Centro Nacional de Supercomputación
y
Red Española de Supercomputación

Mateo Valero
Director

GOBIERNO DE ESPAÑA MINISTERIO DE CIENCIA E INNOVACIÓN

Generalitat de Catalunya
Departament d'Innovació, Universitats i Empresa

UPC UNIVERSITAT POLITÈCNICA DE CATALUNYA

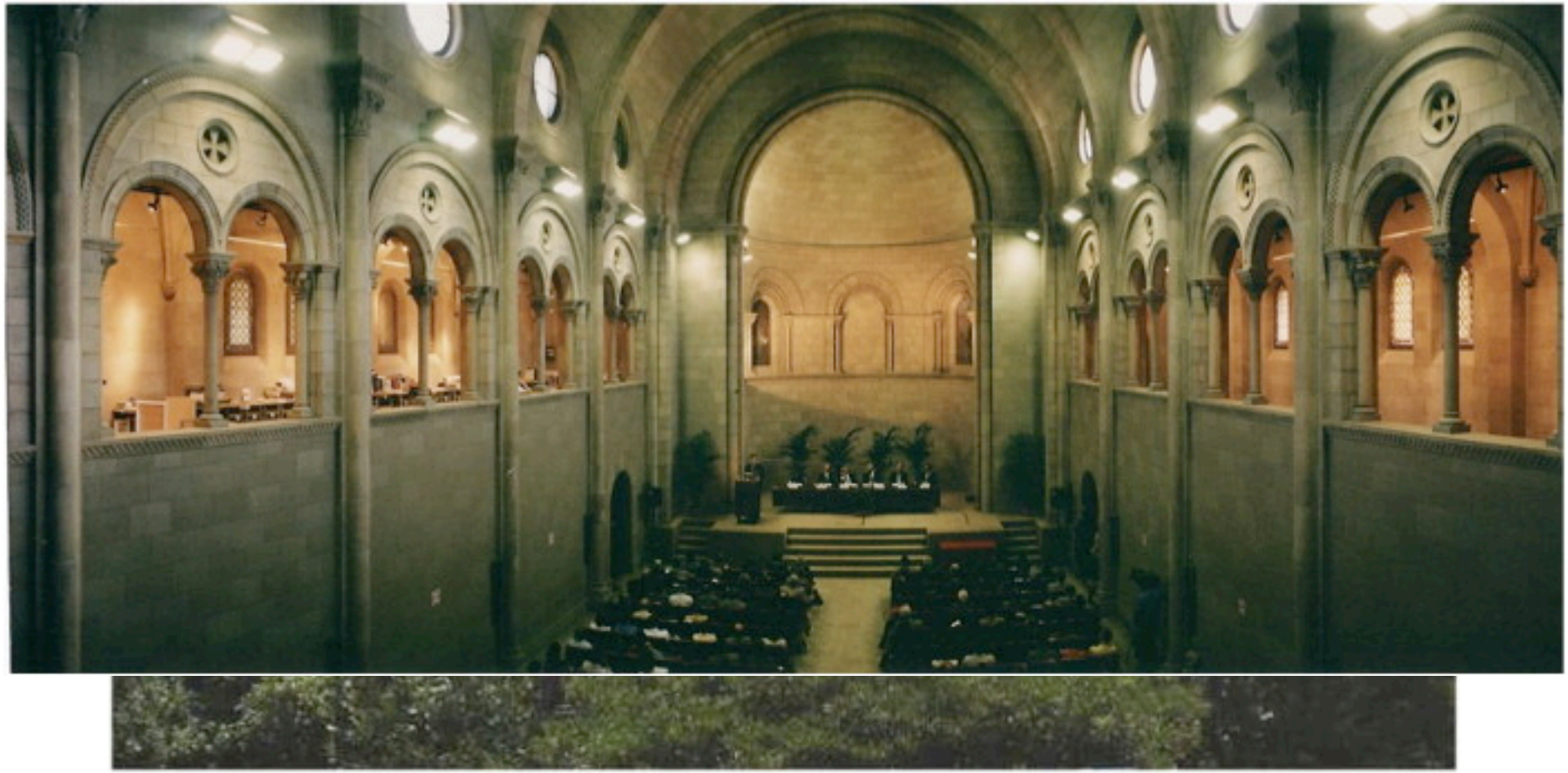
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

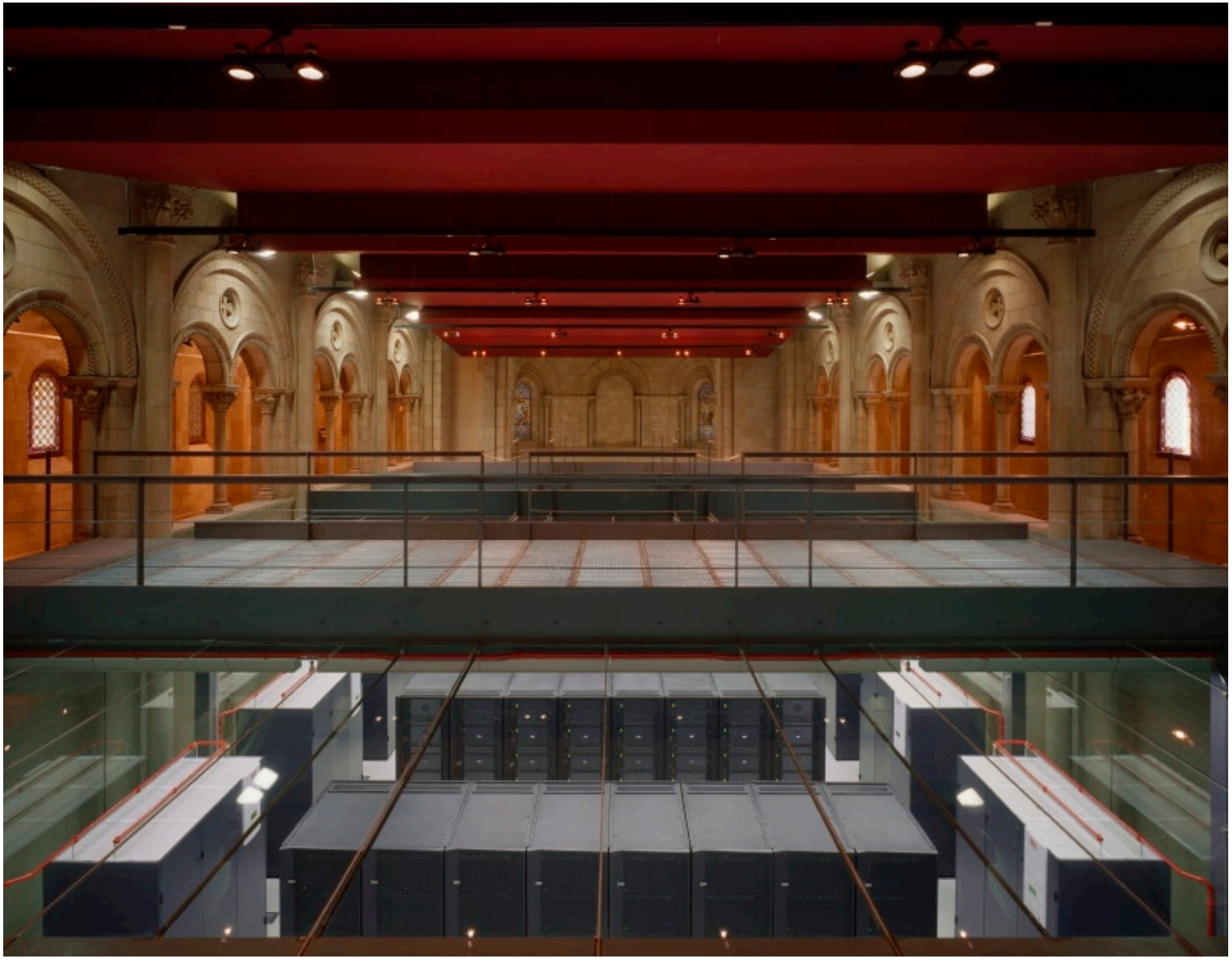
- Misión del BSC-CNS:
  - Investigar, desarrollar, y administrar la tecnología para facilitar el avance de la ciencia

- 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

- MareNostrum 2006
  - 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

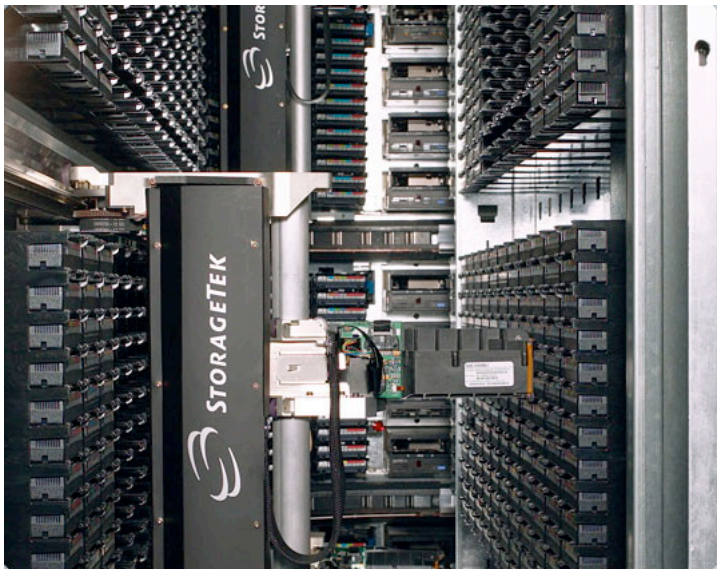
- MareNostrum
  - Procesadores: 10240 PowerPC 970
  - Memoria: 20 Tbytes
  - Disco: 390 + 90 Tbytes
  - Redes: Myrinet, Gigabit, 10/100
  - Sistema: Linux
- UPM
  - Procesadores: 2744 PowerPC 970
  - Memoria: 5.4 Tbytes
  - Disco: 187 + 46 Tbytes
  - Redes: Myrinet, Gigabit, 10/100
  - Sistema: Linux
- 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

Red Española de Supercomputación

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

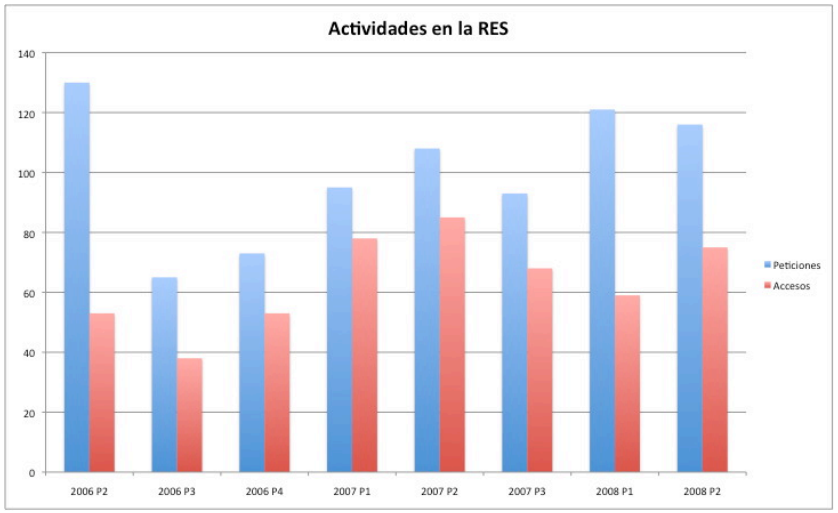
- Sistema de almacenamiento
  - 6 Pbytes sin compresión
  - Tecnología LTO4
  - HSM y backup

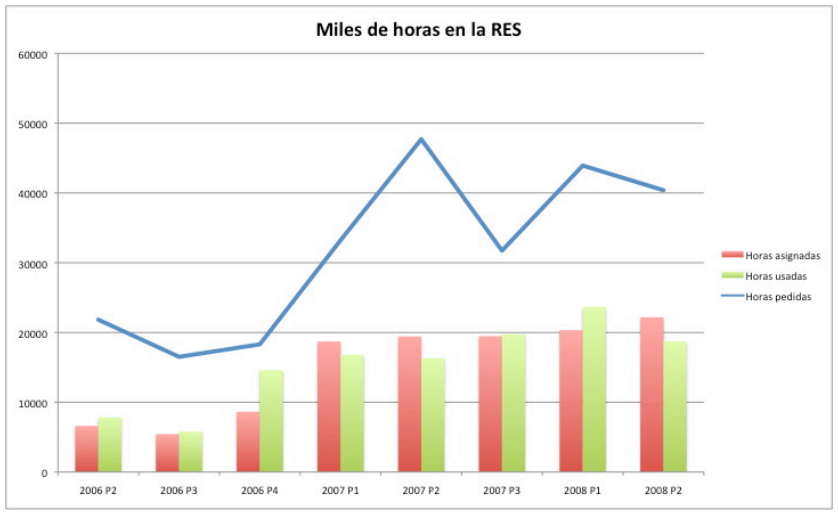


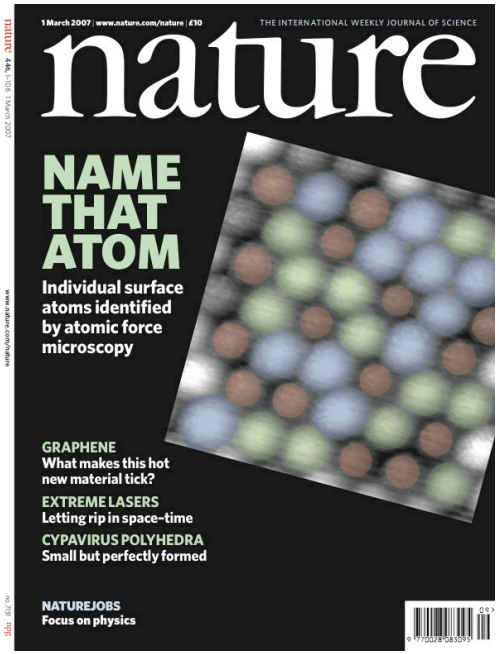
Comité de Acceso único

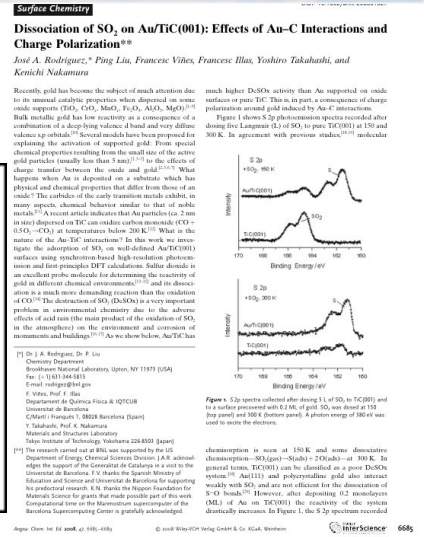
- 44 científicos españoles, renovación cada dos años
- Aprobado por el MEC y la ANEP
- Core Team
    - MEC: Ramón López de Arenosa
    - ANEP: Victoria Ley
    - Experto Supercomputación externo BSC: Pedro de Miguel (UPM)
    - Experto Supercomputación interno BSC: José Maria Cela
  - 4 paneles
    - 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







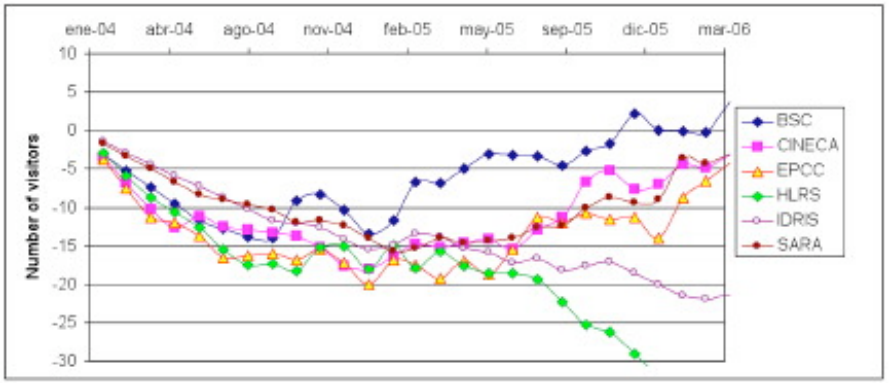

Surface Chemistry

Dissociation of SO_2 on Au/TiC(001): Effects of Au–C Interactions and Charge Polarization**

José A. Rodriguez, Ping Liu, Francesc Viñes, Francesc Illas, Yoshiro Takahashi, and Kenichi Nakamura*

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.

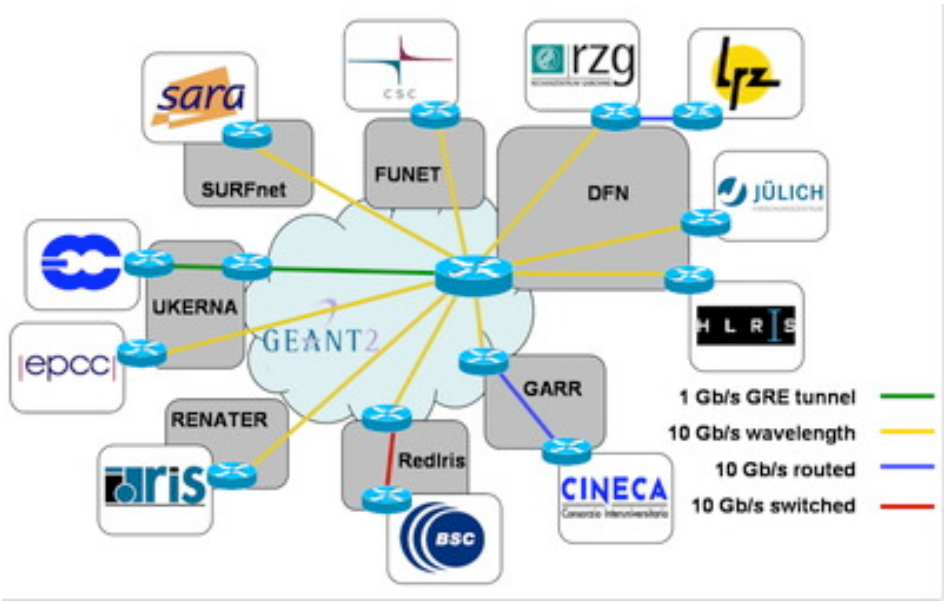


HPC-Europa
Pan-European Research Infrastructure on High Performance Computing

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

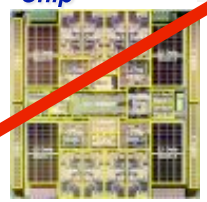
Ciencias de la computación

Computer architecture:

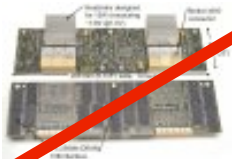
- Highly o-o-o architectures
- Hardware multithreading
- Design space exploration for multicore chips and Hw accelerators
- Transactional memory (Hw, Hw-assisted)
- SIMD and vector extensions/units

Programming models:

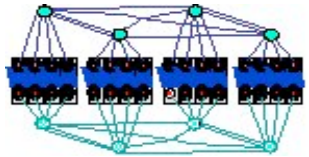
- Scalability of MPI and UPC
- OpenMP for multicore, SMP and ccNUMA
- DSM for clusters
- CellSs
- Transactional Memory
- Embedded architectures



Chip



On-board SMP



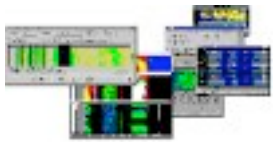
cc-NUMA

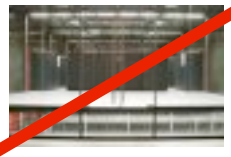
Large cluster systems

Small DMM

Benchmarking, analysis and prediction tools:

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





Future Petaflop systems

The Grid

Grid and cluster computing:

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

Operating environments:

eNANOS

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

Self

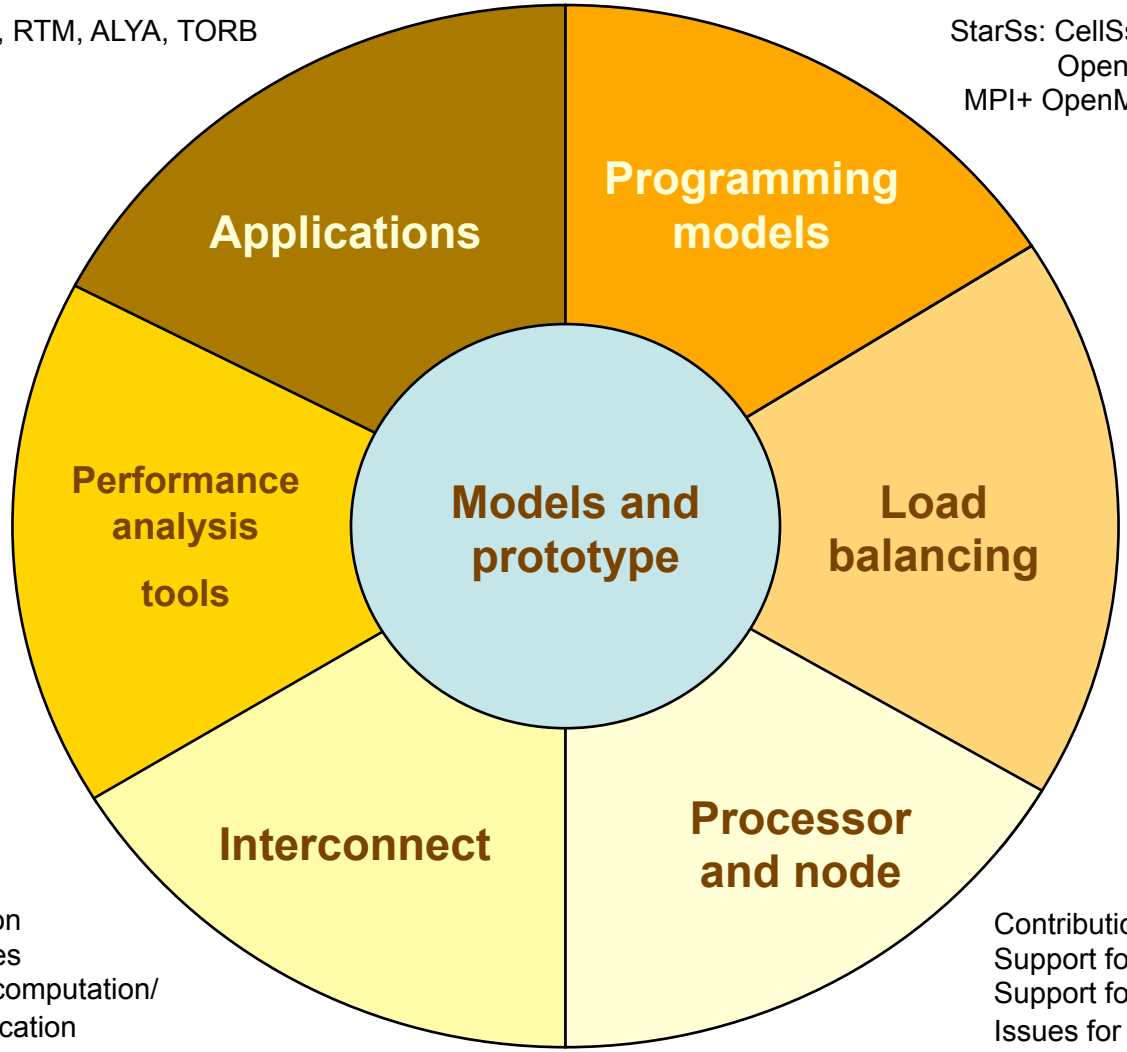
PRACE

SNIC
UNINETT
GRNET
ΕΔΕΤ
GCS
Gauss Centre for Supercomputing
GENCI
EPSRC
BSC
Barcelona Supercomputing Center
Centro Nacional de Supercomputación
NWO
Principal Partners
tier 0
tier 1
Ecosystem
POZMAN
UNIVERSIDADE DE COIMBRA
CSCS
Swiss National Supercomputing Centre
CINECA
Consorzio Interuniversitario
CSC
General Partners

Proyecto MareIncognito: BSC-IBM

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

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



Automatic analysis
Coarse/fine grain prediction
Sampling
Clustering
Integration with Peekperf

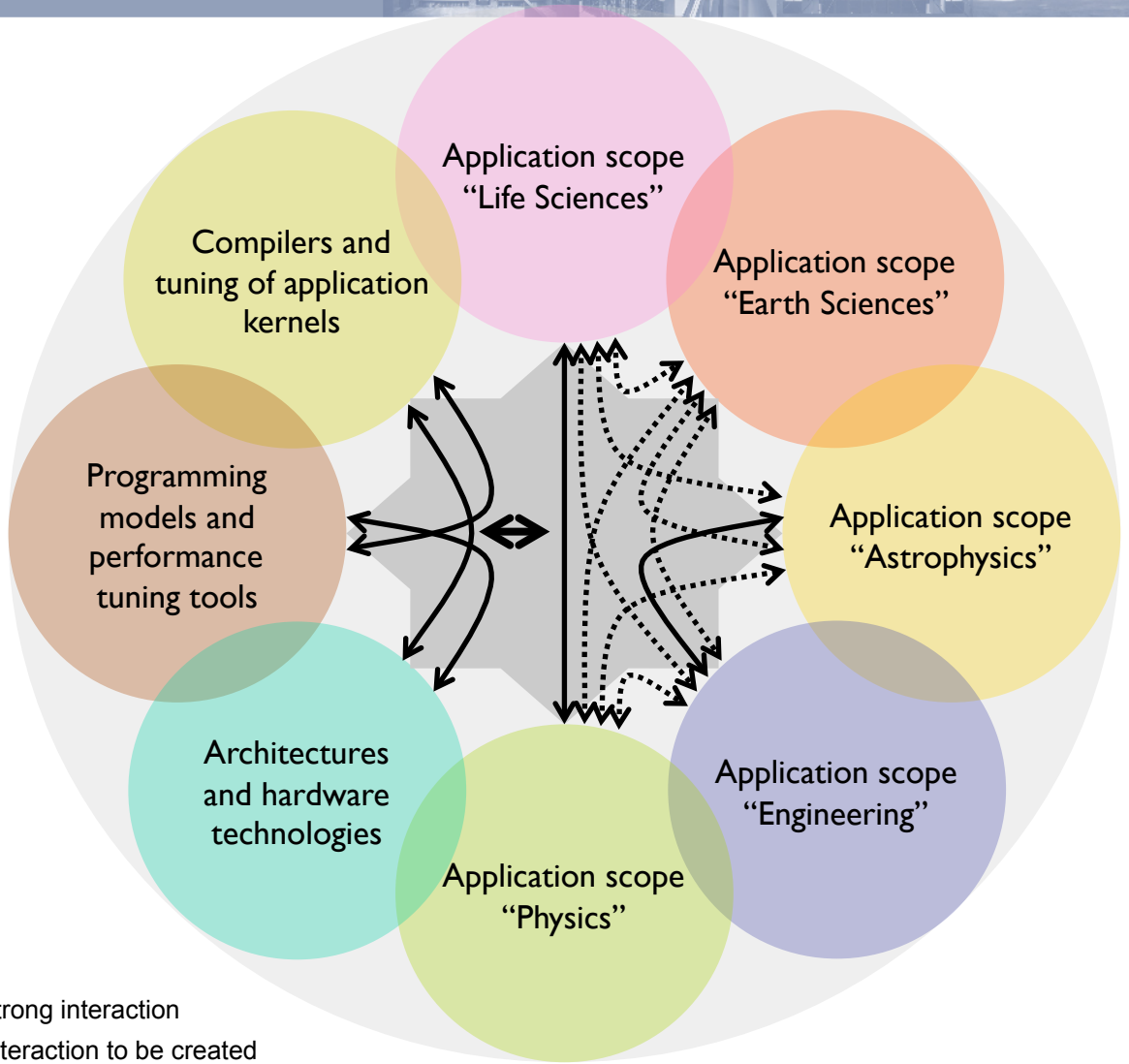
Coordinated scheduling:
Run time,
Process,
Job
Power efficiency

Contention
Collectives
Overlap computation/
communication

Contribution to new Cell design
Support for programming model
Support for load balancing
Issues for future processors

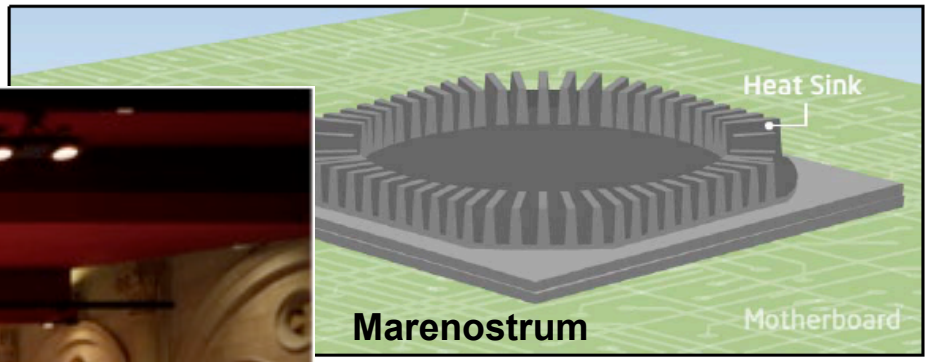
Proyecto Consolider: Supercomputing y e-Science

- 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

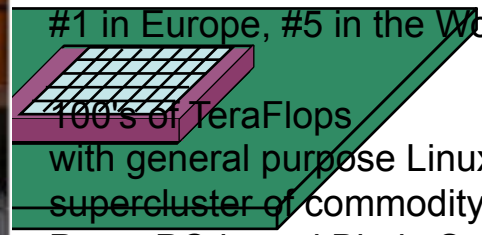
"It is better for Intel to get



s first Tera-scale Research Prototype are a
d supercomputer (above)

Most beautiful supercomputer
Fortune magazine, Sept. 2006

Source: Intel



#1 in Europe, #5 in the World

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

ore type devices,
el,
ional memory

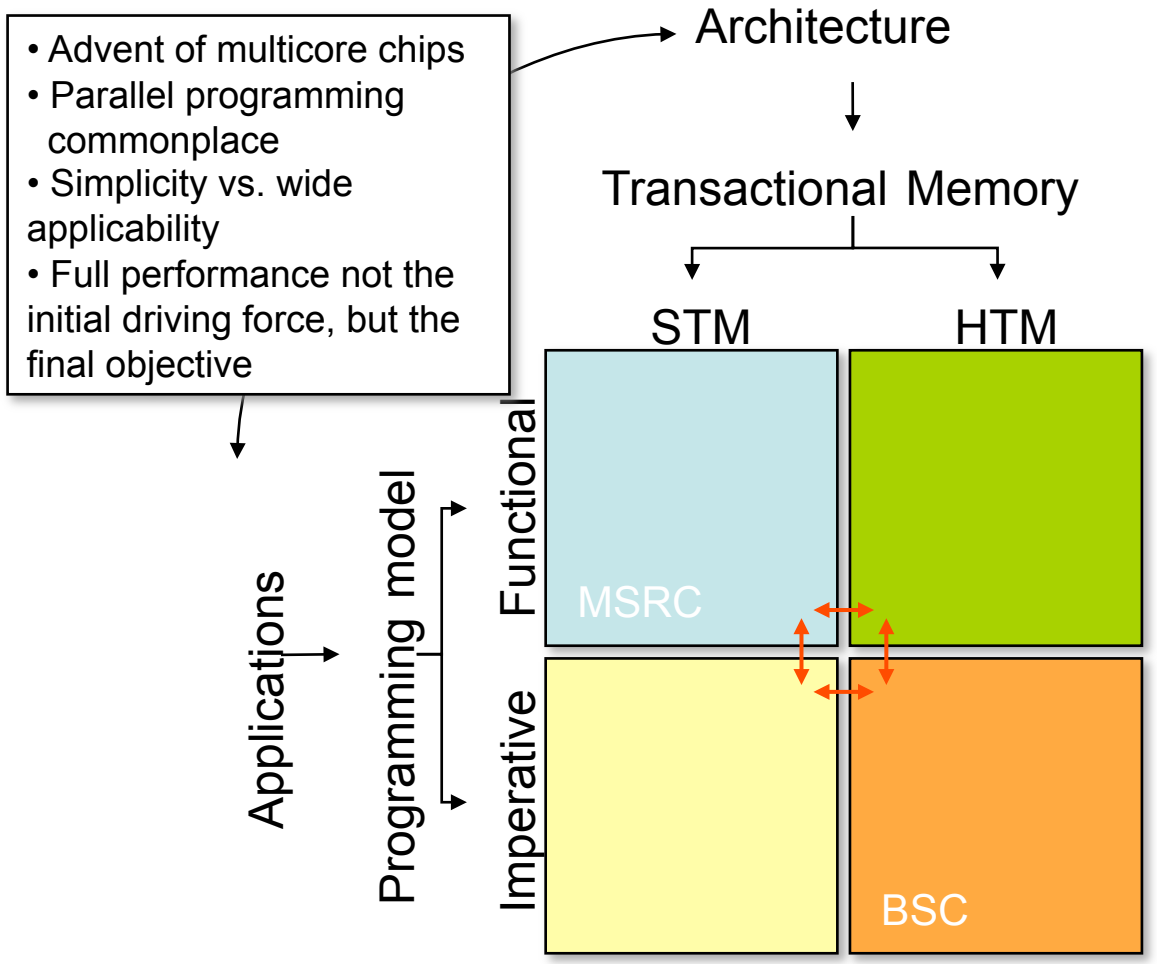
that will allow us to get the full benefit of all those transistors
and map that into higher and higher performance."
Bill Gates, Supercomputing 05 keynote

In 1991 using 10.000 Pentium
Pro processors contained in more than 85 cabinets occupying 200 square meters ☺
•This will be possible in 5 years from now

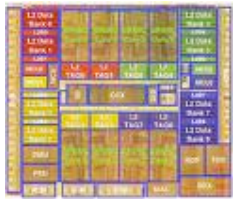
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

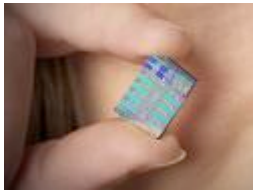
Microsoft - BSC Project: A quick snapshot

- 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



Education for Parallel Programming

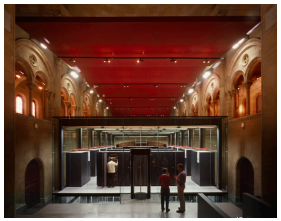




I ♥ many-core programming

I ♥ multi-core programming

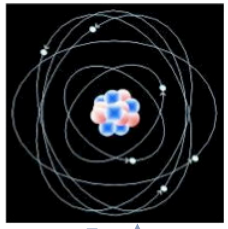
We all ♥ massive parallel prog.



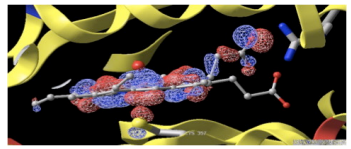
I ♥ games

Multicore-based pacifier

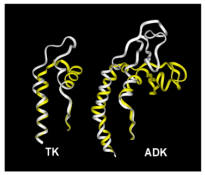
Ciencias de la Vida



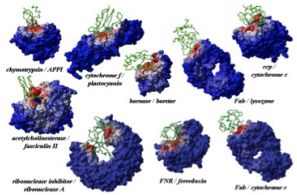
Atomic (and electronic) modeling of protein biochemistry and biophysics



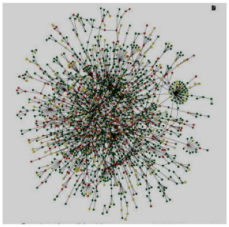
Micro and mesoscopic modeling of macromolecules. Drug Design



Identification of the structural bases of protein-protein interaction

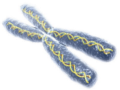


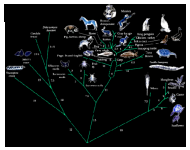
Protein-protein interaction networks
Systems biology



Web services, applications, databases

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

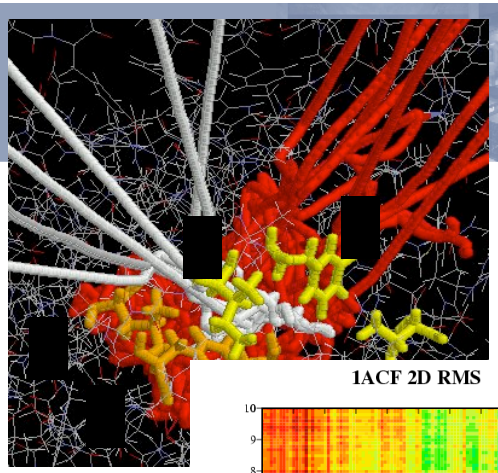


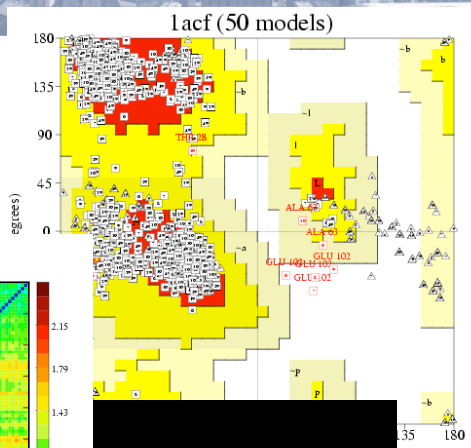


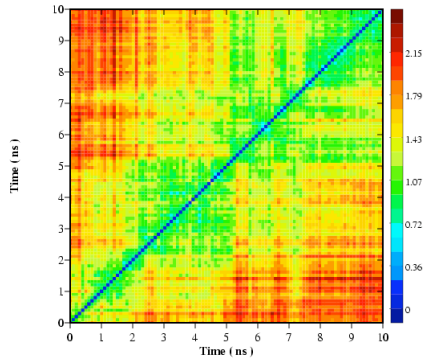
Life Sciences Department

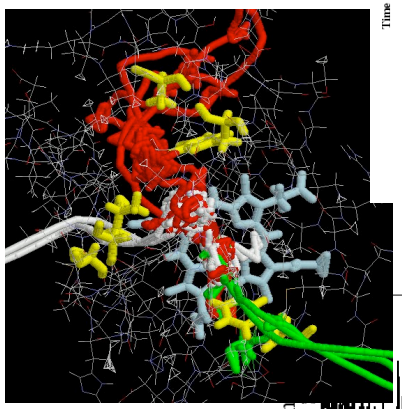
MoDEL

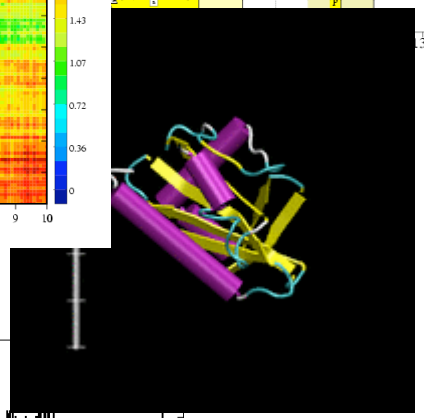
- Library of protein MD simulations
- 1400 at the moment
- >900 CPU years.
- 10 Tb of data

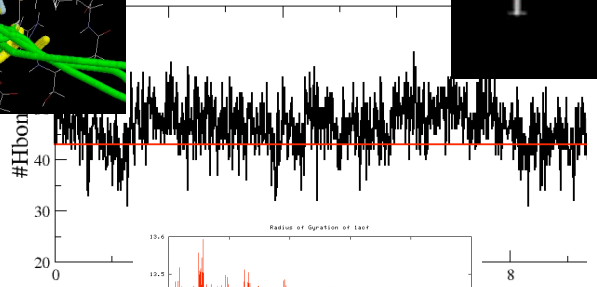


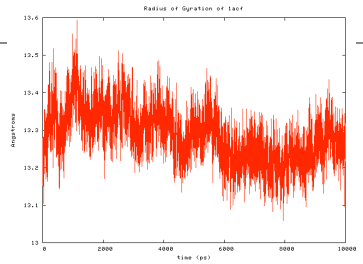


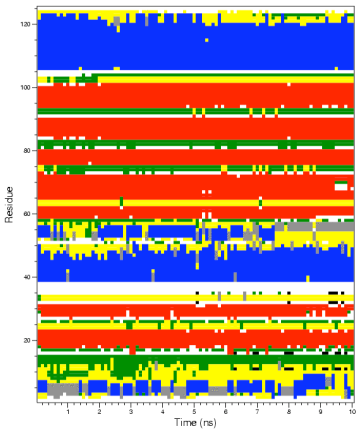


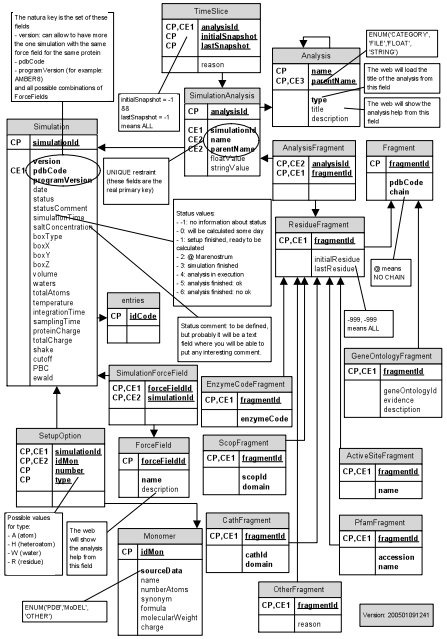












THE ENCODE PROJECT

THE EARTH PROTEOME

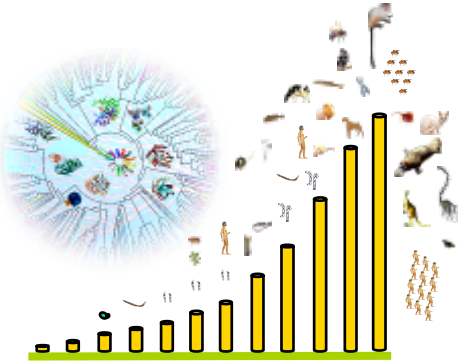
- Genome all organisms + all metagenomes
- $1.4x10^6$ sequences
- 32 Tb of RAM used
- 4000 processors
- 38 CPU years
- 9 Tb of output data
- G-Superscalar
- 3.5 days job!
- 5 DAYS lagtime!!!

EMBL-EBI

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

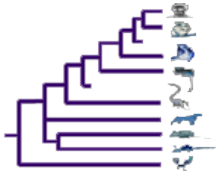
Providing new functional associations and hypothesis for basic research

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

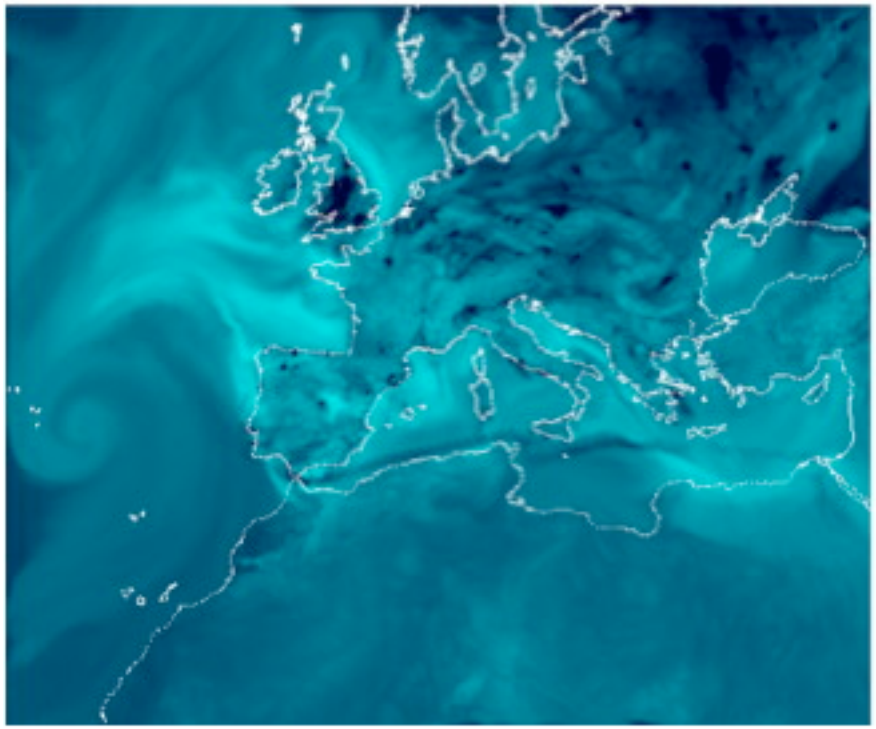
Ecology

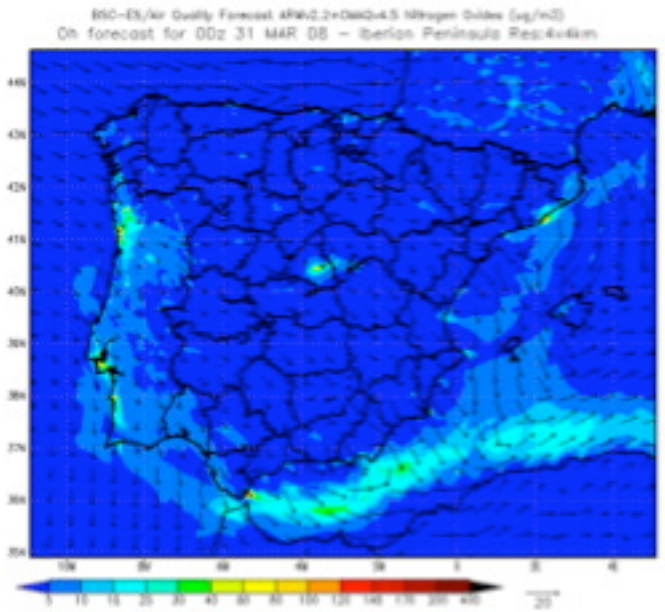
Identification of new pathways and organisms for new possibilities in biodegradation.

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).

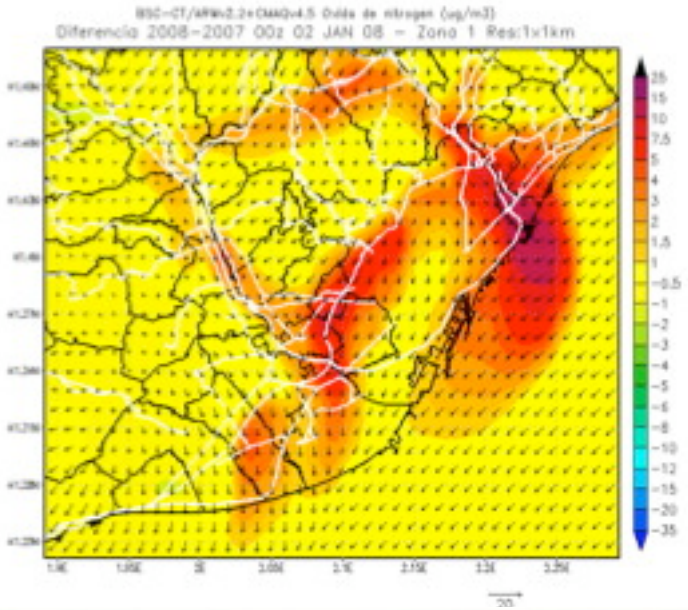




Calidad del Aire

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.

Todos a 80. Paneles que indican la limitación sin excepciones de la velocidad a 80 km/h en un acceso a Barcelona por autopista, en Molins de Rei

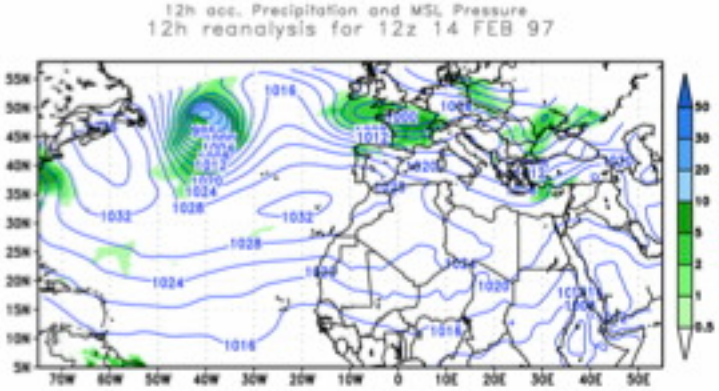
BSC Earth Sciences Department

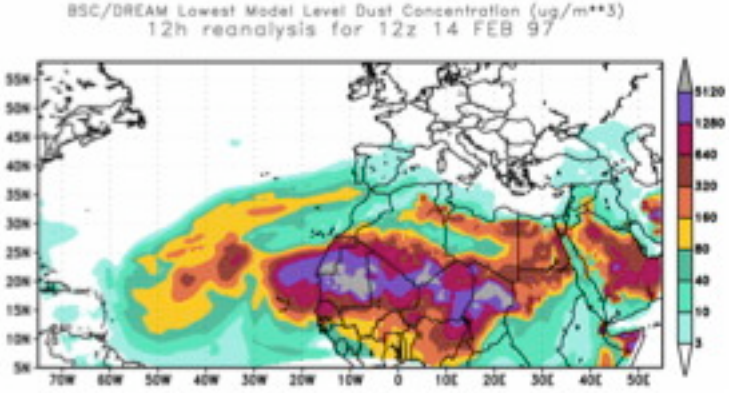
Mineral Dust:

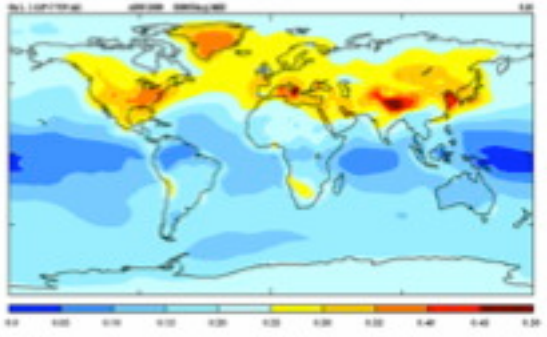
✓ Daily operational forecasts of mineral dust for the Euro-Mediterranean and the East Asia region based DREAM Model (http://www.bsc.es/projects/earthscience/DREAM).

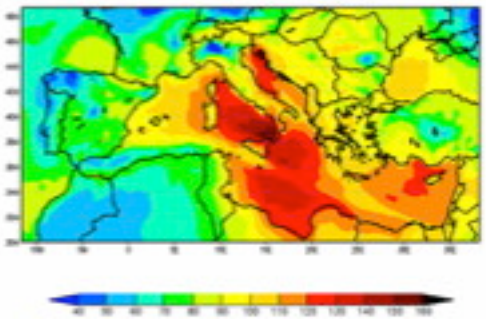
✓ Leading initiative: World Meteorological Organization initiative to create a Regional Centre for Sand and Dust Storm Warning System.

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









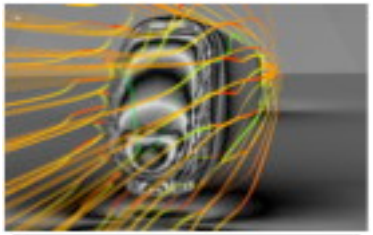
Climate Modelling:

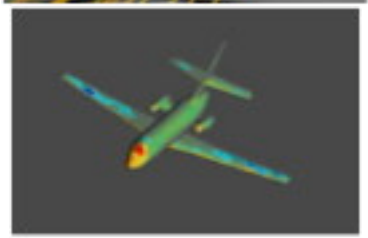
✓ Global Climate Modelling with NASA GISS ModelE and NCAR WACCM in MareNostrum supercomputer with a resolution of 2ºx2.5º.

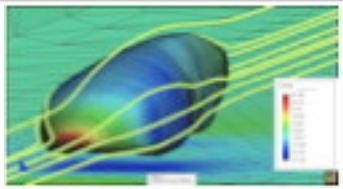
✓ Implementation of a regional climate model (RCM) based on the WRF/CMAQ/DREAM system for the Mediterranean Sea and Europe (20 km resolution) in order to simulations to ascertain the regional impact of climate change in the trends of extreme events.

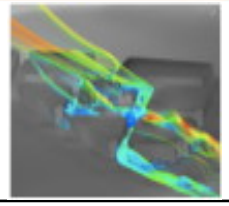
Aplicaciones Científicas y de Ingeniería

Computational Fluid Dynamics

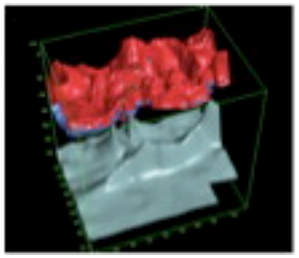


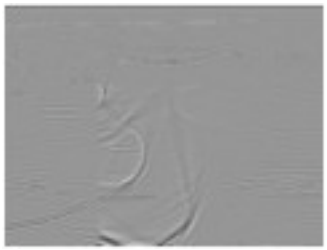






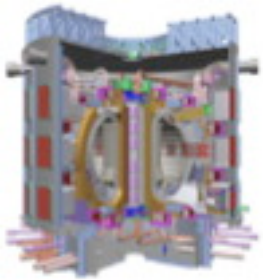
Geophysics

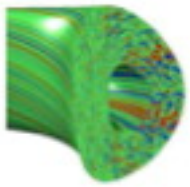




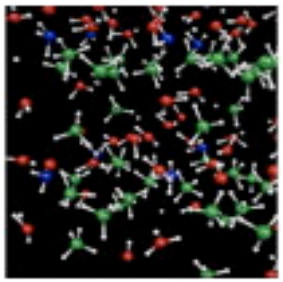
REPSOL

ITER: Plasma physics

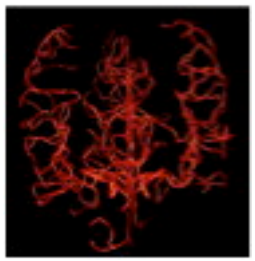




Ab-initio Molecular Dynamics



Bio-mechanics



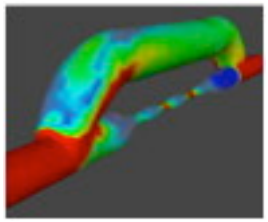
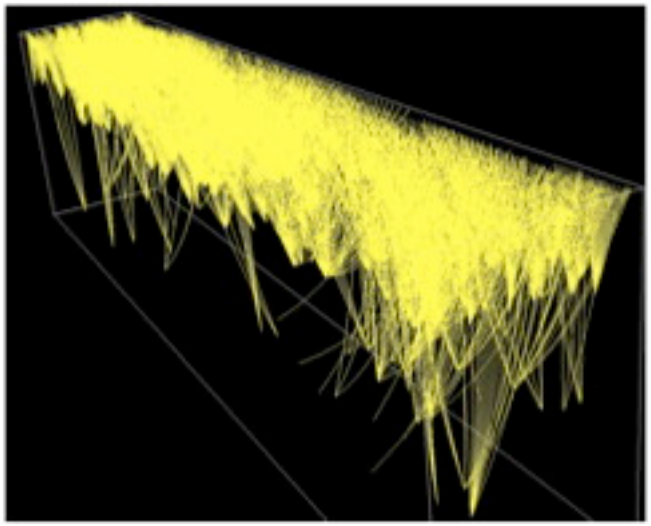
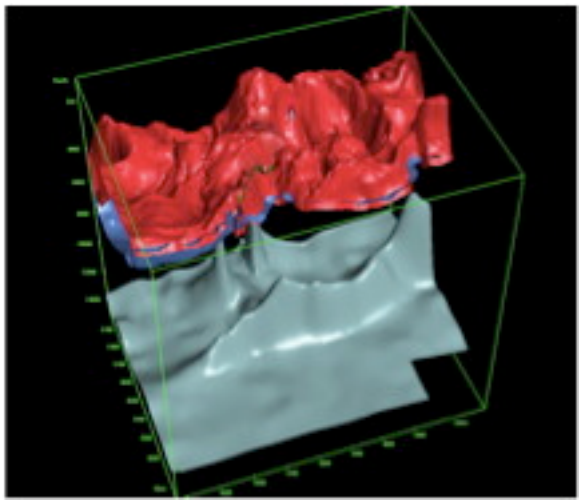


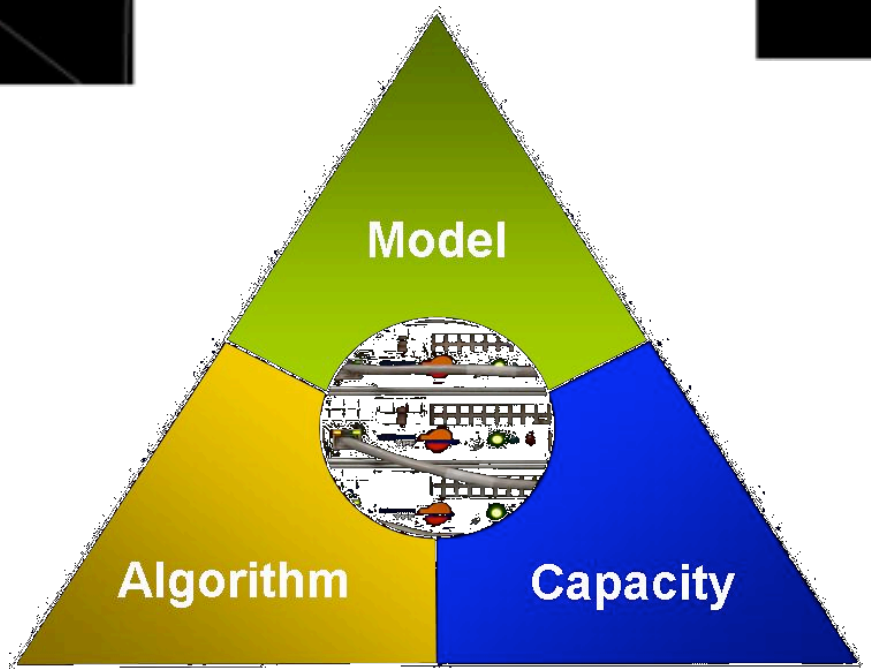
Imagen Sísmica: Proyecto Calidoscopio



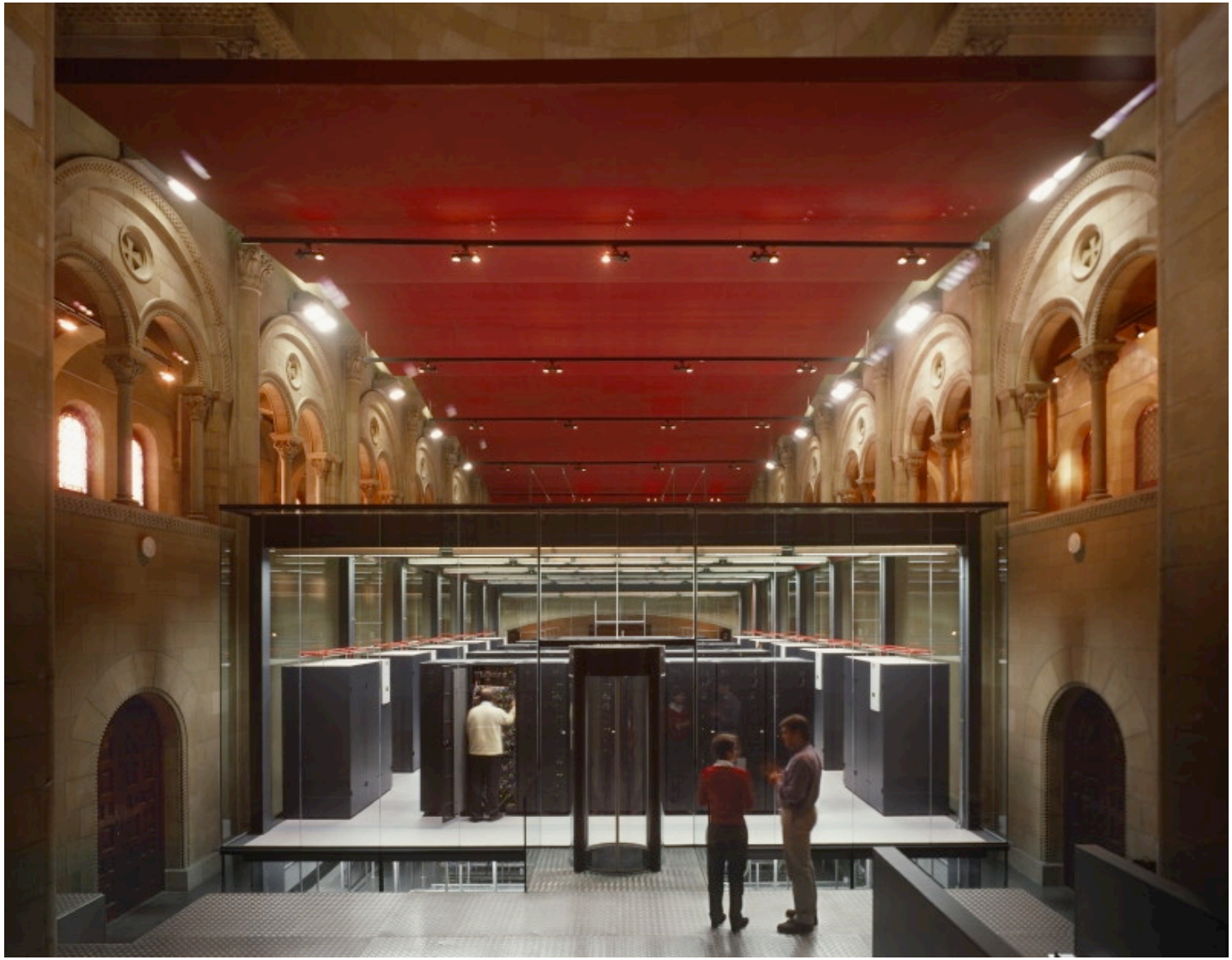


REPSOL YPF

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



3DGEO DEVELOPMENT INC.

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Felicidades!