# ENHANCING HIGH-RESOLUTION AIR QUALITY FORECASTING IN MARENOSTRUM SUPERCOMPUTER

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## INTRODUCTION

One of the topics in which the European Commission has shown a greater concern, through initiatives as GMES is the necessity of developing actions that allow increasing the knowledge on transport and dynamics of pollutants to assure the accomplishment of legislation and to inform the population about the levels of pollutants. The regulation is especially demanding when the threshold levels are exceeded. In this case, it demands a detailed diagnosis of those areas where the exceedances are found and a forecast of the evolution of ground-level concentrations. The development and implementation of an air quality forecasting model using the state-of-the-art techniques in numerical modelling is a challenging topic to accomplish with the European regulations on air quality (Directives 1996/62/EC, 1999/30/EC and 2002/3/EC). According to these directives, air quality modelling, if accurately applied, is a useful tool to understand the dynamics of air pollutants, to analyse and forecast the air quality, and to develop programs to reduce emissions and alert the population when health-related problems take place.

The numerical modelling of air quality represents an essential and strategic tool to inform to the population in advance of the potential exceedances of thresholds (information, alert or protection of human health) when pollution episodes occur. Therefore, it becomes critical to have access to large supercomputing facilities to be able to provide this service to population. The current MareNostrum supercomputer hosted by the Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS) is able to perform more than 94.21 thousand billions operations per second. This capacity, together with the great advances in the parallelization of the numerical codes of air quality models permit the forecast of air pollution with high resolution.

## AIR QUALITY FORECASTING SYSTEM DESCRIPTION

The Barcelona Supercomputing Center currently operates air quality forecasts in Europe and the Iberian Peninsula with MM5-EMEP-CMAQ-DREAM modelling system (http://www.bsc.es/projects/earthscience/aqforecast-en) over the Iberian Peninsula on a daily basis (48-hr forecasting period). The operational products delivered cover 48-hr forecasts of ozone, nitrogen oxides, sulphur dioxide, carbon monoxide or and particulate matter, as well as chemograms in selected cities. The necessity of coupling CMAQ and Eta/DREAM is addressed since nowadays none of the available operational daily forecasts in Europe include the influence of Saharan dust in a non-climatologic basis. As a first approach, the natural dust contribution from Eta/DREAM (http://www.bsc.es/projects/earthscience/DREAM) is added on-line to the output of CMAQ (Figure 1).

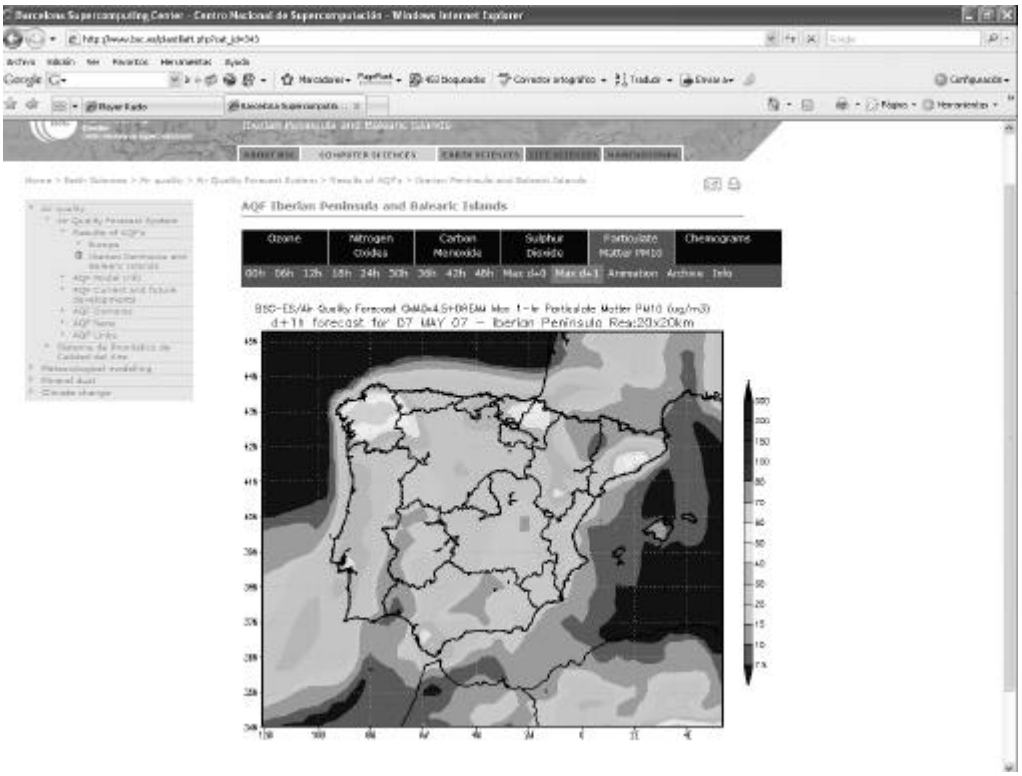


*Fig. 1; Air Quality Forecasting System at BSC-CNS (e.g. maximum concentration of PM10 for day+1 May 7th, 2007 with CMAQv4.5+DREAM models) (http://www.bsc.es/projects/earthscience/aqforecast-en)*

The domain of operational simulations covers an area of 4850 x 4850 km$^2$ for Europe (resolution 50 km) and 1392 x 1104 km$^2$ centred in the Iberian Peninsula (resolution 20 km). The MM5 numerical weather prediction model is used to operationally provide the meteorology parameters to CMAQ chemistry transport model. The MM5 options used are described in detail in Jiménez et al. (2006a; 2006b). Initialisation and boundary conditions are derived from NCEP 1-degree resolution forecast data every 6 hours. Emissions used for the domain of Europe and the Iberian Peninsula are derived from EMEP emissions database on an hourly basis, but biogenic emissions that are estimated following the methods implemented in Parra et al. (2006) using the land-use map derived from CORINE NATure/LANd Cover information. The cells from the European EMEP mesh have a resolution of 50-km in polar coordinates; emissions in the Iberian Peninsula are disaggregated into a grid of 20-km resolution in Lambert coordinates. The emissions of each source are speciated according to the experience of Jiménez et al. (2003) in the categories of the chemical mechanism Carbon Bond-IV (Gery et al., 1989). The Community Multiscale Air Quality Modeling System (CMAQv4.5) represents the state-of-the-science in atmospheric chemistry, simulating the main atmospheric chemistry, transport and deposition processes involved in the domain defined. The particulate matter species included are sulphates, nitrates, ammonia, aqueous aerosols, primary and secondary aerosols of anthropogenic and biogenic origin, elemental carbon and other primary particulate matter.

The model used to provide the concentrations of desert dust is the Dust REgional Atmospheric Model (DREAM) (Nickovic et al., 2001). DREAM is fully inserted as one of the governing equations in the atmospheric NCEP/Eta atmospheric model and simulates all major

processes of the atmospheric dust cycle. Wind erosion of the soil is parameterized by the type of soil, vegetation cover, soil moisture content, and surface atmospheric turbulence. In the operational version, for each texture class fraction four particle size classes (clay, small silt, large silt and sand) are estimated with particle size radii of 0.73, 6.1, 18 and 38 μm, respectively. The resolution is set to 50 km in the horizontal and to 24 layers extending up to approximately 15 km in the vertical. DREAM is a fully operative tool extended and validated by the scientific community (e.g. Ansmann et al., 2003; Pérez et al., 2006a; Pérez et al., 2006b, Balis et al., 2006; Papayannis et al., 2007), nowadays providing accurate forecasts over North Africa, Europe, Middle East and Eastern Asia.

## FUTURE DEVELOPMENTS: CALIOPE AIR QUALITY FORECASTING SYSTEM

The air quality forecasting system is currently being upgraded, in order to be implemented with an unprecedented resolution for Europe (12 km), the Iberian Peninsula (4 km) and some city areas (Madrid and Barcelona, 1 km). In this context, the CALIOPE project has as main objective to establish an air quality forecasting system for Spain coordinated by the Spanish Ministry of the Environment through funded project 441/2006/3-12.1, delivering air-quality related products useful to a wide range of users for reducing the impacts of air pollution on human health.

The estimation for 1-year simulations at this very high resolution is around 328,500 CPU hours. This requires the combined power of over 300 PowerPC 970MP processors and storage capacity of up to 5 TB per year simulated. The huge computing capabilities of MareNostrum supercomputer allows a unique forecasting system with the subsequent improvements with respect to the previous BSC-CNS air quality forecasting system: (1) Change of the meteorological driver to WRF-ARW2.2 (Skamarock et al., 2005) and improvement of initial condition resolution to 0.5º, taken from NCEP high-resolution global forecast system, (2) Upgrade of the High Elective Resolution Modeling Emission System (HERMES); emission model developed at BSC-CNS, for the domain of Spain with a resolution of 1 $km^2$; (3) Increase of the horizontal and vertical resolution of the forecasts for Spain and other hot-spots regions; (4) Operational forecast validation; (5) Improvement of aerosols predictions (secondary organic aerosols, natural dust, re-suspension processes, etc.).

A partnership of four research institutions composes the CALIOPE project: the Barcelona Supercomputing Center (BSC), the CIEMAT, the Earth Sciences Institute 'Jaume Almera' (IJA-CSIC) and the CEAM Foundation. This consortium will deal with both operational and scientific aspects related to air quality monitoring and forecasting (Figure 2). The set of models implemented take into account both anthropogenic and natural pollution. These models are the WRF-ARW meteorological model; the HERMES emission model; the CMAQ and CHIMERE chemistry transport model; and DREAM natural dust model.

The HERMES emission model (Figure 3) has been specifically developed as a high-resolution emission model for Spain under a GIS framework. The emission model focuses in the estimation of gas and particulate matter pollutants, including the ozone precursors and using a high spatial and temporal resolution for Spain. The land has been divided in cells of 1 $km^2$. For that the model uses land-use information (CORINE NATure/LANd Cover information-100 m, population density, industrial location, etc.). The emission model includes biogenic and anthropogenic (on-road, ship and planes traffic, airports and ports, industrial sectors, domestic and commercial) and it is essential when providing data to the air quality models on a hourly, daily, monthly and annual basis. This emission model is currently being parallelised for its implementation in the MareNostrum supercomputer.

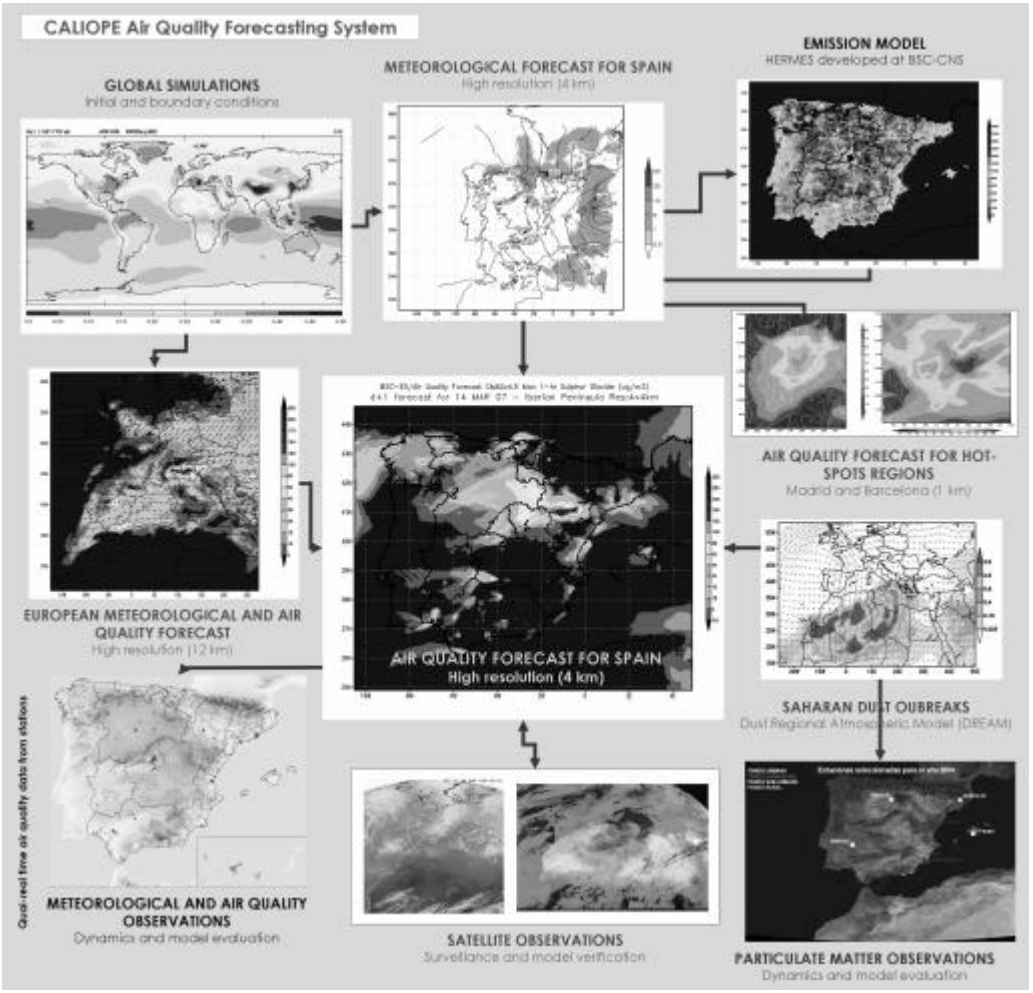


*Fig. 2; Structure of the air quality forecasting system of the project CALIOPE implemented in MareNostrum supercomputer.*

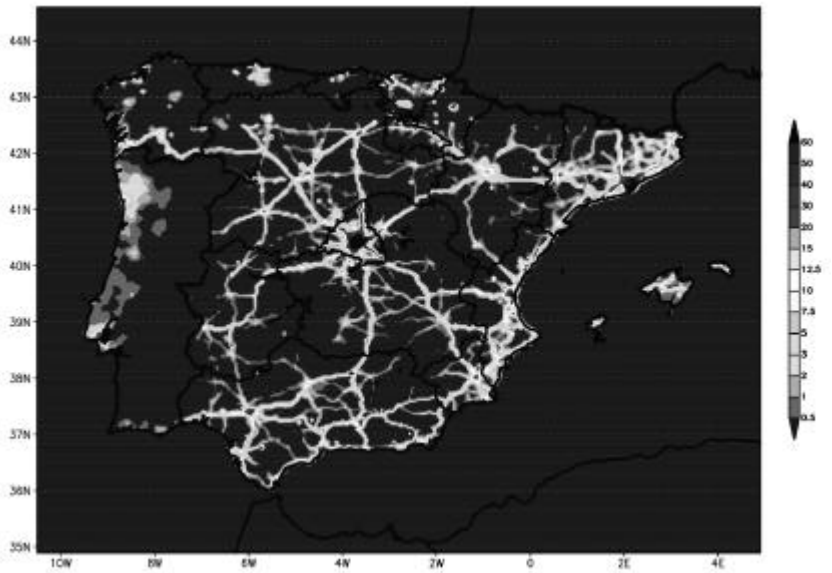


*Fig. 3; HERMES emissions for $NO_2$ (mole $h^{-1}$) at 12 UTC in the Iberian Peninsula aggregated from 1x1km to 4x4km resolution.*

Also, it should be highlighted that the CALIOPE system is useful to complement the data obtained in the present networks of air quality measurements managed by regional and local

authorities, and in certain experimental measurement campaigns or air quality studies performed both in urban or background areas. The results of the CALIOPE system will allow a better level of information for the citizenship related to the forecasting of air quality.

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