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RedIRIS



BSC
**Barcelona
Supercomputing
Center**
Centro Nacional de Supercomputación

Centro Nacional de Supercomputación y Red Española de Supercomputación

Mateo Valero
Director



Generalitat de Catalunya
Departament d'Innovació,
Universitats i Empresa



UNIVERSITAT POLITÈCNICA
DE CATALUNYA

Barcelona Supercomputing Center Centro Nacional de Supercomputación



- Misión del BSC-CNS:

- Investigar, desarrollar, y administrar la tecnología para facilitar el avance de la ciencia



- Objetivos del BSC-CNS:

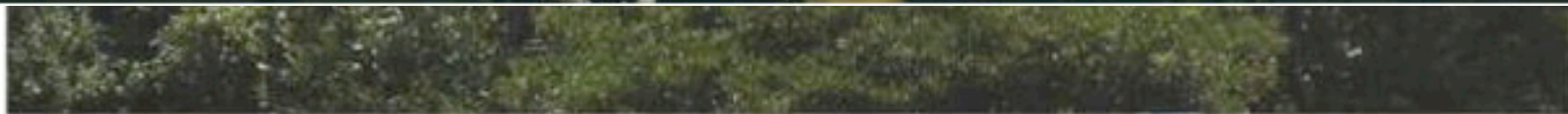
- I+D en Ciencias de la Computación, Ciencias de la Vida y Ciencias de la Tierra.
- Soporte de supercomputación para investigación externa.

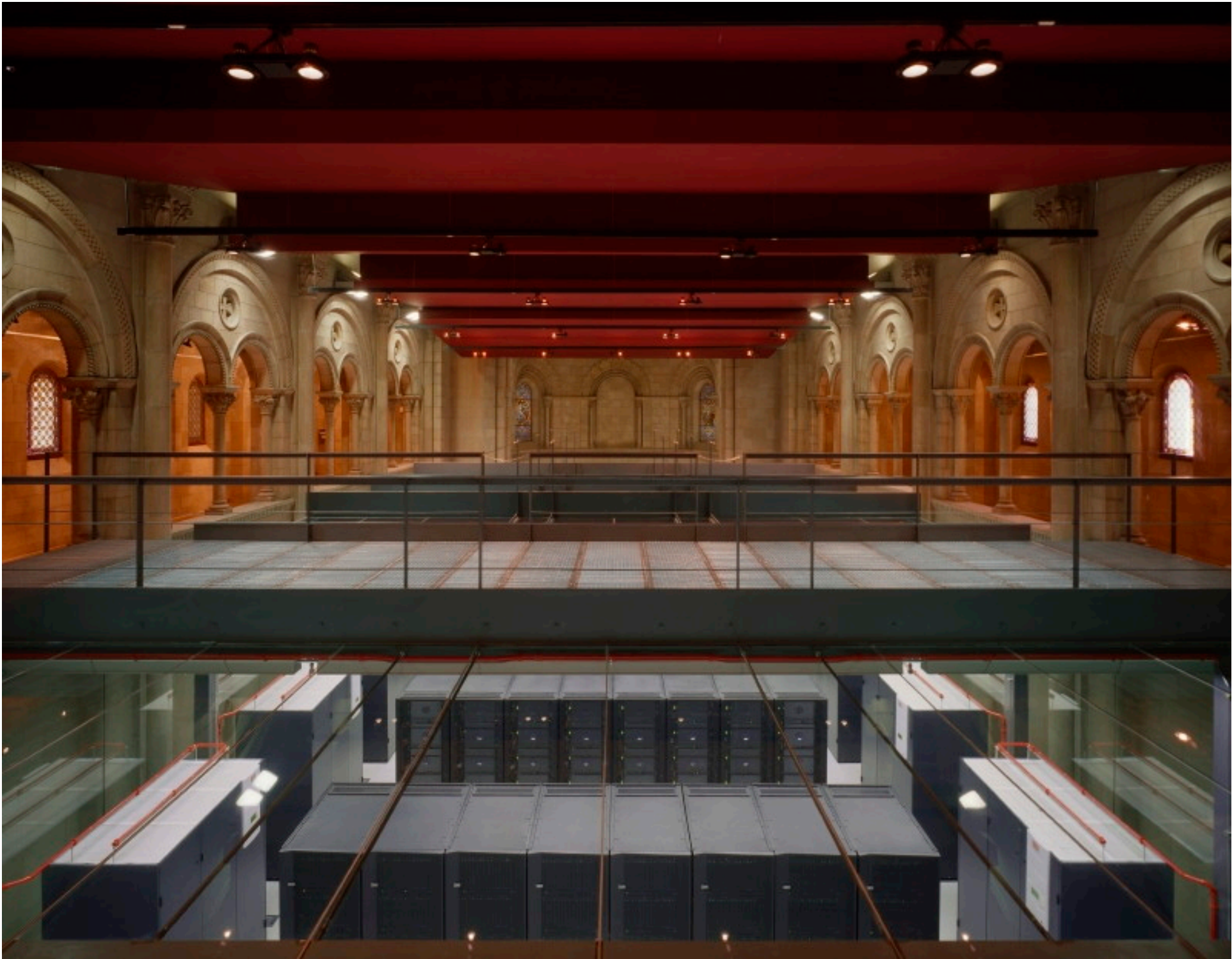
- BSC-CNS es un consorcio formado por :

- Ministerio de Ciencia e Innovación – 51%
- Generalitat de Catalunya (DIUE) – 37%
- Universitat Politècnica de Catalunya – 12%



Un lugar único

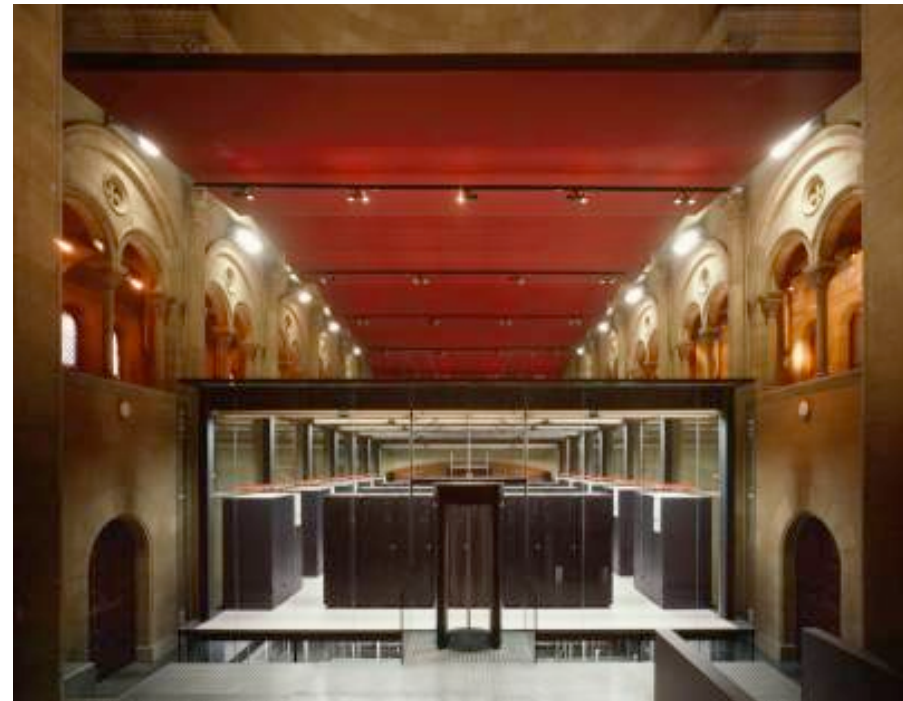




MareNostrum, una mar viva



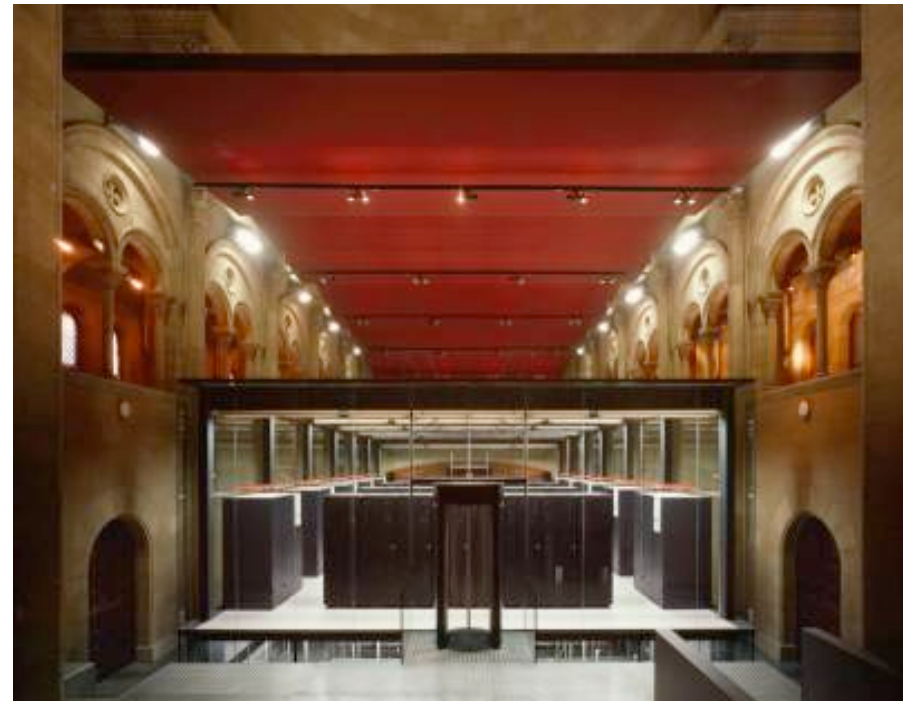
- MareNostrum ₂₀₀₄
 - 4812 PowerPC 970 cores
 - 2406 JS20 2.2 GHz
 - 10 TB of Memory
 - 4 GB per node
 - 270 TB Storage Capacity
 - 3 networks
 - Myrinet
 - Gigabit
 - 10/100 Ethernet
 - Operating System
 - Linux 2.6 (SuSE)



MareNostrum, una mar viva



- MareNostrum₂₀₀₆
 - 10240 PowerPC 970 cores
 - 2560 JS21 2.3 GHz
 - 20 TB of Memory
 - 8 GB per node
 - 480 TB Storage Capacity
 - 3 networks
 - Myrinet
 - Gigabit
 - 10/100 Ethernet
 - Operating System
 - Linux 2.6 (SuSE)



Evolución de MareNostrum



Listado	Posición mundial	Posición europea
Noviembre 2004	4	1
Junio 2005	8	1
Noviembre 2005	5	1
Junio 2006	11	3
Noviembre 2006	5	1
Junio 2007	9	1
Noviembre 2007	13	3
Junio 2008	26	8

Red Española de Supercomputación



- **MareNostrum**
Procesadores: 10240 PowerPC 970
Memoria: 20 Tbytes
Disco: 390 + 90 Tbytes
Redes: Myrinet, Gigabit, 10/100
Sistema: Linux
- **UPM**
Procesadores: 2744 PowerPC 970
Memoria: 5.4 Tbytes
Disco: 187 + 46 Tbytes
Redes: Myrinet, Gigabit, 10/100
Sistema: Linux
- **IAC, UMA, UC, UZ, UV**
Procesadores: 512 PowerPC 970
Memoria: 1 Tbyte
Disco: 14 + 10 Tbytes
Redes: Myrinet, Gigabit, 10/100
Sistema: Linux



Red Española de Supercomputación



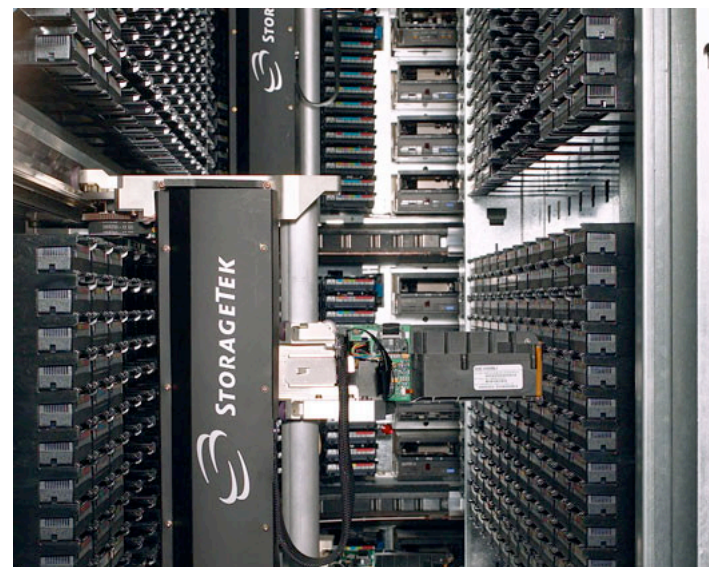
- SGI Altix

- 256 procesadores
 - 128 dual core Montecito
- 2.5 Tbytes de memoria compartida
- Sistema: Linux



- Sistema de almacenamiento

- 6 Pbytes sin compresión
- Tecnología LTO4
- HSM y backup

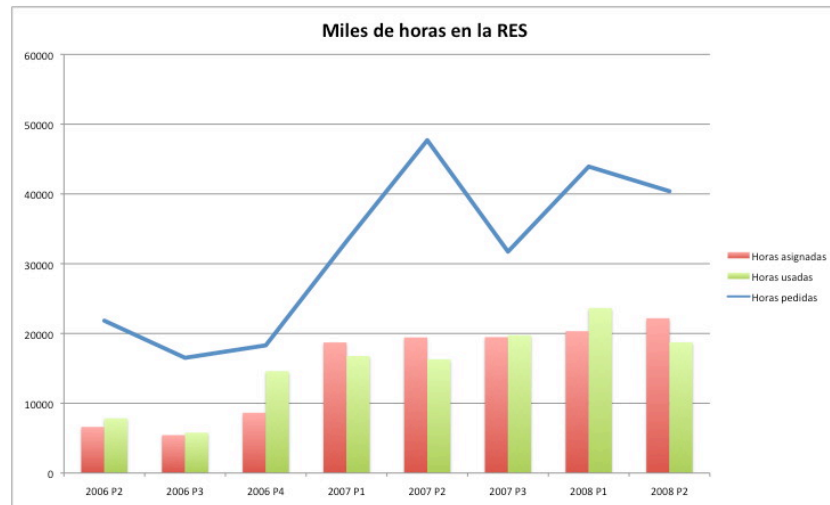
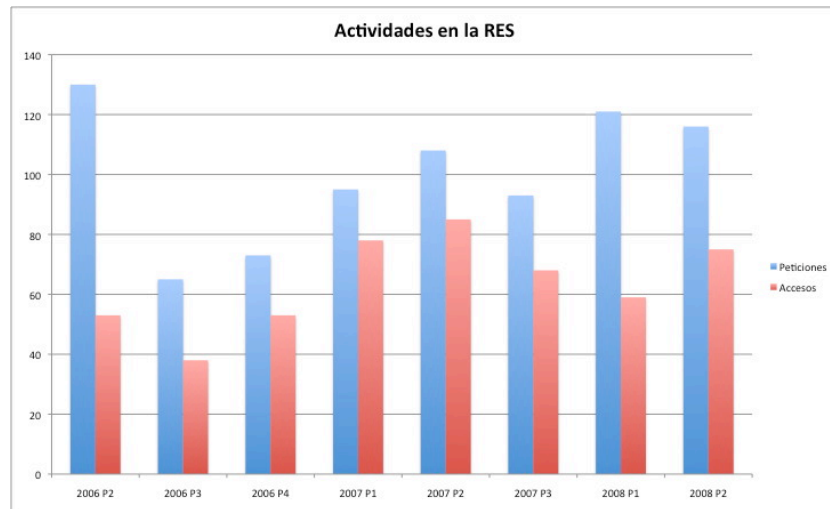


Comité de Acceso único



- 44 científicos españoles, renovación cada dos años
- Aprobado por el MEC y la ANEP
- Core Team
 - MEC: Ramón López de Arenosa
 - ANEP: Victoria Ley
 - Experto Supercomputación externo BSC: Pedro de Miguel (UPM)
 - Experto Supercomputación interno BSC: José Maria Cela
- 4 paneles
 - Astronomía, Espacio y Ciencias de la Tierra
 - José Maria Ibañez, UV
 - Biomedicina y Ciencias de las Vida
 - Alfonso Valencia, CNIO
 - Física e Ingeniería
 - Pablo Ordejón, CSIC
 - Química y Ciencia y Tecnología de los Materiales
 - Agustí Lledós, UB
- Acceso cuatrimestral
- Gestión técnica de la Red conjunta, coordinada por el BSC-CNS.

Satisfacciones de la RES



Surface Chemistry

Dissociation of SO₂ on Au/TiC(001): Effects of Au-C Interactions and Charge Polarization*

José A. Rodríguez,¹ Ping Liu,¹ Francesc Viñes,¹ Francesc Illas,¹ Yoshitro Takahashi,² and Kenichi Nakamura²

Recently, gold has become the subject of much attention due to its unusual catalytic properties when deposited on some oxide supports (TiO₂, CeO₂, MnO₂, Fe₂O₃, Al₂O₃, MgO).¹⁻¹⁵ Bulk metallic gold has low reactivity as a consequence of a combination of a deep-lying valence d band and very diffuse valence sp orbitals.¹⁶ Several models have been proposed for explaining the activation of supported gold: From special chemical properties resulting from the small size of the active gold particles (smaller than 5 nm)^{17,18} to the effects of charge transfer between the oxide and gold.¹⁹⁻²³ What happens when Au is deposited on a substrate which has physical and chemical properties that differ from those of an oxide? The carbides of the early transition metals exhibit, in many aspects, chemical behavior similar to that of noble metals.²⁴ A recent article indicates that Au particles (ca. 2 nm in size) deposited on TiC can oxidize carbon monoxide (CO + 0.5O₂ → CO₂) at temperatures below 200 K.²⁵ What is the nature of the Au-TiC interaction? In this work we investigate the adsorption of SO₂ on well-defined Au/TiC(001) surfaces using synchrotron-based high-resolution photoelectron spectroscopy and first-principles DFT calculations. Sulfur dioxide is an excellent probe molecule for determining the reactivity of gold in different chemical environments,²⁶⁻²⁸ and its dissociation is a much more demanding reaction than the oxidation of CO.²⁹ The dissociation of SO₂ (DSO) is a very important problem in environmental chemistry due to the adverse effects of acid rain (the main product of the oxidation of SO₂ in the atmosphere) on the environment and corrosion of monuments and buildings.³⁰⁻³² As we show below, Au/TiC has

much higher DSO activity than Au supported on oxide surfaces or pure TiC. This is in part a consequence of charge polarization around gold induced by Au-C interactions. Figure 1 shows S 2p photoelectron spectra recorded after dosing the Langmuir (L) of SO₂ in pure TiC(001) at 150 and 300 K. In agreement with previous studies,^{33,34} molecular



*J. A. Rodríguez, Dr. P. Liu, Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973 (USA); E-mail: irrodr@bnl.gov; F. Viñes, Prof. F. Illas, Department of Química Física & IQCIUB, Universitat de Barcelona, C/Quím. Facultat 1, 08035 Barcelona (Spain); Y. Takahashi, Prof. K. Nakamura, National Institute of Advanced Industrial Science and Technology, Tsukuba 226-8503 (Japan)

[†] This research carried out at BNL was supported by the U.S. Department of Energy, Chemical Sciences Division. J.A.R. acknowledges the support of the Generalitat de Catalunya and the Government of Barcelona. Y.V. thanks the Spanish Ministry of Education and Science for a Ramón y Cajal research fellowship and the National Institute of Advanced Industrial Science and Technology for a grant that made possible part of the work. Computational time on the Manosque supercomputer of the Bordeaux Supercomputing Center is gratefully acknowledged.

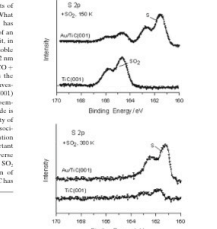


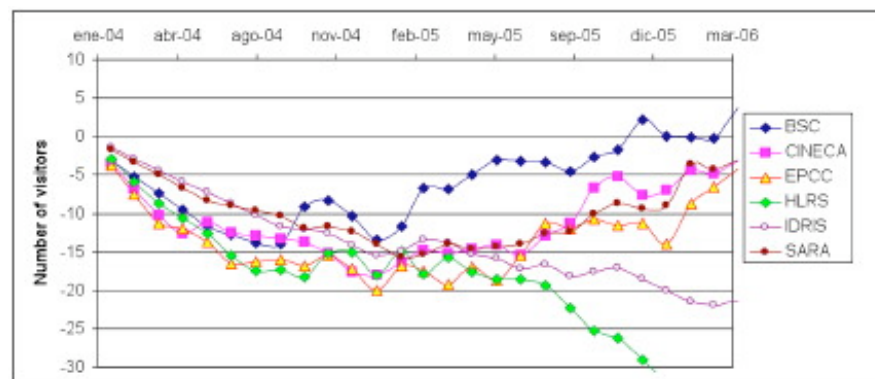
Figure 1. S 2p spectra collected after dosing 1 L of SO₂ in TiC(001) and to a surface pretreated with 0.1 ML of gold SO₂ was dosed at 150 (top panel) and 300 K (bottom panel). A photon energy of 160 eV was used to excite the electrons.

chemisorption is weak at 150 K and some dissociative chemisorption (SO₂ (g) → SO₂ (s) + 2O (s)) at 300 K. In general terms, TiC(001) can be classified as a poor DSO surface.³⁵ Au(111) and silver-supported gold also interact weakly with SO₂ and are not efficient for the dissociation of SO₂ bonds.³⁶ However, after depositing 0.2 monolayers (ML) of Au on TiC(001) the reactivity of the system dramatically increases. In Figure 1, the S 2p spectrum recorded

HPC Europa

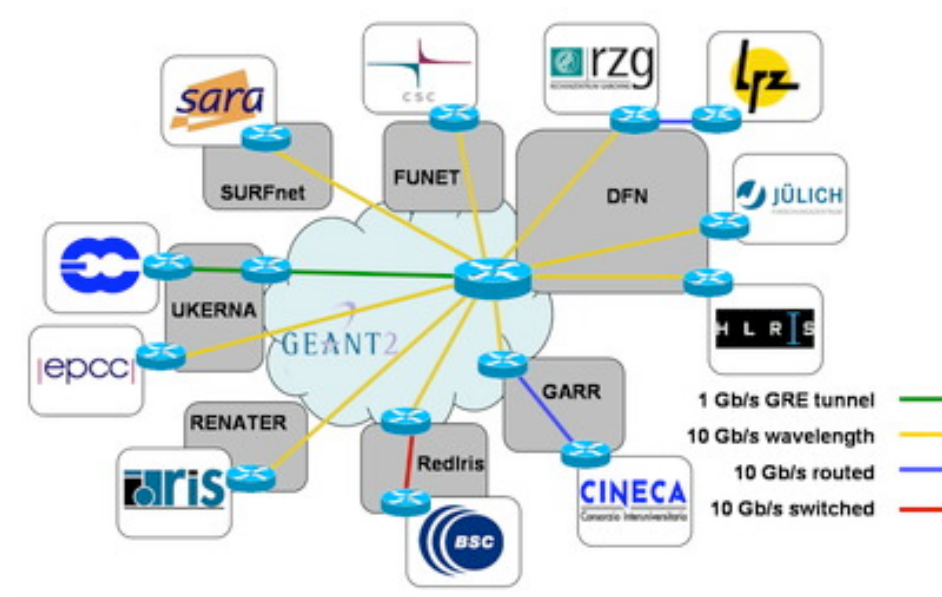


- HPC-Europa is a consortium that aims to provide advanced computational services in an integrated manner to the European research community.
- It enables researchers working in any eligible country in Europe to visit a participating research institute to carry out a collaborative visit of up to 3 months' duration and to gain access to some of the most powerful High Performance Computing (HPC) facilities in Europe.



DEISA

- Consortium of leading national supercomputing centres that currently deploys and operates a persistent, production quality, distributed supercomputing environment with continental scope
- Objectives:
 - To deploy and operate a persistent, production quality, distributed supercomputing environment with continental scope
 - To enable scientific discovery across a broad spectrum of science and technology. Scientific impact is the only criterion for success



Personal del Centro Nacional



Ciencias de la computación

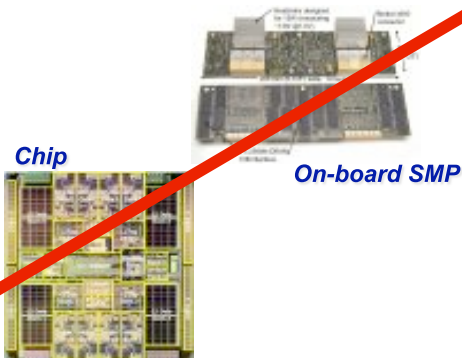
Computer architecture:

- Highly o-o-o architectures
- Hardware multithreading
- Design space exploration for multicore chips and Hw accelerators
- Transactional memory (Hw, Hw-assisted)
- SIMD and vector extensions/units



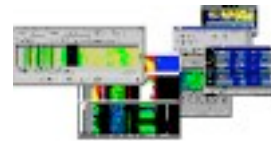
Programming models:

- Scalability of MPI and UPC
- OpenMP for multicore, SMP and ccNUMA
- DSM for clusters
- CellSs
- Transactional Memory
- Embedded architectures

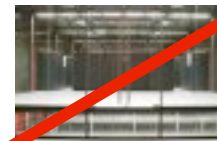


Benchmarking, analysis and prediction tools:

- Tracing scalability
- Pattern and structure identification
- Visualization and analysis
- Processor, memory, network, system



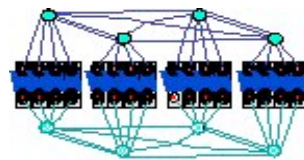
Large cluster systems



Future Petaflop systems



Small DMM



cc-NUMA

The Grid



Grid and cluster computing:

- Programming models
- Resource management
- I/O for Grid



Operating environments:

- Autonomic application servers
- Resource management for heterogeneous workloads
- Coordinated scheduling and resource management
- Parallel file system scalability

eNANOS



PRACE

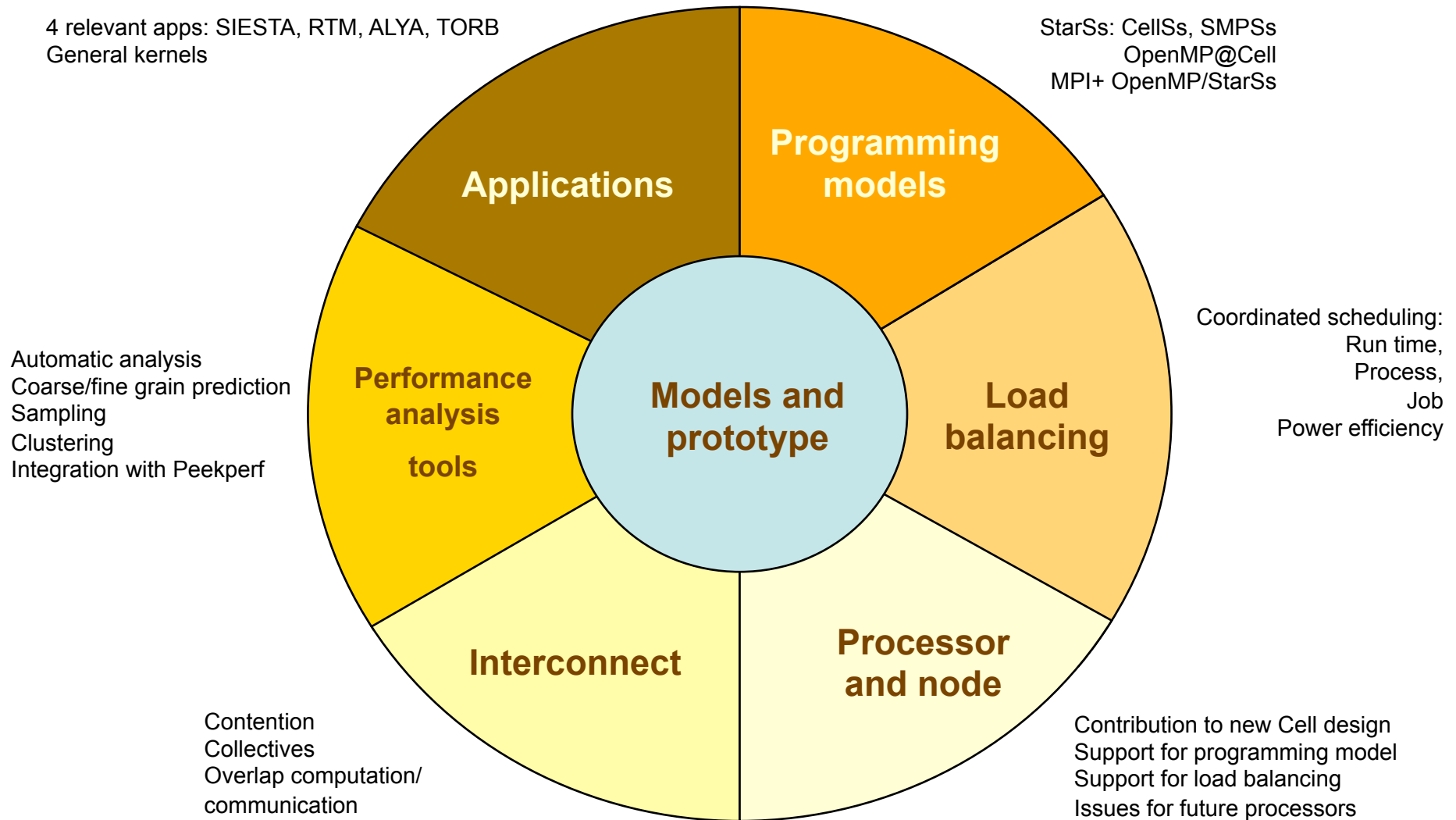


Proyecto MareIncognito: BSC-IBM



4 relevant apps: SIESTA, RTM, ALYA, TORB
General kernels

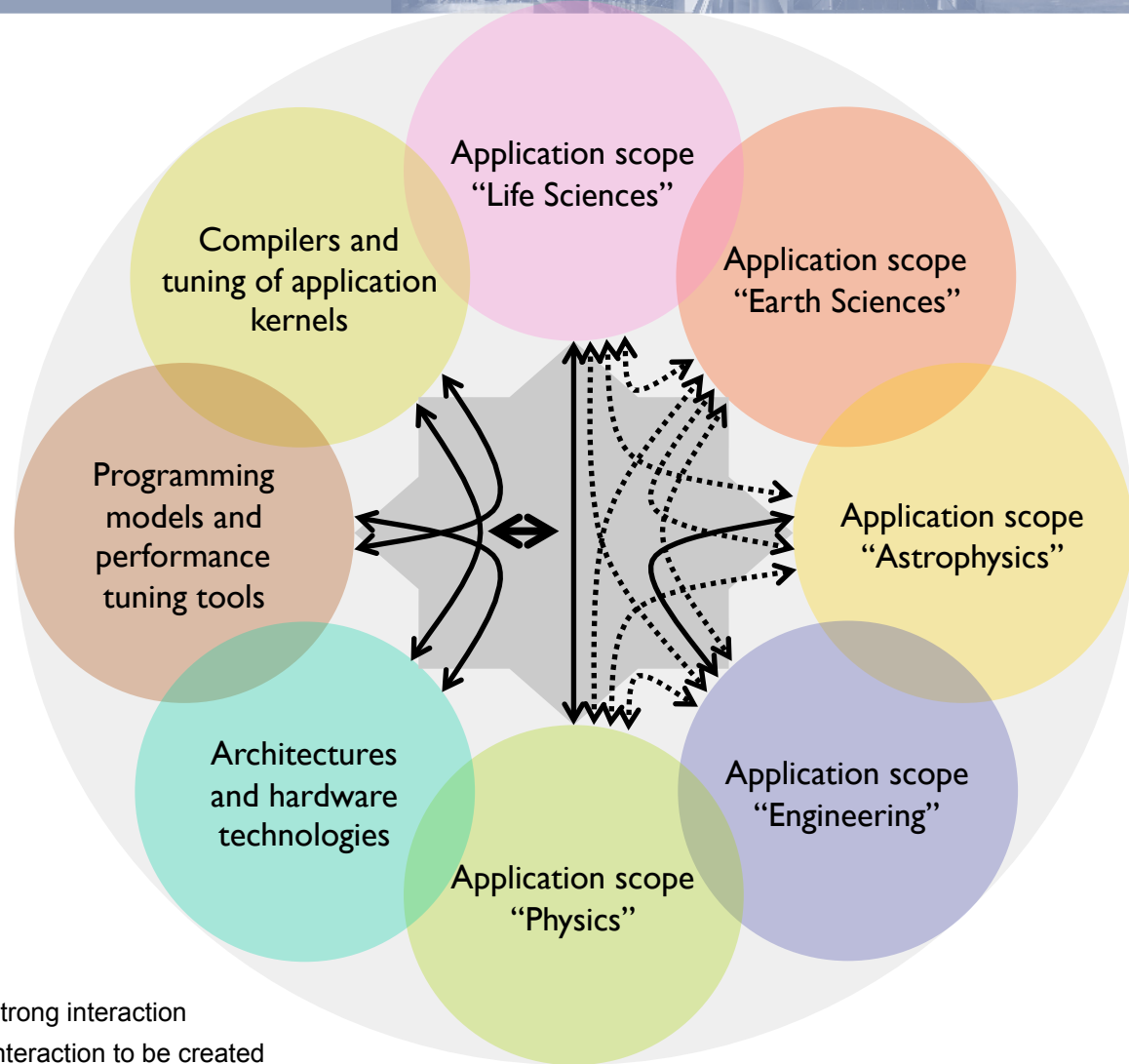
StarSs: CellSs, SMPs
OpenMP@Cell
MPI+ OpenMP/StarSs



Proyecto Consolider: Supercomputing y e-Science



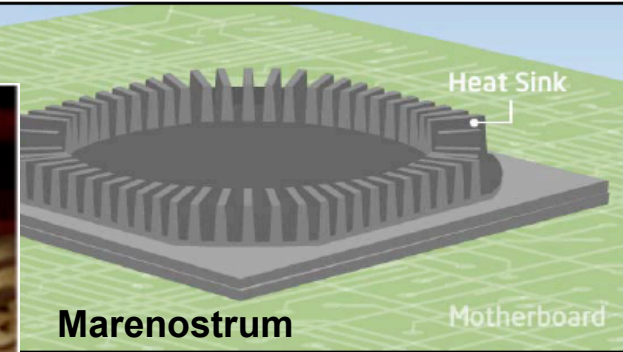
- 21 grupos
- 119 investigadores senior
- 5 Grand Challenges
- 5.000.000 € / 5 años



**Chip Multiprocessors:
Number of cores on chip could double at most every 18 months**

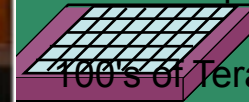


"It is better for Intel to get



Two of the first Tera-scale Research Prototype are a
Most beautiful supercomputer
Fortune magazine, Sept. 2006: Intel

#1 in Europe, #5 in the World



100's of TeraFlops
with general purpose Linux
supercluster of commodity
PowerPC-based Blade Servers

more type devices,
tel,
ditional memory
in 1991 using 10.000 Pentium

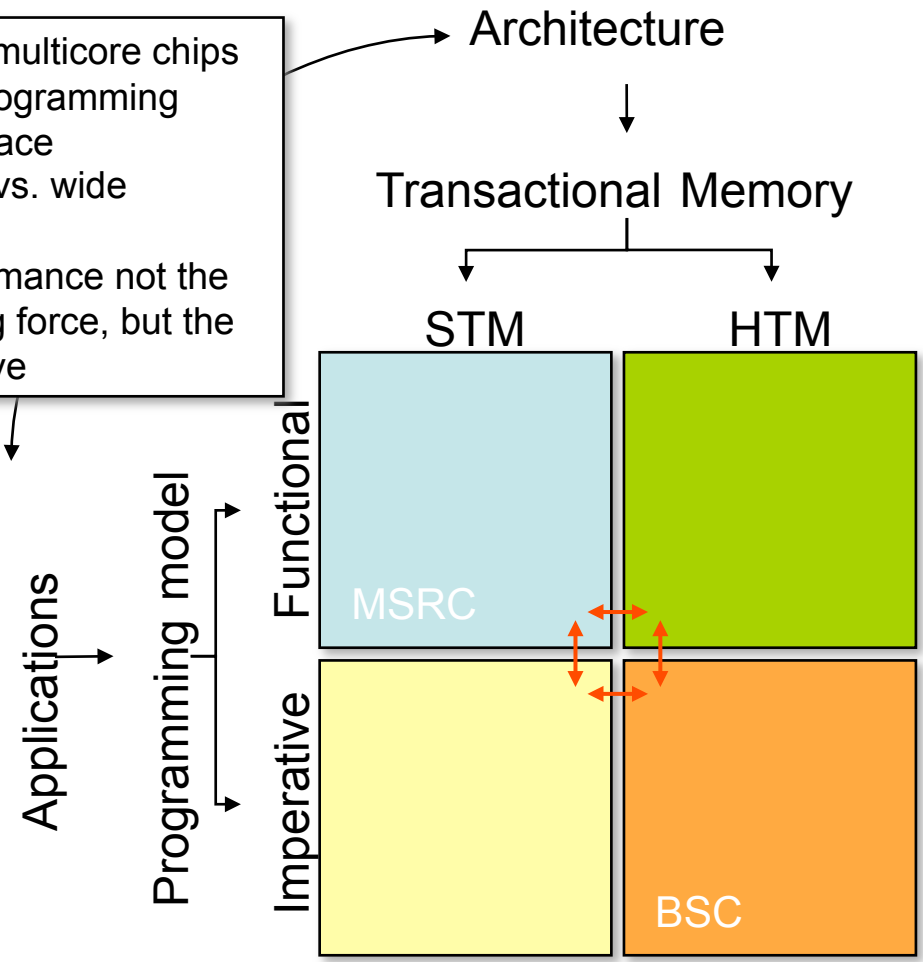
that will allow us to get the full benefit of all those transistors
and map that into higher and higher performance.
Pro processors contained in more than 85 cabinets occupying 200 square meters ☺
• This will be possible in 5 years from now
Bill Gates, Supercomputing 05 Keynote

Microsoft - BSC Project: A quick snapshot



- Project started in April 2006 - 2 years initial duration
- BSC – Microsoft Research Centre inaugurated January 2008
- The Collaboration
 - Barcelona Supercomputing Center (BSC)
 - Computer Architecture
 - Microsoft Research Cambridge (MSRC)
 - Programming Systems
- Initial topic: Transactional Memory

• Advent of multicore chips
 • Parallel programming commonplace
 • Simplicity vs. wide applicability
 • Full performance not the initial driving force, but the final objective



Education for Parallel Programming



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1.4 Data	Blank	1.5 Data	Blank	1.6 Data	Blank
1.7 Data	Blank	1.8 Data	Blank	1.9 Data	Blank
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1.31 Data	Blank	1.32 Data	Blank	1.33 Data	Blank
1.34 Data	Blank	1.35 Data	Blank	1.36 Data	Blank
1.37 Data	Blank	1.38 Data	Blank	1.39 Data	Blank
1.40 Data	Blank	1.41 Data	Blank	1.42 Data	Blank
1.43 Data	Blank	1.44 Data	Blank	1.45 Data	Blank
1.46 Data	Blank	1.47 Data	Blank	1.48 Data	Blank
1.49 Data	Blank	1.50 Data	Blank	1.51 Data	Blank
1.52 Data	Blank	1.53 Data	Blank	1.54 Data	Blank
1.55 Data	Blank	1.56 Data	Blank	1.57 Data	Blank
1.58 Data	Blank	1.59 Data	Blank	1.60 Data	Blank
1.61 Data	Blank	1.62 Data	Blank	1.63 Data	Blank
1.64 Data	Blank	1.65 Data	Blank	1.66 Data	Blank
1.67 Data	Blank	1.68 Data	Blank	1.69 Data	Blank
1.70 Data	Blank	1.71 Data	Blank	1.72 Data	Blank
1.73 Data	Blank	1.74 Data	Blank	1.75 Data	Blank
1.76 Data	Blank	1.77 Data	Blank	1.78 Data	Blank
1.79 Data	Blank	1.80 Data	Blank	1.81 Data	Blank
1.82 Data	Blank	1.83 Data	Blank	1.84 Data	Blank
1.85 Data	Blank	1.86 Data	Blank	1.87 Data	Blank
1.88 Data	Blank	1.89 Data	Blank	1.90 Data	Blank
1.91 Data	Blank	1.92 Data	Blank	1.93 Data	Blank
1.94 Data	Blank	1.95 Data	Blank	1.96 Data	Blank
1.97 Data	Blank	1.98 Data	Blank	1.99 Data	Blank
1.100 Data	Blank	1.101 Data	Blank	1.102 Data	Blank



I ❤️ multi-core programming

I ❤️ many-core programming

We all ❤️ massive parallel prog.

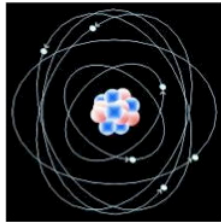


I ❤️ games

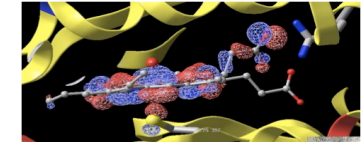
Multicore-based pacifier



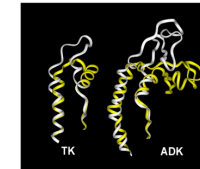
Ciencias de la Vida



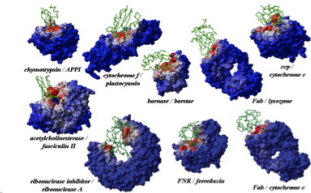
Atomic (and electronic) modeling
of protein biochemistry and
biophysics



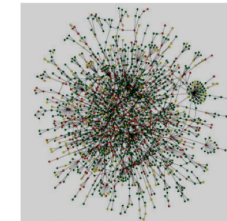
Micro and mesoscopic modeling
of macromolecules. Drug Design



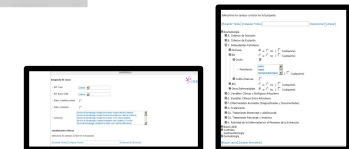
Identification of the structural
bases of protein-protein
interaction



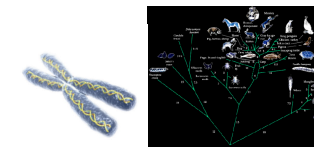
Protein-protein interaction
networks
Systems biology



Web services, applications,
databases



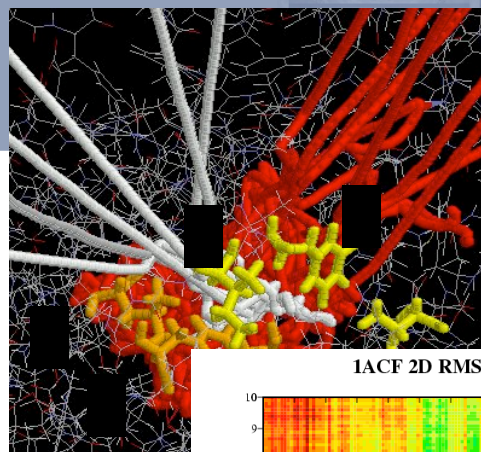
Analysis of genomes and networks
to model diseases, systems and
evolution of organisms



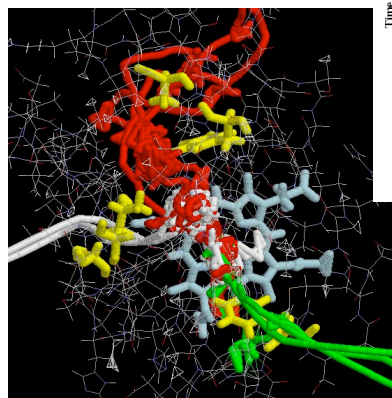
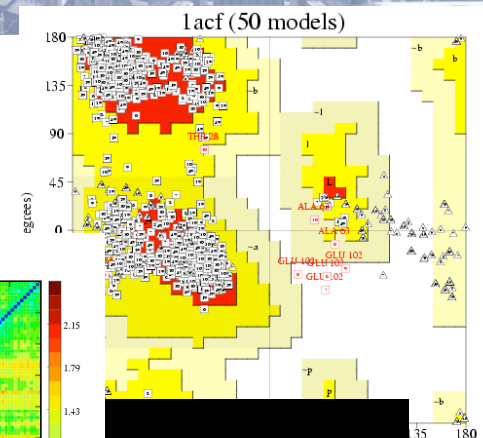
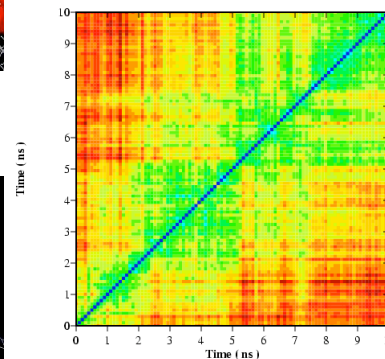
Life Sciences Department



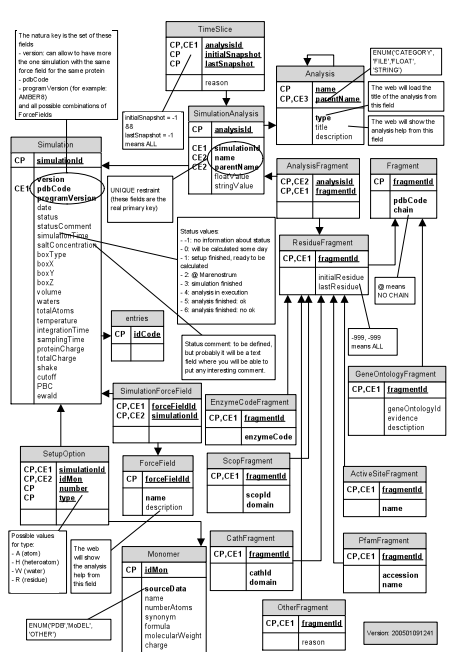
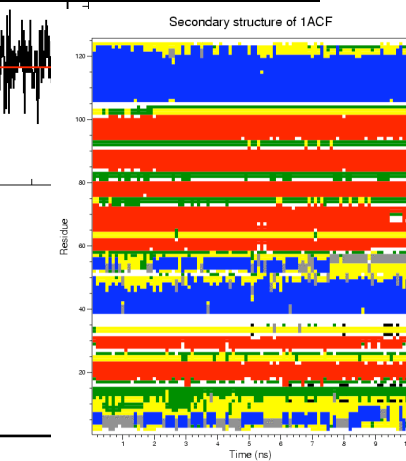
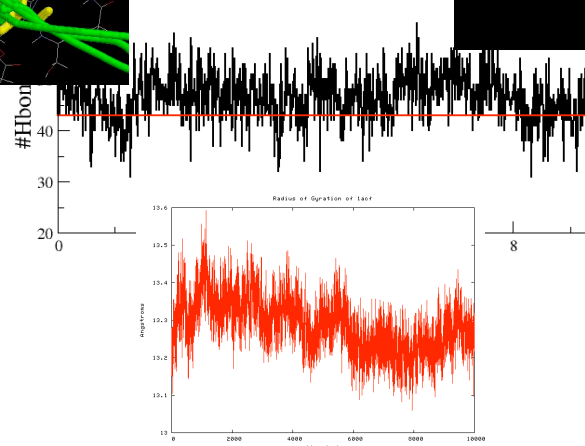
- Library of protein MD simulations
- 1400 at the moment
- >900 CPU years.
- 10 Tb of data



1ACF 2D RMS



Hbonds of lacf





THE ENCODE PROJECT



THE EARTH PROTEOME

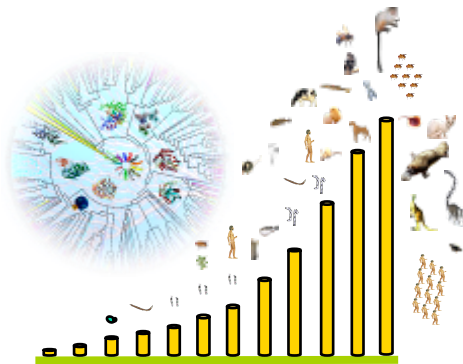
- Genome all organisms + all metagenomes
- 1.4×10^6 sequences
- 32 Tb of RAM used
- 4000 processors
- 38 CPU years
- 9 Tb of output data
- G-Superscalar
- 3.5 days job!
- 5 DAYS lagtime!!!



Analysis of protein and function diversity on earth

Computational genomics group (collaboration with EMBL, Heidelberg)

Identification and classification of new and known proteins from known genomes and metagenomic data



IMPACT FIELDS

Molecular Biology



Providing new functional associations and hypothesis for basic research

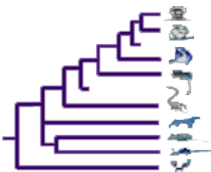
BioMedicine



FP7 European project

Identification of new microorganisms, pathways, proteins and molecules. New therapeutic molecules (antibiotics, protein targets)

Evolution



Understanding the mechanisms of evolution of proteins and organisms

Ecology



Identification of new pathways and organisms for new possibilities in biodegradation.

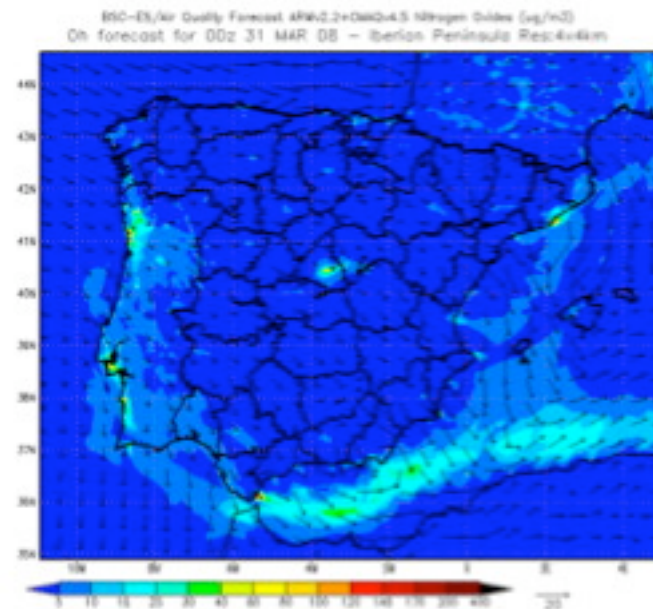
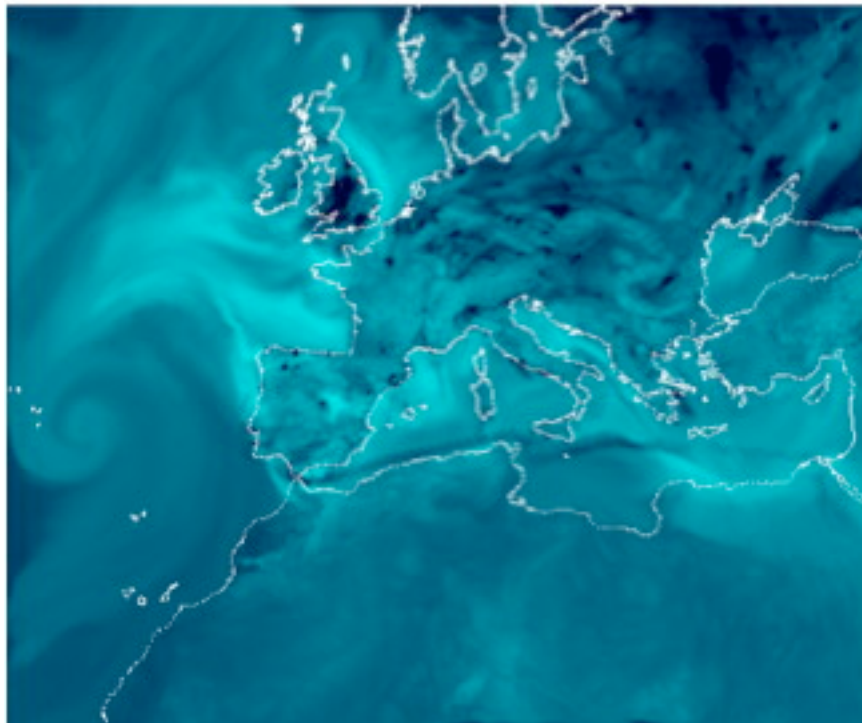


Air Quality and Meteorological Modelling:

✓ The group offers a pan-European (12 km) and Spain (4 km) 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.

(<http://www.bsc.es/caliope>).

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



Calidad del Aire

Efectos en la calidad del aire por la introducción de la limitación de velocidad a 80 km/h en las vías de acceso a Barcelona

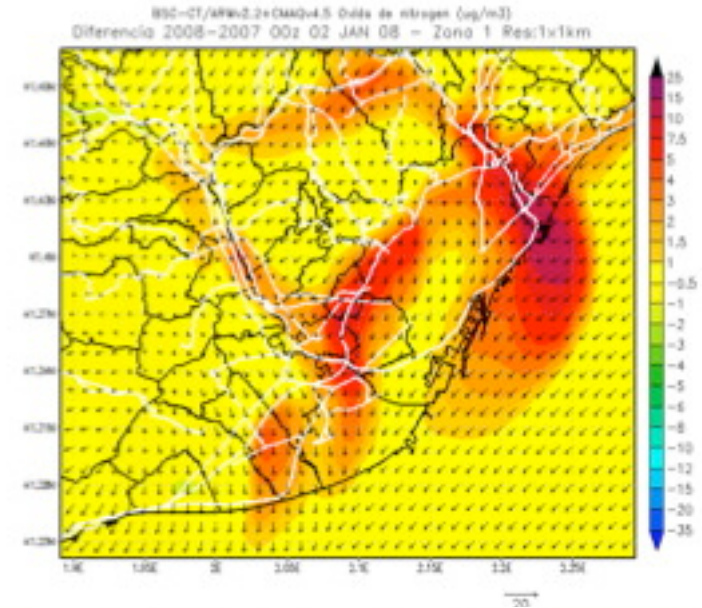
**Evaluación preliminar
1º seis meses 2008**



Vista aérea de Barcelona desde Diagonal Mar en la que se aprecia la capa de contaminación del aire. (MARZO U. SAIZ)



Todas a 80. Póster que indica la limitación sin excepciones de la velocidad a 80 km/h en un acceso a Barcelona por autopista, en Molins de Rei

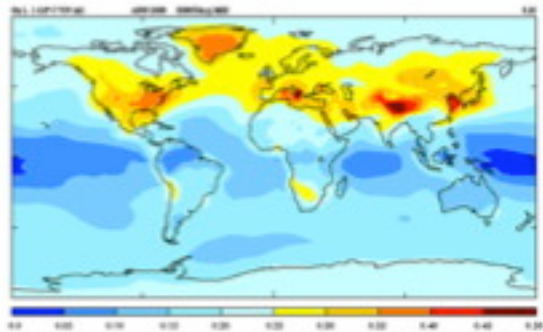


BSC Earth Sciences Department

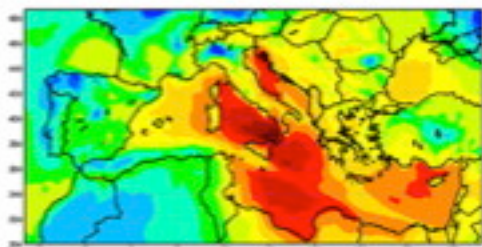


Mineral Dust:

- ✓ 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:** World Meteorological Organization 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.



901-05 Global dust concentration (ug/m³)
August, Scenario 2050 - Mediterranean Res.20x20km

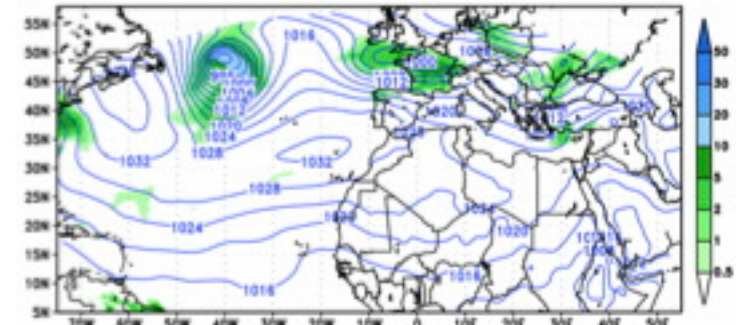


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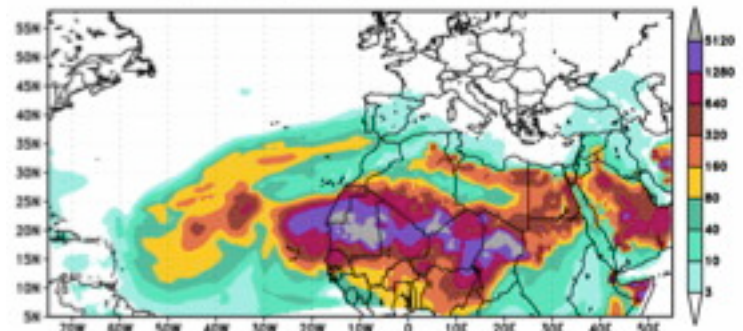
Climate Modelling:

- ✓ **Global Climate Modelling** with NASA GISS ModelE and NCAR WACCM in MareNostrum supercomputer with a resolution of 2°x2.5°.
- ✓ 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.

12h acc. Precipitation and MSL Pressure
12h reanalysis for 12z 14 FEB 97



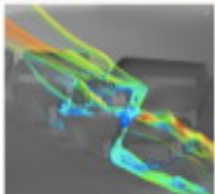
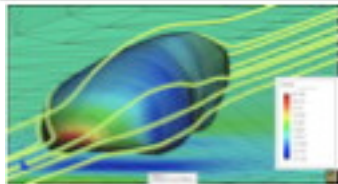
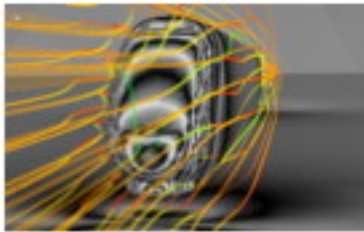
BSC/DREAM Lowest Model Level Dust Concentration (ug/m³)
12h reanalysis for 12z 14 FEB 97



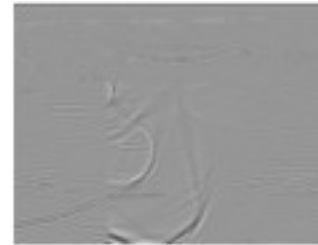
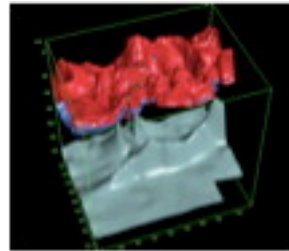
Aplicaciones Científicas y de Ingeniería



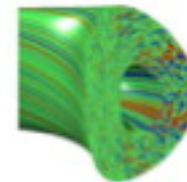
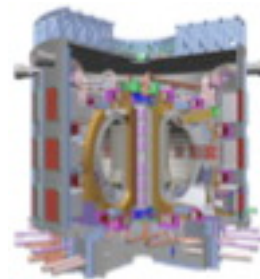
Computational Fluid Dynamics



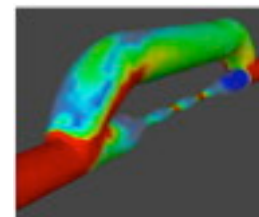
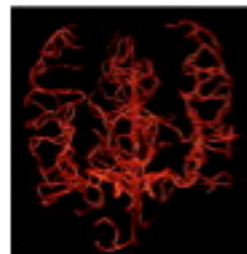
Geophysics



ITER: Plasma physics



Bio-mechanics



Ab-initio Molecular Dynamics

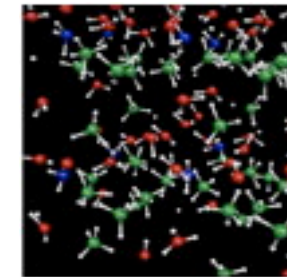
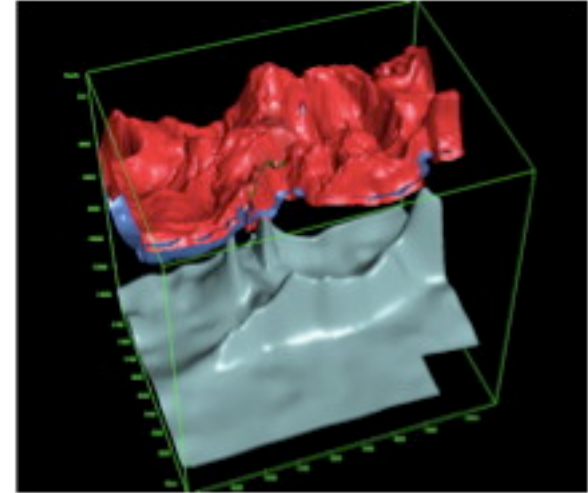
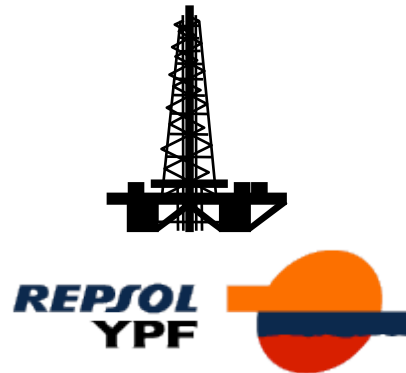
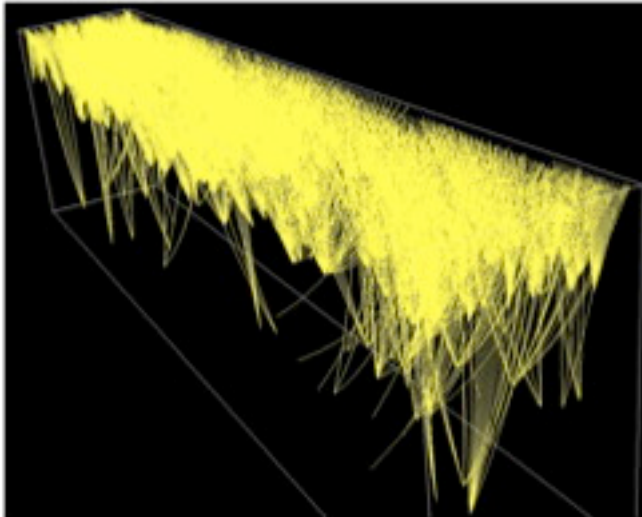
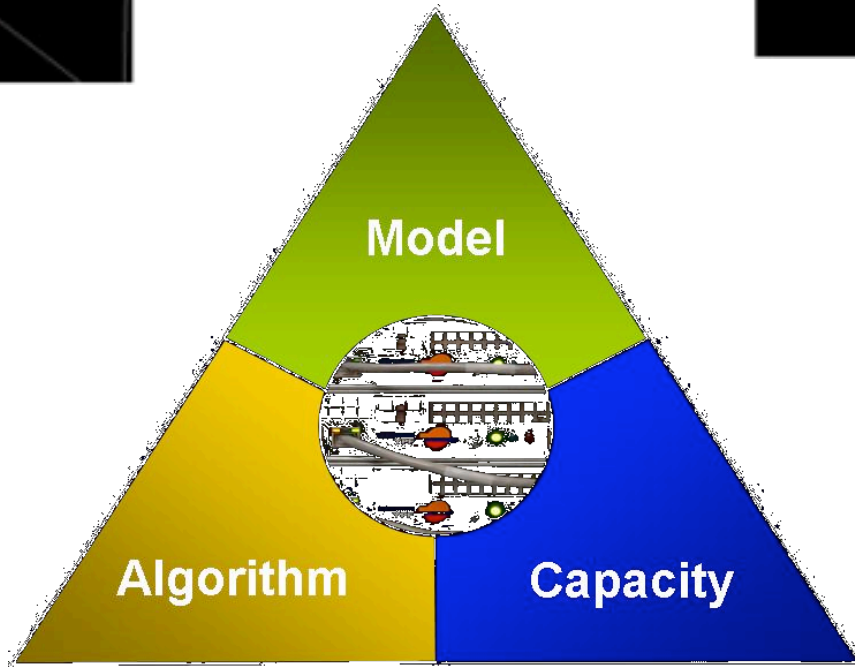


Imagen Sísmica: Proyecto Calidoscopio



Seleccionado por "IEEE Spectrum" como una de las 5 iniciativas mas innovadoras en tecnología del año 2007



Felicidades!

