La modellizzazione dei processi atmosferici: applicazioni alla realta‘ dell’Umbria

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Atmospheric modeling: modeling atmosphere processes

The effects of the emission of pollutants constitute a hazard to human health and to the environment.

EC Directive 96/62/EC recommends a combination of direct measurements and use of models to monitor air quality.

Chemists play a key role in both approaches to understand atmospheric changes and support policymakers.

Models, in particular, are essential to:

- **find out what the contribution of source A at site B is**
- **define cost-effective strategies for reducing pollutants**
- **show the effect of the addition of a pollutant emission**
- **show where to place a future source (industry, freeway)**
- **forecast air quality for the future years**

Atmospheric modeling: pollutants types and quantities

Types of atmospheric pollutants:

- **gas (O_3, C_6H_6, CO, SO_2, NO_x, ...)**
- **solid and liquid: aerosol (e.g. SO_4^{-2}, NH_4^{+}, NO_3^{-}, Fe, C, ...)**

Pollutants quantities depend upon:

- **emissions sources (natural or anthropogenic)**
- **transport and diffusion**
- **physicochemical transformations**

Atmospheric modeling: Chemistry-Transport Model

A Chemistry Transport Model (CTM) should...

start from:

- **localized and quantified emissions**
- **meteorological data (T, P, winds, humidity, ...)**

use tools of:

- **multi-scale interpolation**
- **integration of fluidodynamics equations**
- **kinetics equations**

give:

- **easy to use results for further analysis**

Atmospheric modeling: Chimere

Chimere (chemistry-transport model) code created by the Institute Pierre Simon Laplace (Fr).

http://euler.lmd.polytechnique.fr/chimere/

3D Eulerian Chemistry Transport Model (description of atmospheric physical and chemical processes).

Features:

- **multi-scale, from urban (100 Km) to international scale**
- **resolution from 1-2 Km to 100 Km**
- **long term simulations**
- **free software (GPL license)**
- **several vertical resolutions**
- **several chemical mechanisms**
- **option of aerosol processes**
- **parallel (SPMD, MPI) on linux platform**

Atmospheric modeling: Chimere purposes

What can be done:

- **simulate episodes or long term periods**
- **operational forecasts**
- **study emission scenarios**
- **evaluate strategy effectiveness (reduction plan and pollution control)**

Atmospheric modeling: Chimere input data

What a 3-dimensional atmospheric model needs:

Meteorogical data

- interface to process meteo data
  - data interpolation
  - transformation to Chimere variables
  - creation of a netCDF database

Biogenic emissions

- biogenic emissions preprocessor
  - start from land use and emissions potentials for isoprene, terpene, NO
  - calculate emissions database (meteo dependent)

Atmospheric modeling: Chimere input data

Anthropogenic emissions

- start from annual inventory (CO, NMVOC, NH_3, NO_X, PM10, SO_2)
- aggregation over SNAP97 sector
- temporal apportioning to hourly values
- speciation to required chemical species

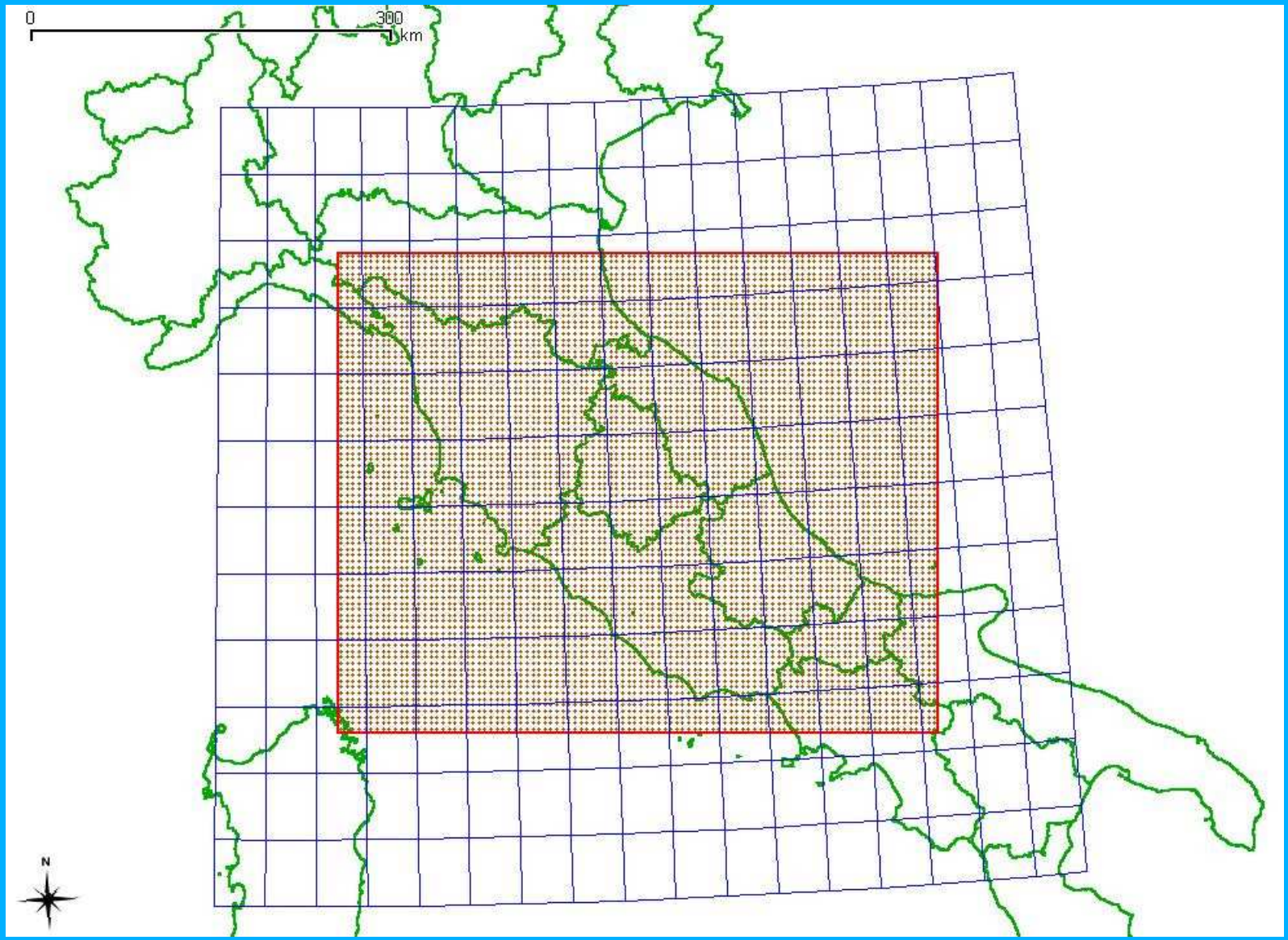
- anthropogenic emissions preprocessor
- creation of a netCDF database

Initial Conditions

- initial concentration of all species
- their influence decays exponentially with the time
- use of a start-up period

Atmospheric modeling: Chimere input data

Boundary Conditions



Atmospheric modeling: Chimere input data

- Initial and Boundary Conditions preprocessor
  - internal (nesting)
  - external (global models: i.e. LMDZINCA2, MOZART2, GOCART)

- time integration of all chemistry-transport equations
  - transport
  - mixing
  - deposition
  - absorption
  - nucleation
  - coagulation
  - photolysis
  - reaction rates

Atmospheric modeling: Chimere input data

Primary (directly emitted) and secondary (through primary photochemical reaction) pollution processes:

- **gas phase; scheme MELCHIOR1 (80 species, 300 reactions) or MELCHIOR2 (44 species, 120 reactions) :**
  - **inorganic (O_3, NO_x, CO, OH, SO_x, ...)**
  - **photolysis**
  - **OH attack to organic comp.**
  - **radical recombination**
  - **radical conversion**
- **solid/liquid phases (PPM, HNO_3, H_2SO_4, NH_3, biog. SOA, anthrop. SOA, water, NaCl):**
  - **red-ox of SO_2, O_3, NO_2, H_2O_2**
  - **catalyzed oxidation**
  - **coagulation, absorption, nucleation**
- **heterogeneous chemistry (HO_2, NO_x):**
  - **gas-liquid interface**

Atmospheric modeling: first results

First results:

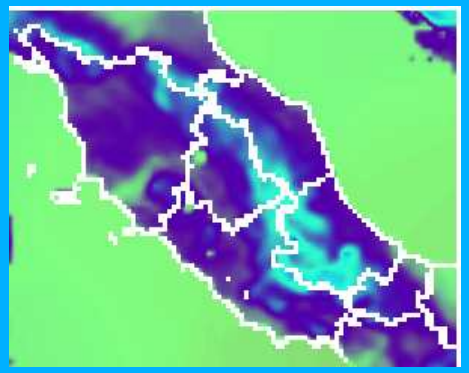
- **implementation of Chimere version V200606A:**
  - **8 Xeon HT biprocessor nodes cluster (dep. Mathematics and Informatics, unipg)**
  - **2 SUN ULTRASPARC biprocessor nodes cluster (dep. Chemistry, unipg)**
- **reproduction of the 2003 benchmark (July-August hot wave)**

Atmospheric modeling: first results

- creation of interfaces to Chimere for:
  - meteo data (LAMI) on Central Italy (CI) domain
    source: Arpa Emilia Romagna
  - Italian biogenic emissions on CI domain
    source: Arpa Emilia Romagna
  - Italian anthropogenic emissions on CI domain
    source: APAT
  - European Boundary Conditions on CI domain
    source: Prevair (France)
  - output visualization (ncview, grads)

Atmospheric modeling: first results

$Temp_{2m}$ (279 to 315 K)



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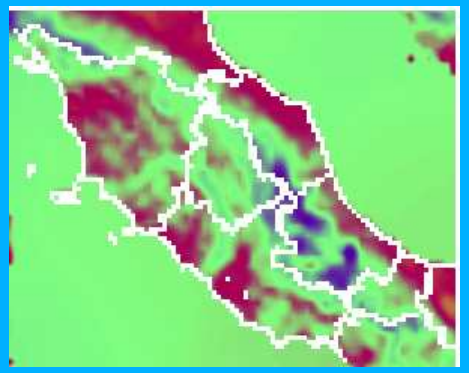

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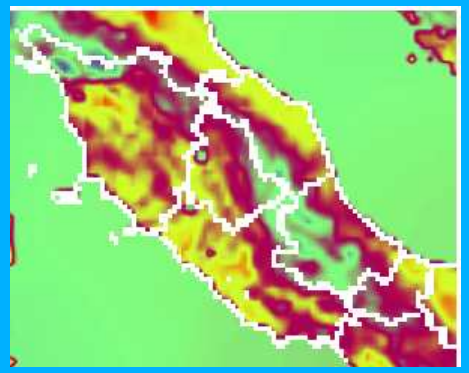

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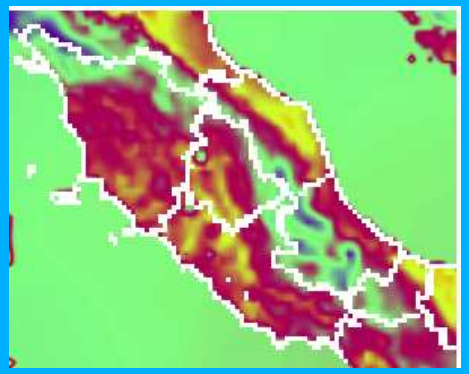

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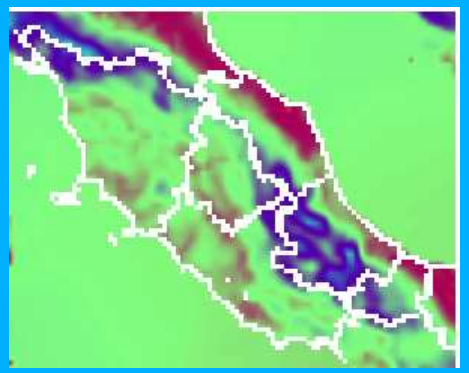

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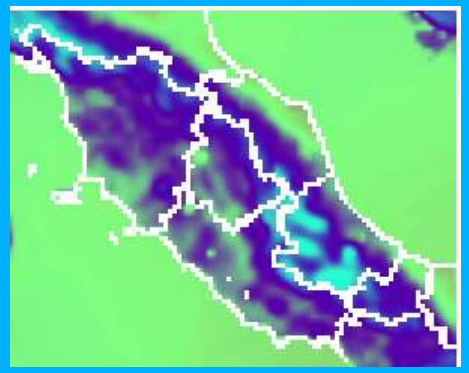

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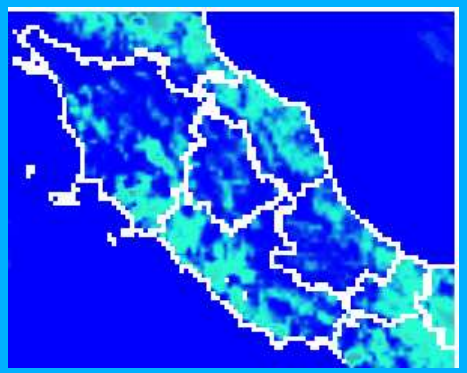
Atmospheric modeling: first results

$NO_{biogenic}$ (0 to $6x10^{11}$ molecules/(cm^2s))



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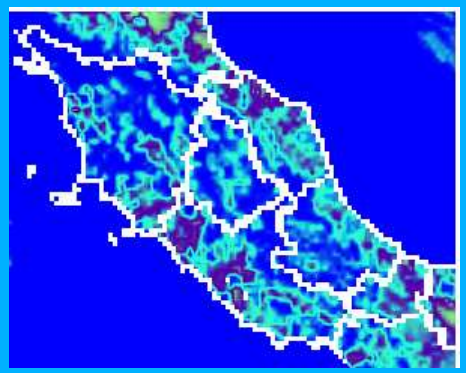

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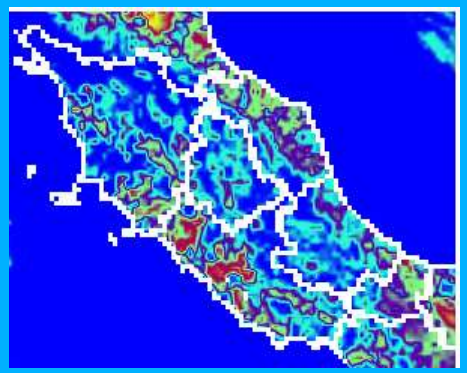

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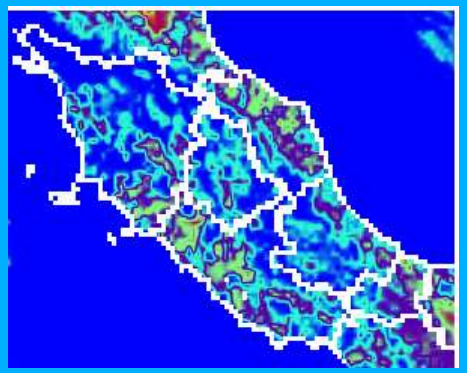

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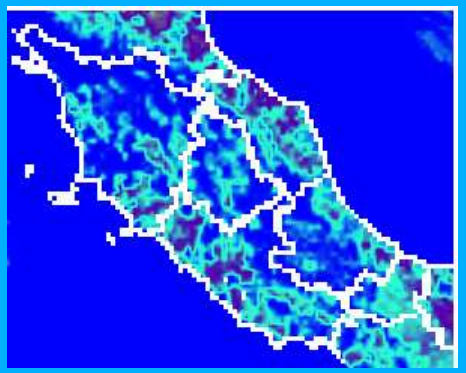

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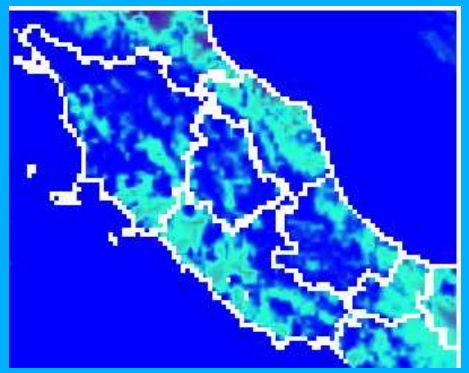

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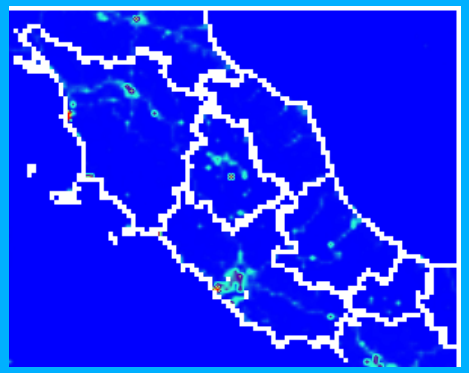
Atmospheric modeling: first results

$NO_{anthropogenic}$ (0 to $3x10^{12}$ molecules/(cm^2s))



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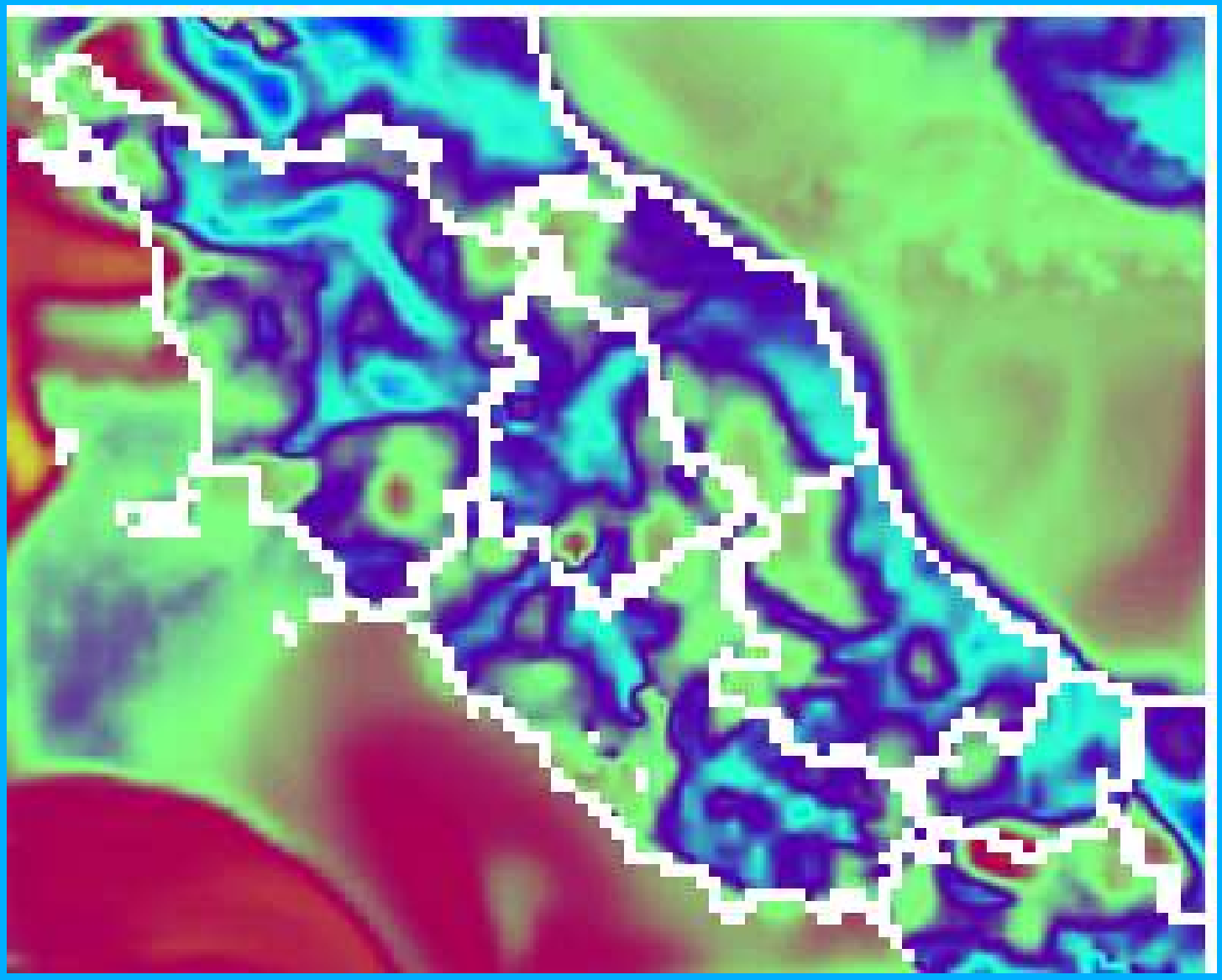
Atmospheric modeling: summer 2004 simulation

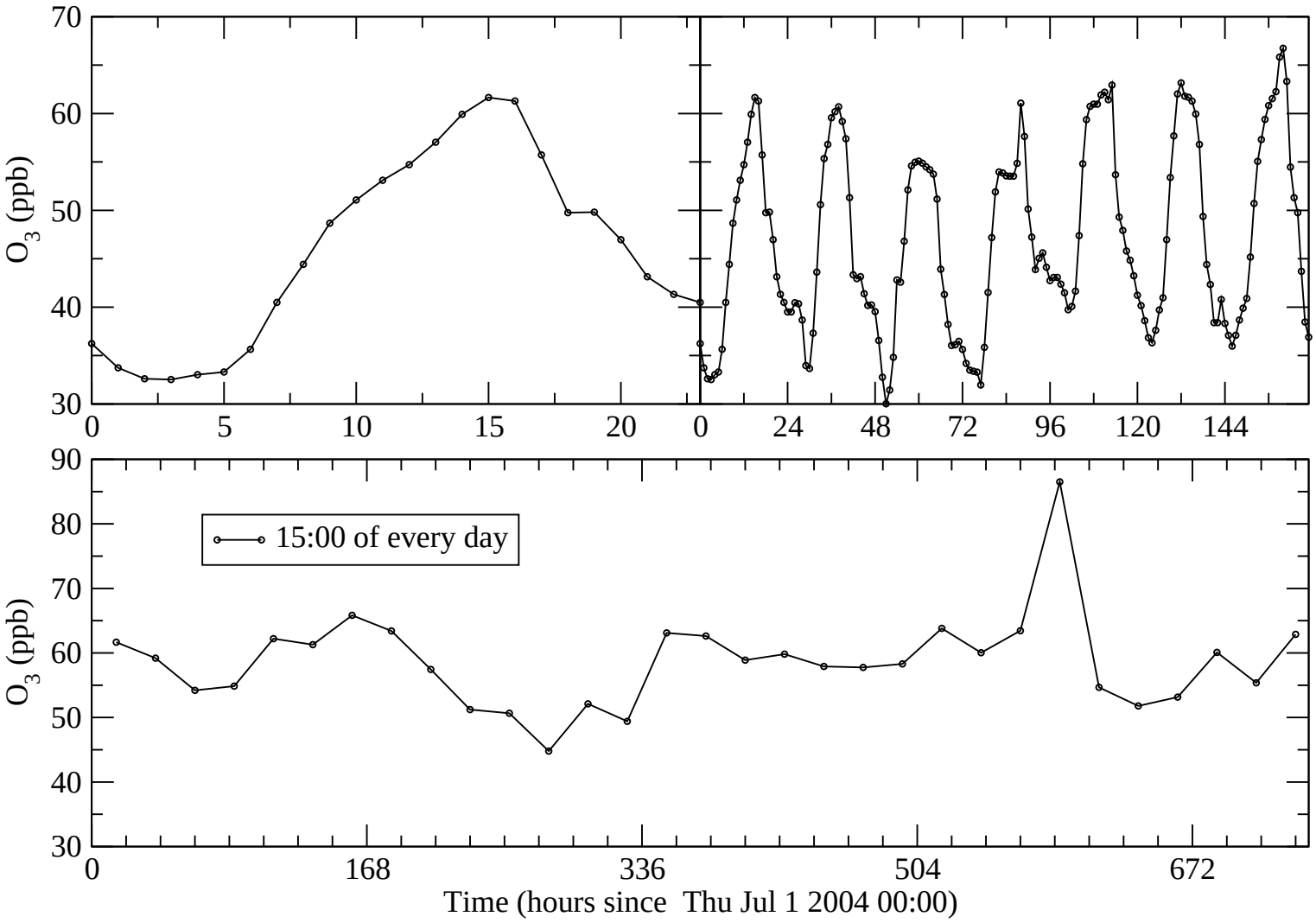
- simulation of Summer 2004 (Central Italy domain)
  - starting 30 Apr 2004; ending 31 Aug 2004
  - 8000 5x5 Km grid cells
  - gas and aerosol phases
  - MELCHIOR2 chemical scheme (44 species, 120 reactions)
  - 8 Intel Xeon processors, 124 hours, 30 GB output
  - 13 (gas/aerosol) + 190 deposition output species

Atmospheric modeling: summer 2004 simulation

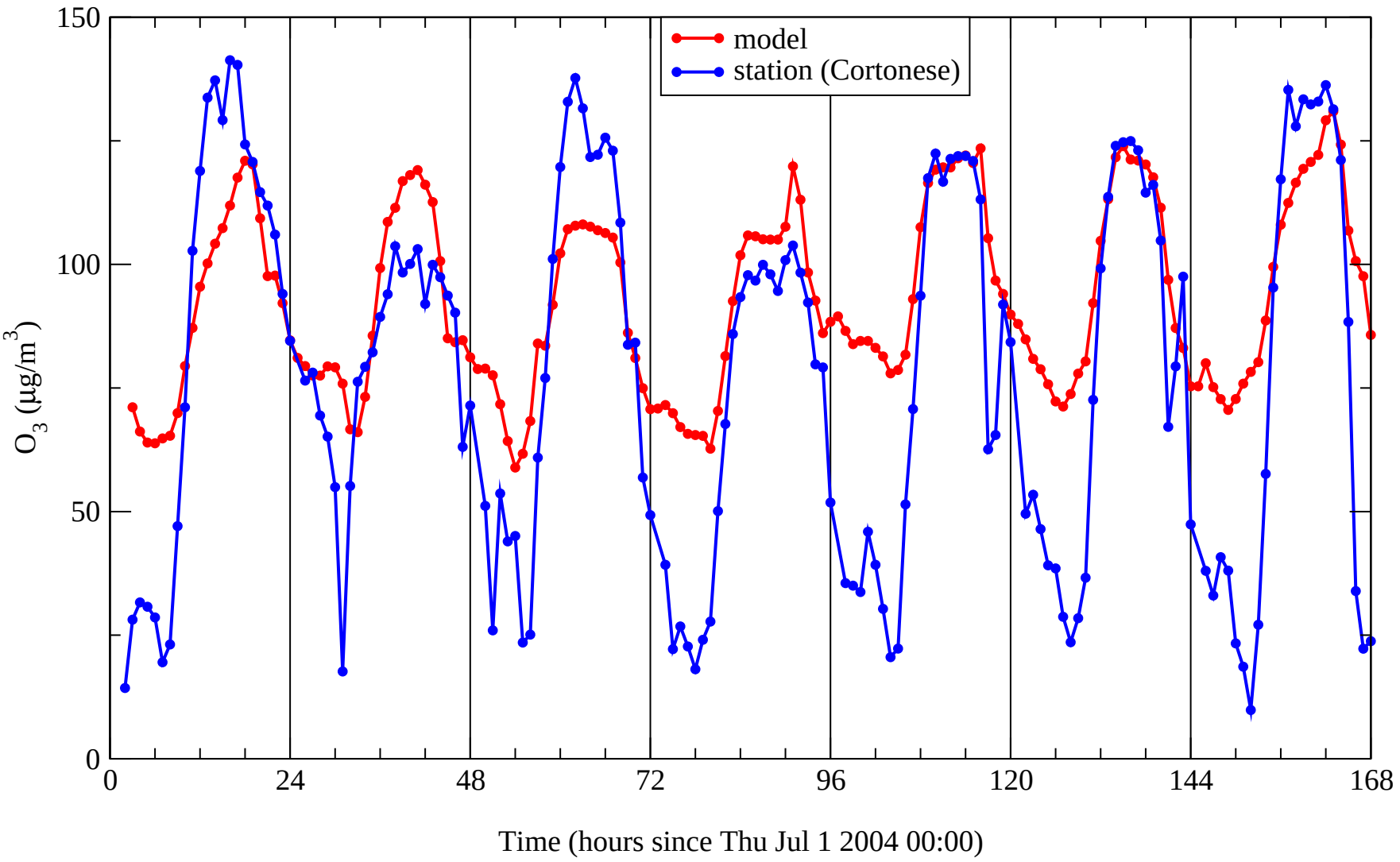
July, the 1st 2004, O_3 distribution: blue= 22.0 ppb, red= 82.8 ppb.



Atmospheric modeling: summer 2004 simulation



Atmospheric modeling: summer 2004 simulation



Atmospheric modeling: Final remark

Work done:

- implemented a Chemistry Transport Model (Chimere)
- applied Chimere to the Air Quality in Umbria

Work in progress:

- paper to be published on Micron (O_3)

in collaboration with Arpa Umbria

- paper to be published on "La chimica e l'industria" (PM)

in collaboration with Arpa Umbria, Dipartimento di Ingegneria Civile ed Ambientale, Dipartimento di Scienze della Terra

Atmospheric modeling: Final remark

Future work:

- one year simulation and law indices calculation
- model validation and sensitivity to anthropogenic emissions
- future emission scenarios
- sensitivity test to chemical mechanisms
- implementation on EGEE (European Computer Grid)
- implementation of other CTM (CAMx) and comparison

Atmospheric modeling: acknowledgments

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