Barcelona Supercomputing Center
Centro Nacional de Supercomputación

PRACE, PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

www.prace-ri.eu

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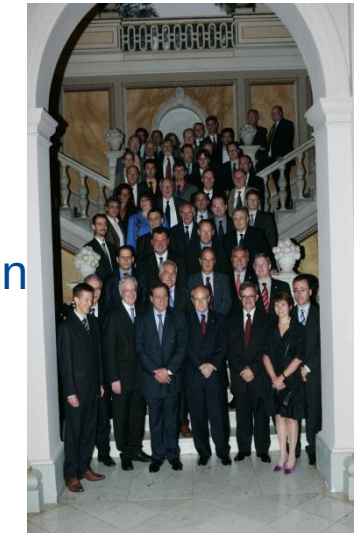
EXCELENCIA SEVERO OCHOA

PRACE Research Infrastructure

- Establishment of the legal framework
  - PRACE AISBL created with seat in Brussels in April (Association Internationale Sans But Lucratif)
  - 24 members representing 20 European countries
    - Hosting members: France, Germany, Italy, Spain
  - Inauguration in Barcelona on June 9, 2010

- Funding secured for 2010 - 2015
  - 400 Million € from France, Germany, Italy, Spain
    Provided as Tier-0 services on TCO basis
  - 70+ Million € from EC FP7 for preparatory and implementation
    Grants INFSO-RI-211528 and 261557
    Complemented by ~ 60 Million € from PRACE members



PRACE AISBL goals

- The development and provision of an Infrastructure at European level which allows the scientific communities, including those within industry, to access European High-end Computing (HeC) systems (Tier-0).

- The management of the coordination between the Infrastructure and existing national computation centres (Tier-1) and also, if agreed, regional computation centres (Tier-2), to allow for the establishment of relationships with the HeC user communities.

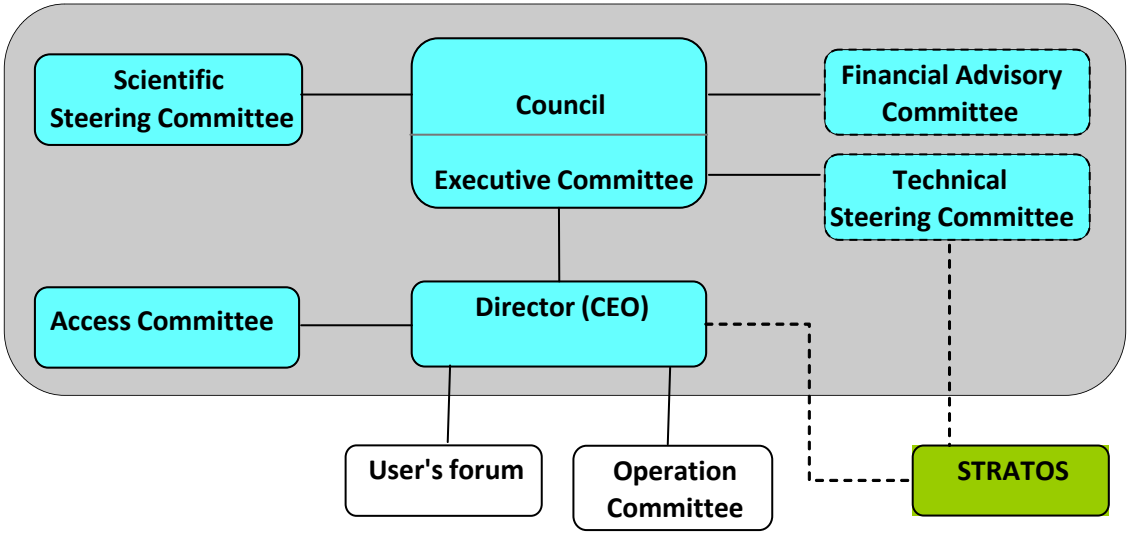
- The provision and rationalization of access to the Infrastructure by qualified European and international scientific communities, either academic or industrial, whose projects may be evaluated for such purpose.

Funding Principles for the Association

- Funding of Tier-0 resources
  - Each hosting member commits to provide Tier-0 resources worth 100 Mio. € based on TCO in the next 5 years
  - National procurements of Tier-0 systems follow an agreed procurement plan
  - Meeting requirements of the user communities with previously identified technology options
- Funding of the HQ operation
  - All partners provide equal cash contributions
- User support, training and other tasks
  - Provided in kind by members on as-needed basis
  - Supported by the planned Implementation Phase project – where eligible

Governance of the Association

- Modelled after successful examples of existing RIs
  - Council as main decision making body
  - Director with strong managing mandate
  - Scientific Steering Committee and Access Committee to give scientific advice and to steer the Peer Review process
  - Further committees will be instantiated by the Council as needed



Scientific Steering Committee

- The SSC is responsible for giving opinions on all matters of a scientific and technical nature
- Maximum of 21 members
- Members appointed by Council based on a list of candidates prepared by the SSC
- Two year term (renewable twice)
- Proposes the members of the Access Committee
- Resolutions by simple majority

Richard Kenway (UK, particle physics), Chair
Jose M. Baldasano (Spain, environment)
Kurt Binder (Germany, statistical physics)
Paolo Carloni (Italy, biological physics)
Giovanni Ciccotti (Italy, statistical physics)
Dann Frenkel (Netherlands, molecular simulations)
Sylvie Joussaume (France, environment)
Ben Moore (Switzerland, astrophysics)
Gernot Muenster (Germany, particle physics)
Risto Nieminen (Finland, materials)
Modesto Orozco(Spain, life sciences)
Maurizio Ottaviani (France, plasma physics)
Michelle Parrinello (Switzerland, chemistry)
Olivier Pironneau (France, mathematics)
Thierry Poinsot (France, engineering)
Simon Portegies Zwart (Netherlands, astrophysics)
Kenneth Ruud (Norway, chemistry)
Wolfgang Schroeder (Germany, engineering)
Luis Silva (Portugal, plasma physics)
Alfonso Valencia (Spain, bioinformatics)

Access Committee

- Responsible for giving opinions on the scientific use of Tier-0 Infrastructure, and providing recommendations on the allocation of Association computational resources based on the Peer Review process
- Proposed by the SSC based on their personal experience in the areas of science
- Appointed by the Council
- Minimum of 5 members
- Two years term (renewable once)
- Half of the members shall be replaced every year

Kenneth Ruud (Chair)
Roberto Capuzzo Dolcetta (Astrophysics)
Peter Nielaba (Chemistry and Materials)
Manuel Peitsch (Life Sciences)
Andreas Schaefer (Particle Physics)
Jean-Claude Andre (Environment)
Hester Bijl (Engineering and applied mathematics)

IBM Blue Gene/P – JUGENE hosted by GCS in Jülich, Germany

- Composed of 294912 processing cores with 4 cores forming a node with 2 GB of memory for a total of 147 TB.

- Performance
  - Peak: 1 PFlop/s
  - HPL: 825.5 TFlop/s

- Will be updated to BlueGene/Q in June'12

- http://www.fz-juelich.de/jsc/jugene

Bull Bullx cluster – CURIE
Hosted by GENCI in TGCC/CEA, Bruyères-Le-Châtel, France

- Composed by 3 different partitions:
  - A fat node partition open to PRACE calls since January 2011 and composed by 360 nodes with 32 cores per nodes, for a peak performance of 105 TeraFlops
  - A thin node partition, open to PRACE calls in Q1 2012 and composed by 5040 blades with 16 cores per node, for a peak performance of up to 1.5 PetaFlops
  - A hybrid node partition, open to PRACE preparatory Access Calls only and composed by 144 blades with 8 scalar cores and 2 GPU per node, for a peak performance of 200 TeraFlops
- http://www-hpc.cea.fr/en/complexe/tgcc-curie.htm

Cray XE6 – HERMIT, hosted by GCS in HLRS, Stuttgart, Germany

- HERMIT has a peak performance of 1 Petaflops and is designed for sustained application performance and highly scalable applications. It is composed of 3552 dual socket nodes equipped with AMD Interlagos Processors leading to overall 113664 processing cores. Nodes are equipped with 32GB or 64GB main memory.

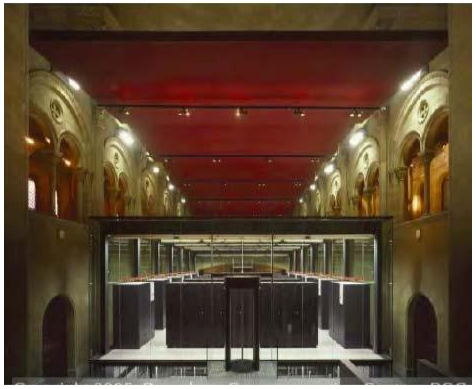
- Performance
  - Peak: 1.045 PFlop/s
  - HPL: 831.4 TFlop/s

- http://www.hlrs.de/systems/platforms/cray-xe6-hermit/

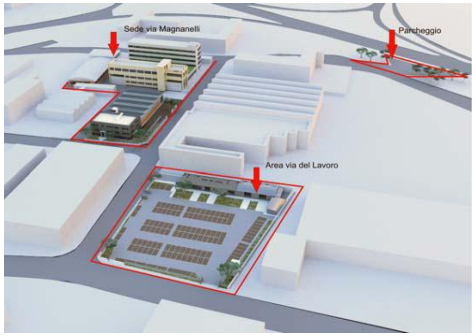
Systems coming 2012Q2

- SuperMUC – hosted by GCS in LRZ, Garching, Germany
  - http://www.lrz.de/services/compute/supermuc/systemdescription/
  - SuperMUC is based on the Intel Xeon-Architecture and will provide a peak performance of about 3 Petaflops

- MareNostrum – hosted by BSC in Barcelona, Spain
  - Details will be made available at http://www.bsc.es/MareNostrum
  - MareNostrum will be announced shortly. It will be a system with 1 PetaFlops peak performance, equipped with general-purpose processors.



- FERMI – hosted by CINECA in Casalecchio di Reno, Italy
  - BlueGene/Q, 163,840 cores, 1,6 GHz, 1 GB/core
  - FERMI will deliver 2.1 PetaFlops peak performance www.cineca.it/en/hardware/FERMI



Call for proposals

- Preparatory Access
  - Intended for preliminary resource use required to prepare proposals for Project Access
  - Technical review
  - 3 types:
    - Type A: Code scalability tests
      - 2 months
    - Type B: Code development and optimization
      - 6 months
    - Type C: Code development and optimizations with the support of PRACE experts
      - 6 months
  - 3 Tier-0 machines:
    - IBM BlueGene/P “JUGENE”, (GCS@Jülich, Germany)
    - BULL Bullx cluster “CURIE”, (GENCI@CEA, France)
    - Cray XE6 “HERMIT”, (GCS@HLRS, Germany)

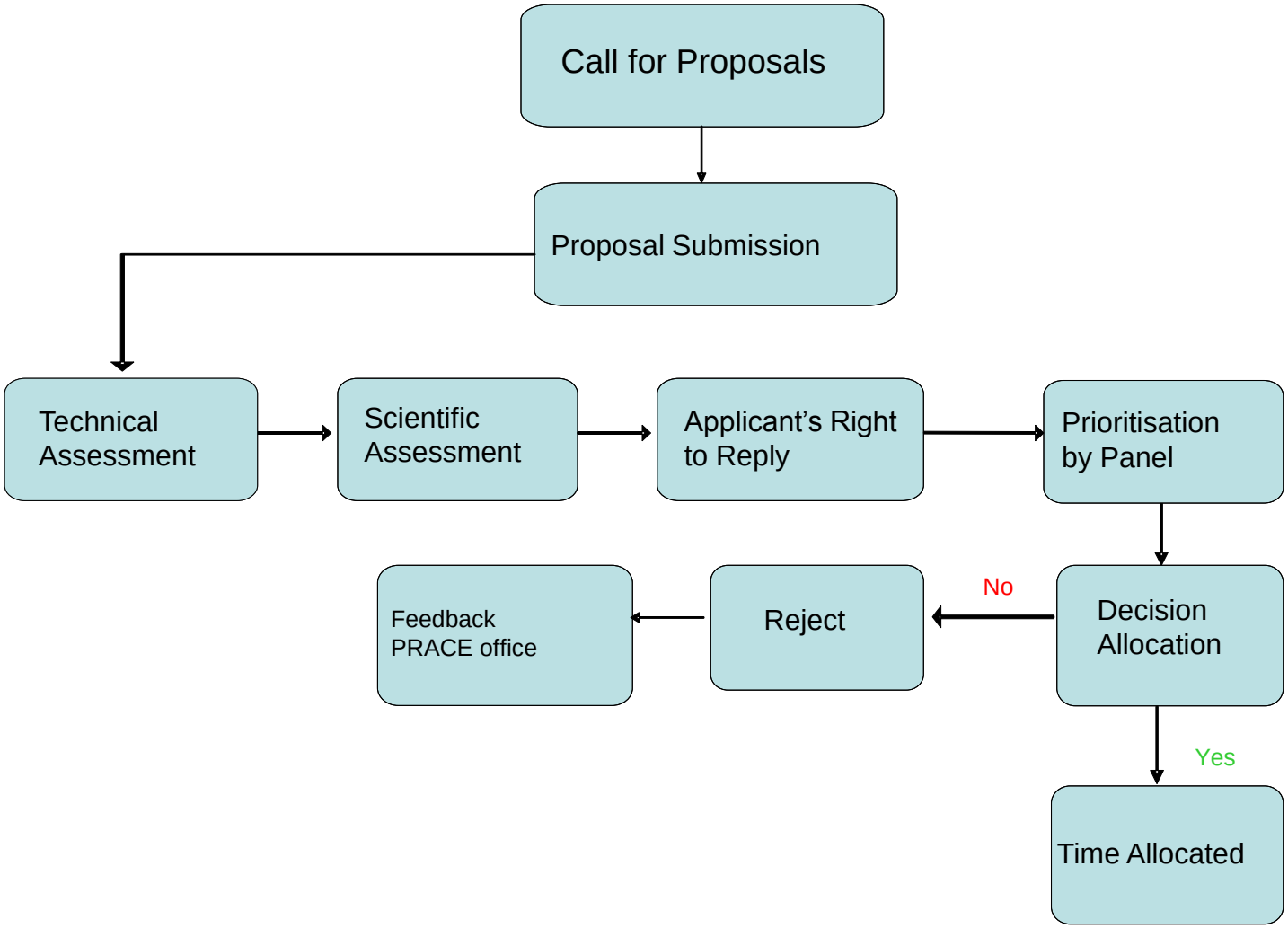
Call for proposals

- Project Access
  - Intended for individual researchers and research groups including multi-national research groups
  - Technical and Scientific review
- Multi year access
  - Available to major European projects or infrastructures that can benefit from PRACE resources
  - Technical and Scientific review
  - Planned for 2 years allocation

Peer review principles

- Transparency
- Fairness
- No parallel assessment
- Avoiding conflict of interests
- Reviews by non-conflicted experts
- Confidentiality
- Right to appeal technical and scientific evaluations

Peer Review Process



Technical Assessment

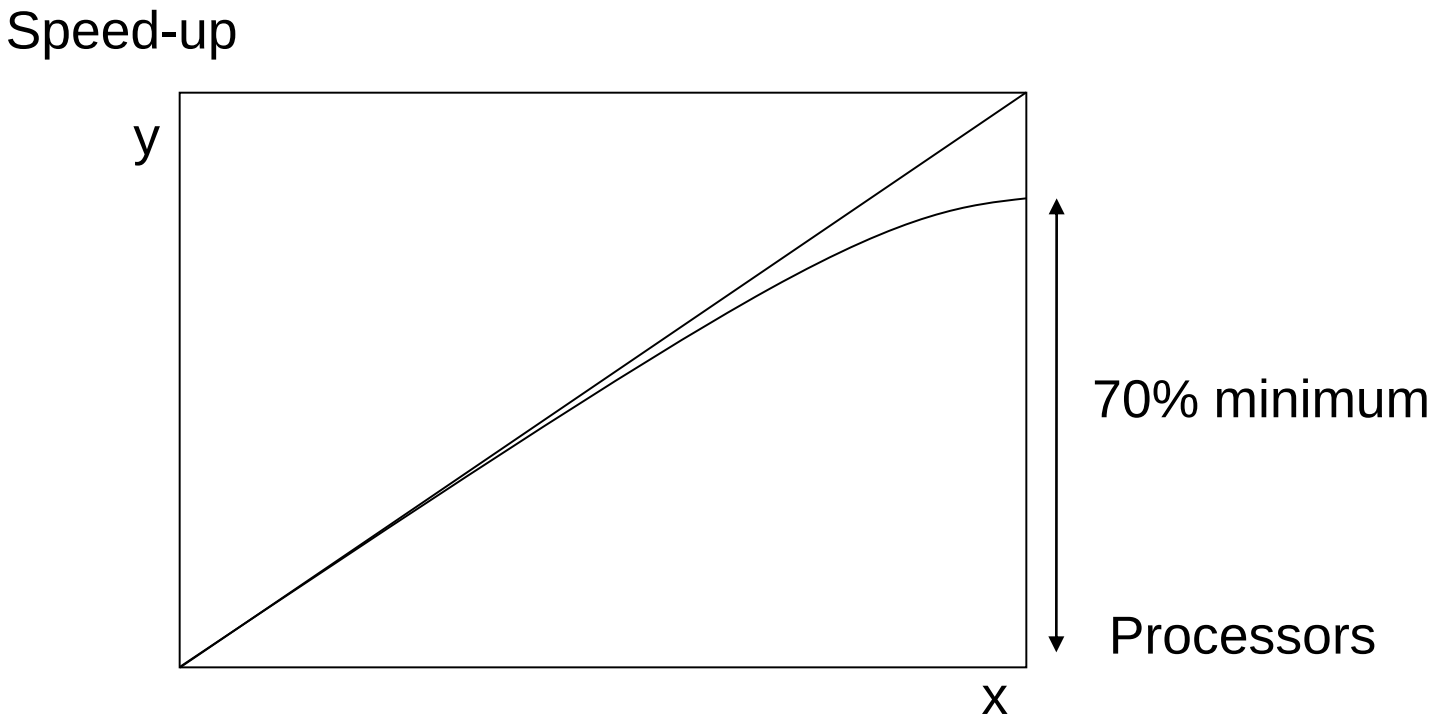
- All proposals will undergo a technical assessment. The technical assessment can result in three outcomes:
  - Feasible, very well suited
  - Feasible, not ideal for the requested resources
  - Proposal for rejection

Criteria for technical assessment

- The **need** to use a PRACE resource
- **Software availability** on the requested resource
  - The codes necessary for the project must be available on the system requested and/or, in case of codes developed by the applicants and Project and Programme Access proposals sufficiently tested for efficiency, high scalability, and suitability.
  - For Project and Programme Access Proposals proof of successful tests must be submitted together with the proposal;
- **Feasibility** of the requested resource. The requested system must be suitable for the proposed project. The technical assessment may redirect projects to a more appropriate system.
- These criteria should be **fully addressed** in the application.

5th regular call: Tier-0

- Scalability is a relative measure
  - We need to show it in the proper frame
    - Processor number
    - Problem size



Scientific Assessment

- Scientific review is performed by internationally recognized experts in the field of research of the proposal
- Maximum one expert selected from the proposed by the applicant
- During the scientific assessment an increase or decrease in the requested resources can be recommended for consideration in resource allocation.
- Technical assessment is available to scientific reviewers

Criteria for scientific assessment

- **Scientific excellence**. Demonstrate scientific excellence and a potential for high European and international impact
- **Novelty and transformative qualities**.
  - Proposals should be novel, develop an important scientific topic of major relevance to European research
  - describe possible transformative aspects, and expected advances
- **Relevance** to the call if a specific scope is stated in the call
- **Methodology**
- **Dissemination**
  - The planned channels and resources for dissemination and knowledge exchange
  - List of recent publications relevant to the proposed project.
- **Management**. Solid management structure in the project

Resource Allocation

- Access Committee makes a recommendation for resource allocation to the PRACE Board of Directors
- Composed of eminent scientists
- Analyse
  - Technical and scientific review reports
  - Applicants' response
- Produce
  - A single and unique ranked list for each call
  - Project and Programme proposals are ranked in the same list
  - Takes into account the advice regarding amounts of resources
  - Possible decision on cut-off threshold for granting of proposals

Propuestas españolas

- Preparatory Access: Type A:
  - Marzo 2012:
    - Project name: Abl kinase activation: free energy calculations on the interplay between SH2 domain coordination and kinase dynamics
      - Leader: Francesco L. Gervasio, Spanish National Cancer Research Center
  - Septiembre 2011:
    - Project name: Large-scale O(N) DFT simulations of defects in metal oxides
      - Leader: Pérez Rubén, Universidad Autónoma de Madrid, Madrid, Spain
  - Julio 2011
    - Project name: NMMB/BSC-CTM porting and scalability test – extension
      - Leader: Oriol Jorba, Barcelona Supercomputing Center - Centro Nacional de Supercomputación, Barcelona, Spain
  - Marzo-Mayo 2011
    - Project name: NMMB/BSC-CHEM
      - Leader: Oriol Jorba, Barcelona Supercomputing Center, Barcelona, Spain
    - Project name: First principles design of a biocatalyst for water oxidation
      - Leader: Carme Rovira, Parc Científic de Barcelona, Barcelona, Spain
    - Project name: Linear-scaling Density Functional Theory of heterogeneous proteins with Conquest
      - Leader: Antonio Sánchez Torralba, Spanish National Cancer Research Centre (CNIO), Madrid, Spain

Propuestas españolas

- Preparatory Access: Type B:
  - Marzo 2012:
    - Project name: Optimization of new algorithms in Octopus for methods to calculate the electrostatic potentials created by charge distributions
      - Leader: Joseba Alberdi Rodríguez, Universidad del País Vasco, Spain
    - Project name: Scalable and Dynamic Performance Tuning for Large-Scale Applications
      - Leader: Tomás Margalef, Universidad Autónoma de Barcelona, Spain
    - Project name: Nested hybrid MPI/OpenMP iterative substructuring domain decomposition methods for computational fusion
      - Leader: Santiago Badía, CIMNE, Universidad Politécnica de Cataluña, Spain
    - Project name: Broadening scalability of TermoFluids code
      - Leader: Ricard Borrell, Termo Fluids, S.L., Spain

Propuestas españolas

- Preparatory Access: Type C:
  - Marzo-Mayo 2011
    - Project name: Self organization, pattern formation and morphological instabilities in suspensions of microswimmers
      - Leader: Ignacio Pagonabarraga, University of Barcelona, Barcelona, Spain
    - Project name: New algorithms in Octopus for Petaflop computing
      - Project leader: Joseba Alberdi Rodriguez, Universidad del Pais Vasco/Euskal Herriko Unibertsitatea, Donostia-San Sebastian, Spain
  - Primera y segunda ronda de evaluación:
    - Project name: Parallel uniform mesh subdivision in Alya
      - Leader: Guillaume Houzeaux, Barcelona Supercomputing Center, Spain

Propuestas españolas

- 4th Regular Call:
  - Project name: The domain interplay in protein kinases: free energy calculations on the allosteric effect of the SH2 domain on kinase activation
    - Leader: Francesco L. Gervasio, CNIO, Spain
  - Project name: Numerical simulation of air flow in the human large airways
    - Leader: Guillaume Houzeaux, BSC-CNS, Spain
  - Project name: Extreme Star-Formation Modeling: From the Galactic Fountain to Single Stars in One Run
    - Leader: Paolo Padoan, ICREA and University of Barcelona (ICC), Spain

Propuestas españolas

- 3rd Regular Call:
  - Project name: Modeling gravitational wave signals from black hole binaries
    - Leader: Sascha Husa, Universitat de les Illes Balears, Spain
  - Project name: Branch point motion in star polymers and their mixtures with linear chains
    - Leader: Angel Rubio, CSIC-UPV/EHU, Spain
  - Project name: Ligth quark mass dependence of two-hadron energies in Lattice QCD
    - Leader: Assumpta Parreño, University of Barcelona, Spain
  - Project name: First principles design of a biocatalyst for water oxidation
    - Leader: Carme Rovira, University of Barcelona, Spain

Propuestas españolas

- 2nd Regular Call:
  - Project name: Large Scale simulations of Ly-alpha and Ly-break galaxies in the high-z universe: Probing the epoch of reionization.

    Leader: Gustavo Yepes, Universidad Autonoma de Madrid, Spain

  - Project name: The molecular bases of the transport cycle of APC antiporters

    Leader: Modesto Orozco, Institute for Research in Biomedicine Structural and Computational Biology, Spain
- 1st Regular Call:
  - Project name: Entrainment effects in rough-wall boundary layers

    Leader: Javier Jimenez, Universidad Politecnica Madrid, Madrid, Spain

  - Project name: Non diffusive transport in ITG plasma turbulence

    Leader: Edilberto Sánchez, EURATOM-CIEMAT Association, Madrid, Spain

5th regular call: Tier-0

- Evaluation process similar to 5th call, submission via web
- IBM Blue Gene/Q “JUQUEEN” (GCS@Jülich, Germany)
  - Scalability: at least 8192 compute cores
  - Available capacity in this call is 312 million compute core hours
- Bull BULL Bullx cluster “CURIE” (GENCI@CEA, France)
  - Scalability: at least 512 cores for the fat nodes partition and above 2048 cores for the thin nodes partition
  - Available capacity
    - On the thin nodes partition: 201 million compute core hours
    - On the fat nodes partition: 28 million compute core hours
- Cray XE6 “HERMIT” (GCS@HLRS, Germany)
  - Scalability: at least 2048 compute core
  - Available capacity in this call is 160 million compute core hours.
- “SuperMUC” (GCS@LRZ, Germany)
  - Scalability: at least 4096 compute core
  - Available capacity in this call is 200 million compute core hours.
- “FERMI” (CINECA, Italy)
  - Scalability: at least 2048 compute core
  - Available capacity in this call is 300 million compute core hours.
- “MareNostrum” (BSC, Spain)
  - Scalability: at least 2048 compute core
  - Available capacity in this call is 135 million compute core hours.

5th regular call: Tier-0

- Eligibility for Tier-0 resources
  - For this call, proposals from academia are eligible, as long as the project leader is a senior researcher employed in a research organisation. The employment contract of the project leader with the research organisation must be valid at least 3 months after the end of the allocation period.
  - Industry will be eligible for access through collaborations with academia, i.e. industry must have the role of collaborators in academic projects.
- For this call, proposals asking for resources on a single machine or on multiple machines are allowed.
- Please note that a proposal asking for resources on multiple machines has to justify the need to access several machines. The proposal will be awarded or rejected in totality (no subpart of the proposal will be awarded).
- It is also possible to request a Multi-year access (1+1)

Past project access calls for proposals (in million core hours)

Call	Access time	Requested Hours	Requested Projects	Awarded Hours	Awarded projects
Early Access	July 2010 March 2011	1870	65	324	10
1st Call	Nov. 2010 Oct. 2011	2874	59	362	9
2nd Call	May. 2011 April 2012	1251	46	397	17
3rd Call	Nov. 2011 Oct. 2012	1687	63	721	29
4th Call	May 2012 April 2013	1931	102	1134	55
Total		**9615**	**335**	**2940**	**120**

Soporte desde el BSC-CNS

- Preparación técnica de solicitudes
  - Mejorar el *success ratio* de las solicitudes
- Realización pruebas de escalabilidad en supercomputadores del Centro
- Ayuda en el acceso y ejecución
  - Porting de código
  - Transferencia de entrada/salida
  - Acceso a sistema de colas
  - Rendimiento de aplicaciones
- Transferencia de datos
  - Durante y después del acceso

Gracias