Earth Sciences

Modelling of global and regional climate.

Current Developments at MareNostrum Supercomputer

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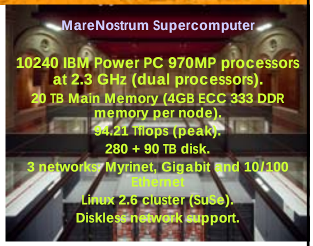
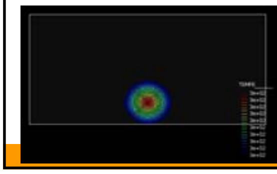
Research is devoted to: high-resolution meteorological modelling, air quality modelling (photochemical and aerosol pollution); global and regional climate modelling (feedback with air quality and radiative forcing); and global and regional modelling of desert dust.



Computational Earth Sciences:



✓ Performance studies of the cores of the WRF meteorological model using Paraver software developed at BSC-CNS.

✓ Initial steps: application of current numerical methods to atmospheric models based on finite-volume schemes to be implemented in large HPC facilities.

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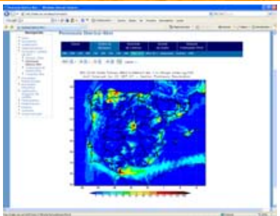
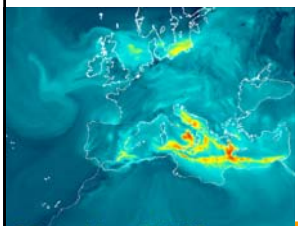
Air Quality and Meteorological Modelling:

✓ The group offers a pan-European Air Quality forecasting and assessment service to end-users that takes advantage of the high spatial and temporal resolution of the air quality modelling system.

✓ Daily operational forecasts for meteorology and air quality (12 km for Europe and 4 km for the Iberian Peninsula) (http://salam.upc.es/caliope).





✓ High-resolution long-term modelling for Europe and the Iberian Peninsula to describe the dynamics of air pollution and the relationship between emissions and atmospheric physico-chemical processes.

✓ Development of the HERMES high-resolution emission model for Spain (1 km and 1 hr).

✓ WRF model used for severe weather impact studies (e.g. the extra-tropical storm Delta was modelled at high-resolution,1 km).

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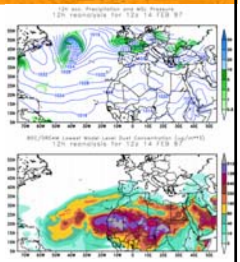
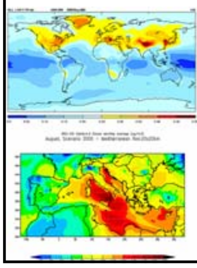
Mineral Dust:

✓ Daily operational forecasts of mineral dust for the Euro-Mediterranean and the East Asia region based DREAM Model (http://www.bsc.es/projects/earthscience/DREAM).

✓ Leading initiative: WMO initiative to create a Regional Centre for Sand and Dust Storm Warning System.

✓ Initial steps for the development of a global-to-regional / hydrostatic-non hydrostatic dust model based on the UMO.





Climate Modelling:

✓ Global Climate Modelling with NASA GISS ModelE and NCAR WACCM in MareNostrum supercomputer with a resolution of 2ºx2.5º.

✓ Implementation of a regional climate model (RCM) based on the WRF/CMAQ/DREAM system for the Mediterranean Sea and Europe (20 km resolution) in order to simulations to ascertain the regional impact of climate change in the trends of extreme events.

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Outline

1. Climate models: formulation and supercomputing needs
2. Global circulation models (GCMs): applications of NASA's GISS ModelE and NCAR's WACCM at MareNostrum Supercomputer
3. Regional climate models (RCMs): what information can we get from them compared to GCMs? WRF/CMAQ applied to regional climate studies
4. High-resolution applications of atmospheric modelling implemented in supercomputers: the CALIOPE project
5. A parallel performance study of a RCM: the WRF framework

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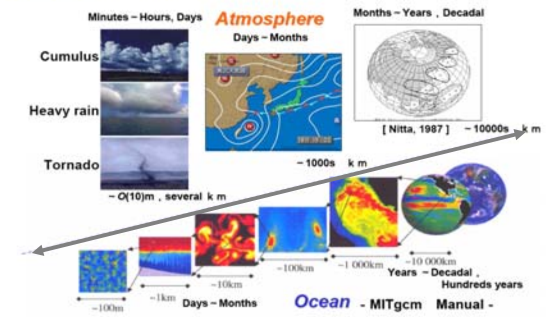
Atmospheric Earth System Time/Space Scale



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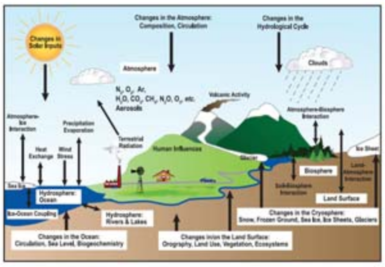
Source: IPCC AR4, 2007.



FAQ 1.2, Figure 1. Schematic view of the components of the climate system, their processes and interactions.

CLIMATE SYSTEM:

- ✓ The atmosphere: circulation, the heat transfer to and from the sun, formation of clouds and atmospheric reactive flows that determine the concentrations of its chemicals.
- ✓ The ocean: interaction of ocean and atmpsphere through exchange of momentum, heat and water. The ocean is a heat sink and it is a medium of transport of energy from continent to continent.
- ✓ Land: vegetation, man and soil play an important role in terms of air dynamics and chemicals transport.
- ✓ Cryosphere: snow, ice and sea-ice influence on the large-scale circulation.
- ✓ Biosphere: life on earth and in the water has an important impact on the CO_2 cycle.

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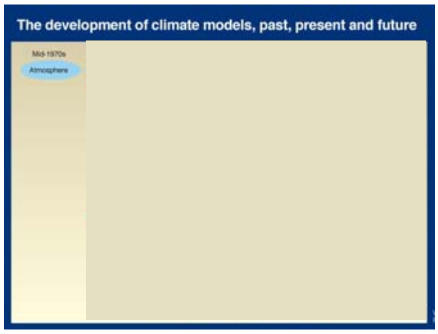
Present situation: global circulation models



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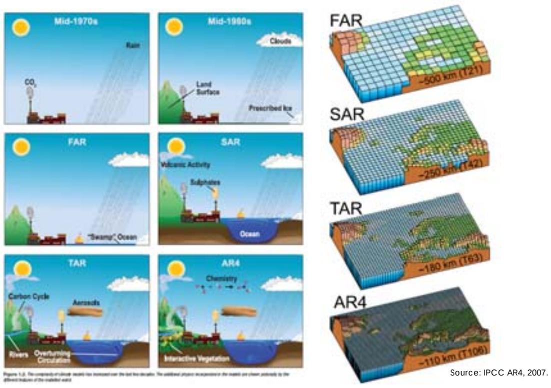

Source: IPCC AR4, 2007.

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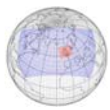
- ✓ Current operational models:
  - NWP:
    - Global models: 50-25 km – spectral models
    - Limited area models – Regional scale: 20-12 km – grid cell models
  - Air quality models:
    - Limited area models – Regional scale: 50 km
    - Limited area models – Local scale: 10 km
- ✓ Current climate models:
  - Global resolution – 4ºx4.5º to 2ºx2.5º
  - Regional applications – 50 to 20 km
- ✓ Scalability limitations of actual codes:
  - NWP:
    - Global resolution:
      - 1º horizontal resolution scales up to 64 cpus
      - 0.5º horizontal resolution scales up to 120 cpus
      - 0.25º horizontal resolution scales up to 240 cpus
      - Some test applications of global resolutions of 3 km with 6000 cpus
    - Limited area model:
      - Function of the domain dimensions and resolution

Global model



Limited area model (blue,red)

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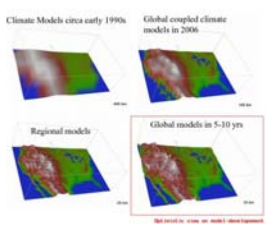
- ✓ Needs for enhanced atmospheric modelling systems:
  - Improvements of scalability of actual atmospheric codes for higher-resolution applications and climate simulations.
    - Towards grid cell global unified models at finer resolutions:
      - Global simulations at 20 - 3 km
        - Consistent simulations of processes of a large range of scales.
        - Ability for developing nonhydrostatic processes.
- ✓ Increasing resolutions of actual climate simulations
  - To 1º degree global simulations for reliability comparisons with actual results.
  - Capacity for regional higher resolution simulations:
    - To improve simulations of mesoscale processes in region with strong surface forcing (complex topography, land-use heterogeneity, sea-land interface, etc.)
    - Trends in the extreme episodes of air pollution (especially ozone and particulate matter)
- ✓ Needs for increasing supercomputing resources in capacity applications, better codes for capability applications.



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ECMWF Supercomputer History

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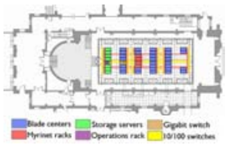
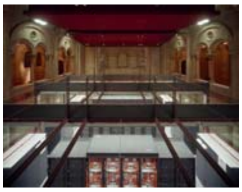
MareNostrum Supercomputer

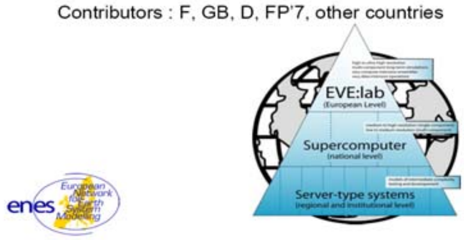
- ✓ 10240 IBM Power PC 970MP processors at 2.3 GHz (2560 JS21 blades).
- ✓ 20 TB Main Memory.
- ✓ 94,21 Tflops (peak performance).
- ✓ 280 + 90 TB disk.
- ✓ Interconnection networks:
  - ➢ Myrinet
  - ➢ Gigabit
- ✓ Linux cluster (SuSe).
- ✓ Diskless network support.





The ENES proposal

60 TFE in 2008 for Europe (EVE:lab)
Sustained effort until 10 PFE
Contributors : F, GB, D, FP'7, other countries



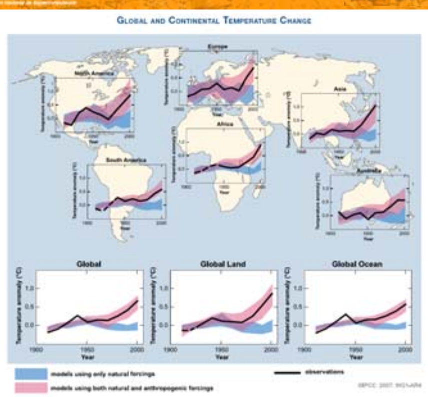
Enhancing supercomputing capabilities

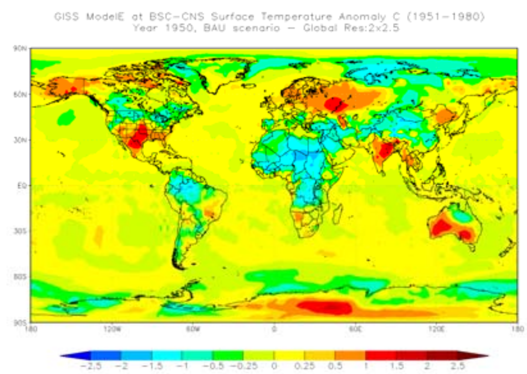
Challenge	1TF sustained	10-100 TF sustained	100-1000 TF sustained	>1 PF sustained
Weather and air quality	Preliminary studies on limited domains	Cloud resolving models and high resolution air quality forecast on limited domains	1 km resolution model for the area of EU member state	1 km resolution models, including more processes and coupling (aerosols, land surface, ...)
Climate Extreme events, Impacts		Modified regime for extreme events (5 to 10 200-year medium-resolution coupled simulations) ->		Tropical phenomena (high-vertical resolution O/A coupling, 10cm, 1°A, 0.5°O)
Climate Earth System Modelling		Increase the number of species/variables (->200)	Oceanic CO2 absorption (1/12° & biogeochemistry)	Oceanic CO2 absorption (1/20° & biogeochemistry)
Climate Quantifying uncertainties	IPCC-type « crude » estimations	1. Estimate climate sensitivity with "super-parameterizations" (2D at each grid point) 2. Estimate the range of possibilities Ensemble of 1.000 simulations at today resolution with Earth System models	Quantify the probabilities Ensemble of 1.000 simulations at increased resolution	Estimate climate sensitivity with high-resolution NH model (Grid-size of ≈3km)
Climate surprises Slow-down of the Gulf Stream	Preliminary studies have shown such events are possible within the next couple of centuries	Define probabilities : More numerous simulations	Better estimation of the time horizon : Longer simulations Increase resolution	Toward real prediction: Increase spatial resolution (1 PF and beyond)

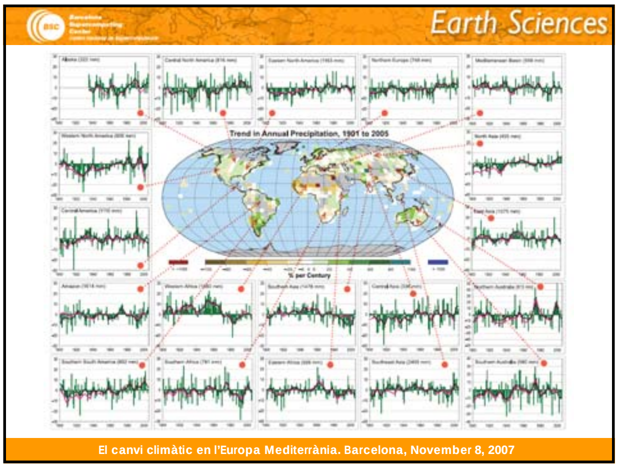
Global circulation models (GCM)

Some models built upon the philosophy "modeling-by-components"

- ✓ *Goddard Institute for Space Studies* (GISS) GCM, NASA, U.S.A.
- ✓ *Whole-Atmosphere Community Climate Model* (WACCM), *National Center for Atmospheric Research* (NCAR), Boulder, Colorado, U.S.A.
- ✓ *Hamburg General Circulation Model, version 4* (ECHAM-4), Max Plank Institute, Hamburg, Germany
- ✓ *Hadley Centre Coupled Model, version 3* (HadCM3), Met Office, Reading, UK
- ✓ *Geophysical Fluid Dynamics Laboratory,* Princeton (CDG1), U.S.A.



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Trend in Annual Precipitation, 1901 to 2005
% per Century
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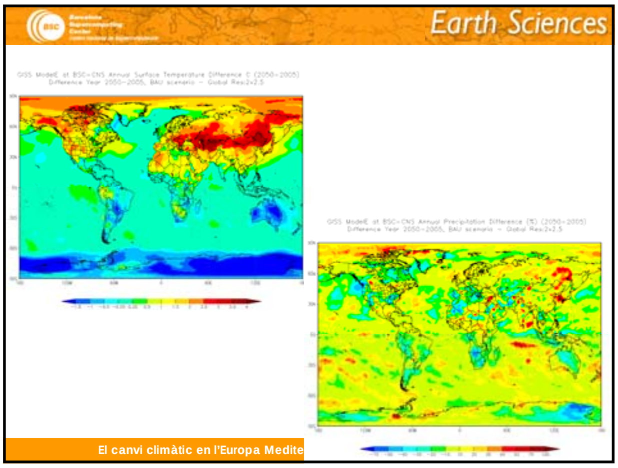
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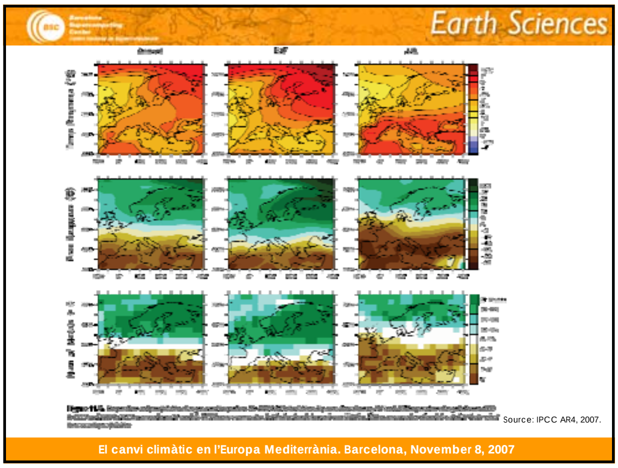
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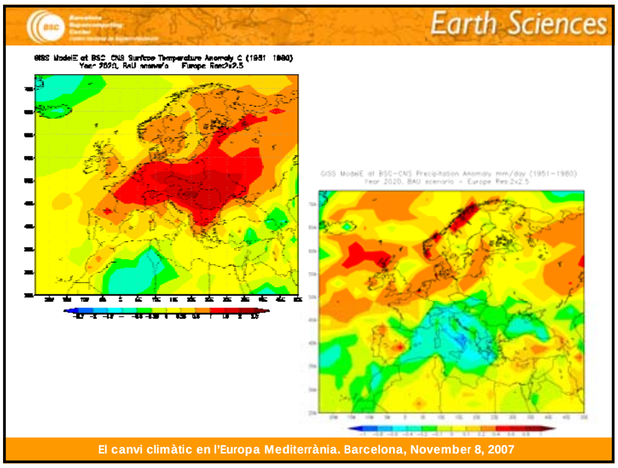
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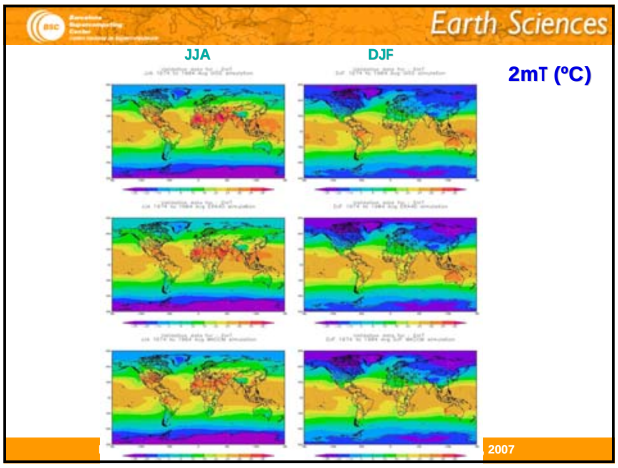
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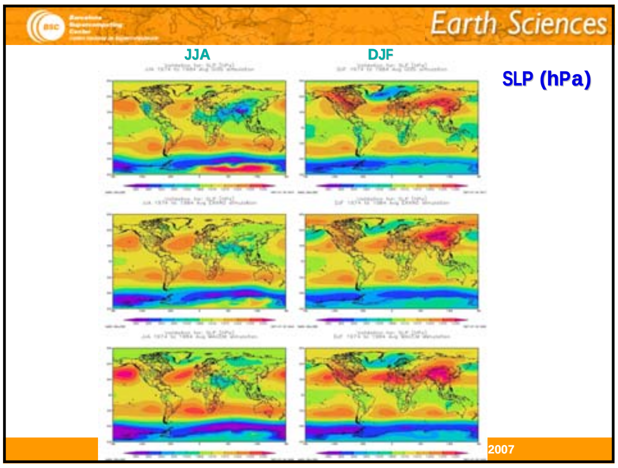
JJA
DJF
2mT (ºC)
2007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JJA
DJF
SLP (hPa)
2007

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		GISS	WACCM	ERA40
SLP [hPa]	σ	8.449	11.127	9.395
	R	0.871	0.957	
2mT [°C]	σ	18.321	19.848	20.011
	R	0.996	0.998	
tcc [%]	σ	12.47	N.A.	16.142
	R	0.25384	N.A.	
Geop. Height [m] at 700 mb	σ	199.88	233.79	216.53
	R	0.988	0.9947	
Geop. Height [m] at 500 mb	σ	339.86	373.44	348.82
	R	0.99467	0.9973	

		GISS		WACCM	
		BIAS	RMSE	BIAS	RMSE
World	SLP [hPa]	-0.5578	13.237	-1.118	14.322
	2m T [°C]	0.8662	11.237	-0.1797	11.840
	tcc [%]	13.567	22.324	N.A.	N.A.
	Geop. Height [m] at 500 mb	2.775	41.851	14.484	43.032
	Geop. Height [m] at 700 mb	-2.676	38.508	4.856	32.799

1957-2002 time-space avaraged values for standard deviation (s) and correlation coefficient *R (left)*; and bias and root mean square error (RMSE) *(down)* for sea-level pressure, surface temperature, total cloud cover and geopotential height.

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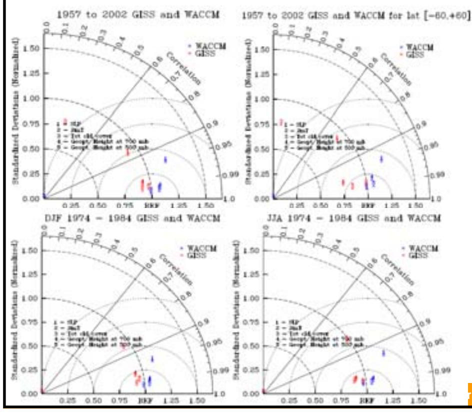

Taylor diagrams showing the difference in performance of the GISS and WACCM for selected quantities. Sea-level pressure, 2mT, Geopotential height at 700 and 500mb and Total cloud cover: entire global domain (left) and from 60 degrees south to 60 degrees north. The standard deviation was normalized With respect to the ERA-40.

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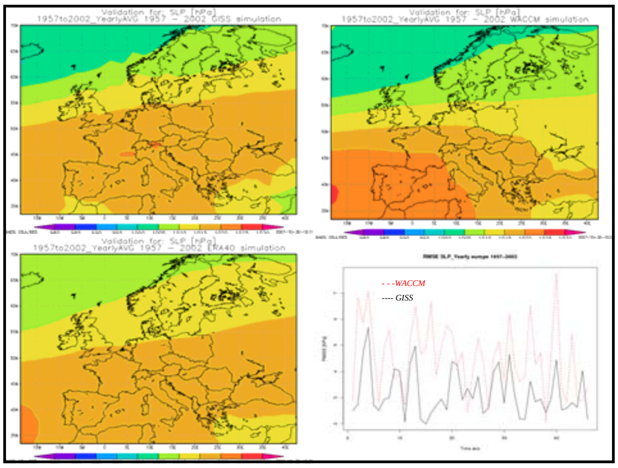

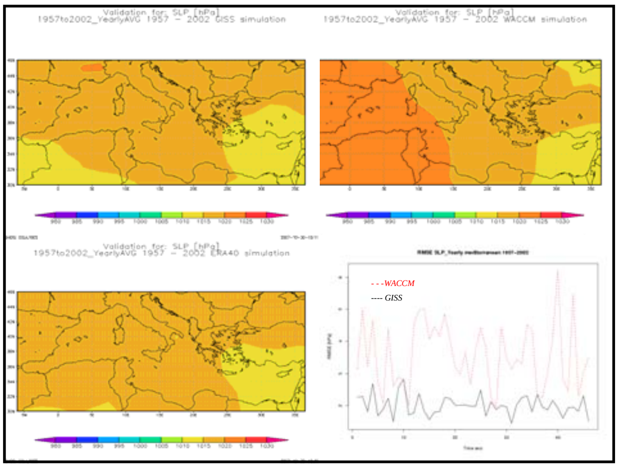

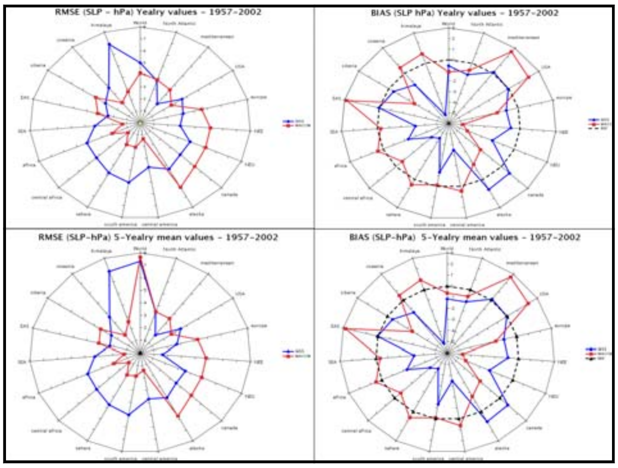

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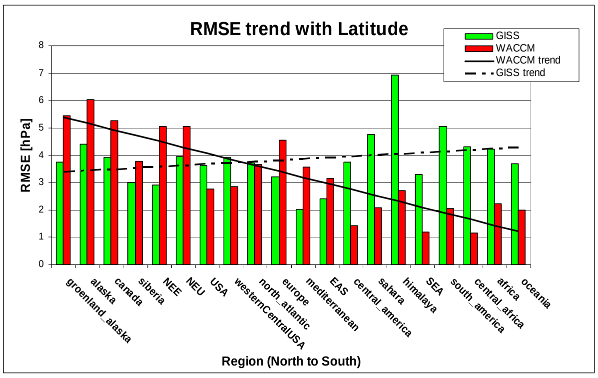

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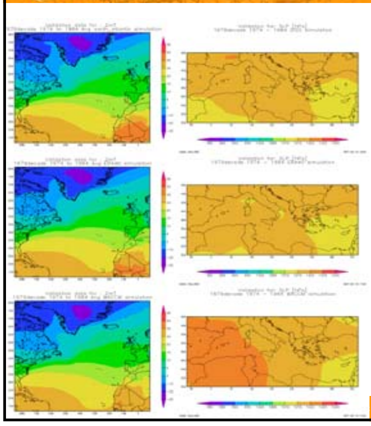
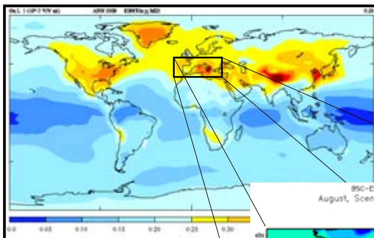


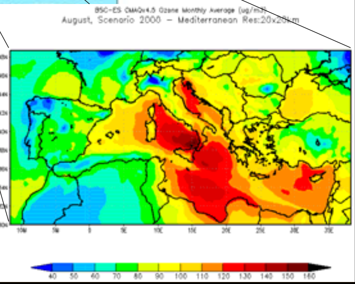
Regional Climate

Present-day difficulties for very high-resolution modelling come conditioned not only by HPC limitations (scalability, I/O), but also by physical constrains and limitations with global circulation models. That leads to the use of REGIONAL CLIMATE MODELS (RCMs).

RCMs applications in well resolved domain use a grid at least one order of magnitude finer (10-20 km) and temporal scales of hours. Therefore, this forces to the use of high performance computational resources.

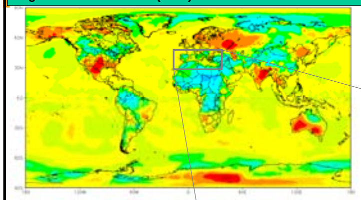


WHAT INFORMATION CAN WE GET FROM REGIONAL CLIMATE MODELS (RCM) THAT IS NOT EXPLAINED BY GLOBAL (GCM) MODELS?



- **RCM have been shown to improve simulations of mesoscale processes in region with strong surface forcing (complex topography, land-use heterogeneity, sea-land interface, etc.)**
- **Convective precipitation for extreme (torrential) episodes of rain and changes in the period under study**
- **Fine-scale resolving processes (mesoscale circulations)**
- **Trends in the extreme episodes of air pollution (especially ozone and particulate matter)**

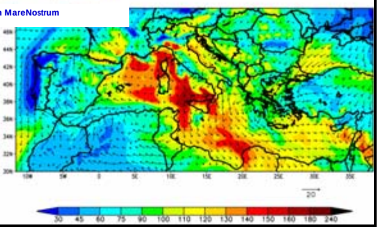
High-performance computing: coupling of NASA-GISS global chemistry-climate model with a Regional Climate Model (RCM)



GISS NASA Global Model implemented in MareNostrum

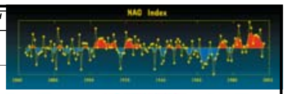
RCM can help explaining trends in extreme events: torrential precipitations, heat waves, droughts, air pollution episodes, affecting human health

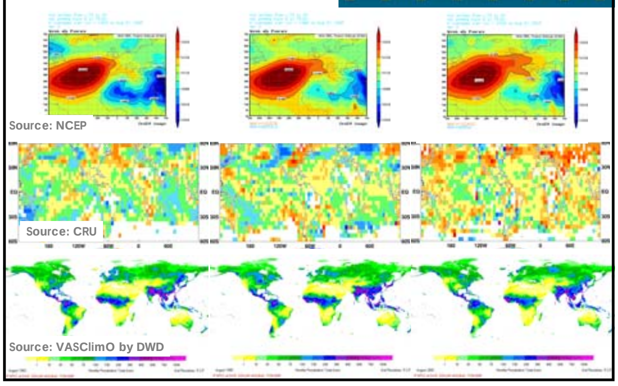
RCM based on WRF-ARW/HERMES/CMAQ/DREAM



The computation time (just RCM) for each day of one climate scenario is about 3.5h per day (using 200 MareNostrum processors). Therefore, the total computation time for each climate scenario is around **260400 h·cpu** for 1-year simulations. In a single-processor computer, the simulations would take over **10850 days (29.72 years).**

	Monthly station based NAO index (August)	Seasonal station based NAO index (JAS)	Annual station based NAO index
1960	-3.5	-2.6	-1.88
1980	-2.1	-1.0	-1.58
2000	0.4	3.3	1.18





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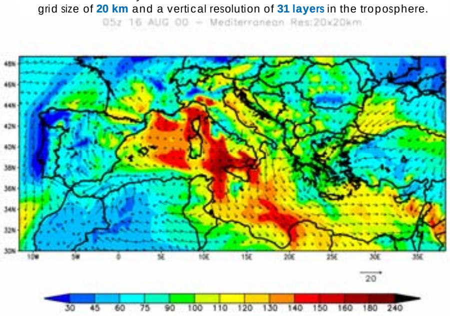
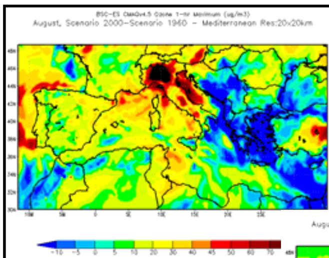
The domain of study covers an area of 4940 km x 2640 km with a horizontal grid size of 20 km and a vertical resolution of 31 layers in the troposphere.



In order to isolate the possible effects of climate variability on the ground concentrations of photochemical pollutants in the Mediterranean, the assumption of unchanged anthropogenic emissions was implemented.



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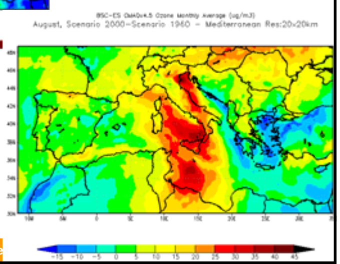
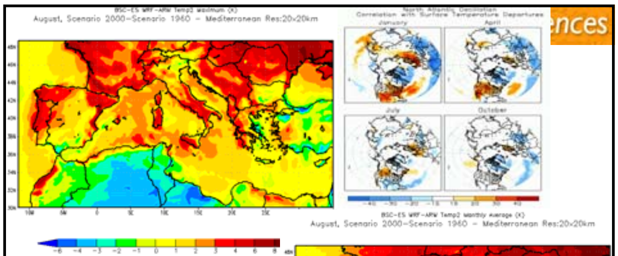
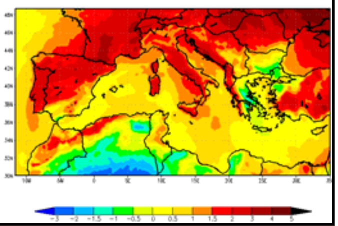
The assumption of unchanged emissions leads to an increase of the concentrations of pollutants in central regions, mainly in northern Italy (over 70 μg m^{-3} for maximum 1-hr levels)

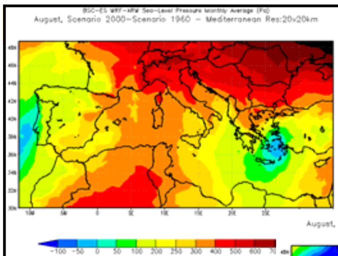


The August average concentration depicts a marked gradient from the central Mediterranean (where increases in the ground-level ozone mixing ratio reach 30 μg m^{-3}) to the extremes of the domain, where no noticeable increases or even slight decreases are modelled.



The increase of pollutants' concentrations may be driven by an enhanced secondary production as a consequence of the temperature increase in central Europe for the period of study...





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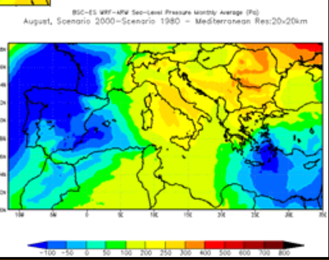
...and the higher pressures extending towards central Europe and eastern regions observed for August 1960, 1980 and 2000.



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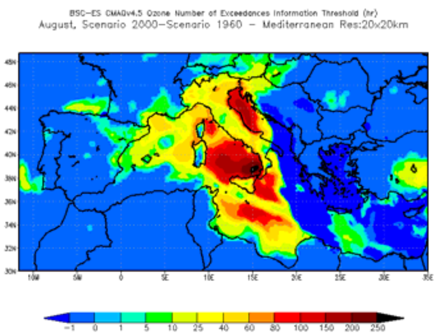
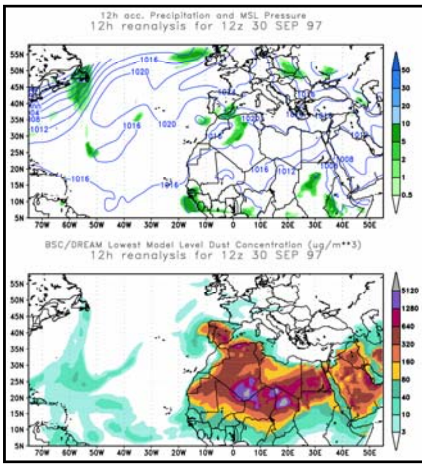


The number of exceedances of the maximum 1-hr ozone threshold (180 μg m^{-3}) has progressively increased in the months of August of the years 1960-1980-2000 in the central Mediterranean meanwhile the number of exceedances has decreased over the eastern coast and the Aegean Sea.



Resolution: 1/3º x 1/3º horizontal and 24 levels
- Time step: 120 s
- Vegetation cover and soil properties constant

- Computing time single processor for 24 h simulation: ~ 70 min
- Computing time single processor for 48 years: ~ 851 days (~ 28 months)
- 116 processors: ~ 7 days

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WRF simulation - computational requirements

Domain: Europe 12 km 401x401x23

	Simulation 1950-1980	*Simulation 1980-2006*	*Simulation 2006-2030*
Storage Capacity - hourly base (Tbytes)	8,95	7,76	7,16
Storage Capacity - daily mean (Tbytes)	0,37	0,32	0,30
Storage Capacity - monthly mean (Gbytes)	12,23	10,60	9,79
Simulation time - 128cpus - (days)	74,61	64,66	59,69
Simulation time - 2560cpus - (days)	3,73	3,23	5,47
Simulation time - 5120cpus - (days)	1,87	1,62	

CMAQ simulation - computational requirements

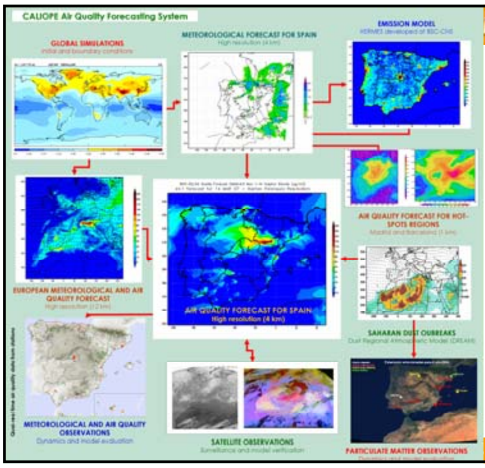
Domain: Europe 12 km 401x401x12

	Simulation 1980-2006	*Simulation 2006-2030*
Storage Capacity - hourly base (Tbytes)	16,45	15,19
Storage Capacity - daily mean (Tbytes)	0,69	0,63
Storage Capacity - monthly mean (Gbytes)	22,47	20,74
Simulation time - 128cpus - (days)	137,09	126,54
Simulation time - 2560cpus - (days)	6,85	6,76
Simulation time - 5120cpus - (days)	3,43	

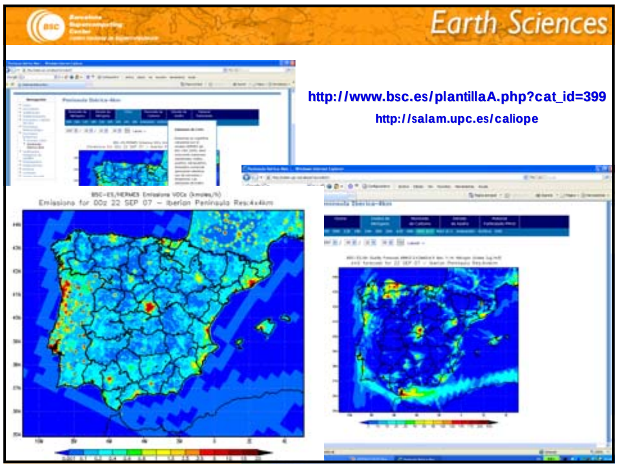
DREAM simulation - computational requirements

Domain: Europe - North Africa 1/4º 250x180x24

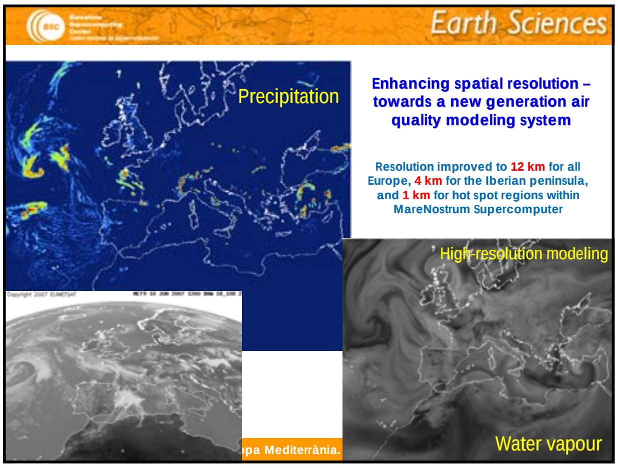
	Simulation 1980-2006	*Simulation 2006-2030*
Storage Capacity - hourly base (Tbytes)	5,92	5,47
Storage Capacity - daily mean (Tbytes)	0,25	0,23
Storage Capacity - monthly mean (Gbytes)	8,22	7,59
Simulation time - 128cpus - (days)	5,76	5,32
Simulation time - 256cpus - (days)	3,10	2,86
Simulation time - 512cpus - (days)	1,76	1,63



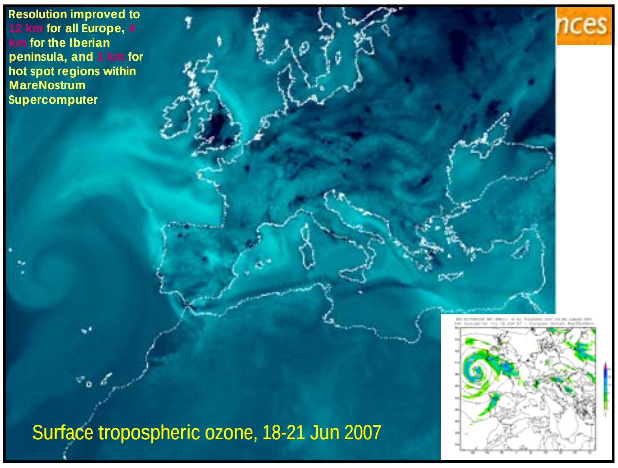
CALIOPE Air Quality Forecasting System



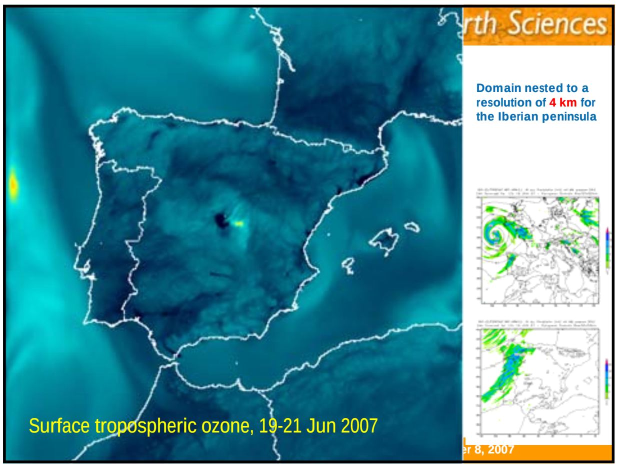
Earth Sciences
http://www.bsc.es/plantillaA.php?cat_id=399
http://salam.upc.es/caliope



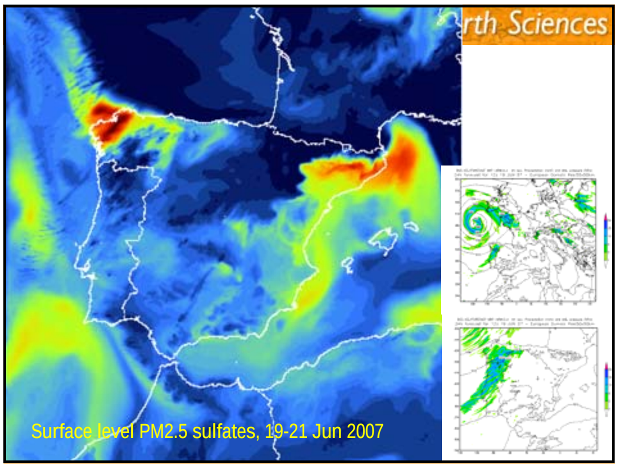
Earth Sciences
Precipitation
Enhancing spatial resolution – towards a new generation air quality modeling system
Resolution improved to 12 km for all Europe, 4 km for the Iberian peninsula, and 1 km for hot spot regions within MareNostrum Supercomputer
High-resolution modeling
Water vapour



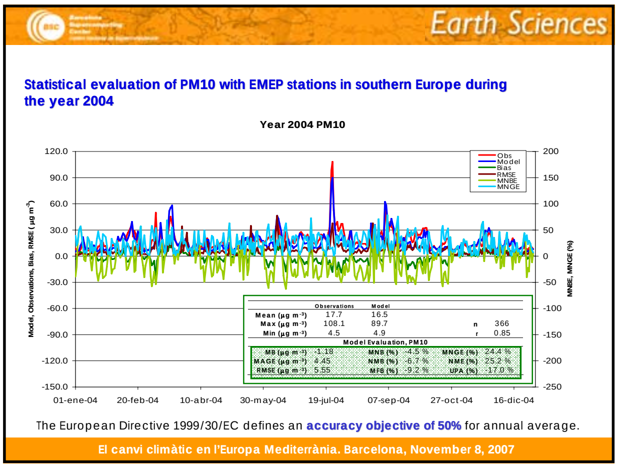
Resolution improved to 12 km for all Europe, 4 km for the Iberian peninsula, and 1 km for hot spot regions within MareNostrum Supercomputer
Surface tropospheric ozone, 18-21 Jun 2007



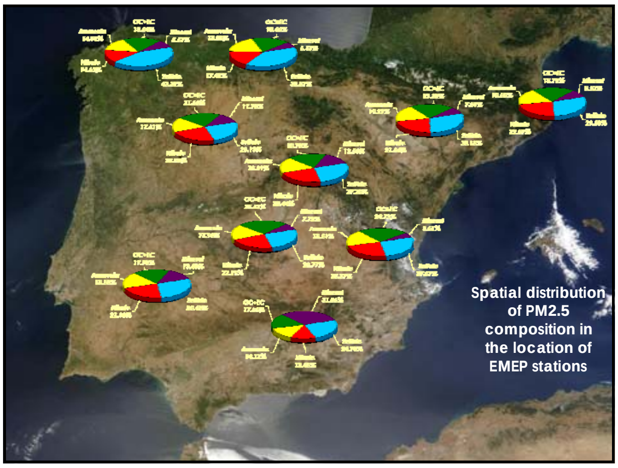
Domain nested to a resolution of 4 km for the Iberian peninsula
Surface tropospheric ozone, 19-21 Jun 2007

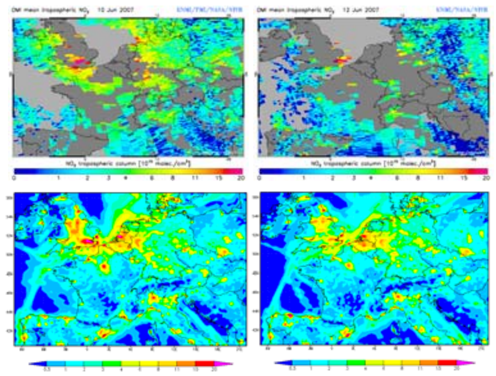


Surface level PM2.5 sulfates, 19-21 Jun 2007



Earth Sciences
Statistical evaluation of PM10 with EMEP stations in southern Europe during the year 2004
Year 2004 PM10
Obs
Model
Bias
RMSE
MNBE
MNGE
Model, Observations, Bias, RMSE (μg m⁻³)
MNBE, MNGE (%)
01-ene-04
20-feb-04
10-abr-04
30-may-04
19-jul-04
07-sep-04
27-oct-04
16-dic-04
Observations / Model
Mean (μg m⁻³) 17.7 16.5
Max (μg m⁻³) 108.1 89.7 n 366
Min (μg m⁻³) 4.5 4.9 r 0.85
Model Evaluation, PM10
MB (μg m⁻³) -1.18 MNB (%) -4.5 % MNGE (%) 24.4 %
MAGE (μg m⁻³) 4.45 NMB (%) -6.7 % NME (%) 25.2 %
RMSE (μg m⁻³) 5.55 MFB (%) -9.2 % UPA (%) -17.0 %
The European Directive 1999/30/EC defines an accuracy objective of 50% for annual average.
El canvi climàtic en l'Europa Mediterrània. Barcelona, November 8, 2007

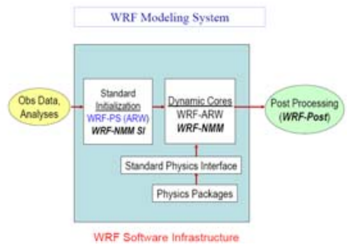




Parallel performance of WRF

- ✓ **The Barcelona Supercomputing Center has performed a parallel performance study of the WRF model by applying the Paraver analysis tool (Computer Science Department – Earth Science Department).**
- ✓ **Weather Reasearch & Forecasting (WRF) Model v2.1.2**
  - Next-generation mesocale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs.
  - Suitable for a broad spectrum of meteorological applications across scales ranging from meters to thousands of kilometers.
- ✓ **Developed by:**
  - National Center for Atmospheric Research (NCAR)
  - National Oceanic and Atmospheric Administration
  - National Centers for Environmental Prediction (NCEP)
  - Forecast Systems Laboratory (FSL)
  - Air Force Weather Agency (AFWA)
  - Naval Research Laboratory
  - Oklahoma University
  - Federal Aviation Administration (FAA).

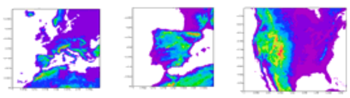
- ✓ **The current WRF (Weather Research and Forecasting Model) software framework (WSF) supports two dynamical solvers:**
  - The nonhydrostatic Mesoscale Model (NMM) developed by the National Centers for Environmental Prediction with user support provided by the Developmental Testbed Center, and currently operational Numerical Weather Prediction model for USA.
  - The Advanced Research WRF (ARW) developed and maintained by the Mesoscale and Microscale Meteorology Division of NCAR.



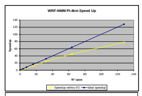
Definition of study cases

- ✓ **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 4 km domains

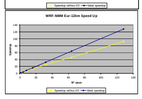
	Domain				
	Europe	Iberian peninsula	Europe	Iberian peninsula	USA
Model	WRF-ARW	WRF-ARW	WRF-NMM	WRF-NMM	WRF-ARW
NX	400	400	400*	400*	425
NY	400	400	400*	400*	300
NZ	38	38	38	38	35
Resolution (km)	12	4	12	4	12
Simulation day	08/11/2005	13/09/2006	08/11/2005	13/09/2006	25/10/2001
Hours of simulation	9-12h	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



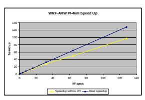
NMM Spain 4Km



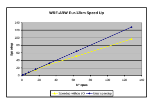
NMM Europe 12Km



ARW Spain 4Km



ARW Europe 4Km



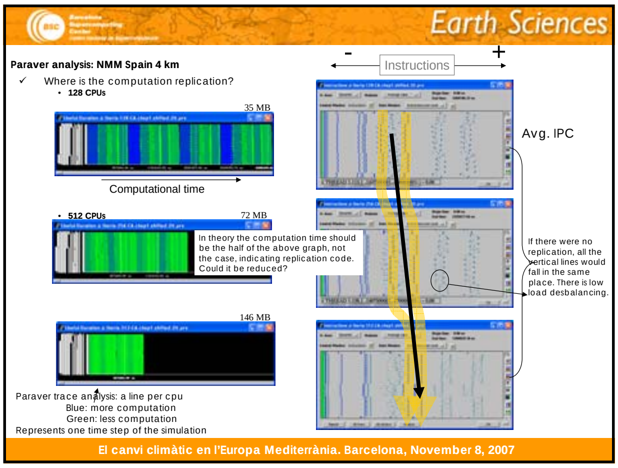
Speedup – 1 to 128; 128 to 512 cpus

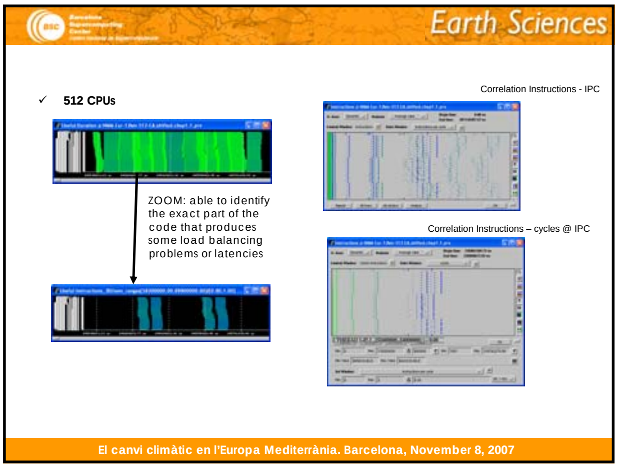
	Proc	512	256	128
NMN Iberia 4Km	LB	0.94	0.94	0.95
	Comm	0.95	0.96	0.97
	1/Complexity	0.88	0.94	1.00
	Avg IPC	0.75	0.75	0.76
	Speedup model	3.36	1.81	1.00
	Efficiency model	0.84	0.91	1

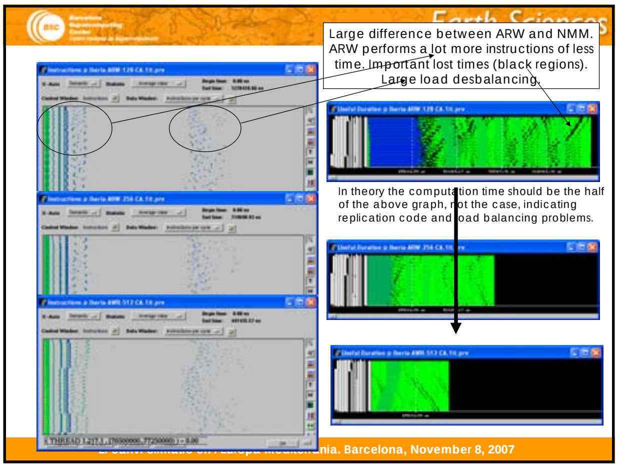
The major problem with NMM is related to code replication when doubling the nº of cpus. Inherent to the code structure? There are no load balancing problems, and no communications problems. Low IPC ratio – related to the code programming?? It could be improved, although ARW presents even lower values.

Major communication problems with ARW, and larger load balancing problems.

	Proc	512	256	128
ARW Iberia 4Km	LB	0.85	0.91	0.94
	Comm	0.70	0.79	0.81
	1/Complexity	0.91	0.95	1.00
	Avg IPC	0.51	0.50	0.50
	Speedup model	2.90	1.77	1.00
	fficiency model	0.73	0.88	1







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Summary: Climate and supercomputing

- ✓ Climate modelling:
  - Current codes require high computational resources – capacity
  - For Regional Climate Simulations several efforts need to be with actual codes: needs for better speed-up, related with above aspects.
  - High demanding computational resources for regional climate applications.
  - CPU intensive application.
  - Intensive I/O – disk storage requirements.
  - Need efforts to improve parallel performance:
    - Ongoing studies: I/O improvement, scalability.
- ✓ Parallel performance:
  - Benchmark study of WRF meteorological model
    - Scalability related to domain dimensions and resolution – test cases presents good scalability up to 128 cpus
  - Parallel performance study of WRF
    - Analysis with Paraver tool shows a well structured parallelization of WRF-NMM, more load balancing problems appears with WRF-ARW.
  - Valuable information about how to proceed to improve actual codes.

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