Earth Science Research at the Barcelona Supercomputing Center

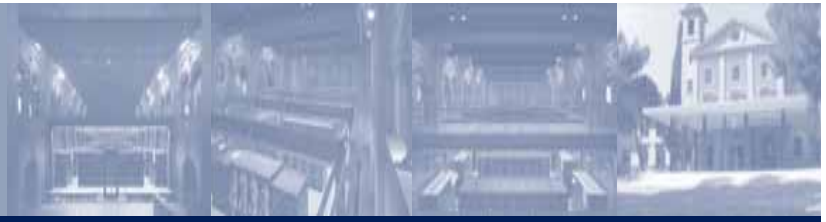
Dr. José M. Baldasano
jose.baldasano@bsc.es

Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS)
Earth Sciences Department. Barcelona, Spain

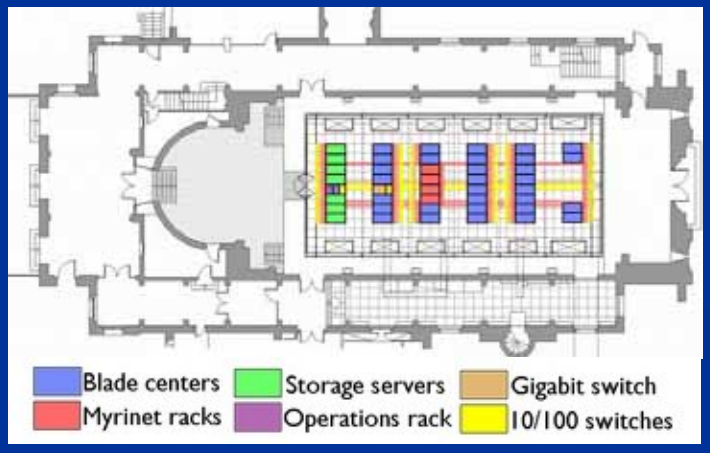
29th HPC User Forum -- September 8 to 10, 2008 -- In Tucson, Arizona

A unique place ……

MareNostrum



- 10240 IBM Power PC 970MP processors at 2.3 GHz (2560 JS21 blades).
- 20 TB Main Memory.
- 94,21 Tflops (peak performance).
- 280 + 90 TB disk.
- Interconnection networks:
  - Myrinet
  - Gigabit
- Linux cluster (SuSe).
- Diskless network support.



MareNostrum

- MareNostrum's evolution:

TOP500® SUPERCOMPUTER SITES

List	World Position	Europe Position
November 2004	4	1
June 2005	5	1
November 2005	8	1
June 2006	11	3
November 2006	5	1
June 2007	9	1
November 2007	13	3

Spanish Supercomputing Network (RES)

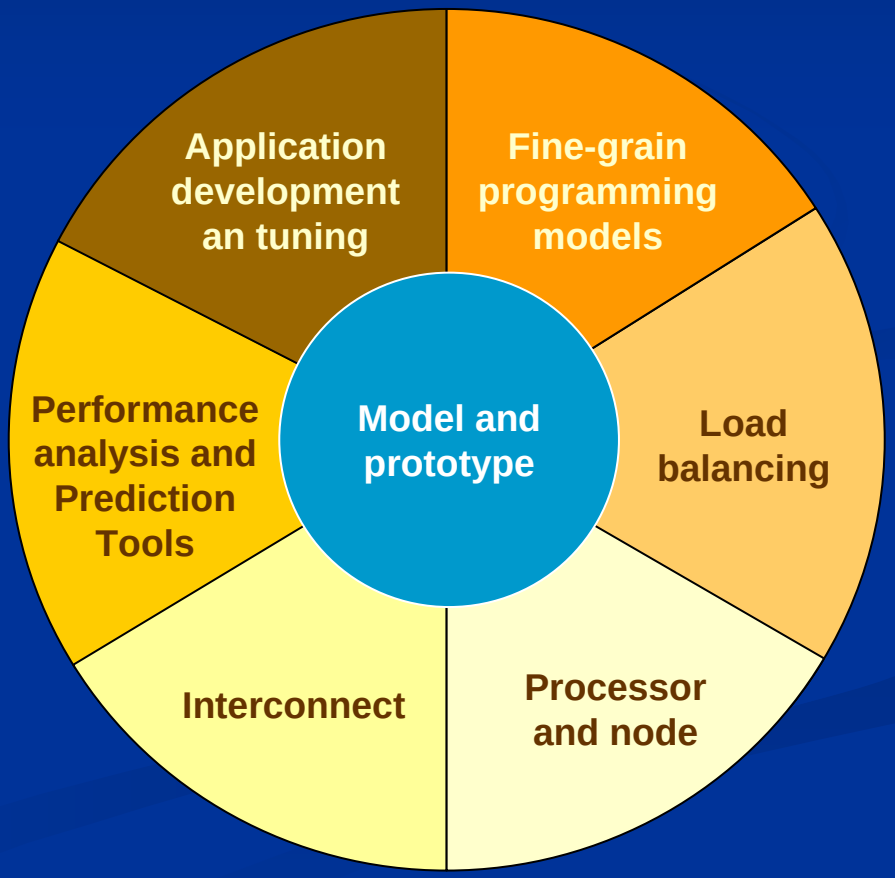
MareNostrum
Processors: 10240 PowerPC 970 2.3 GHz
Memory: 20 Tbytes
Disc: 280 + 90 Tbytes
Networks: Myrinet, Gigabit, 10/100
Operating System: Linux

CeSViMa
Processors: 2408 PowerPC 970 2.2 GHz
Memory: 4.7 Tbytes
Disc: 63 + 47 Tbytes
Networks: Myrinet, Gigabit, 10/100
Operating System: Linux

IAC, UMA, UNICAN, UNIZAR, UV
Processors: 512 PowerPC 970 2.2 GHz
Memory: 1 Tbyte
Disc: 14 + 10 Tbytes
Networks: Myrinet, Gigabit, 10/100
Operating System: Linux

The BSC-IBM MareIncognito project

- 10 Petaflop research project (2010)
- Port/develop applications to reduce time-to-production once installed
- Programming models
- Tools for application development and to support previous evaluations
- Evaluate node architecture
- Evaluate interconnect options



Which countries joined PRACE

HPC NEWS

PRACE selects Petaflop/s HPC sites

1 September 2008

PRACE (Partnership for Advanced Computing in Europe) has selected a broad coverage of promising architectures for Petaflop/s-class systems to be deployed in 2009 and 2010. Prototypes will be installed at six partner sites starting in 2008.

PRACE analysed key scientific applications and mapped them to suitable architectures. As a result six prototypes were selected including more advanced hybrid systems.

'Our objective is to build the best set of prototypes for preparing a timely and seamless deployment of production systems in 2009 and 2010 – not to attempt to select the best individual prototypes', said François Robin, from CEA/GENCI. The prototypes will be installed at the following PRACE partner sites:

- BSC (Barcelona Supercomputing Center, Spain), installs a hybrid prototype combining IBM Cell and Power6 processors. The Cell processors are used for computation and the Power6 processors for service.
- CEA (French Atomic Energy Commission, France) and FZJ (Forschungszentrum Jülich, Germany) jointly use Intel Nehalem/Xeon processors in their systems. Two shared-memory multiprocessors (thin node clusters) will be distributed over the two sites; a prototype produced by Bull at CEA and a larger system of the same architecture at FZJ.
- CSC (The Finnish IT Center for Science, Finland) and CSCS (Swiss National Supercomputing Centre, Switzerland) jointly evaluate the Cray XT5 architecture. This Massively Parallel Processing (MPP) prototype will be installed at CSC's facilities.
- FZJ provides its already installed IBM BlueGene/P system, as a Massively Parallel Processing prototype.
- HLRS (High Performance Computing Center Stuttgart, Germany) offers a NEC SX-9 and an x86 based cluster as a hybrid prototype.
- NCF (Netherlands Computing Facilities Foundation, The Netherlands) evaluates the IBM Power6 architecture, a shared-memory multiprocessor (fat node cluster). This prototype will be installed in SARA Computing and Networking Services facilities in Amsterdam.

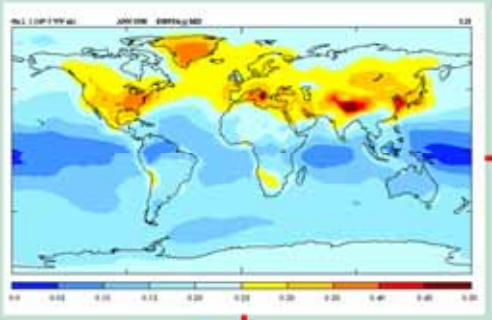
These prototypes will be used to evaluate the architectures in near-production situation with regard to application performance and scalability, as well as total cost of ownership and energy consumption. They will make also possible the evaluation of software for managing the distributed infrastructure, the preparation of benchmarks for future Petascale systems allowing better understanding of user requirements, the scaling and optimisation of libraries and codes and the definition of technical requirements and procurement procedures for the PRACE Petaflop/s production systems for 2009/2010.

Related internet links

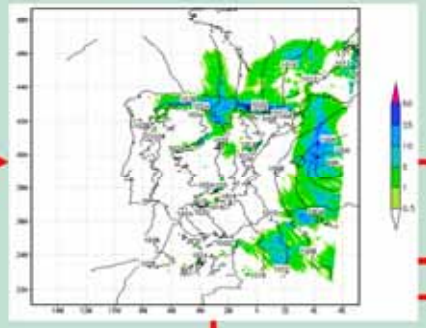
PRACE

CALIOPE Air Quality Forecasting System

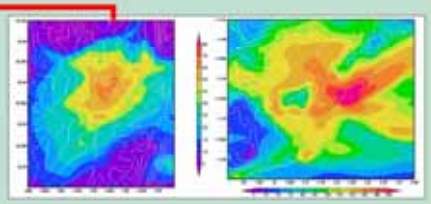
GLOBAL SIMULATIONS
Initial and boundary conditions



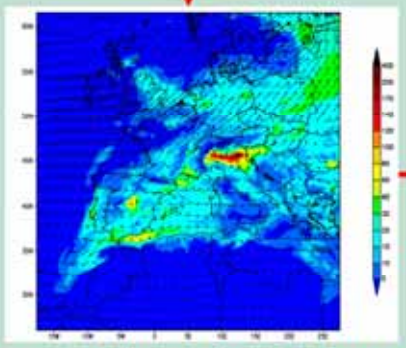
METEOROLOGICAL FORECAST FOR SPAIN
High resolution (4 km)



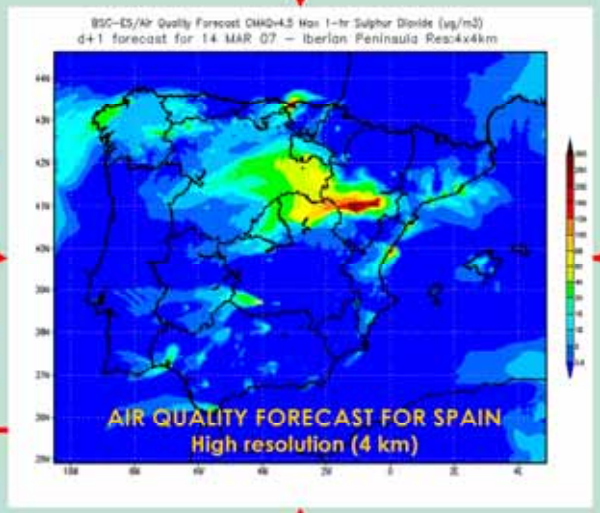
EMISSION MODEL
HERMES developed at BSC-CNS

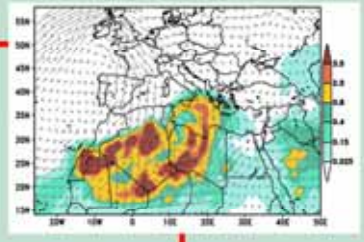


AIR QUALITY FORECAST FOR HOT-SPOTS REGIONS
Madrid and Barcelona (1 km)



EUROPEAN METEOROLOGICAL AND AIR QUALITY FORECAST
High resolution (12 km)

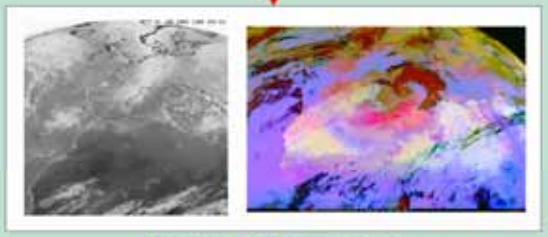




SAHARAN DUST OUBREAKS
Dust Regional Atmospheric Model (DREAM)

Quasi-real time air quality data from stations

METEOROLOGICAL AND AIR QUALITY OBSERVATIONS
Dynamics and model evaluation



SATELLITE OBSERVATIONS
Surveillance and model verification

PARTICULATE MATTER OBSERVATIONS
Dynamics and model evaluation

CALIOPE: Air Quality Forecasting System

MINISTERIO DE MEDIO AMBIENTE

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

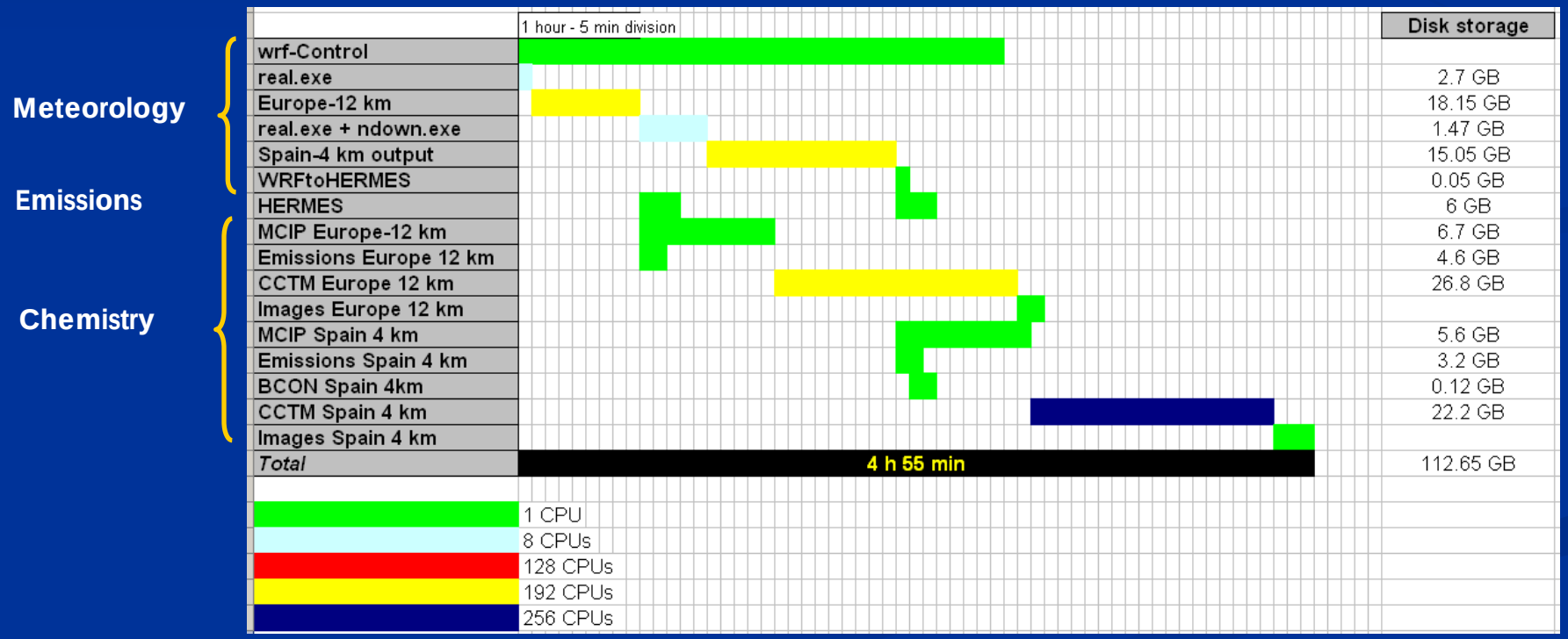
MINISTERIO DE EDUCACIÓN Y CIENCIA
Ciemat
Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

MINISTERIO DE EDUCACIÓN Y CIENCIA
CSIC

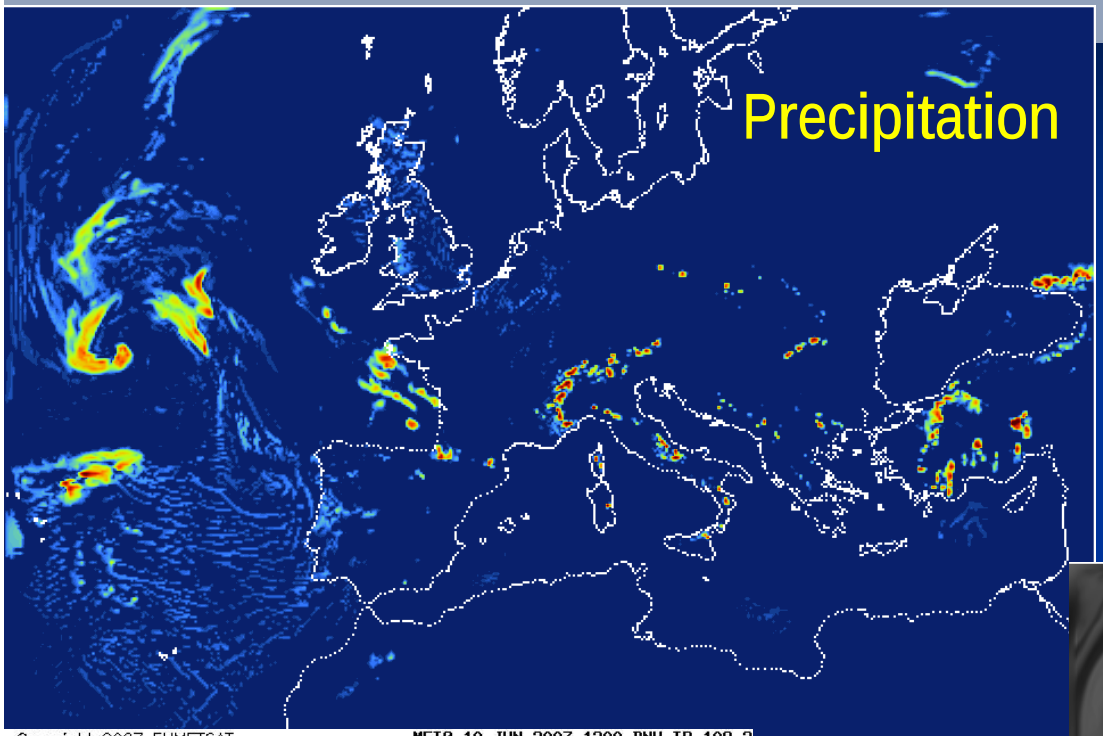
CEAM
FUNDACION CENTRO DE ESTUDIOS AMBIENTALES DEL MEDITERRANEO

Computational requirements

- Workflow of a 48 h high-resolution simulation of Europe at 12 km and Spain at 4 km

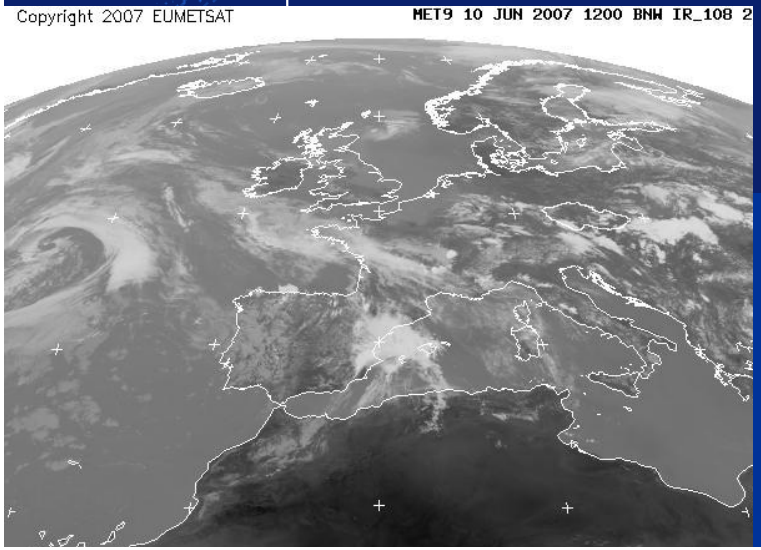


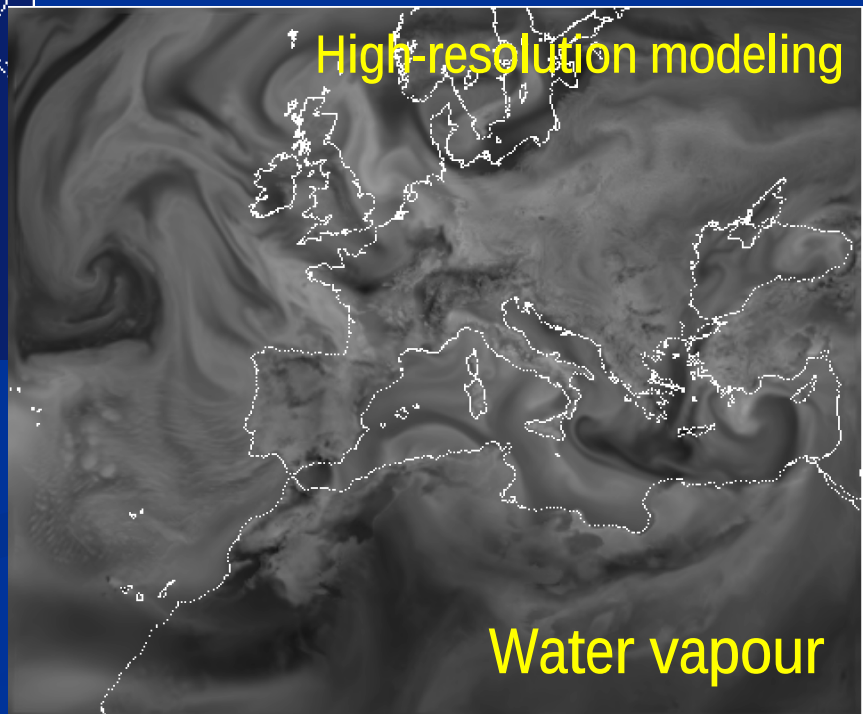
http://salam.upc.es/caliope



Enhancing spatial resolution – towards a new generation air quality modeling system

Resolution improved to 12 km for all Europe, 4 km for the Iberian peninsula, and 1 km for hot spot regions within MareNostrum Supercomputer





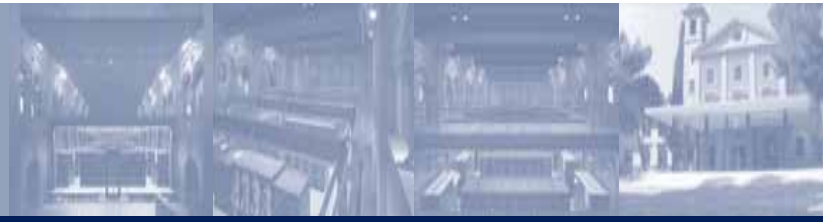
Parallel performance study of the WRF model by applying the Paraver analysis tool

- **Definition of the study cases:**
  - Europe at 12 km horizontal resolution: WRF-ARW, WRF-NMM
  - Iberian peninsula at 4 km horizontal resolution : WRF-ARW, WRF-NMM
  - North America at 12 km horizontal resolution : WRF-ARW
  - Analysis of European and Iberian peninsula domains

- **WRF computational needs depend of:**
  - 1) Domain size
  - 2) Topography
  - 3) Meteorological conditions

	Domain				
	Europe	Iberian peninsula	Europe	Iberian peninsula	USA
Model	WRF-ARW	WRF-ARW	WRF-NMM	WRF-NMM	WRF-ARW
NX	400	400	400*	400*	425
NY	400	400	400*	400*	300
NZ	38	38	38	38	35
Resolution (km)	12	4	12	4	12
Simulation day	08/11/2005	13/09/2006	08/11/2005	13/09/2006	25/10/2001
Hours of simulation	9-12h	15-18h	9-12h	15-18h	0-3h
Microphysics	WSM 3class	WSM 6class	Ferrier	Ferrier	Ferrier
LSM	Noah	Noah	Noah	Noah	5-layers
PBL	YSU	YSU	MYJ	MYJ	YSU
Cu	KF	Explicit	BMJ	Explicit	KF

Main results



Performance in MareNostrum Supercomputer:

- Reduced scalability of atmospheric WRF codes (30-40%) in current HPC environments
  - Over 128 cpus, reduced speedup
- Similar codes have large difference in performance computing. Differences between NMM and ARW dynamical cores:
  - ARW: load balancing and communications problems. Low Instructions per cycle. Sensitive to contention.
  - NMM: code replication major point.
- Limitation of coding paradigm finite difference schemes
  - Replication of code for communication exchange
  - Strong scalability limitation in current HPC environment

HERMES2004: High-Elective Resolution Modelling Emission System (Baldasano et al 2008)

Database information management

Biogenic emissions

- Land use map
- Emission factors and biomass
- Meteorological information (air temperature, solar radiation)

On road, ships and aircrafts traffic

- Roads (urban streets, roads, etc.), LTO cycles and ships routes
- Hourly, weekly and monthly profiles
- Distribution of the vehicles
- Velocity by road type
- Meteorological information (air temperature)
- Type of combustibles

Industry and electric generation

- Location (point/area)
- Production / electric generation
- Emission factors – energetic intensity
- Chimney height / diameter

Residential and commercial

- Density population map
- Combustibles consume
- Emission factors
- Solvent use
- Waste generation

Emission computation and speciation

BVOCs	NO_x, VOCs, CO, SO_2, particulate matter, CO_2, CH_4 and N_2O	NO_x, VOCs, CO, SO_2, particulate matter, CO_2, CH_4 and N_2O	NO_x, VOCs, CO, SO_2, particulate matter, CO_2, CH_4 and N_2O

Speciation

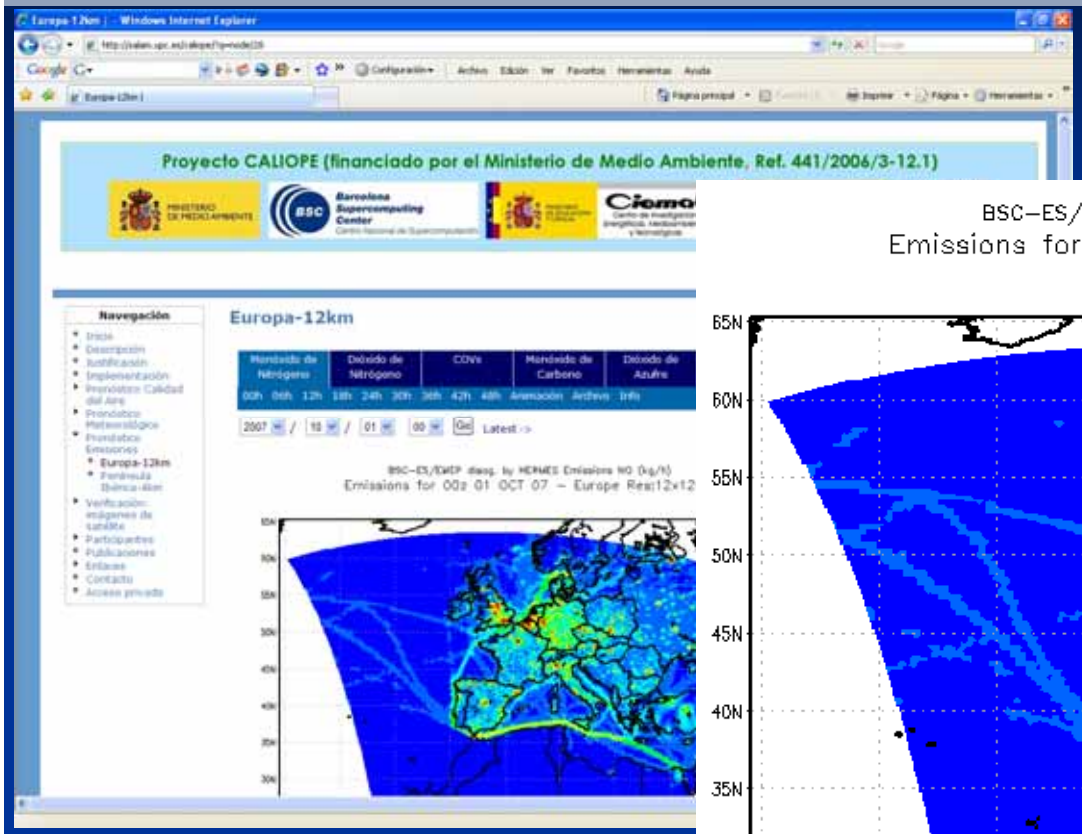
Management of the emission information

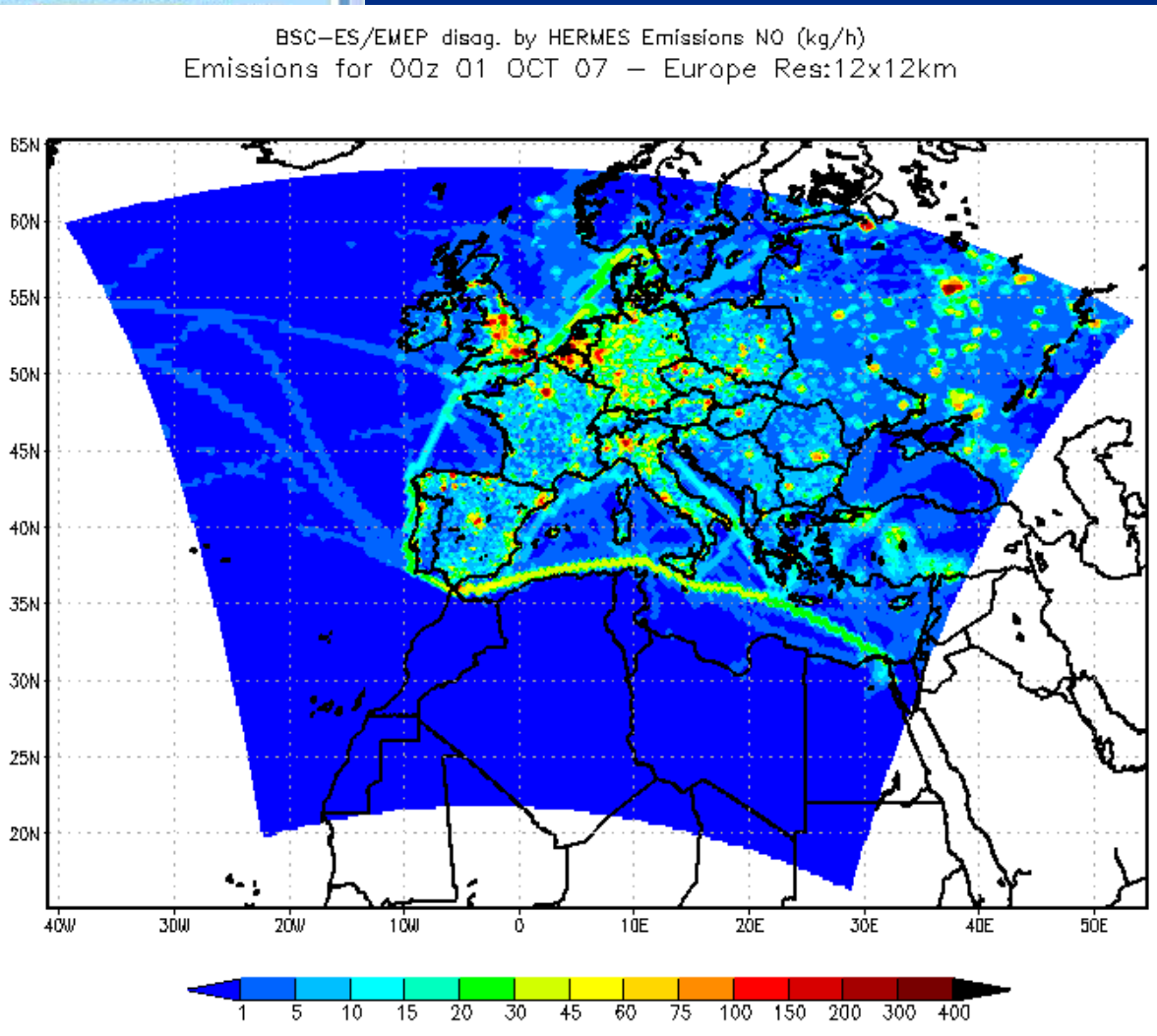
- Visualization and analysis of the results
- Management information tool

Management of emission data for air quality modelling

- Hourly aggregation of archives (4x4 km, 1x1 km grid size)
- Height desaggregation (vertical layers)
- Database resolution (1 - 4 km grid size)
- Generation of netCDF emission files

HERMES: Emissions for Europe, 12 km, disaggregated from EMEP (50 km), 01-02 October 2007, pollutant: NO

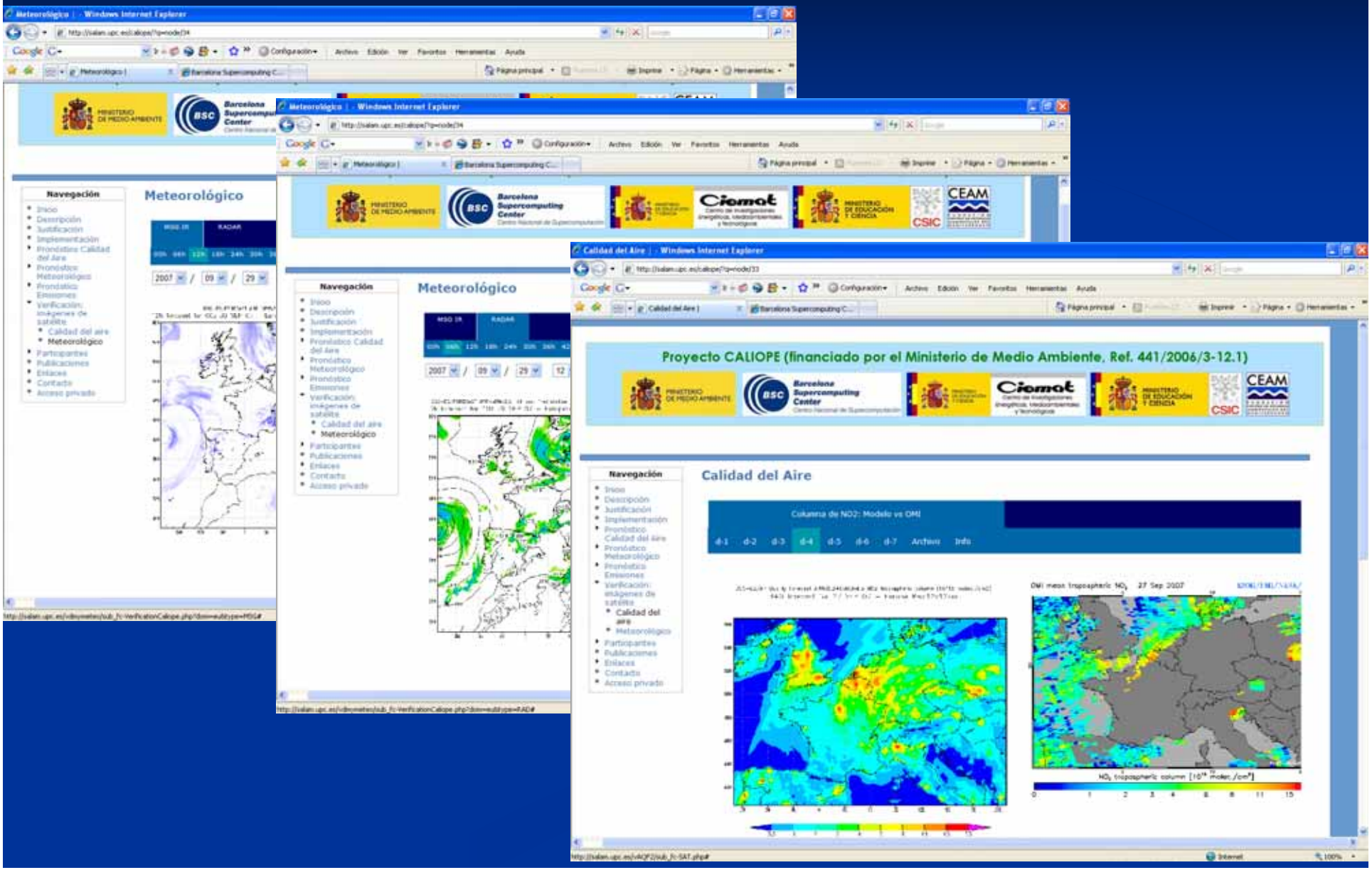




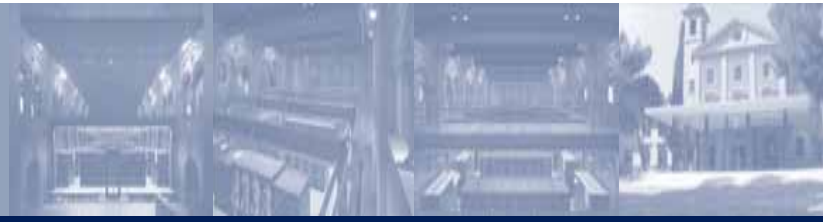
1. Operational meteorological validation: MSG

2. Operational meteorological validation: RADAR

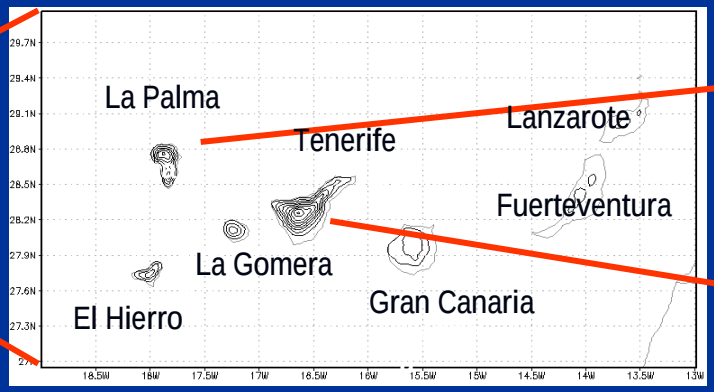
3. Operational air quality validation: OMI NO_2 tropospheric column



Canary Islands archipelago

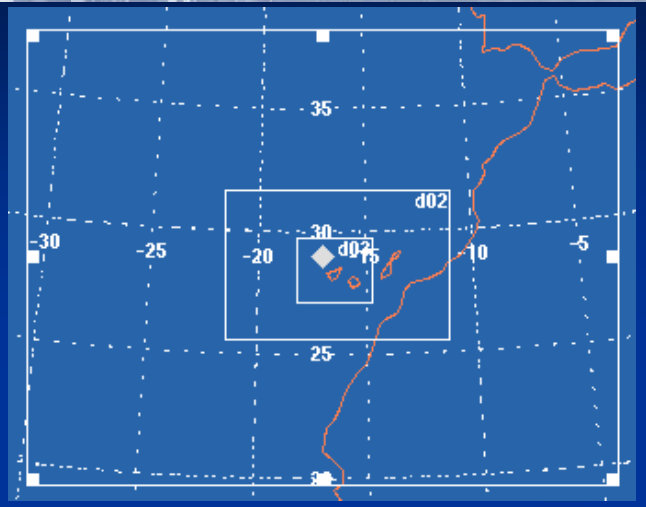


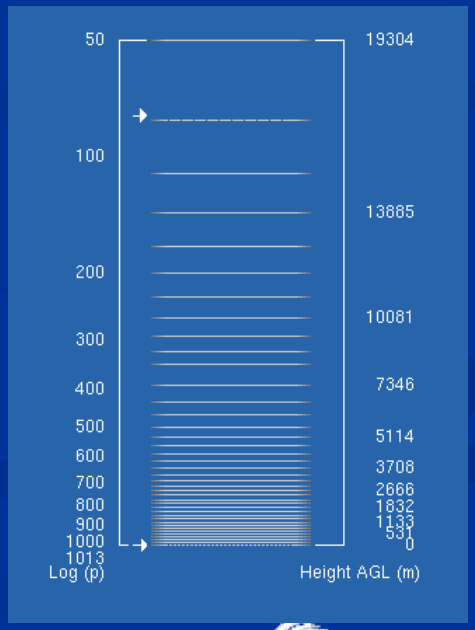
The Canary Islands are located in the middle-east of the Atlantic Ocean in front of the southern coast of Morocco. They are the most distant archipelago of Spain constituted of seven islands of volcanic origin with very complex topography. La Palma, which is a very steep island, and Tenerife, the largest island (1929 km^2) with the highest peak (3718 m a.s.l.) of Spain (Teide volcano), were the most affected for the synoptic situation of Delta storm.



Methods

- Weather Research and Forecasting (WRF) Model
  - ARW dynamics solver
  - Microphysics: single-moment 3-class scheme
  - Cumulus: Kain-Fritsch
  - PBL: Yonsei University PBL scheme
  - LSM: Rapid Updated Cycle LSM
  - Radiation: RRTM for LW, Dudhia scheme for SW
  - IC & BC: ECMWF IFS-0.25º forecast, BC every 3h.
- Conducted numerical simulations:
  - Base case run: three nested high-resolution domains 9, 3, 1 km
  - Experimental run without Canary Islands topography
  - 00 UTC 28 November 2005 – 00 UTC 30 November 2005
- Domains:
  - D1: 300 x 230 grid points at 9 km
  - D2: 340 x 226 grid points at 3 km
  - D3: 337 x 292 grid points at 1 km
  - 40 sigma vertical levels;
  - model top at 50 hPa





Operational forecast products

SDS WS Operational products

http://www.bsc.es/projects/earthscience/DREAM/

Model predictions (72-h):

Horizontal distribution

- ➢ PM2.5, PM10, TSP at surface and height
- ➢ Total column mass (dust load)
- ➢ Dust aerosol optical depth
- ➢ Wet, dry, total deposition
- ➢ Visibility (soon available)
- ➢ Meteorological variables

✓ Vertical distribution

- ➢ Cross sections
- ➢ Fixed point/time profiles

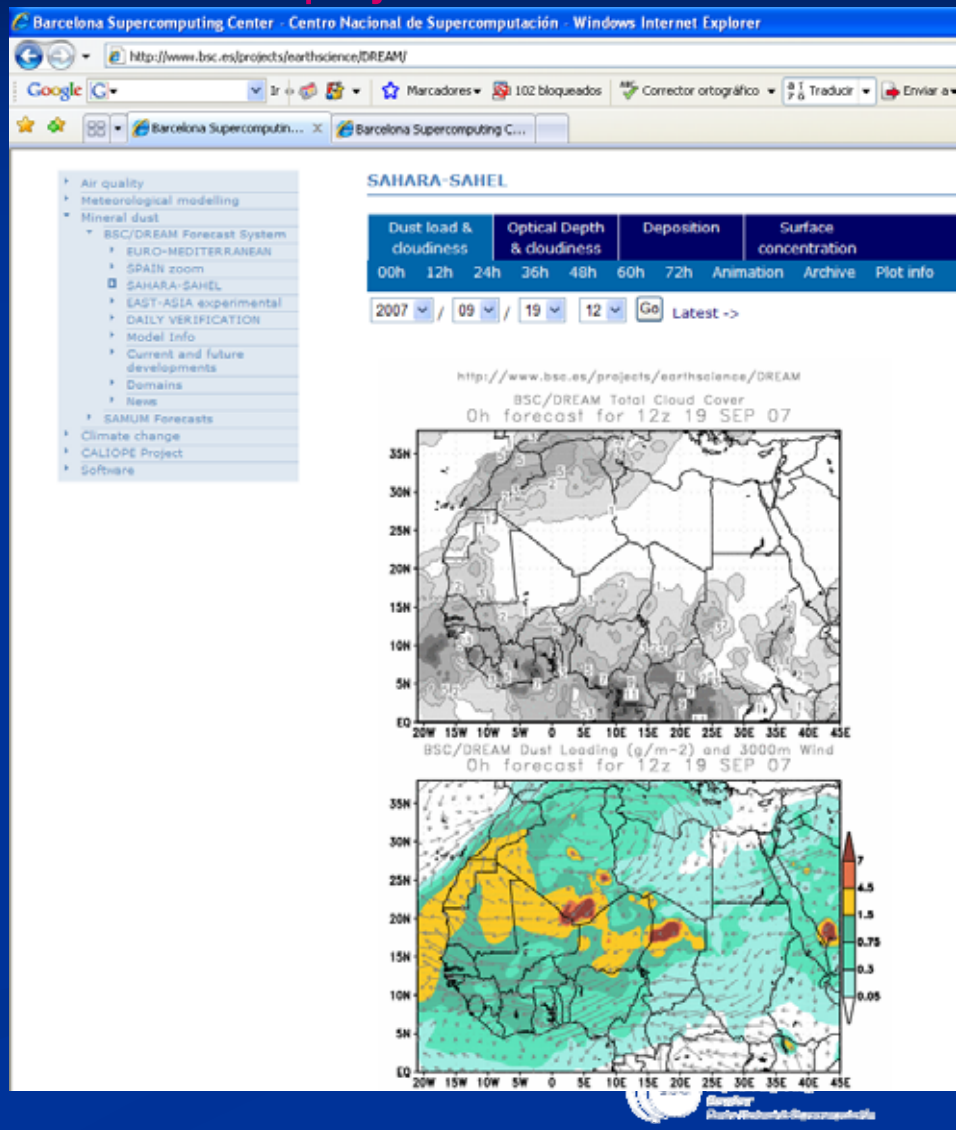
✓ Fixed point (selected sites/cities)

- ➢ Dustgrams
- ➢ Meteograms

Request-only basis:

✓ Numerical data

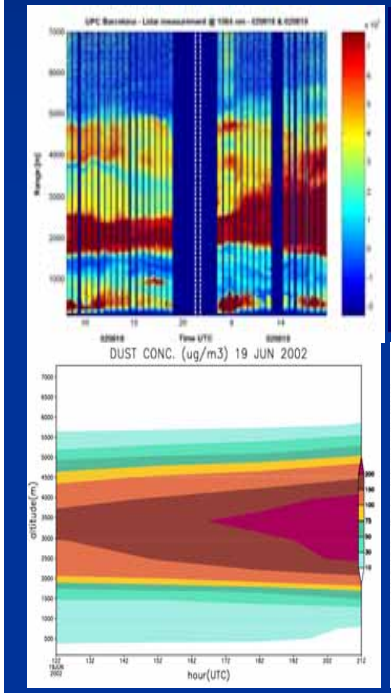
✓ Climatology



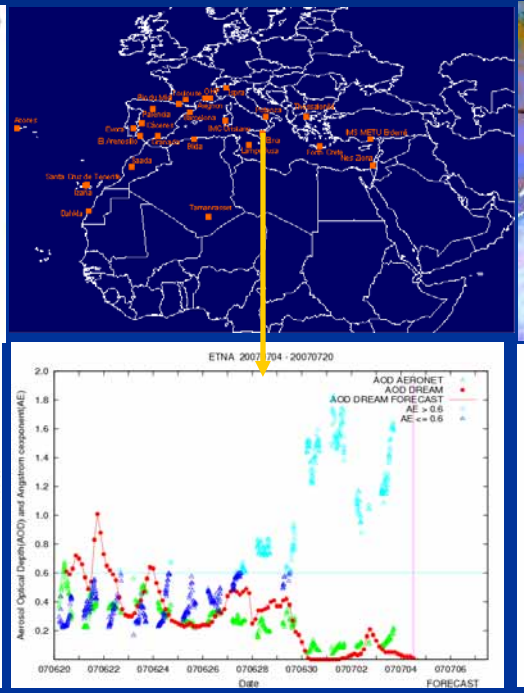
Dust forecast and validation system

Model has shown very good agreement with observations in a number of studies of single events (e.g., *Ansmann et al.*, 2003, *Papayannis et al.*, 2005; *Pérez et al*., 2006a;b; *Jiménez et al,* 2006 ….)

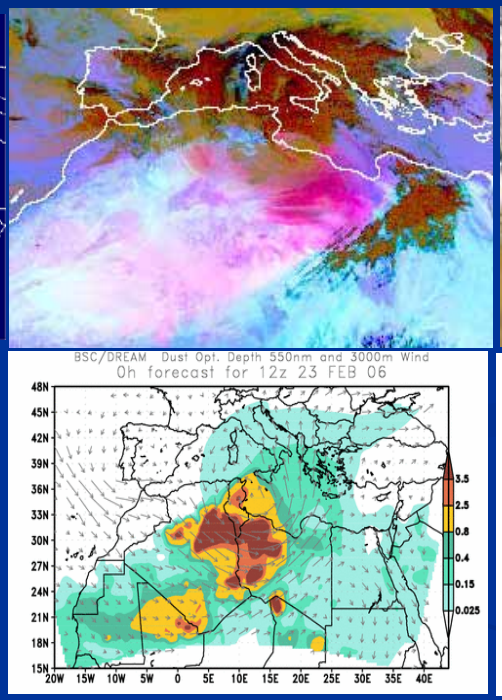
Lidars - EARLINET



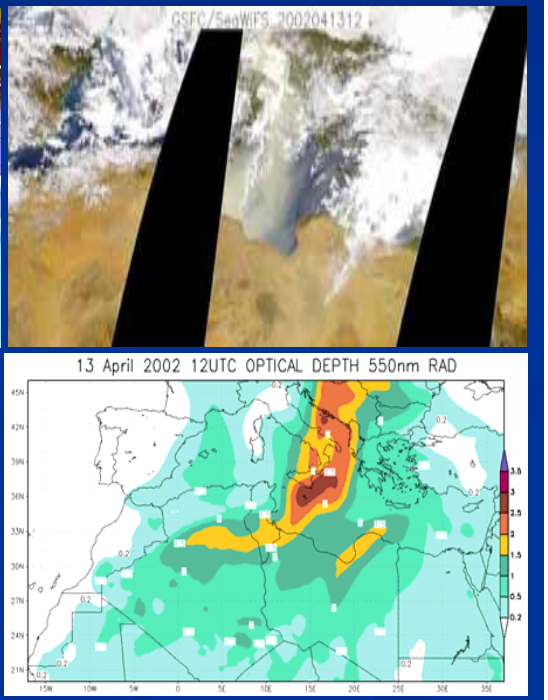
AERONET - ONLINE



Meteosat Second Generation



SeaWIFS



Current users of the system:

- Scientific (aerosols, ocean, health, …)
- Experimental campaigns (TROMPETA, SAMUM, …)
- Observational Networks: Earlinet (European Lidar Network), AERONET and in-situ observations
- Satellite community
- Spanish administration: alert system

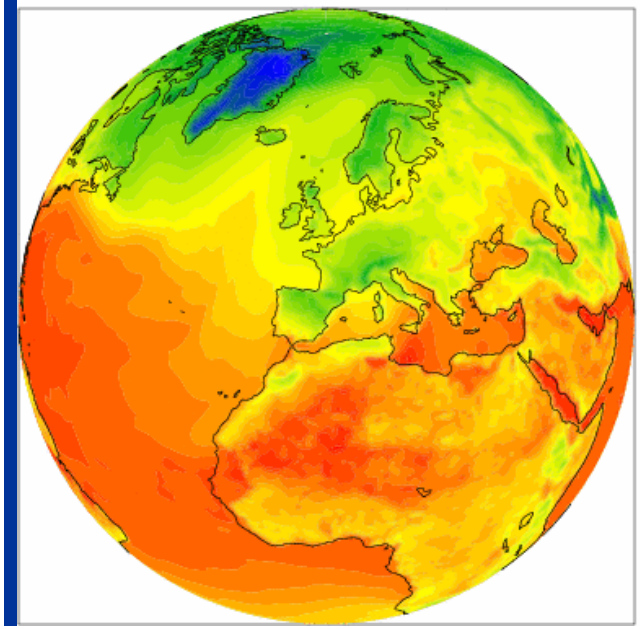
New model development: Global / Regional ESMF/NMM-b (2007-2010)

Implementation of aerosol and chemistry module into the most recent parallelized and non-hydrostatic version of the NMM/ NCEP model, with application either as a limited area or global model

→ Increasing resolution
→ Global model domain
→ High resolution dust forecast

Eta model	ESMF/NMM-b model
Regional model	Global/Regional model
Hydrostatic	Non-hydrostatic
Eta coordinate	Sigma coordinate
Arakawa E-grid	Arakawa B-grid
Convection parameterization	Microphysical convection

Temperature field from UMO



•NEW GENERATION OF EARTH SYSTEM MODELLING FRAMEWORK (ESMF) IN MARENOSTRUM PARALLELIZED ENVIRONMENT

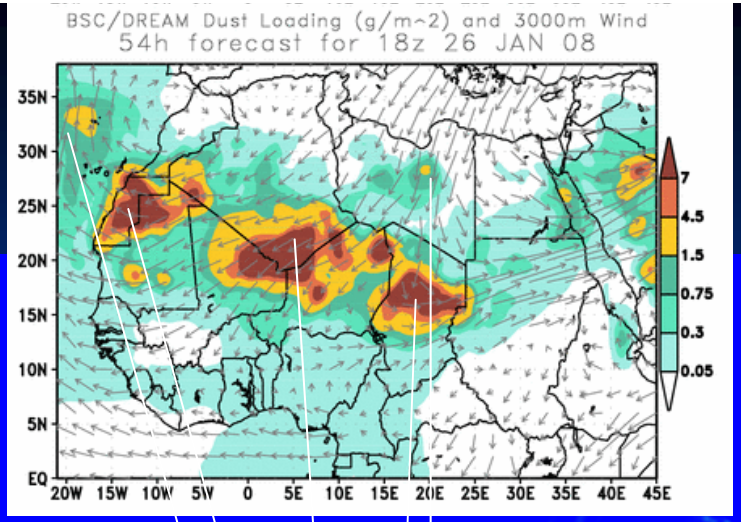
•IMPLEMENTATION OF MINERAL DUST MODULE

•IMPLEMENTATION OF FULL CHEMISTRY COMPONENT ON-LINE

•CODE IMPROVEMENT AFTER BENCHMARK AND PERFORMANCE STUDIES

PRELIMINARY RESULTS WITH DUST COMPONENT

Simulation set-up:
Global
Cycle 20080124 12 UTC
60 hours forecast
160 CPU's
8 dust bins
769x541 64 sigma layers



Cycle 20080124_12
54h forecast

Dust conc bin 4
Sigma layer 52

kg/m^3

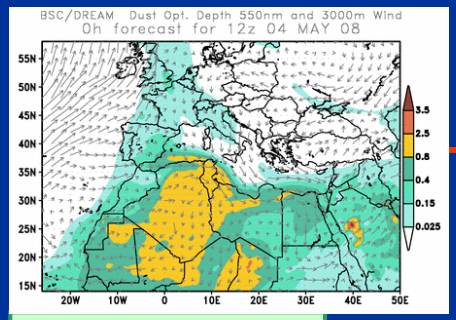
WMO Sand and Dust Storm Warning and Assessment System (SDS WAS)

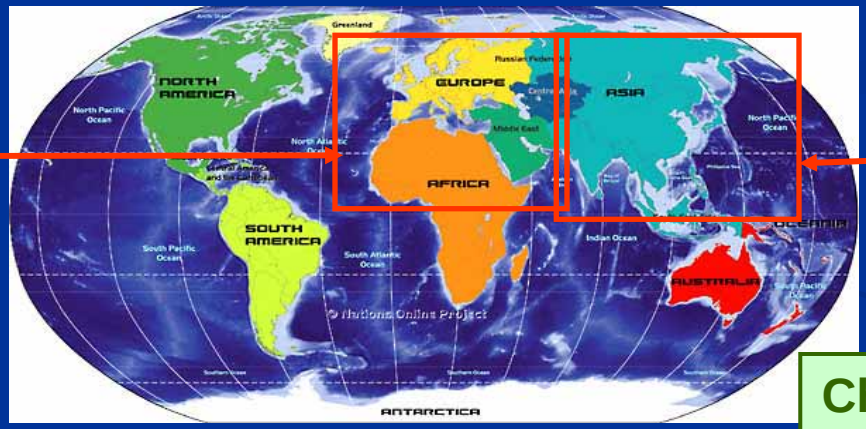
- To enhance the ability of participating countries to establish and improve systems for forecasting and warning to suppress the impact of Sand and Dust Storm

by

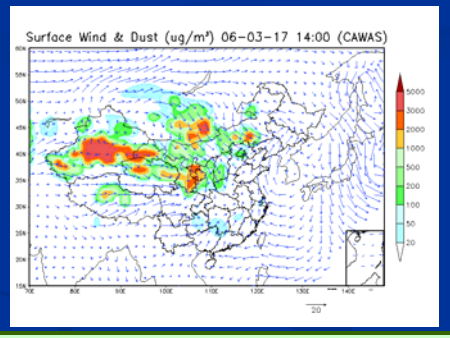
- Establishing a coordinated global network of Sand and Dust Storm forecasting centers delivering products useful to a wide range of users in understanding and reducing the impacts of SDS

North Africa, Middle East and Europe





Asia

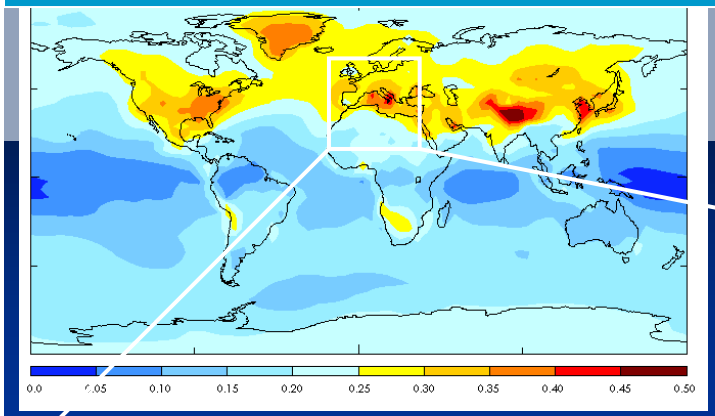


BSC-CNS
AEMET
CSIC, Spain

China Meteorological Administration (CMA)
Xiao Ye Zhang
xiaoye@cams.cma.gov.cn

WMO REGIONAL CENTRES

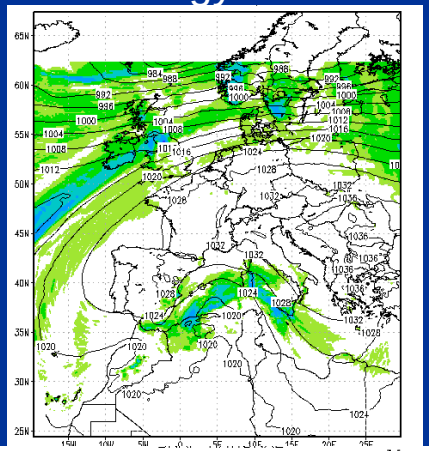
Global Circulation Model: EC-Earth (ECMWF), GISS ModelE (NASA)

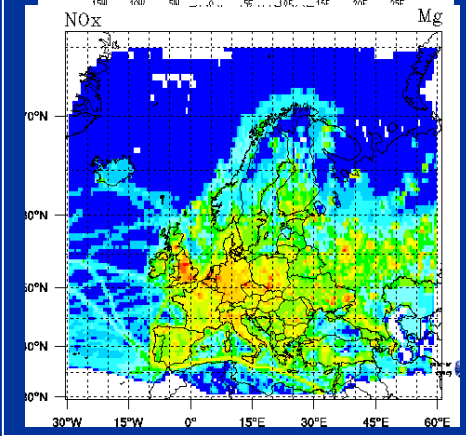


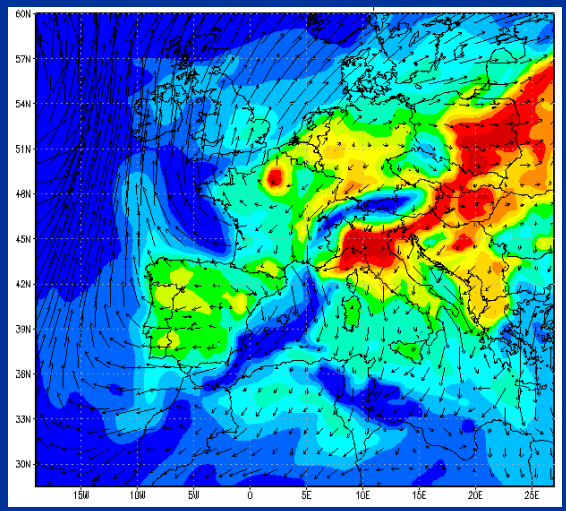
Climate modeling system at BSC-CNS:
Global Circulation Model
Regional Climate Model

Regional modelling system

Meteorology: WRF-ARW / WRF-NMM

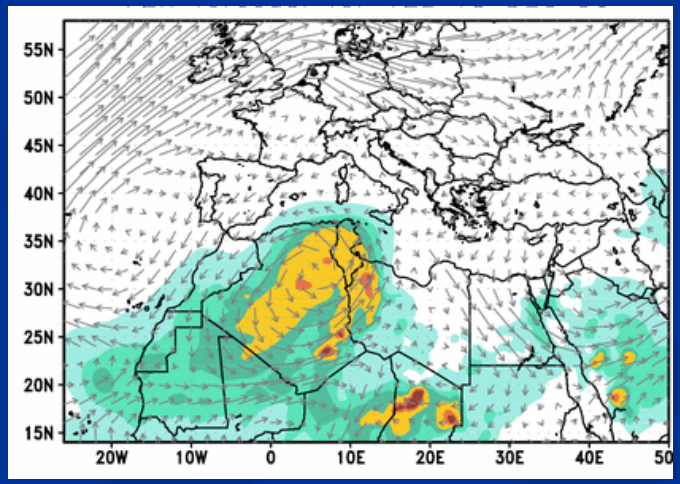




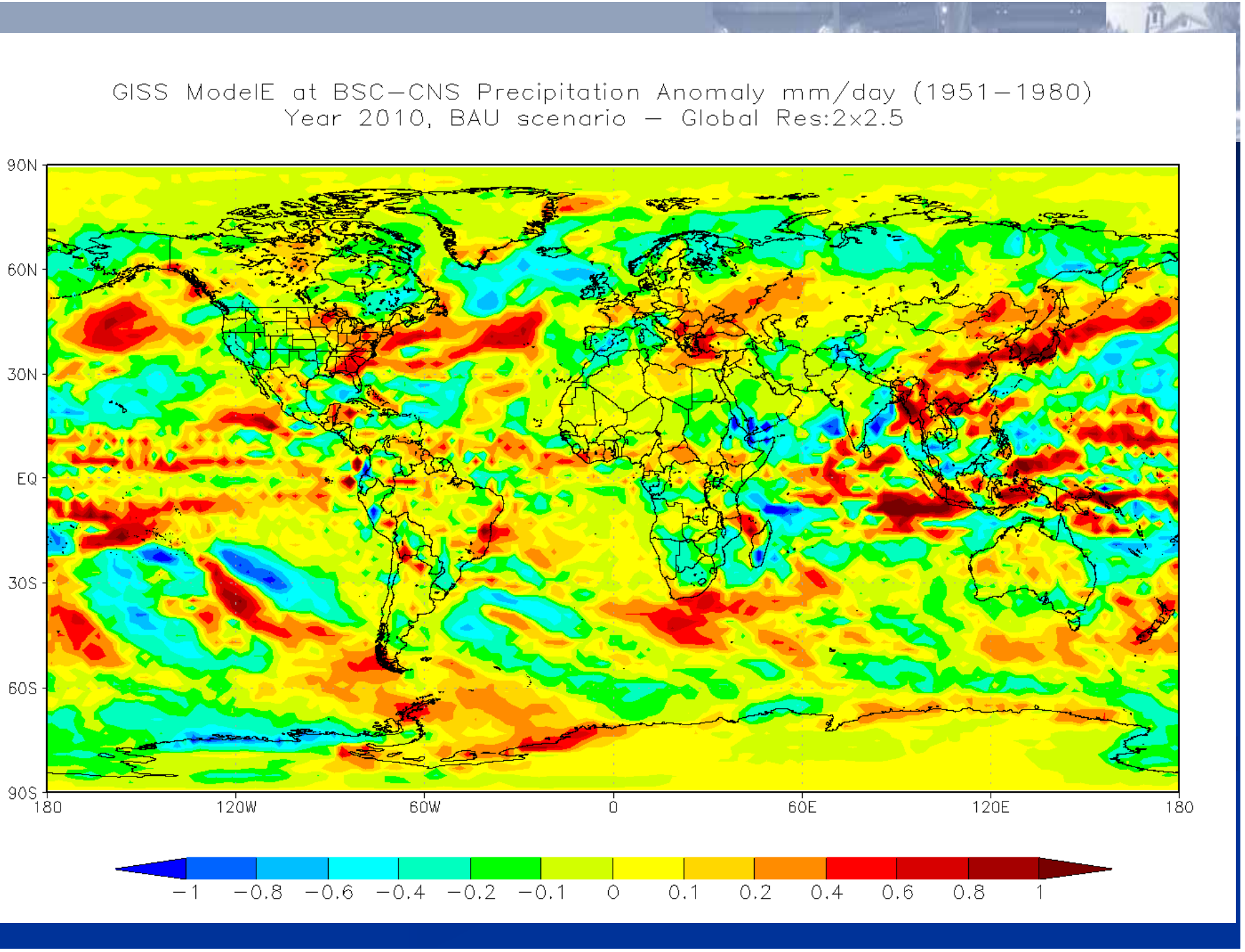


Chemistry Transport: CMAQ / CHIMERE

Mineral Dust: DREAM

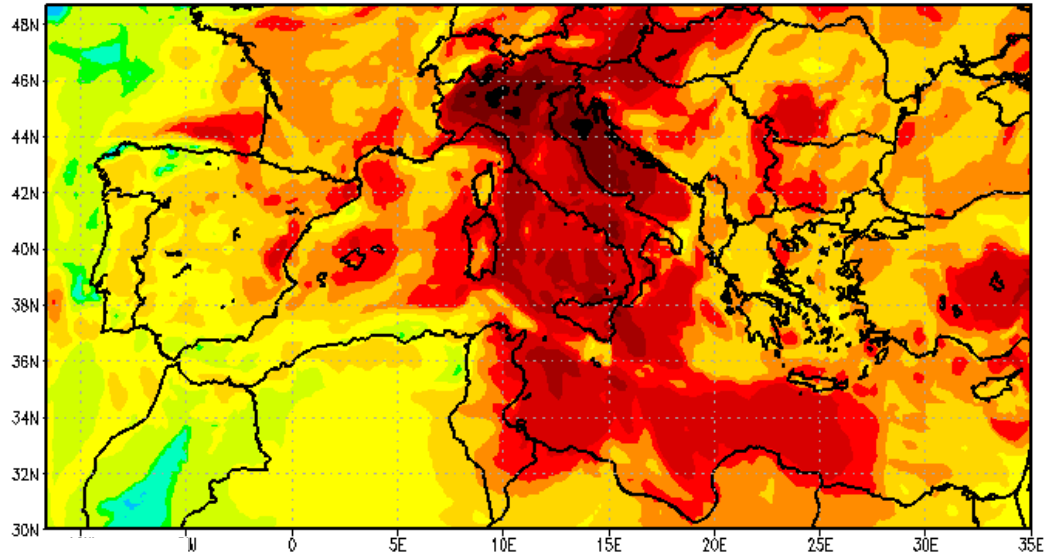


Emissions: HERMES, EMEP


GISS ModelE at BSC-CNS Precipitation Anomaly mm/day (1951-1980)
Year 2010, BAU scenario - Global Res:2x2.5
90N
60N
30N
EQ
30S
60S
90S
180
120W
60W
0
60E
120E
180
-1
-0.8
-0.6
-0.4
-0.2
-0.1
0
0.1
0.2
0.4
0.6
0.8
1

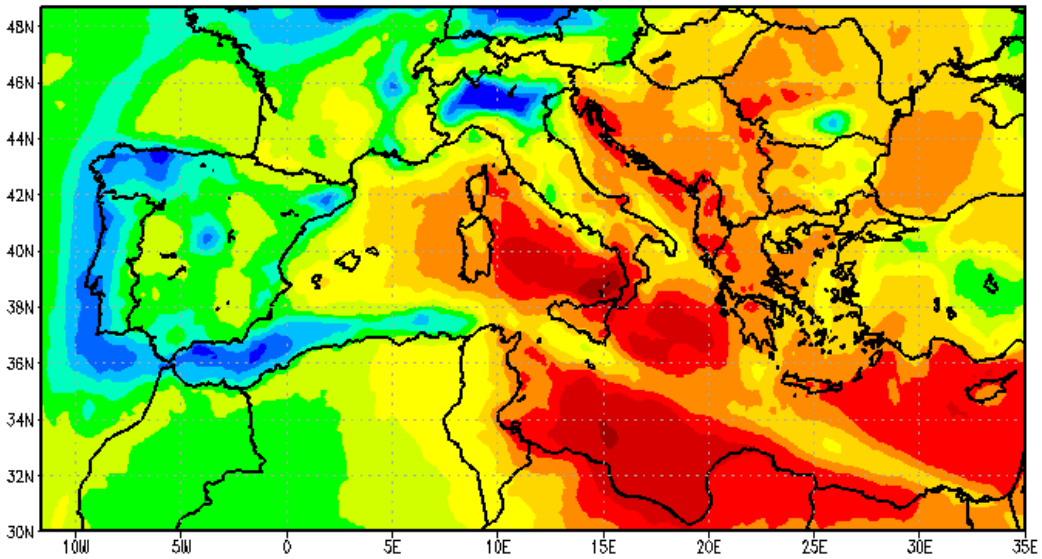
BSC-ES CMAQv4.5 Ozone 1-hr Maximum (ug/m3)

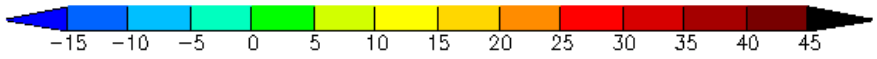
August, Scenario 2000-Scenario B1 2030 - Mediterranean Res:20x20km

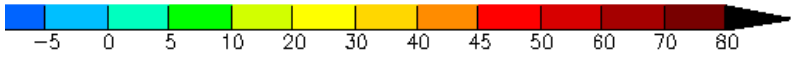


BSC-ES CMAQv4.5 Ozone Monthly Average (ug/m3)

August, Scenario 2000-Scenario B1 2030 - Mediterranean Res:20x20km







Combination of Collaborative Project and Coordination and Support Action for Integrating Activities

FP7-INFRASTRUCTURES-2008-1
INFRA-2008-1.1.2: Targeted approach: Integrating Activities

INFRA-2008-1.1.2.21:
"Establishing an European e-Infrastructure for earth system's understanding and modelling"

InfraStructure for the European Network for Earth System Modelling

IS-ENES

Coordinator: Dr Sylvie Joussaume

Participant no.	Participant organisation name	Part. Short Name	Country
1 (Coordinator)	Centre National de la Recherche Scientifique - IPSL	CNRS - IPSL	France
2	Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V.	MPG	Germany
3	Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique	CERFACS	France
4	Deutsches Klimarechenzentrum GmbH	DKRZ	Germany
5	Finnish Meteorological Institute	FMI	Finland
6	University of Manchester	UNIMAN	United Kingdom
7	Academy of Athens – Centre for Atmospheric, Physics and Climatology	AA - CAPC	Greece
8	Science and Technology Facilities Council	STFC	United Kingdom
9	Centro Euro-Mediterraneo per i Cambiamenti Climatici	CMCC	Italy
10	METOFFICE	METOFFICE	United Kingdom
11	Koninklijk Nederlands Meteorologisch Instituut	KNMI	Netherlands
12	Météo France - Centre National de Recherches Météorologiques	MF - CNRM	France
13	Sveriges Meteorologiska och Hydrologiska Institut	SMHI	Sweden
14	NEC Laboratories Europe - IT Research Division	NLE-IT	Germany
15	Linköpings Universitet	LIU	Sweden
16	Barcelona Supercomputing Centre	BSC	Spain
17	Wageningen Universiteit	WU	Netherlands
18	Institutul National de Hidrologie si Gospodarire a Apelor	INHGA	Romania
19	Deutsches Zentrum Für Luft- und Raumfahrt in der Helmholtz Gemeinschaft	DLR	Germany
20	Program for Climate Model Diagnosis and Intercomparison	PCMDI	United States of America

Thanks you for the attention

CONTACT
jose.baldasano@bsc.es