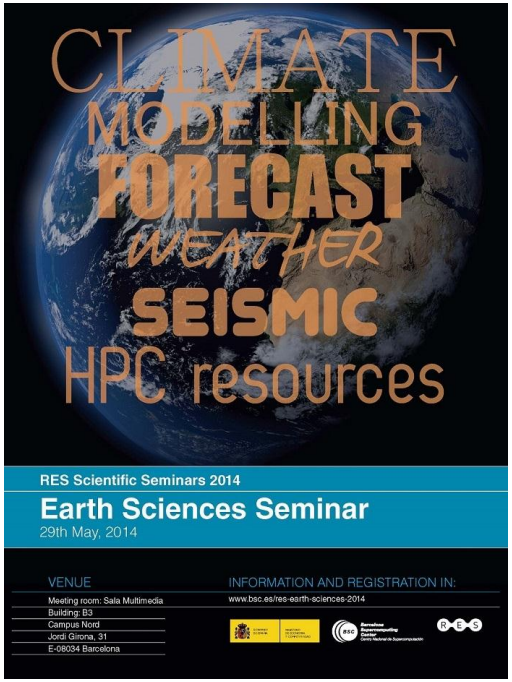
PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

Supercomputing resources in BSC-CNS, RES & PRACE



Sergi Girona
BSC Operations Director &
PRACE Director

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

BARCELONA SUPERCOMPUTING CENTER

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

- BSC-CNS objectives:
  - R&D in Computer, Life, Earth and Engineering Sciences
  - Supercomputing services and support to Spanish and European researchers

- BSC-CNS is a consortium that includes:
  - Spanish Government 51%
  - Catalonian Government 37%
  - Universitat Politècnica de Catalunya (UPC) 12%

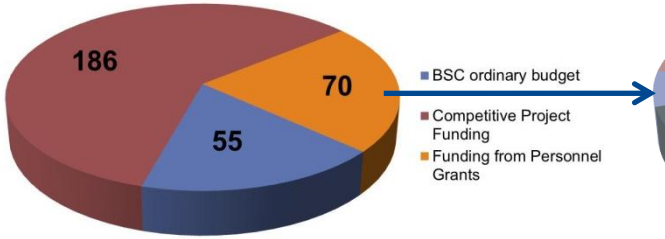
GOBIERNO DE ESPAÑA · MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

Generalitat de Catalunya
Departament d'Economia i Coneixement

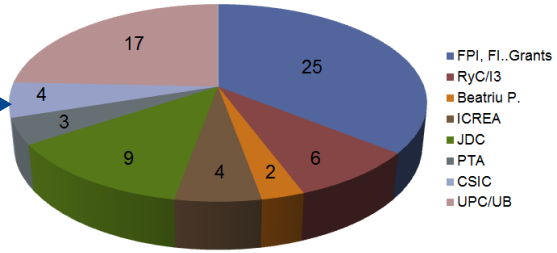
UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

- +300 people, 40 countries

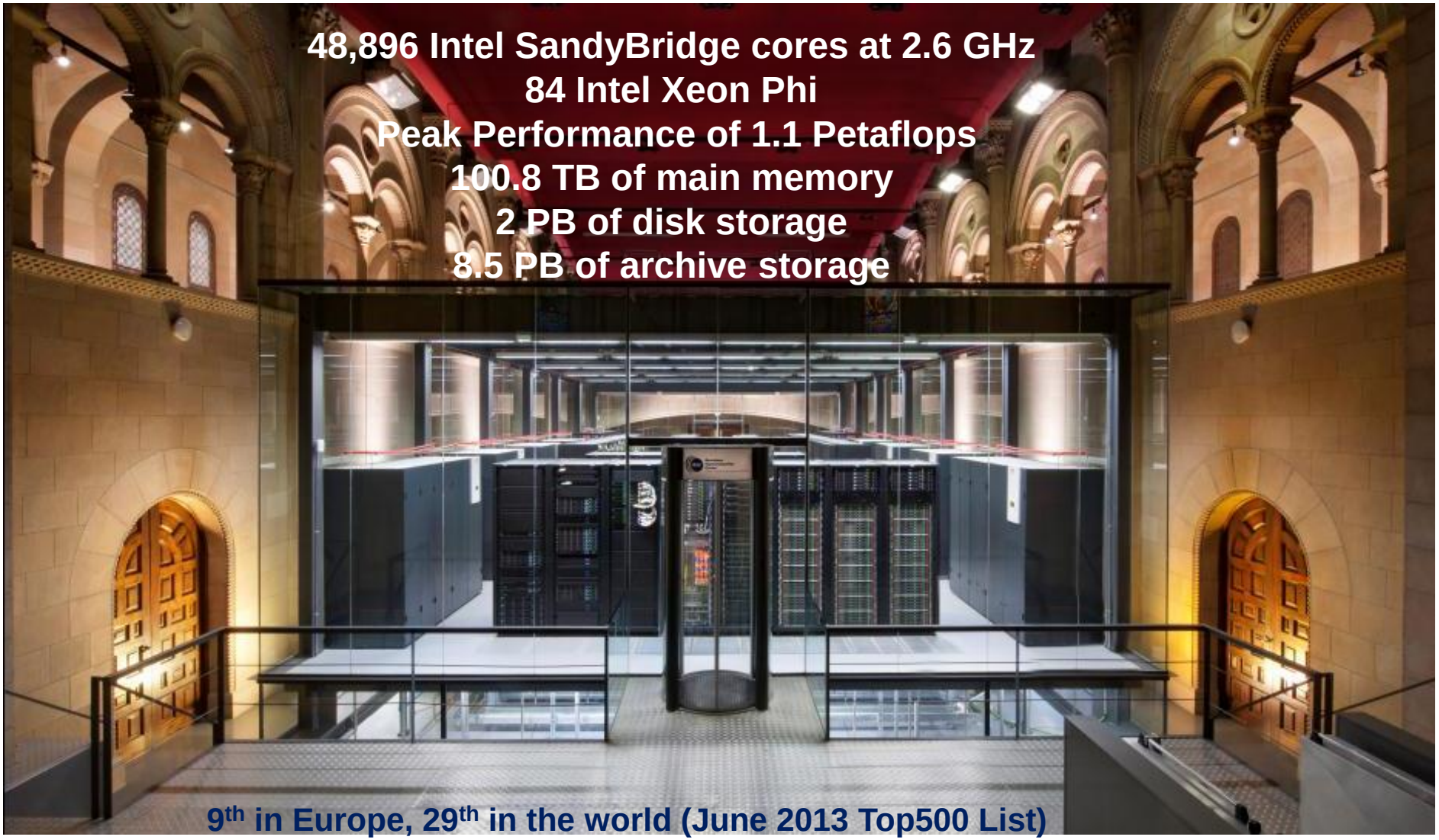
BSC STAFF 2012



Funding from Personnel Grants 2012



MareNostrum 3



BSC at a glance

EXCELENCIA SEVERO OCHOA

One of only 13 centres recognised with prestigious Severo Ochoa award for excellence

GOBIERNO DE ESPAÑA · MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

Generalitat de Catalunya Departament d'Economia i Coneixement

UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH

National & European HPC Infrastructure

- *Spanish national HPC lab*
- *PRACE Tier-0 Hosting Partner*

Bridge to Latin America

- *Extensive network of contacts*
- *Coordinator, RISC and OpenBio projects*

Computer Sciences

- *Architecture, Programming Models, Tools, Cloud and Grid*

Education & Training

- *UPC, PATC, BMW, Pumps*

Life Sciences

- *Molecular and protein modelling, computational genomics etc.*

BSC

+300 staff from +40 countries

Key European Research partner

- *Participation in 79 FP6/7 projects, 14 as coordinator*

Earth Sciences

Atmospheric processes and climate change modelling

Solid Partnerships with Industry

- *Repsol, Microsoft, IBM, Intel, Iberdrola, NVIDIA, Samsung*
- *Leading role in ETP4HPC*

Computer Applications

- *Simulation of complex problems on High Performance Computers*

RES

- La RES es una infraestructura virtual distribuida consistente en la interconexión de supercomputadores que gestionan su capacidad de cálculo y proporcionan servicio a investigadores españoles.

RES: Solicitud de acceso

Solicitud, protocolo de acceso y publicación de convocatorias cada 4 meses en

www.bsc.es/RES

Información en solicitud:

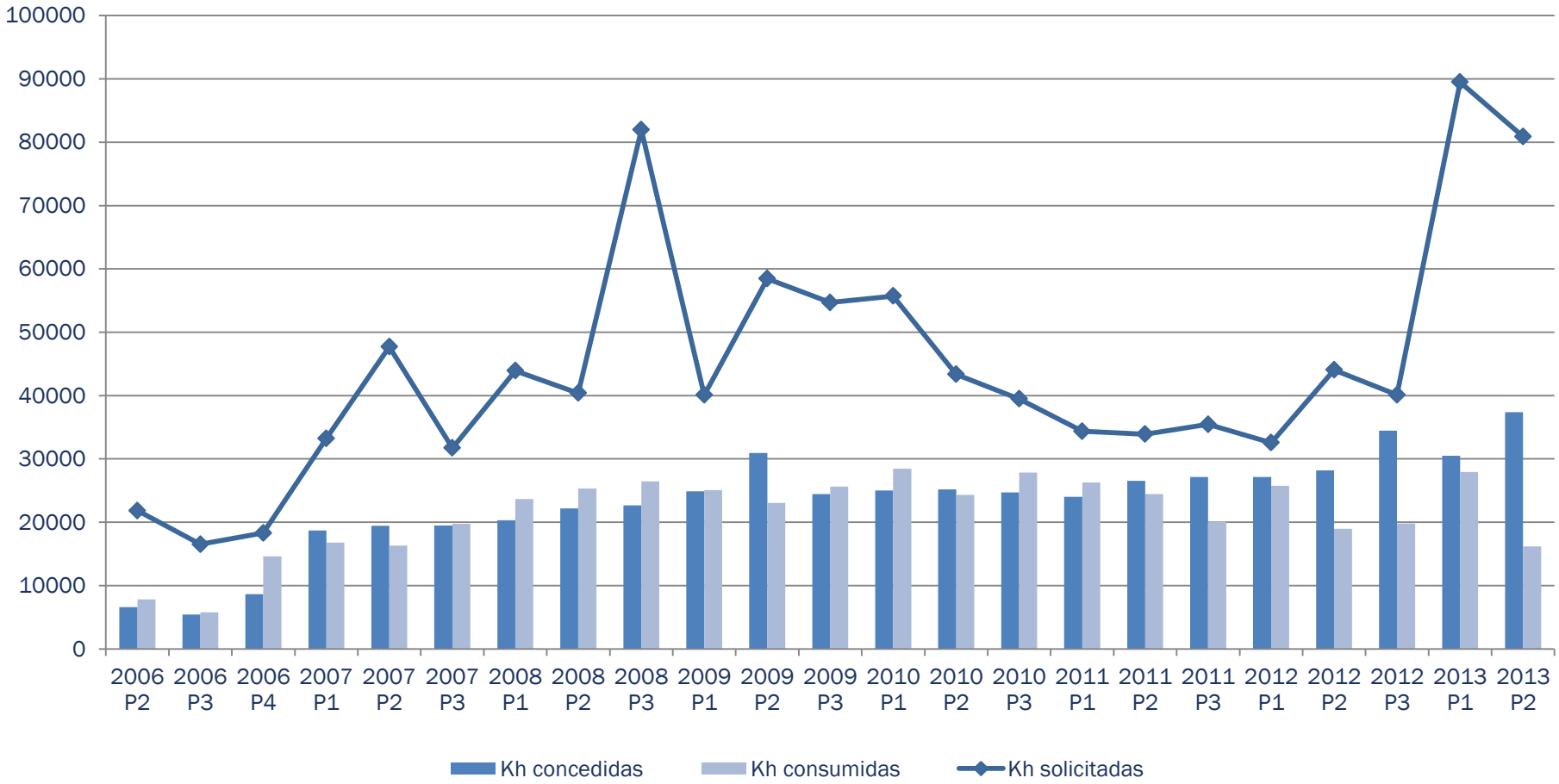
Descripción del proyecto y su objetivo

Librerías numéricas y software necesario

Descripción del equipo de investigación

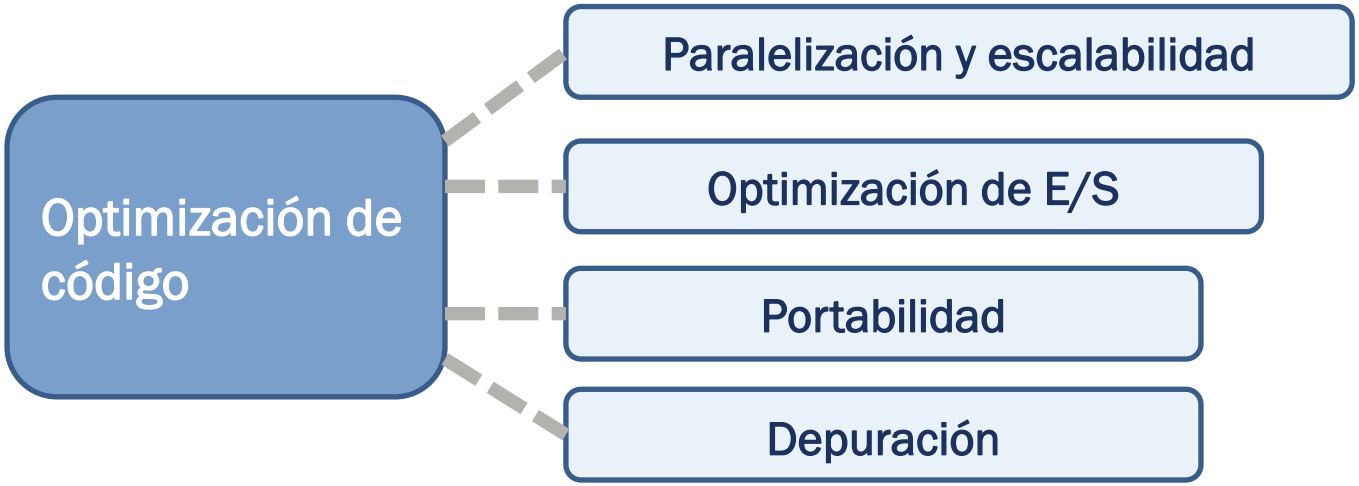
Horas de cómputo y memoria necesaria

RES: Solicitudes, acceso y consumo



** En 2013 se contabilizan sólo los 2 primeros periodos de acceso (el 2º aún sin finalizar) debido a que aún no ha terminado el año.*

RES: Soporte



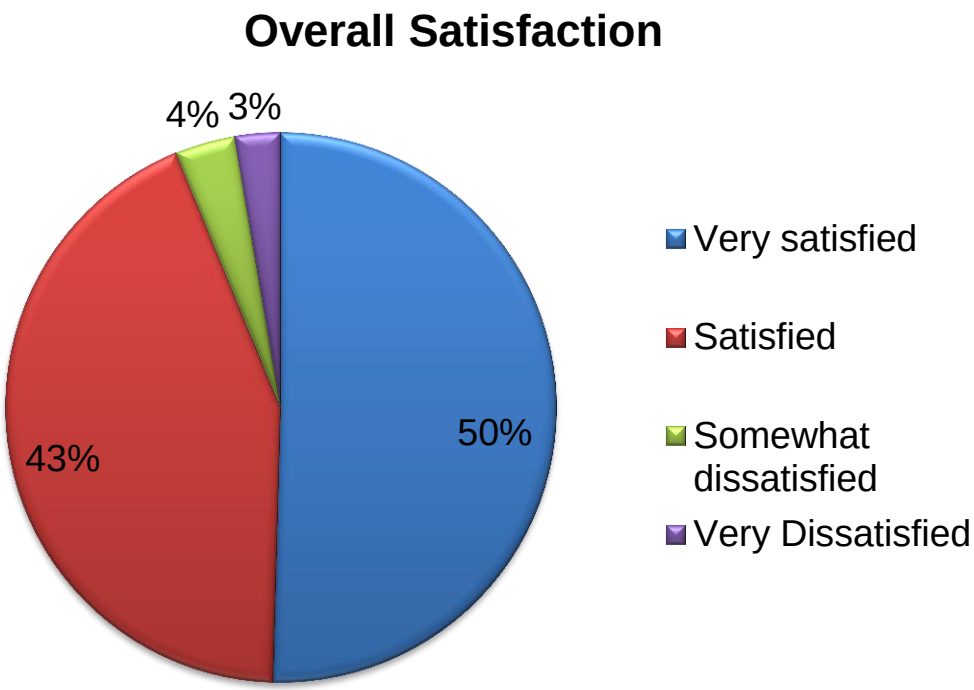
Almacenamiento de datos

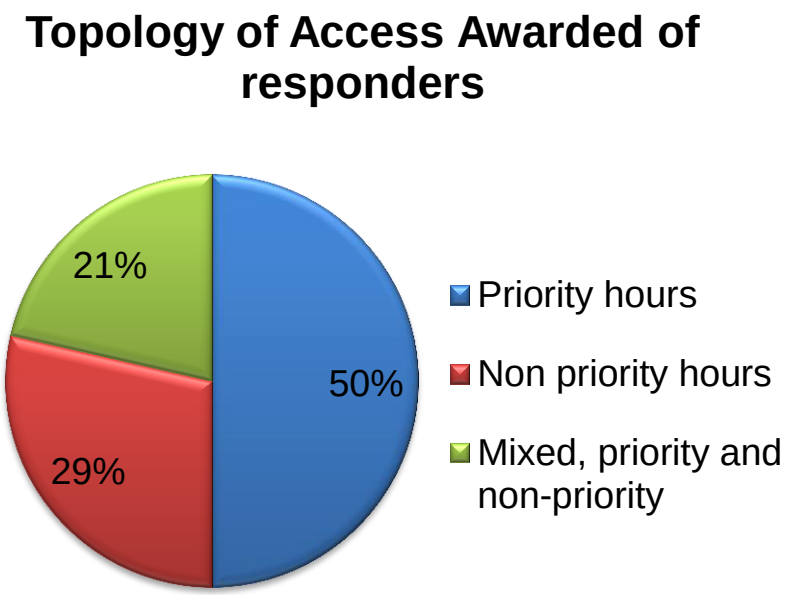
Actividades de test

Difusión científica

Organización de jornadas, cursos/formación y seminarios

RES, user survey results





PRACE days15

PRACE SCIENTIFIC AND INDUSTRIAL CONFERENCE 2015

Combining the PRACE Scientific Conferences and PRACE Industrial Seminars, this conference will bring together experts from academia and industry who will present their advancements in HPC-supported science and engineering.The programme will include keynote speeches, parallel and poster sessions as well as a meeting of the PRACE User Forum.

The PRACE Scientific and Industrial Awards as well as a prize for Best Poster will be presented and we are looking forward to making this event a tradition for the European HPC communities!

AVIVA STADIUM
Lansdowne Road, Dublin, Ireland
26 - 28 May 2015

www.prace-ri.eu/pracedays15

www.linkedin.com/company/prace

@PRACE_RI

ENABLE SCIENCE FOSTER INDUSTRY

The Implementation Phase of PRACE receives funding from the EU's Seventh Framework Programme (FP7/2007-2013) under grant agreements RI-283493 and RI-312763.

PRACE: the European HPC Research Infrastructure

- Enabling **world-class science** through large scale simulations
- Providing **HPC services on leading edge capability** systems
- Operating as a **single entity** to give access to **world-wide supercomputers**
- **Attract**, **train** and **retain** competences
- **Lead** the **integration** of a highly effective **HPC ecosystem**
- Offering its resources through a **single** and **fair** pan-European **peer review process** to academia and industry

- **25** members, since 2010
- **6** supercomputers in **4** hosting countries, nearly **15 Pflop/s**
- Common operation procedure between **35** centers in Europe
- **22** prototypes evaluated
- **169** white papers produced
- **1500** communications from our users
- **166** Thesis
- HPC Community building: **183** events

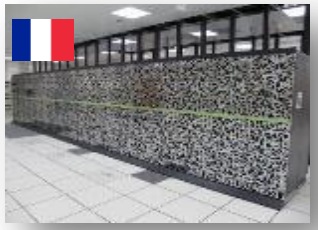
- **8 billion** hours granted since 2010 (a system with 900k cores for 1 year)
- **303** scientific projects enabled from **38** countries
- More than **20 SME** and **industries** access in first year
- **360** PATC Training days
- **2734** Trained people
- **170** applications enabled

PRACE systems

From 2013, more than 16 Pflop/s provided

MareNostrum: IBM IDPX at BSC, >48 000 cores

JUQUEEN: IBM BlueGene/Q at GCS partner FZJ, >458 000 cores



CURIE: Bull Bullx at GENCI partner CEA >90 000 cores.

SuperMUC: IBM IDPX at GCS partner LRZ, >155 000 cores

FERMI: IBM BlueGene/Q at CINECA, >163 000 cores

HERMIT: Cray at GCS partner HLRS, >113 000 cores

How can researchers are accessing the HPC resources?

1. The Preparatory Access call
2. The Project access call

How can researchers are accessing the HPC resources?

1. Preparatory Access

- Permanently open with quarterly cut-off dates (03/06/09/12)
- Intended to prepare proposals for Project Access
  Not for production runs nor research activities
  - Testing scalability: **Type A**, allocation for 2 months
  - Code development or optimisation:
    - **Type B**, allocation for 6 months
    - **Type C**, allocation for 6 months, including expert support
- Fixed amount of resources, depending on the system
- Technical review only
- Start date of awarded projects approx. 45 days after the cut-off date

Preparatory Access: Resources per type of Preparatory Access

(2014)	Type A – 2 months	Type B/C – 6 months
Curie FN/TN Curie H	50.000 CPU 50.000 GPU	200.000 CPU 100.000 GPU
Hermit	50.000 CPU	50.000 CPU
Fermi	50.000 CPU	250.000 CPU
JUQUEEN	100.000 CPU	250.000 CPU
MareNostrum MareNostrum H	50.000 CPU 5.000 MIC	100.000 CPU 20.000 MIC
SuperMUC	100.000 CPU	250.000 CPU

How can researchers are accessing the HPC resources?

2. Project Access

- 2 calls a year
  - Call open in February > Access starting in September
  - Call open in September > Access starting in March
- 12 months award period
- “On demand” resource request, usually above 5Mio CPU hours
- Proposals requesting resources on multiple machines are allowed
- Technical and Scientific peer review
- Start date of awarded projects approx. 15 weeks after call closed

Project Access:
Resources per Project Access (in MioH)

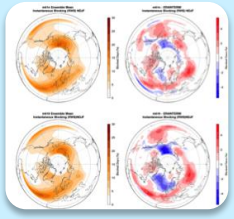
(8th call)	Total available resources	Average awarded resources per project
Curie FN/TN Curie H	201/28 CPU 0,5 GPU	15/11 CPU 0,3 GPU
Hermit	120 CPU	23 CPU
Fermi	360 CPU	47 CPU
JUQUEEN	100 CPU	20 CPU
MareNostrum	120 CPU	25 CPU
SuperMUC	170 CPU	19 CPU

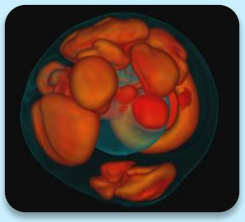
Terms of Access

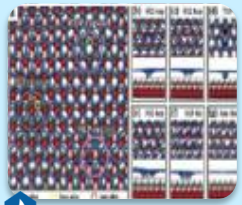
- **REPORTING**: providing a final report on the results obtained* is a mandatory condition to access PRACE resources
- No **EXTENSION** : exception possible in time only & only in case of unforeseen technical issues
- **ACKNOWLEDGEMENT**: applicants must **acknowledge PRACE** in all publications that describe results obtained using PRACE resources, using the text specified in the "Guide for Applicants to Tier-0 Resources" section 4.2.
- **DISSEMINATION**: applicants allow PRACE to publish the final report of the project (please check specific conditions), and should provide some material for additional dissemination activities (slides, pictures, reference of publications with work executed in PRACE systems).

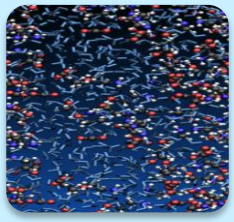
PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

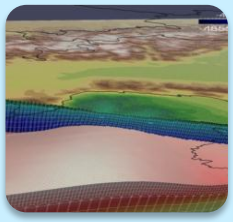
PRACE serves academic and industrial competitiveness

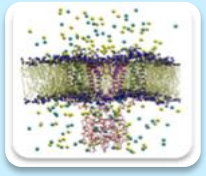












Earth System Sciences

88 million core hrs on Marenostrum (ES) for ES

The project aims at developing **new climate models** for preparing the 6th IPCC campaign in relation with ENES.

Astrophysics

million core hrs: 98 on CURIE (FR) + 49 on SuperMUC (DE) for Germany

The objective is to understand the **explosion of massive stars into supernovae** and understand the origin of the heaviest of the chemical elements, such as gold, platinum, lead, and uranium.

Materials

10 million core hours on CURIE(FR) for Finland

The goal of this project was to study using DFT simulations the effects of **irradiation on Graphene nanostructures**, especially vacancies and their coalescence into holes/defects.

Chemistry

59,8 million core hrs on JUQUEEN (DE) for Switzerland

The goal is to **catch CO_2 in a solvent before it is released into the air,** making the **exhausts from e.g. power plants significantly cleaner** – and then to reduce the cost of regenerating the solvent by optimizing the regeneration process

Seismology

53.4 million core hrs on SuperMUC (DE) for Italy

The massive allocation of computing resources awarded via PRACE can be used to explore the non-linearity involved in the dependence **of local ground shaking on geological structure**.

Life Science

56 million core hours on CURIE (FR) and 82 million core hours on SuperMuc for FR

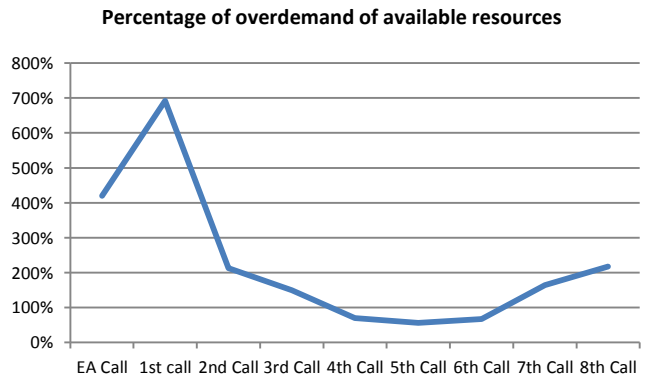
The project aims at understanding how a **nervous impulse is transported with neurons**, and especially the function of the ion channels, to contribute to the design of drugs that will modulate their activity.
This allocation is 30 times larger than a typical allocation.

PRACE impact on research:

Resources supply and demand & European collaborations

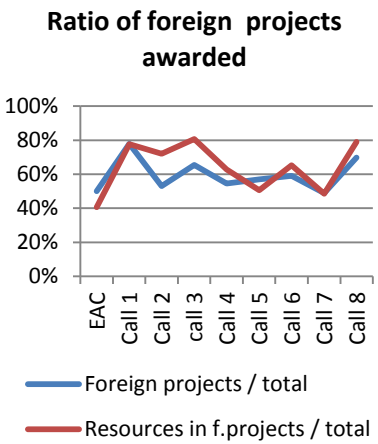
Request for core hours = 2 x the resources available

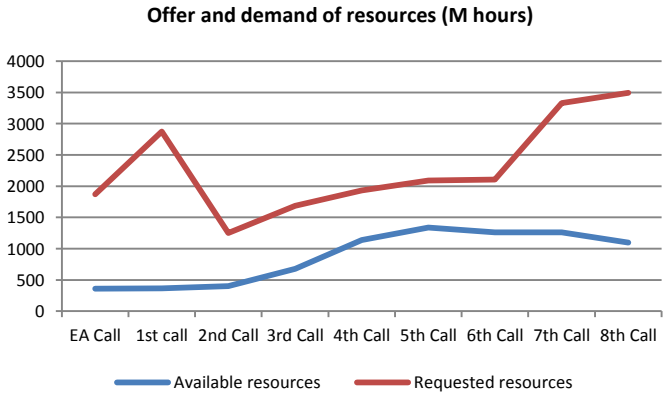
- → average over demand in PRACE = 162%.
- → Significant increase of the demand over the last 3 calls (218% in the 8th call).
- → **Demand for Tier-0 resources exists and evolves positively!**



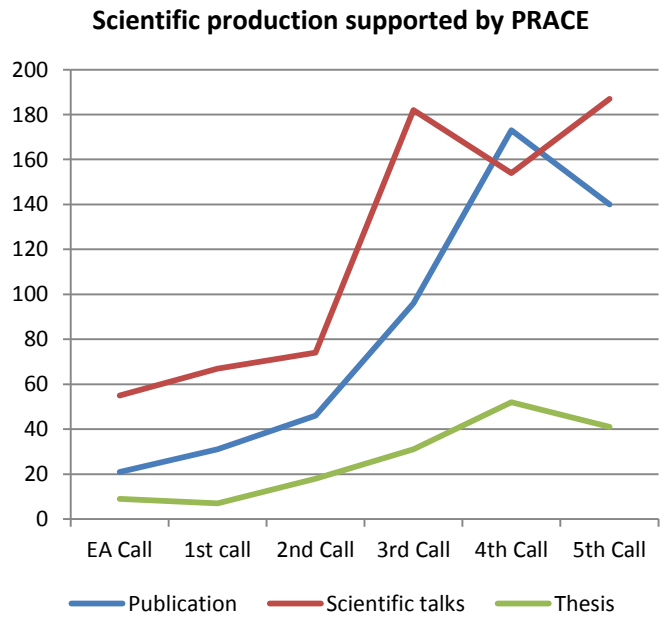
PRACE and European collaboration

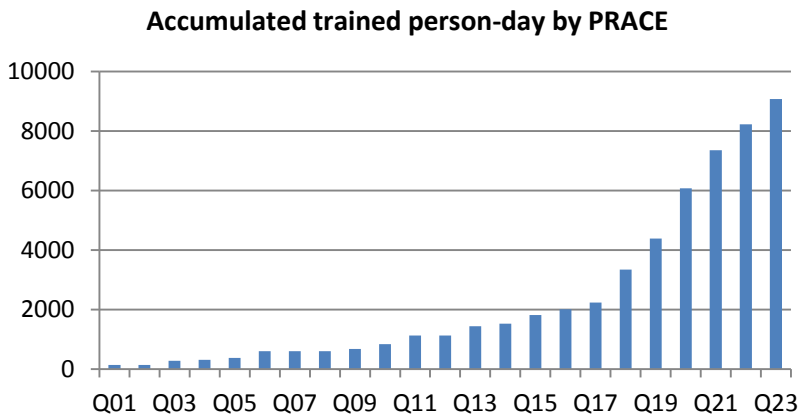
→ **63% of the PRACE resources** awarded to projects led by a **different country** than the machine providing the resources.





PRACE impact on scientific production and know-how in Europe





Until call n°5 PRACE has supported:

- 158 PhD Thesis
- 507 publications
- 719 scientific talks
- 2 patents

- In 5 years PRACE provided to **9079 training person-days** of attendance-based courses.

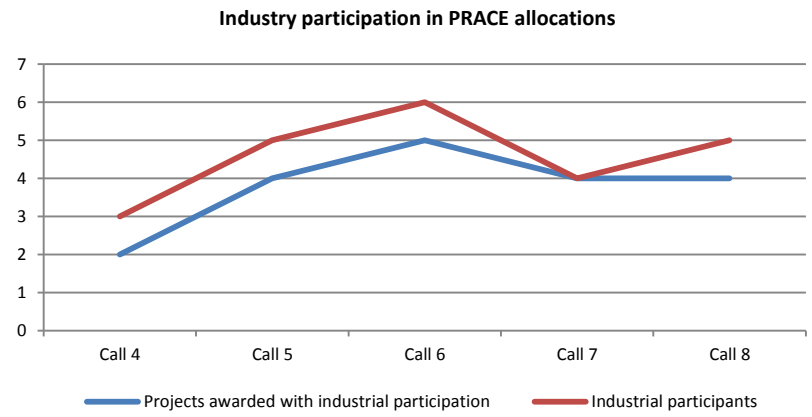
→ **PRACE has increased the European HPC know how to 2874 people.**

- Average **rate of recurring participation** in training = 30% → PATCs are not a closed circuit.

PRACE impact on the the industrial sector

Increasing trend both in:

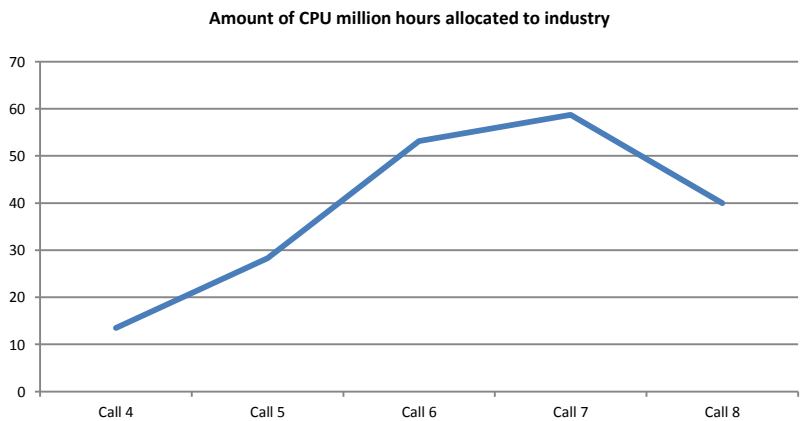
- **participation** (number of projects awarded with industry participation + and number of industrial participants)
- amount of resources awarded to industrial users



SHAPE
SME HPC Adoption Programme in Europe

In the **SHAPE pilot**:

- 10 success cases of **SMEs** from 6 different countries **benefitting not only from PRACE resources but from the know how in the PRACE centers**.



Barcelona Supercomputing Center
Centro Nacional de Supercomputación
www.bsc.es

Gracias!