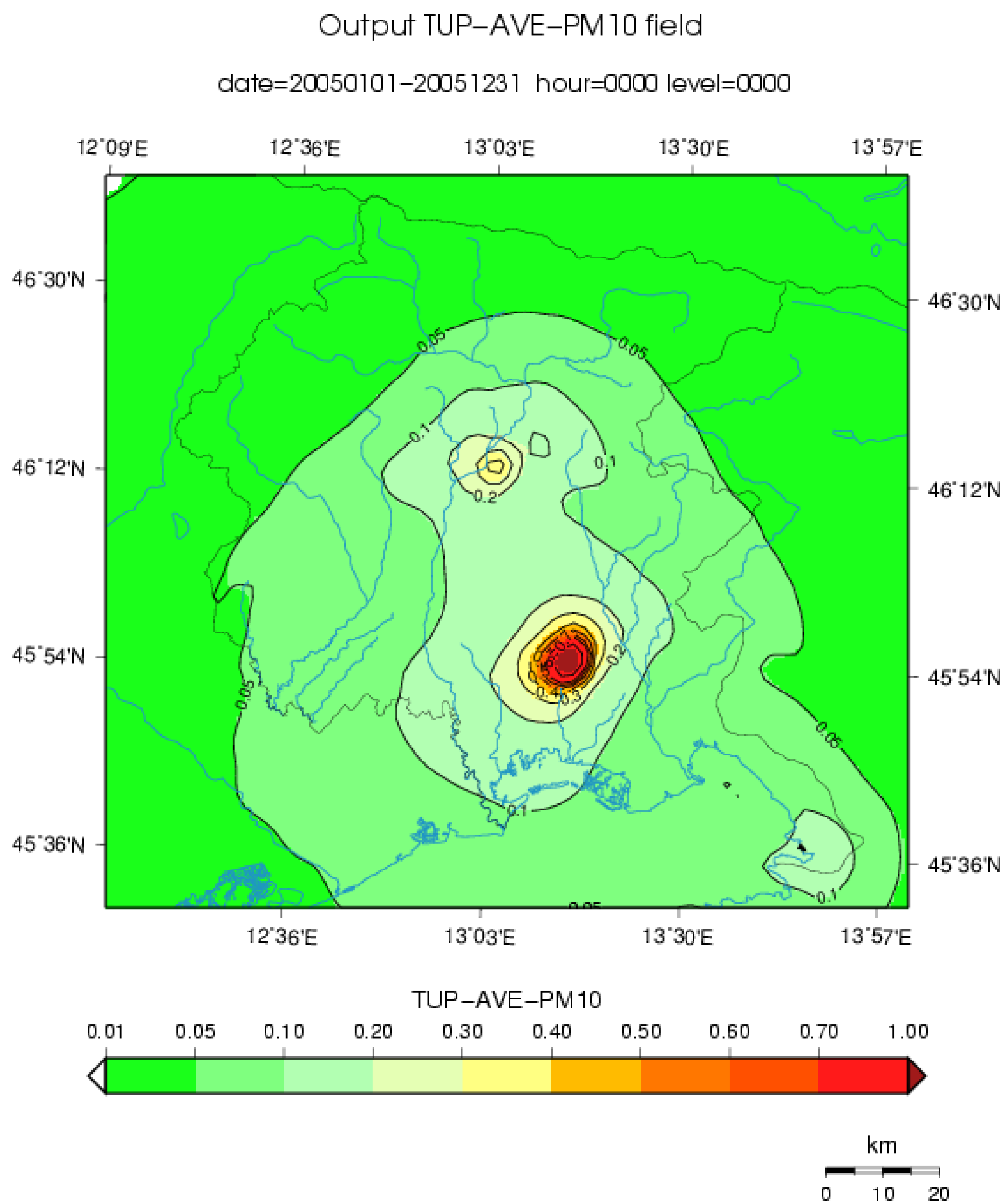


Environmental monitoring: daily run over past 24 hours



Impact evaluation: one (or more) yearly run over past weather (climate)

Diagnostic simulations for PM10: big industrial plants impacts evaluation



Model

CALMET-CALPUFF chain (off-line)

Emissions

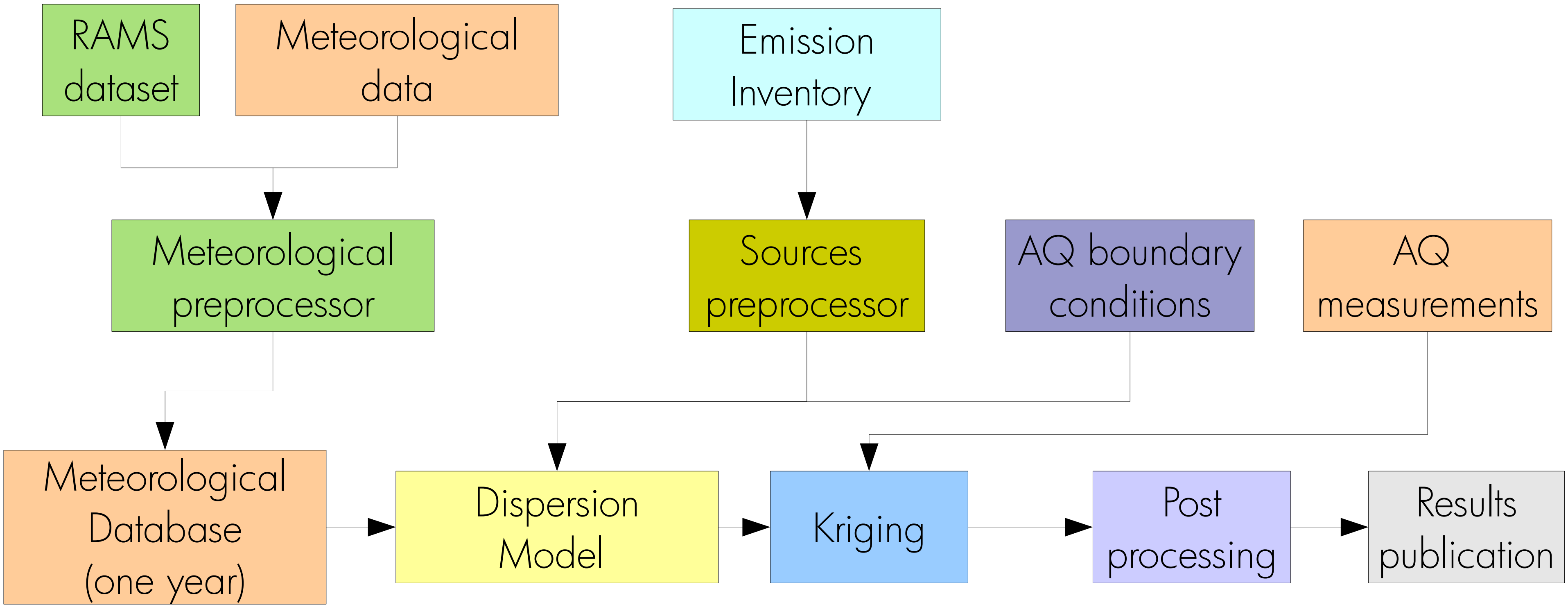
Industrial plants emission model

Meteorology

2005 mesonetwok measurements, sea temperature, radiosounding WMO 16044, ECMWF reanalysis boundary conditions and cloud cover, sea surface temperature

Diagnostic simulations for PM10: air quality evaluation – workflow

Off-line model simulations are suitable for air quality evaluations in regional domains



Diagnostic simulations for PM10: air quality evaluation – daily average concentration

Model

FARM (off-line) + kriging on air quality measurements

Emissions

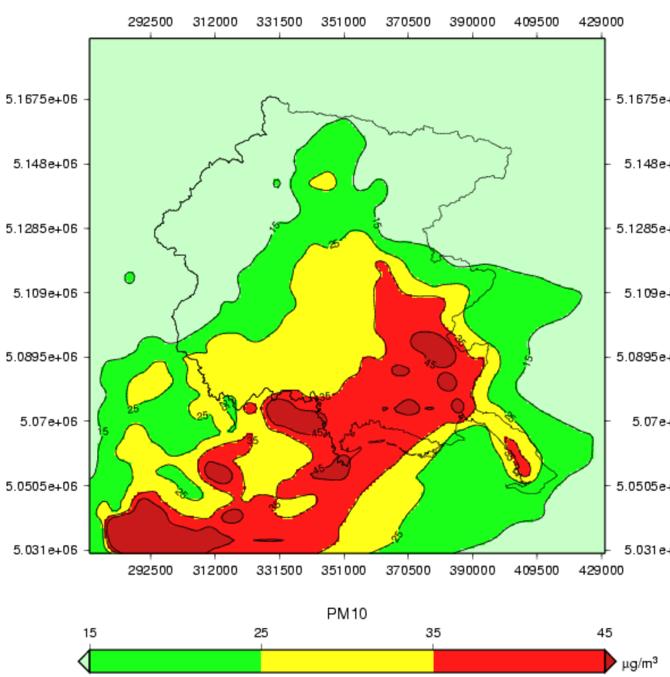
Whole regional inventory (point sources, traffic, diffuse, etc)

Meteorology

RAMS simulations and 2005 mesonetwok measurements

Boundary conditions

National dataset + EU dataset



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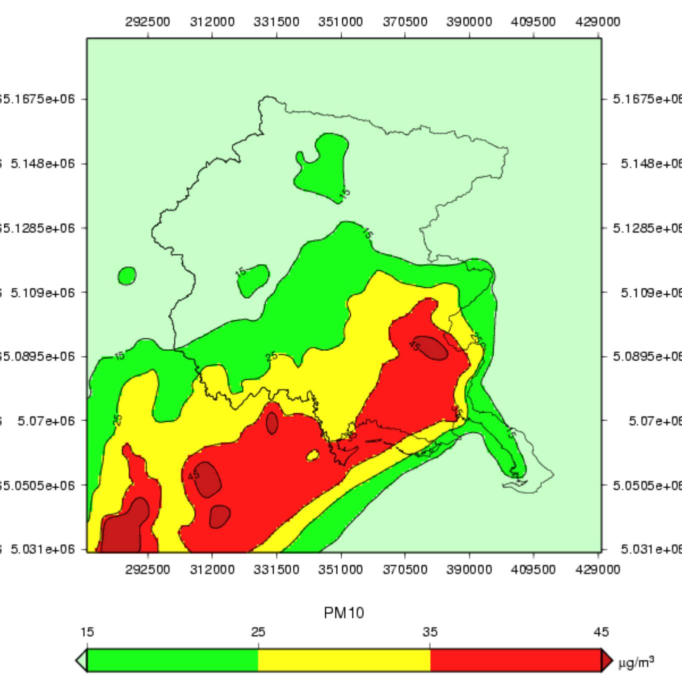

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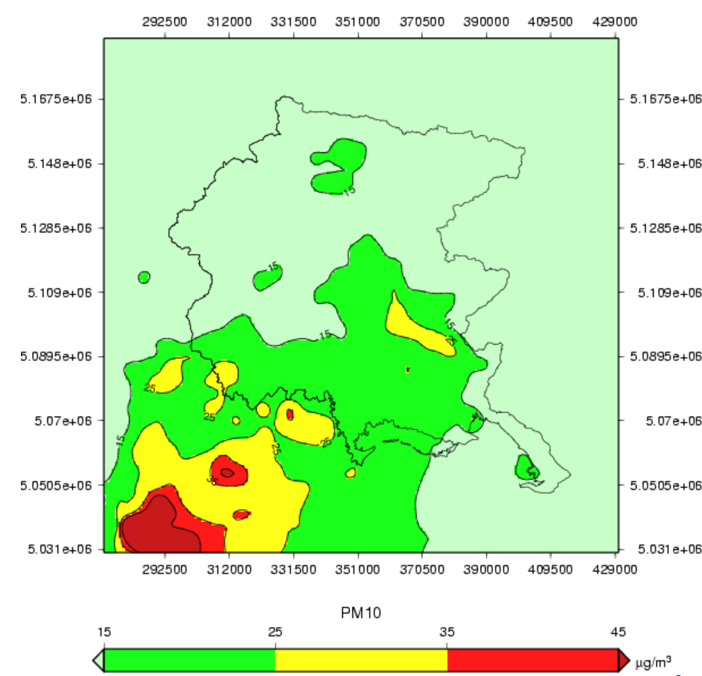

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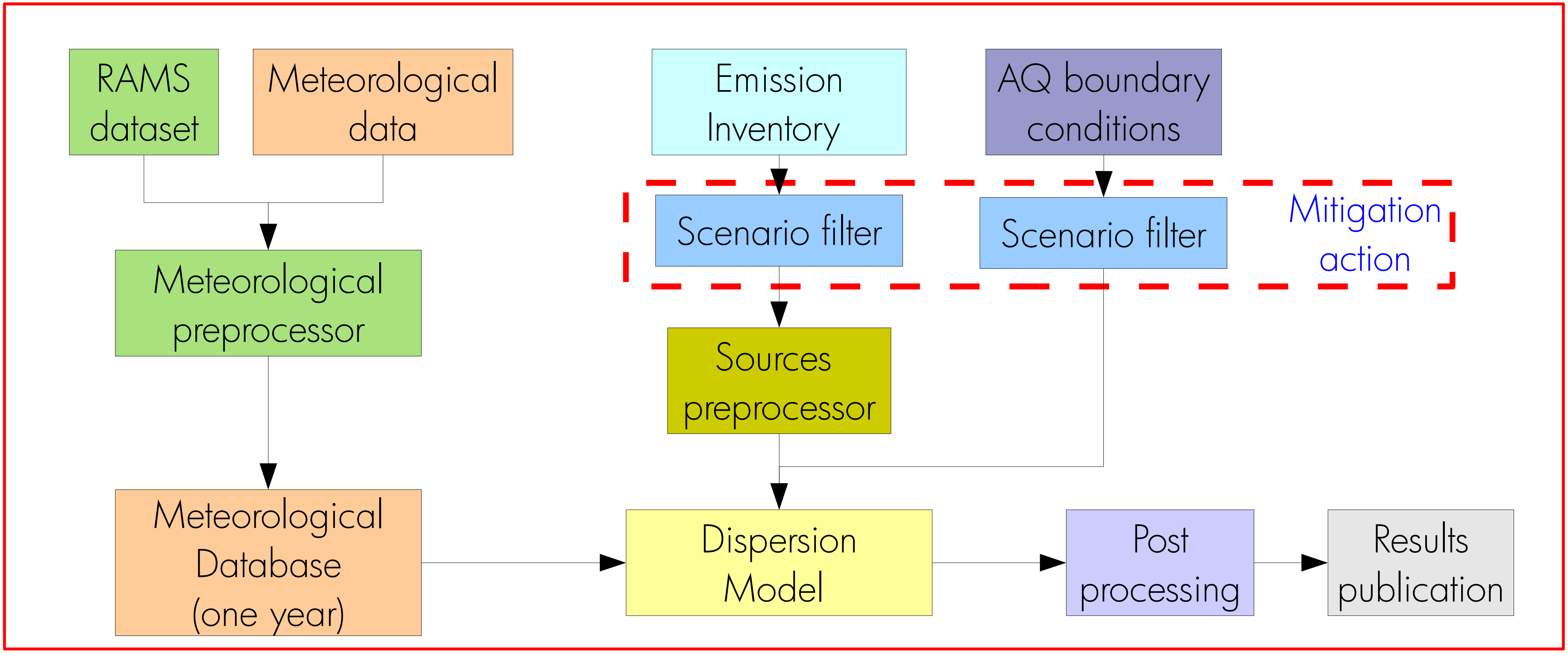
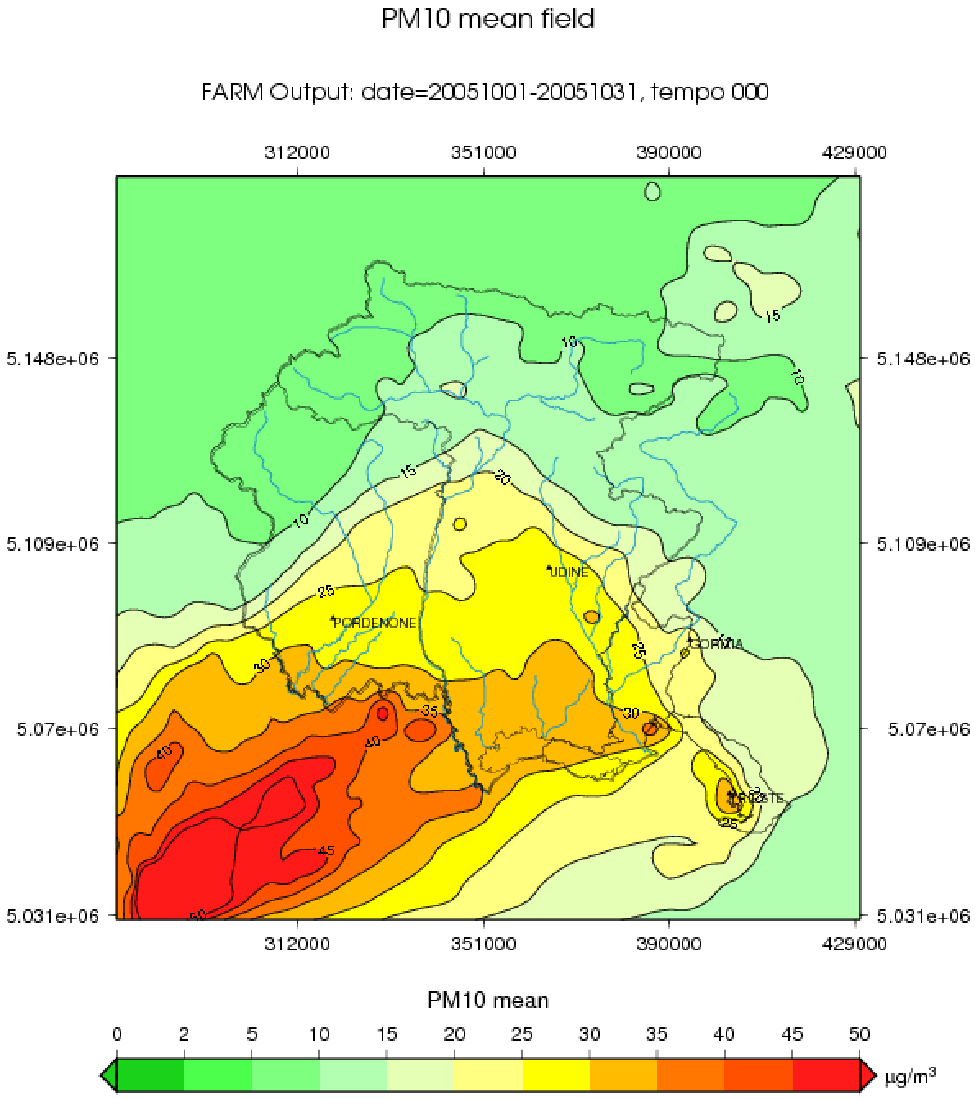
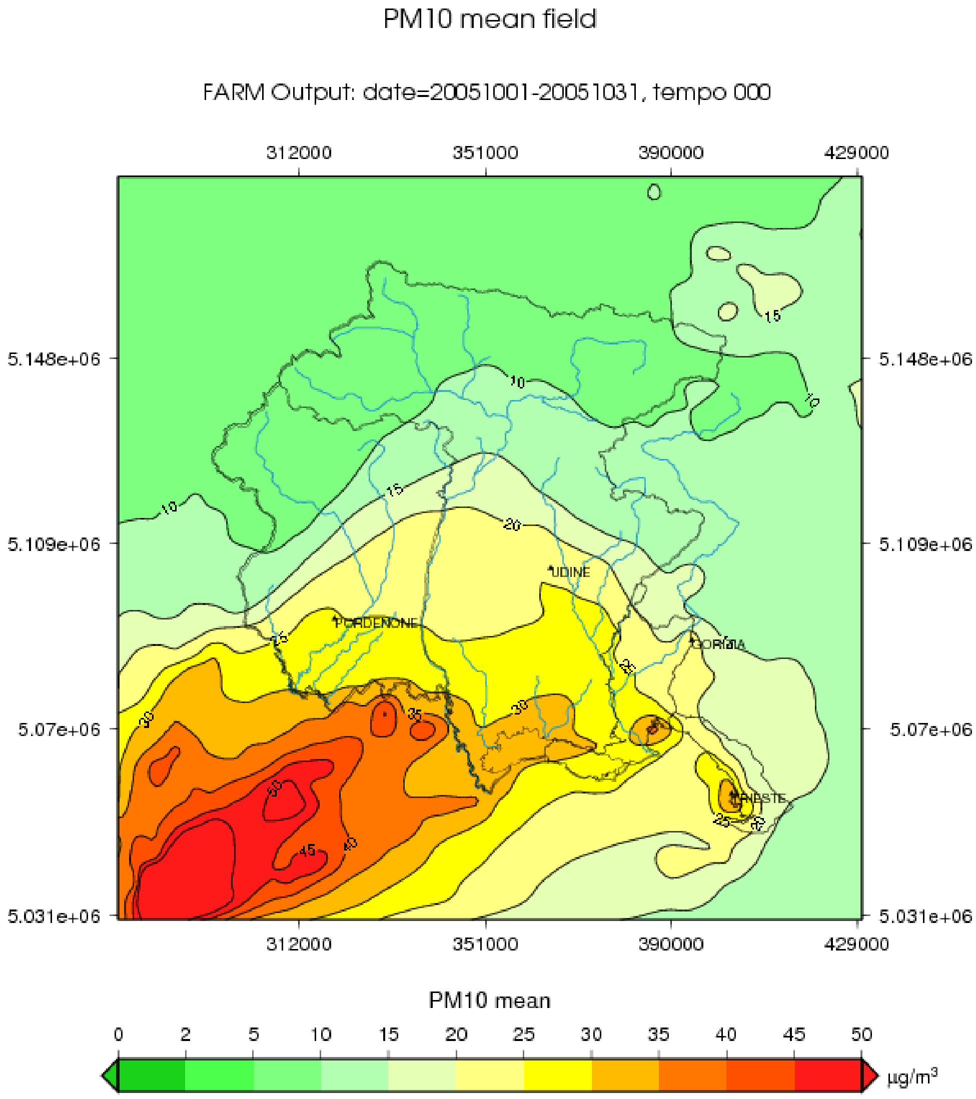
Air quality scenario for mitigation actions - Workflow

Off-line model simulations are suitable for air quality evaluations in regional domains



Air quality scenario for mitigation actions – domestic wood fires removed

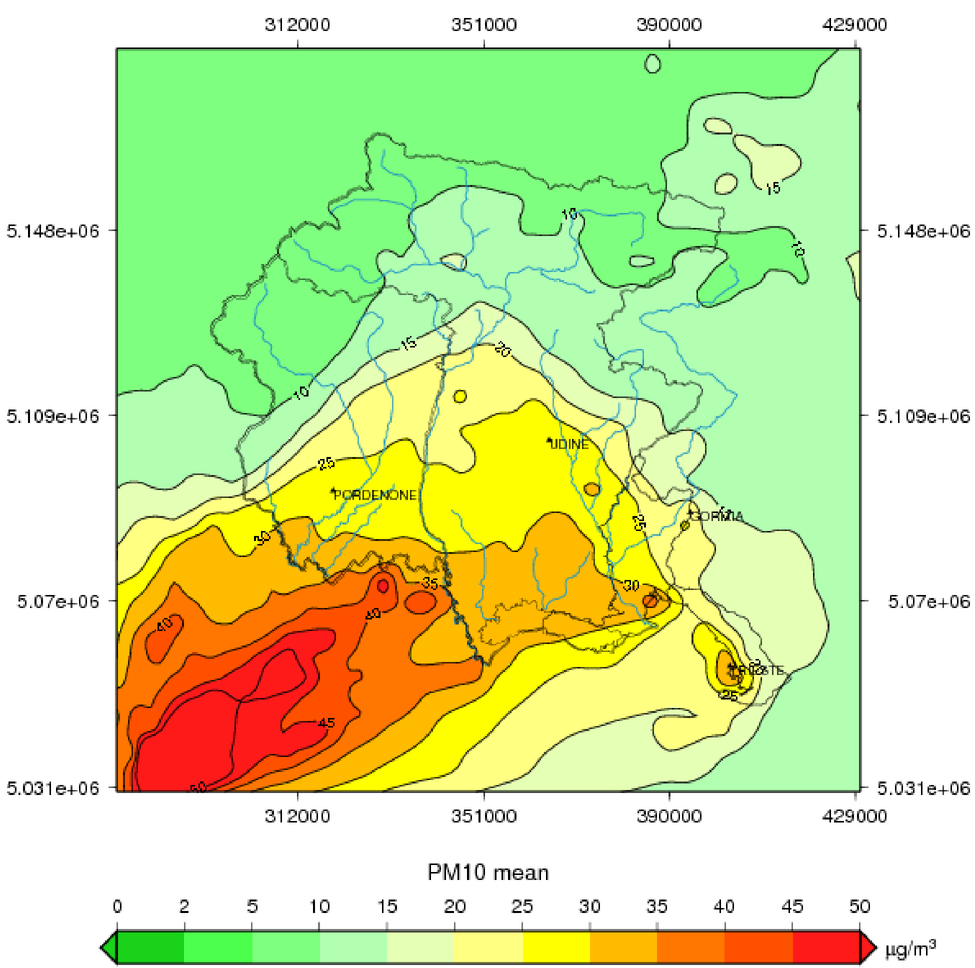




Air quality scenario for mitigation actions – house heading reduced by 2C

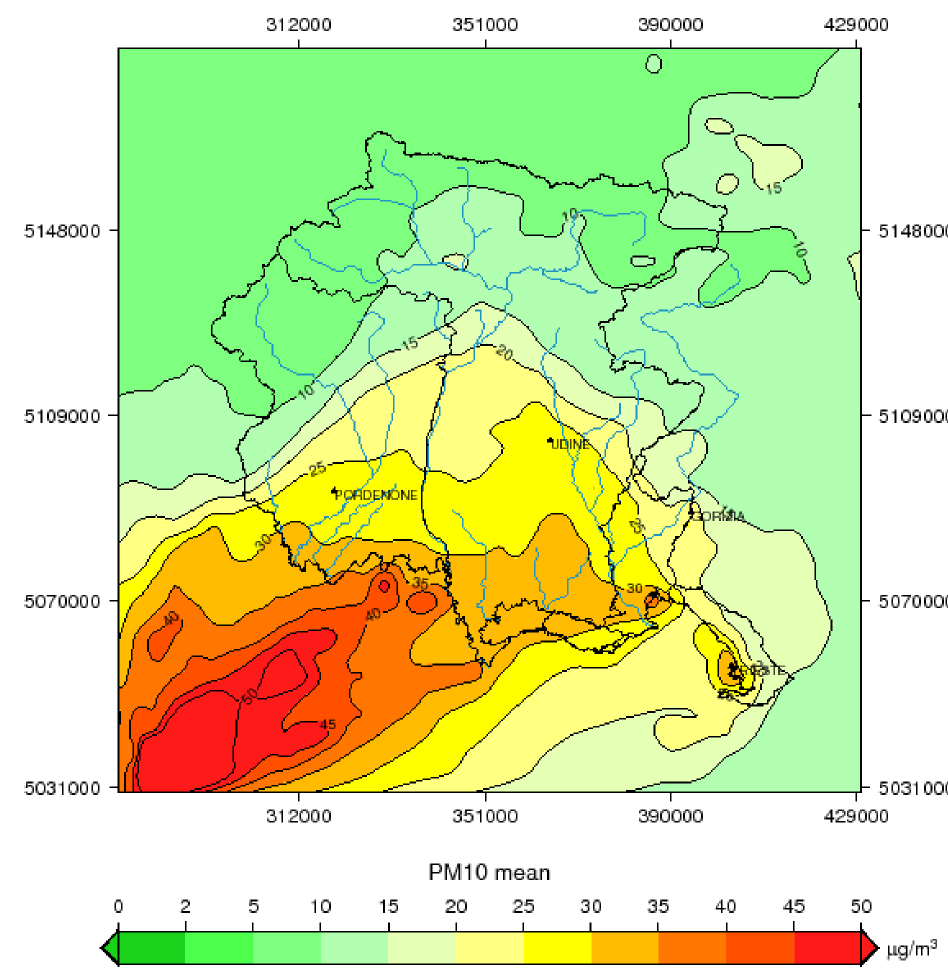
PM10 mean field

FARM Output: date=20051001-20051031, tempo 000

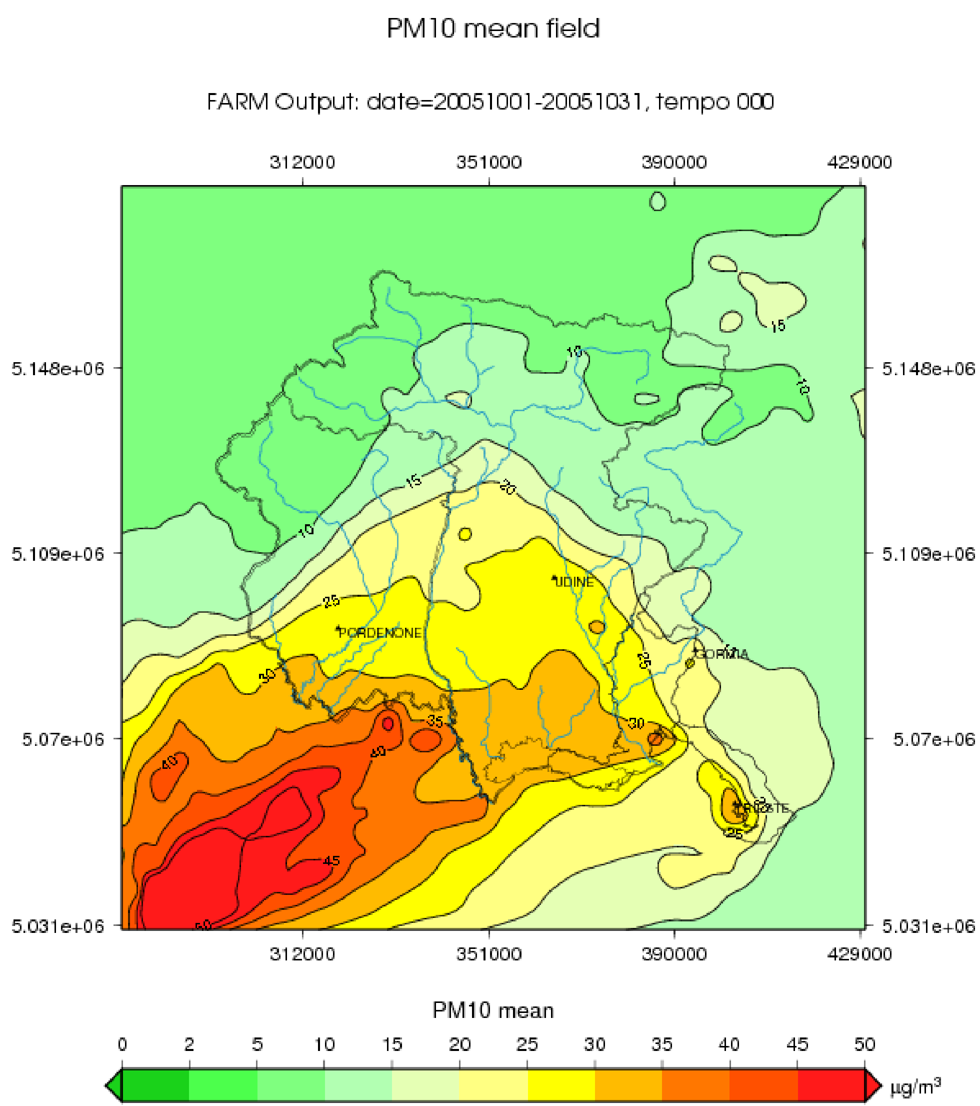


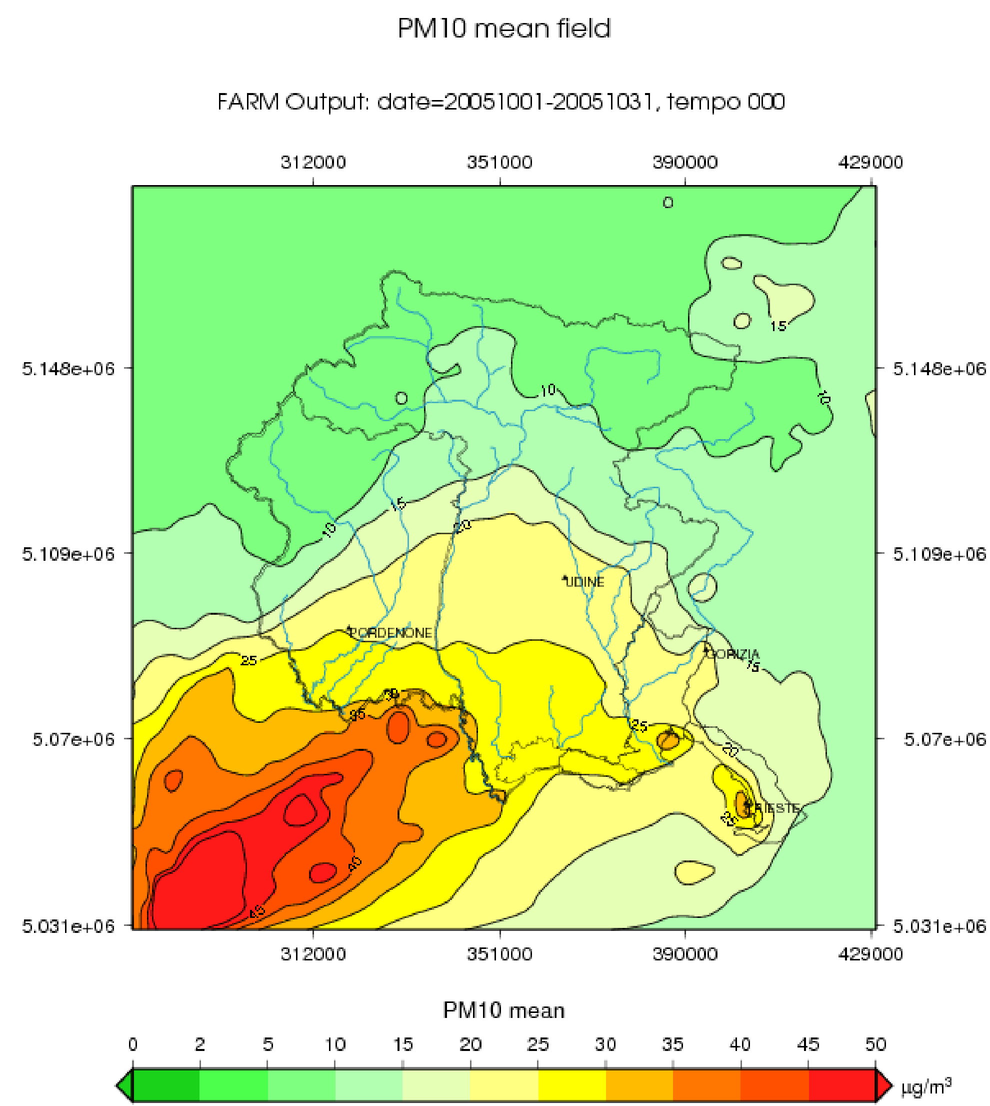
PM10 mean field 01C081B0B1_2005

FARM Output: date=20051001-20051031, tempo 000

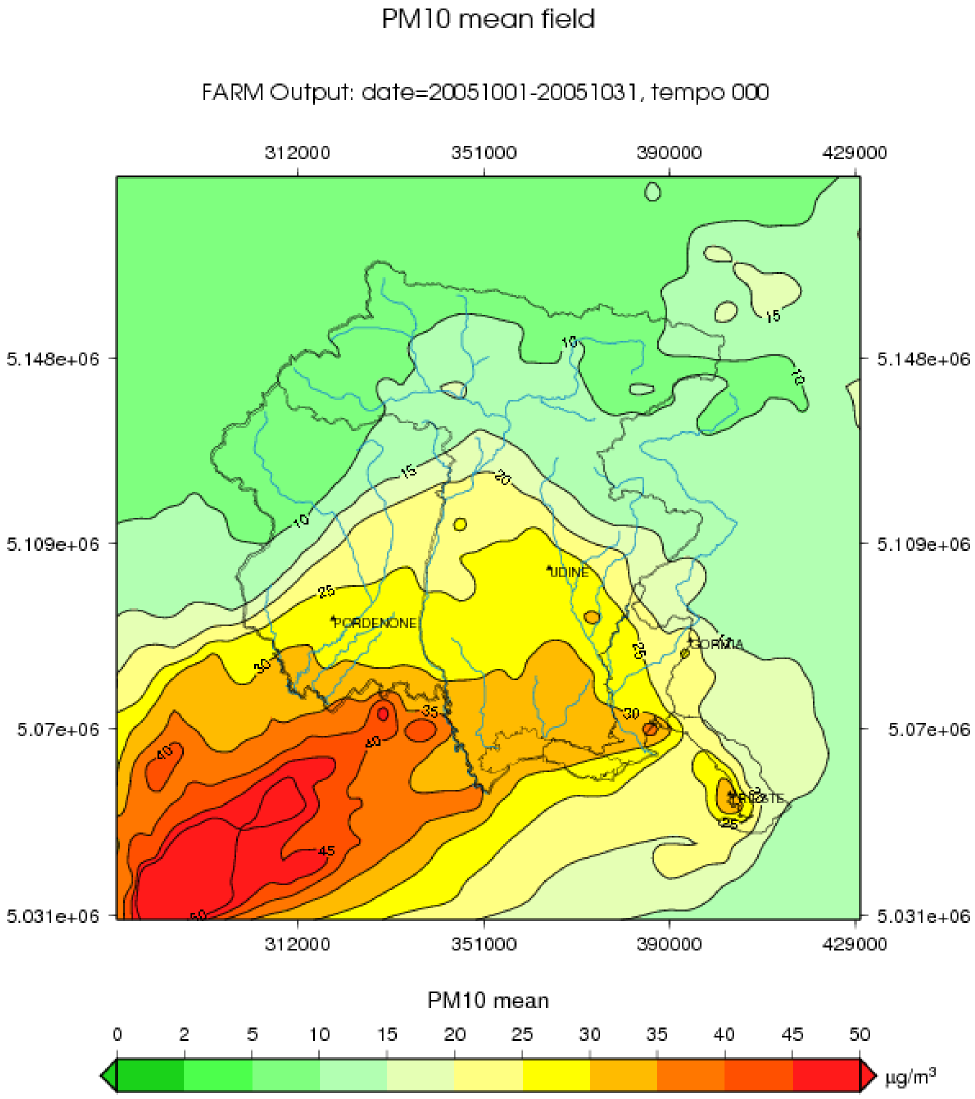


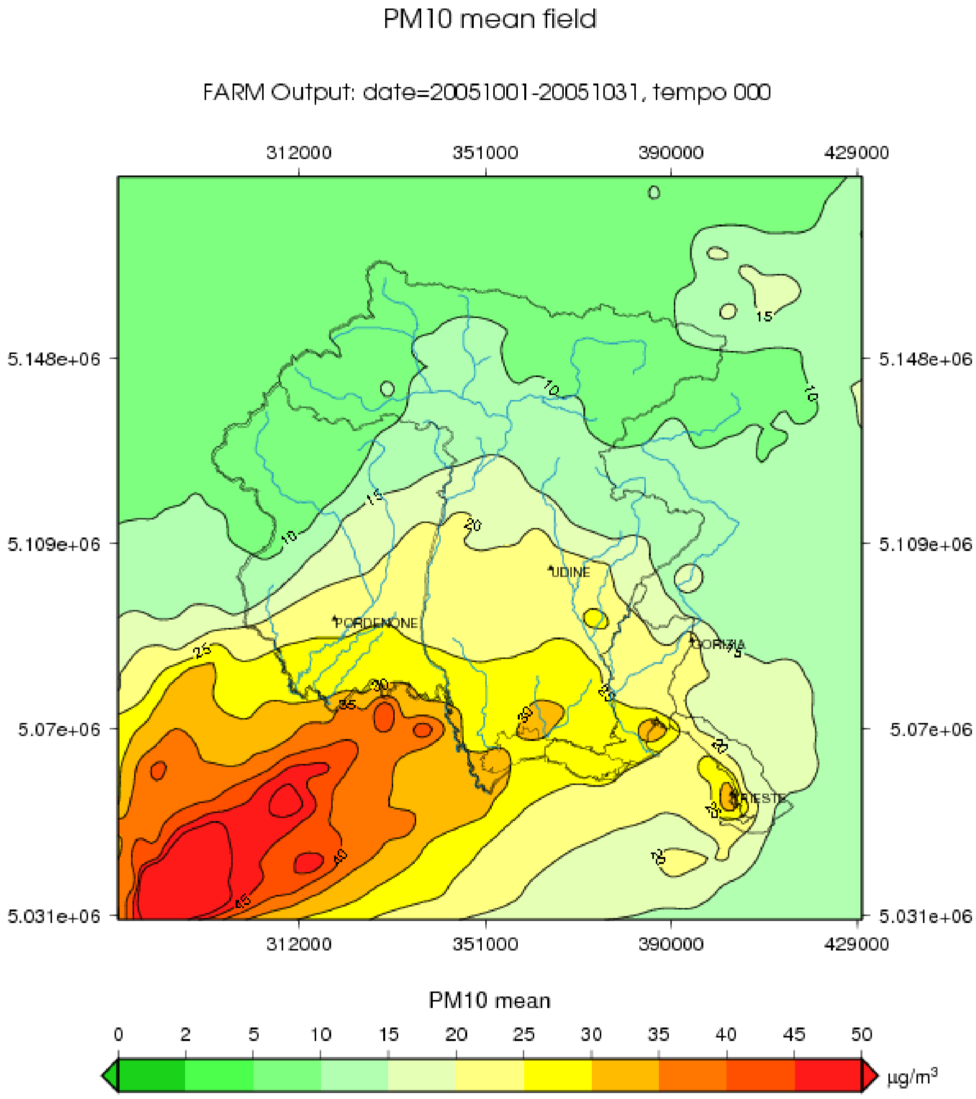
Air quality scenario for mitigation actions – industries removed



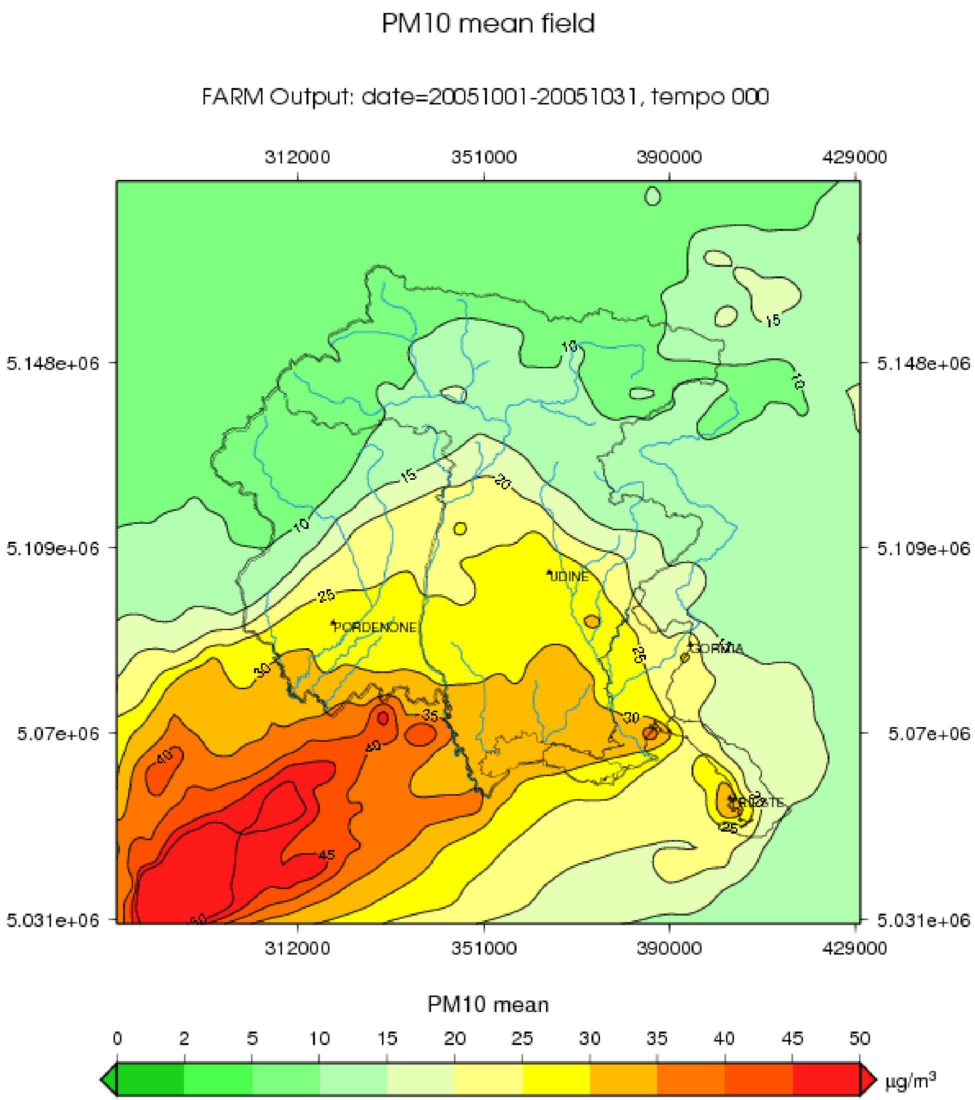


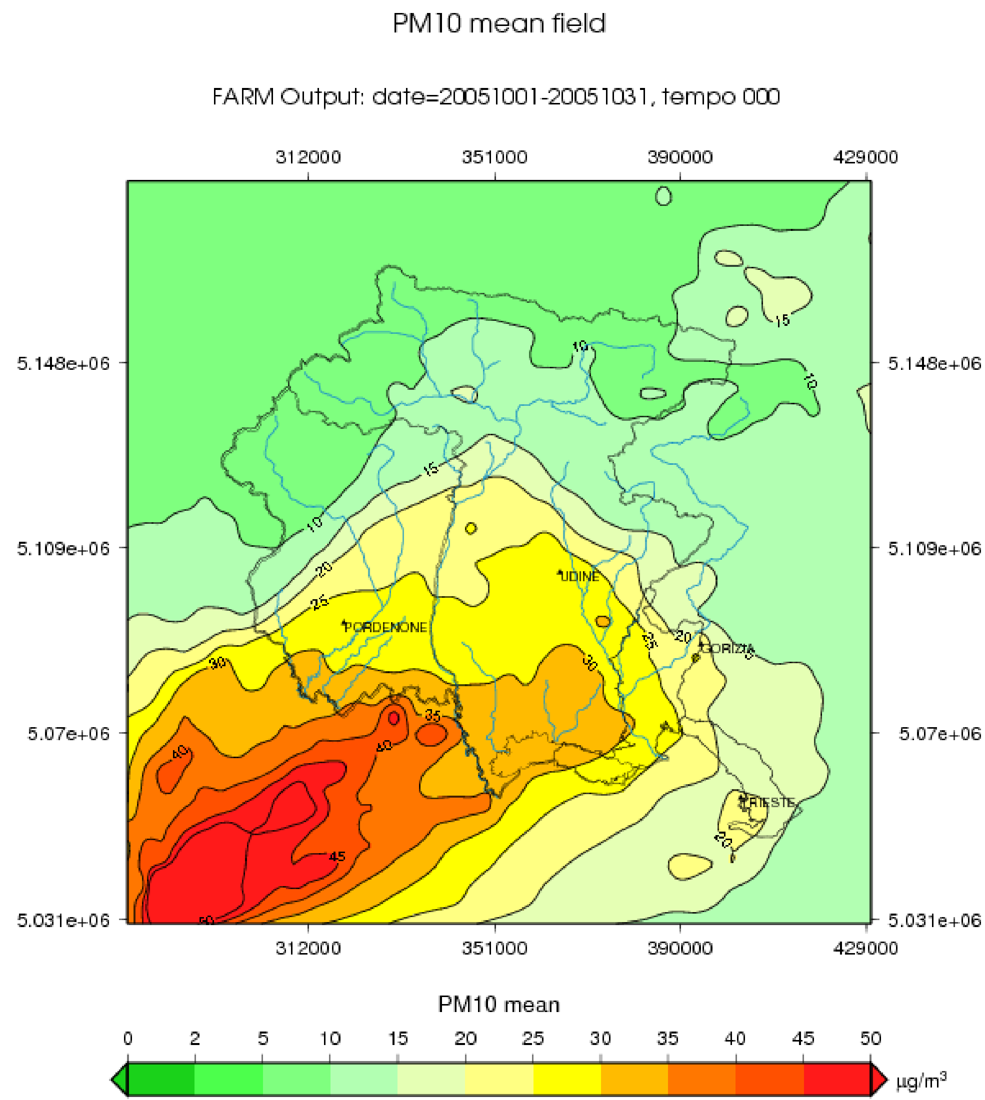
Air quality scenario for mitigation actions – traffic on all roads removed



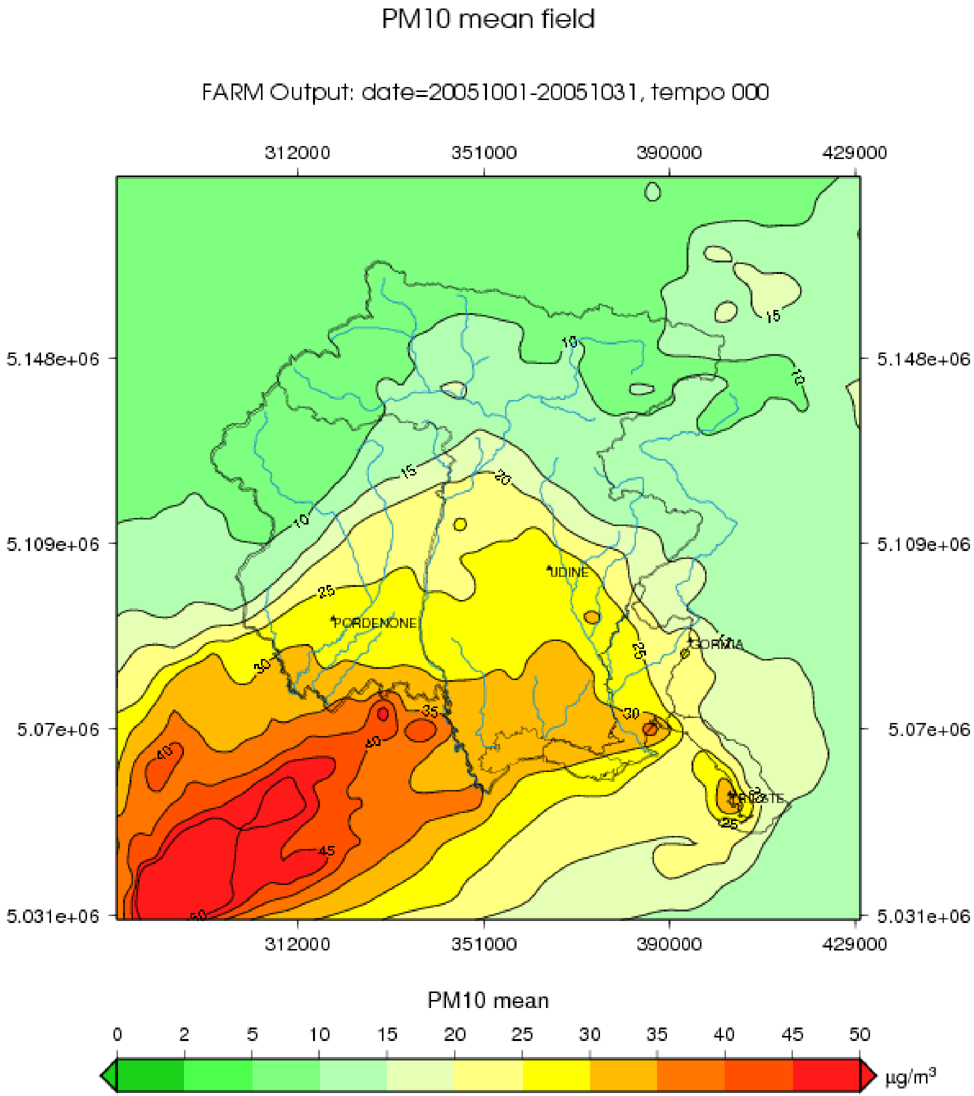


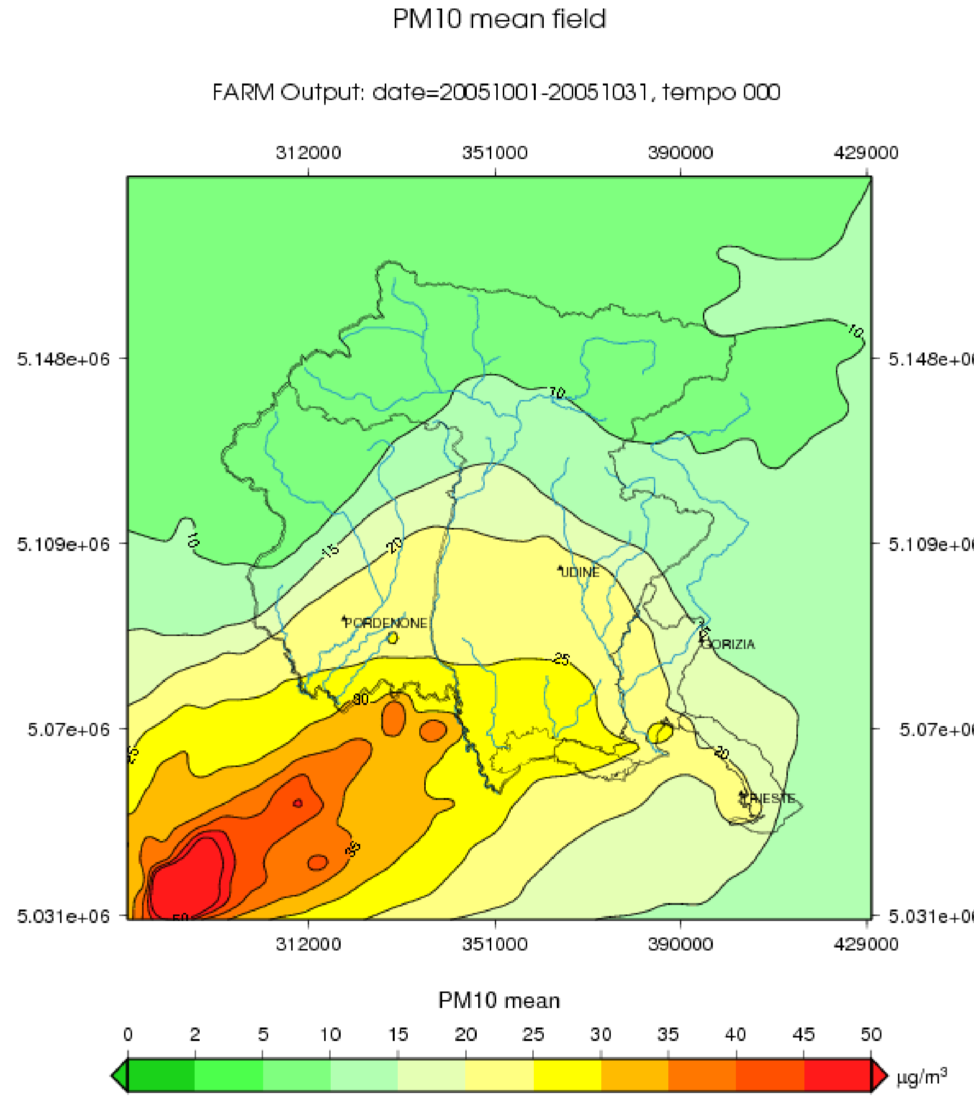
Air quality scenario for mitigation actions – without harbors emissions





Air quality scenario for mitigation actions – primary particulate emissions removed





New computational approach – GRID computing

Heavy consuming simulations and complex work flows can be distributed on computational GRIDS

Advantages: larger computational resources, data storage and work flow facilities
Requirements: e-infrastructure (user support and knowledge)

Example from project **MADBAG**: Monitoraggio Ambientale Distribuito BAsato su Grid

Grid computing is a form of distributed computing where a "virtual super computer" is built by many distributed computing and storage resources, integrated via a network middleware in order to optimize resource load and usage and provide higher throughput. GRIDCC and DORII add to Grid computing the capability to integrate distributed instruments and databases.

New computational approach – MADBAG project and GRID computing for AQ

Project **MADBAG**: Monitoraggio Ambientale Distribuito BAsato su Grid

- Regional Project (Friuli Venezia Giulia)
- Partners: Sincrotrone Trieste (coordinator), ARPA-FVG, UNITS

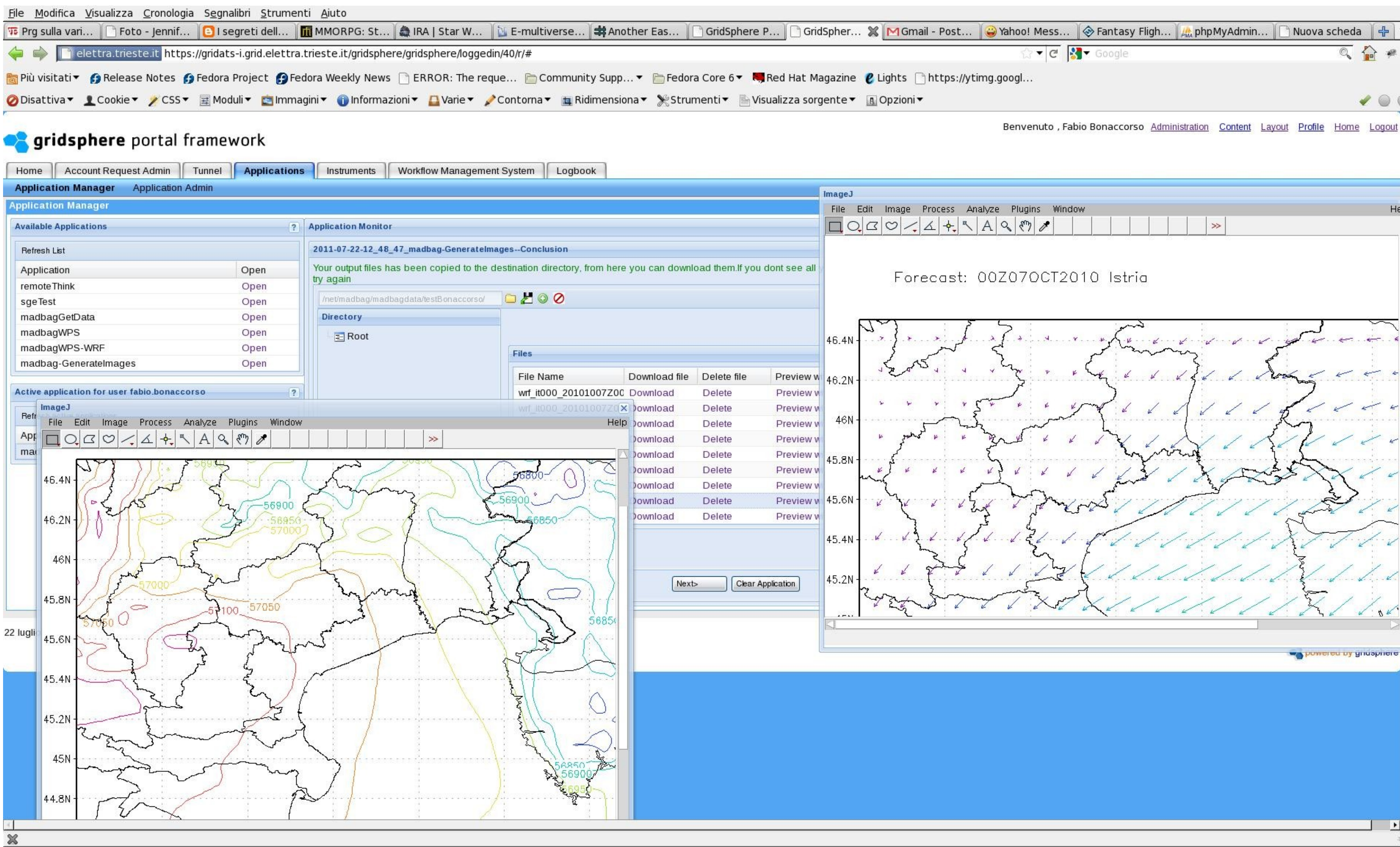
Objectives:

- Development of a distributed research infrastructure for environmental monitoring and capable of integrating meteo data, air quality data, databases of pollution sources and advanced computing resources.

- Provide the researchers with a powerful instrument to perform scenario analysis both on meteo and on air quality.

Air quality forecasts on GRID: the MADBAG project experience

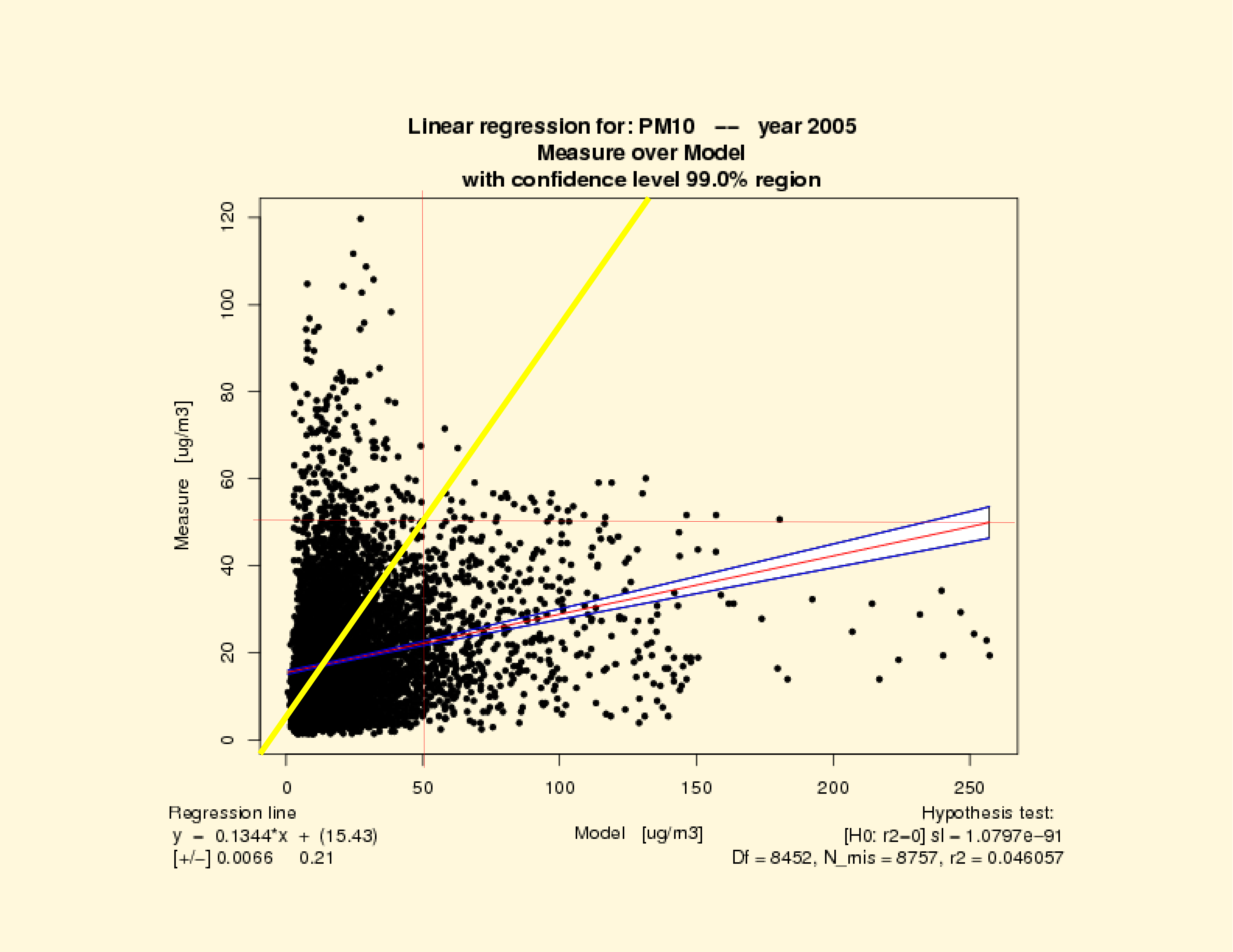
A virtual control room allows to generate and monitor the complete simulation from the beginning to the end (based on web)



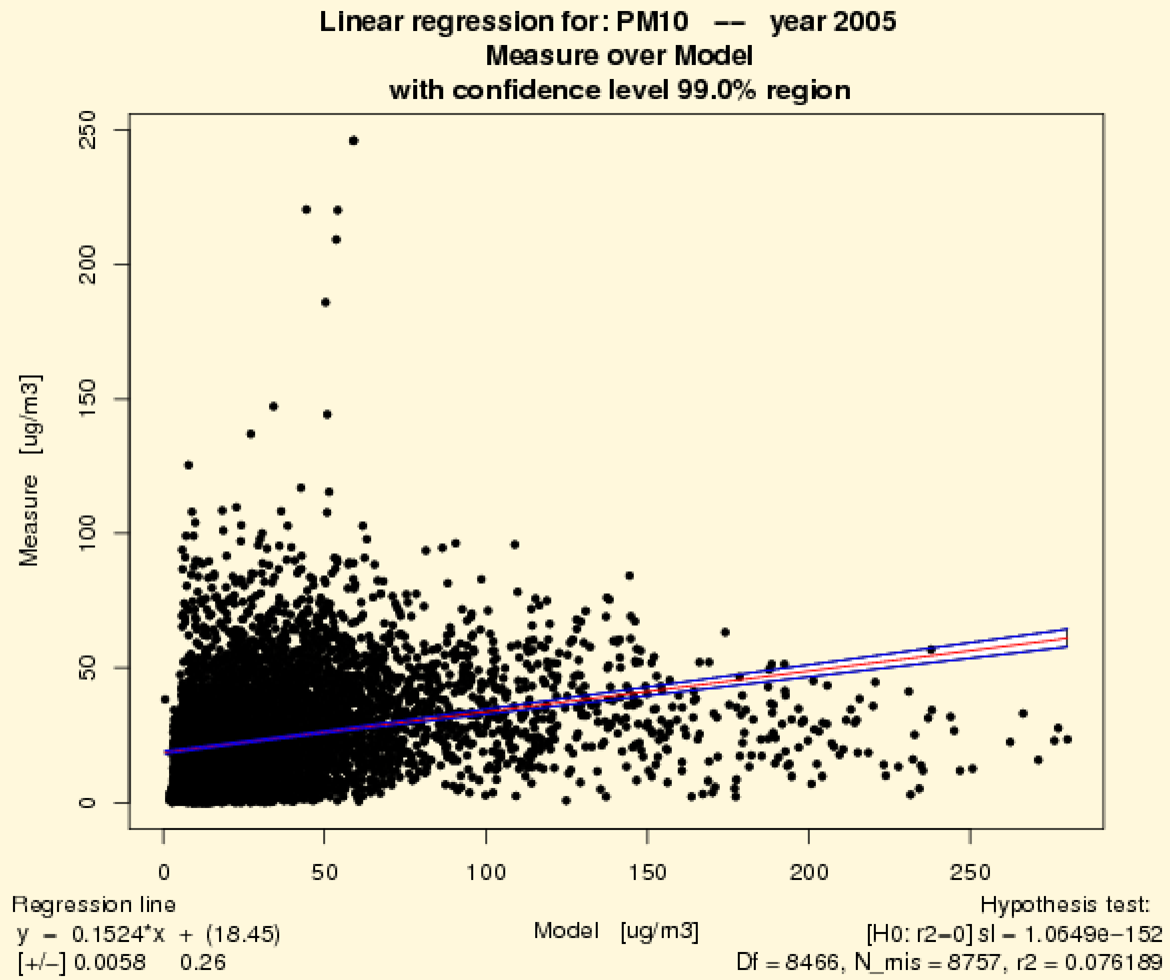
Thanks

Thanks for your attention

Air quality forecasts verification examples



Air quality forecasts verification examples



Air quality forecasts verification examples