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2011 Annual Report





The 2011 Combined Annual Report of the Barcelona Supercomputing Center - Centro Nacional de Supercomputación (BSC-CNS) and the Spanish Supercomputing Network (RES) summarises the various support and research activities for the year and provides a short description of the two organisations.





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» 2011 Review



Mateo Valero, Director of the BSC-CNS and
Francesc Subirada, Associate Director of the BSC-CNS

We are extremely proud to once again present the results of the activities of BSC-CNS during 2011. A major highlight of the year was the tremendous honour of being recognised as an inaugural Severo Ochoa centre. A new initiative launched in 2011 by the Spanish Ministry for Science and Innovation, the award recognises Spanish centres of international excellence with a track record of cutting edge science as well as an ambitious current project of frontier research. Only eight centres in all Spain received the award, which provides €4 million over 4 years to support the development of the project, which in BSC-CNS is to develop green, energy efficient and low cost computer systems and software applied to personalised medicine, modelling of human organs using computational biomechanics, and multi-scale air quality and climate modelling. The specific objectives of the programme are: to improve world-class research centres' capacity to organise and carry out research; to improve their capacity to attract, recruit, train and retain human resources; to further develop their relationships with other leading international centres; and to disseminate their research results to broader society.

Mission

The mission of BSC-CNS is to investigate, develop and manage information technology in order to facilitate scientific progress.

As the national supercomputing infrastructure, and one of the Tier-0 nodes in the Europe-wide supercomputing network (PRACE), BSC-CNS has the difficult task of ensuring that its computing systems remain at the technological and performance forefront of computational capabilities. The long-term strategy of BSC-CNS to develop and implement low-cost, energy efficient systems is bearing fruit, with the installation in 2011 of MinoTauro. MinoTauro is not only the fastest supercomputer in Spain, ranked at 114 in the world by the Top500 list, but is also the most efficient HPC cluster in Europe, ranked 7th in the world by the Green500 list.

This installation is just a forerunner of the much larger supercomputer that will be installed in 2012, which will serve the European supercomputing initiative (PRACE) as one of its principal nodes, with an update cycle funded collaboratively by the 22 member nations.

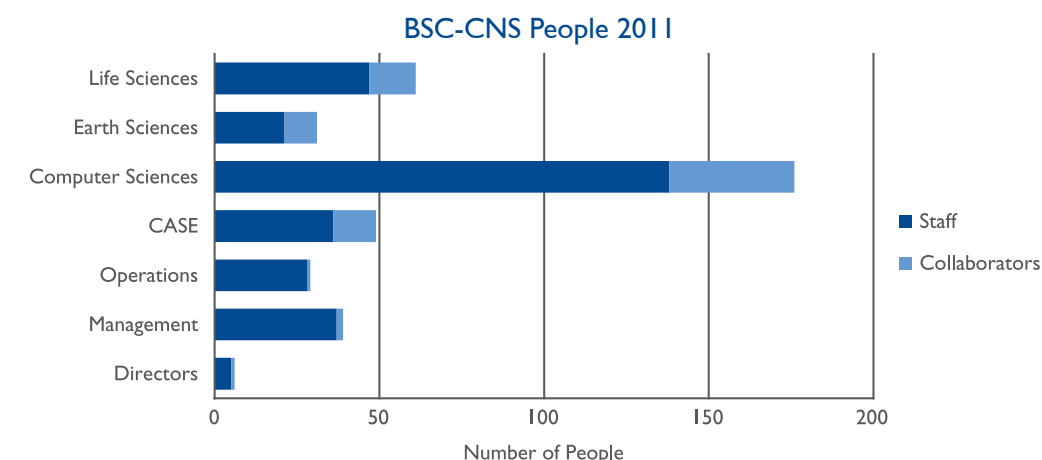
The installation of MinoTauro, together with an upgrade to the Magerit node in Madrid, saw the Spanish Supercomputing Network (RES) significantly increase in capacity during 2011. In addition to expanding infrastructure, BSC-CNS devoted increasing efforts to outreach to scientists via a growing program of technical workshops and user meetings, with the objective of facilitating scientists from all disciplines to expand the application of supercomputing in their respective fields.

Powerful Computing

BSC-CNS is the National Supercomputing Facility in Spain and manages the MareNostrum, as well as the MinoTauro supercomputer, newly installed in 2011. MinoTauro is not only the fastest supercomputer in Spain, ranked at 114 in the world by the Top500 list, but is also the most efficient HPC cluster in Europe, ranked 7th in the world by the Green500 list.

Based on its experience in establishing and managing the RES, BSC-CNS conceived and initiated RISC - the IberoAmerican Supercomputing Network (www.risc-project.eu), whose aim is to deepen strategic R&D cooperation between Europe and Latin America in the field of High Performance Computing, to identify common needs, research issues and opportunities for cooperative R&D on HPC between EU and Latin America, thus setting the basis for the formulation of a global strategy for future research.

The year also saw the formalisation of several major collaborations with private industry, notably the establishment of the Repsol-BSC Research Center to further develop algorithms to process seismic images, and the establishment of the Intel-BSC Exascale Laboratory to develop next generation programming models and tools for exascale systems. BSC-CNS was also named by NVIDIA as a CUDA Center of Excellence, the recognition meaning that NVIDIA will provide financing to support BSC-CNS's growing number of research and training programs relating to GPU computational technologies. Existing major collaborations were further developed: with Iberdrola to model wind flows around windfarms in order to optimise energy output and efficiency, with IBM to define hardware and software components for new generations of petascale supercomputers, and with Microsoft to design multicore architectures and software stacks for next generation mobile and desktop markets.



BSC-CNS continues to grow in international reputation, successfully attracting some of the best and brightest young researchers from across the globe. During 2011, some 391 people performed research or provided support at the centre. Over 38% of staff are of foreign nationality, with over 42 countries represented including: Algeria, Argentina, Austria, Belgium, Brasil, Bulgaria, Canada, Colombia, Cuba, Denmark, Ecuador, France, Germany, Greece, Hungary, Chile, China, India, Iran, Ireland, Israel, Italy, Japan, Mexico, Montenegro, Netherlands, Pakistan, Peru, Poland, Portugal, Russia, Serbia, Slovakia, South Africa, Switzerland, Syria, Thailand, Turkey, Ukraine, United Kingdom and USA.

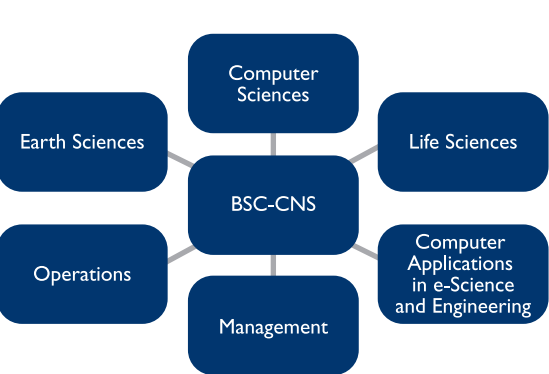


World Map of Countries of Origin

BSC-CNS is not only a singular supercomputing infrastructure, but also a cutting-edge research centre. Key achievements in 2011 of the Computer Sciences department were the creation of joint centres with Intel and Nvidia to pursue research in topics related to software technologies for Exascale computing and accelerator-based architectures, and the design and assembly of an energy-efficient cluster based on low-power components to serve both as a PRACE prototype and seed for the EU Exascale Mont-Blanc project.

Support and Research

BSC-CNS, which provides both Support to other research institutes, as well as undertaking primary Research in its own right, is organised into 6 core departments; Computer Sciences, Life Sciences, Earth Sciences, Operations, Computer Applications in Science & Engineering (CASE), and Management.



The Support functions provide technical and operational support to internal and external researchers and scientists, collaborators and other institutions and industrial partners. In particular, the Operations Department also manages all activities relating to the MareNostrum supercomputer and access to the other nodes of the RES. The various departments have a number of scientific research groups, each headed by a Team Leader, which focus their activities on the study of hardware and system software for the supercomputers of the future and on the application of computer simulation to the underlying physical processes of nature, with particular focus on Life, Earth and Engineering sciences.

Life Sciences continued to grow their fruitful Joint Research program with the IRB, with research highlights including significant advances in the development of HPC technologies for datamining of genomic data, with particular impact in the analysis of the genomic nature of chronic lymphocytic leukaemia, and also in the description of functionally-relevant protein flexibility, describing for the first time the conformational ensemble defining molten globule proteins, and determining the conformational transitions associated to membrane transporters.

Earth Sciences achieved a milestone in 2011 with the development and implementation of the new pre-operational state-of-the-art model, NMMB/BSC-Dust, for the prediction of the mineral dust cycle at global and regional scales, providing 72 hour forecasts for the North African, Middle Eastern, and European/Mediterranean domains. The model, developed in collaboration with NOAA/NCEP and NASA GISS, is based on the incorporation of dust physics and dynamics in the NCEP-NMMB atmospheric framework, which allows for parallel and high resolution modeling at multiple spatial scales.

The CASE department established the REPSOL-BSC Research Center to develop the most advanced tools in seismic imaging, and numerous collaborations were initiated or further developed in fields across the scientific and industrial spectrum, ranging from biomechanics modelling of human organs, to wind farm optimisation, to the recycling of cement.

As part of its on-going program to support the growing demands of Spanish supercomputing users, and its critical role in the commissioning of new systems and prototypes, during 2011 the Operations department installed and commissioned MinoTauro, the most power efficient supercomputing system in Europe and undertook a major upgrade of the power line at BSC-CNS.

In addition to the projects undertaken by the BSC-CNS research departments, over 255 external projects utilised over 70 million hours of computation on RES systems. These activities, representing fields of science as diverse as medicine, astrophysics and social sciences, are evaluated for merit and prioritised by an independent Access Committee. Requests for access come from all over Spain, and indeed all over Europe, testifying to both the quality of the RES facilities and the ever increasing demand for supercomputing resources. Requests for access continue to increase each year, and despite increases in computing capacity remain steadily at around double the available computing time.

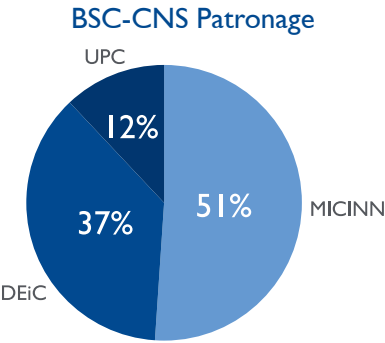
The work carried out by the scientists at BSC-CNS resulted in over 83 journals and book chapter publications, and some 156 key conference presentations. Additionally, BSC-CNS researchers presented numerous workshops at both national and international levels, and the centre hosted a number of key international events.

Broad Access

The powerful resources of the MareNostrum Supercomputer and the RES nodes are accessed by a broad spectrum of Spanish and international scientists. Computing time is allocated by the Access Committee, composed of a Core Team and four Expert Panels of prestigious Spanish scientists external to the BSC-CNS. Additionally, a percentage of computing time is reserved for commercial projects to enable Spanish companies to maintain international competitiveness.

Patrons of the BSC-CNS

The BSC-CNS is a legally autonomous, public consortium, with three founding partners: the Spanish Ministry of Science & Innovation (MICINN), the Departament d'Economia i Coneixement (DEiC) of the Catalan government and the Universitat Politècnica de Catalunya (UPC). The voting representation is divided between MICINN (51%), DEiC (37%), and UPC (12%).



The income of BSC-CNS in 2011 was €20.1 M, of which €5.3 M corresponded to ordinary budget, and €7.3 M were derived from competitive projects. Of particular note, almost €2 M of funding was derived from projects with private companies, an increase of 40% on 2010. In 2011, BSC-CNS participated in 19 collaborative projects with industry, 22 national projects, and 42 competitively funded EU projects, consolidating BSC-CNS involvement in the FP7, where BSC-CNS has achieved the 3rd highest return from FP7* of any Spanish public research organisations - after CSIC and CNIO (with 31 projects, 6 as coordinator).

* Source CDTI: Spanish Participation FP7 - provisional results 2007-2010.

Despite the difficult economic times, 2011 was in all respects an excellent year for BSC-CNS with continued growth in personnel, capacities and activities, and increasing recognition both nationally and internationally as a key centre of reference in High Performance Computing and e-Science. This is due, first and foremost, to the dedication, hard work, and brilliant minds of the staff, students, collaborators and visiting researchers who are the BSC-CNS. The Directors wish to express their profound gratitude to all who worked with BSC-CNS throughout the year, and also give thanks and recognition to the patrons of BSC-CNS; MICINN, DEiC and UPC for their continued strong support, and to the European Commission and other funding agencies and private companies who sponsored research and development activities during 2011.

Mateo Valero, Director

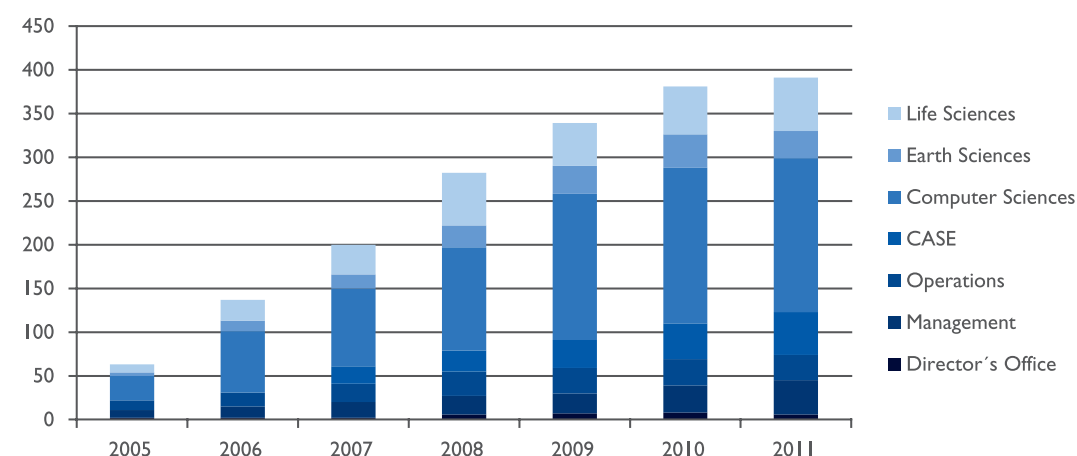
Francesc Subirada, Associate Director

Key to the success of BSC-CNS are the many people of different backgrounds that work and collaborate with the center. These include contracted staff, visiting academics, students, and collaborators from other institutes and private industry, amongst others.

As at 31st December 2011, the core staff of BSC-CNS included 94 permanent positions, 107 dedicated to specific projects and 67 scholarship students. These numbers were significantly augmented by additional staff who participated in the BSC-CNS via a number of programs.

Total personnel who worked at BSC-CNS throughout the year increased slightly from 381 during 2010 to 391 during 2011, mainly through new temporary and shared staff, resident students, and collaborating and visiting researchers.

Annual BSC-CNS Staff and Collaborators



Shared Staff and Human Resource Programs In addition to its own staff, BSC-CNS hosts shared staff from other public institutions such as the Technical University of Catalonia (UPC), the Institute for Research in Biomedicine (IRB) and the Consejo Superior de Investigaciones Científicas (CSIC). In 2011, BSC-CNS also welcomed high level scientific personnel from special human resources public programs such as the Ramón y Cajal Program, the ICREA Program and other personnel training research programs sponsored by various Spanish Ministries.

The BSC-CNS Fellowship Program The BSC-CNS Fellowship program invites applicants from relevant scientific disciplines to participate in several European research projects and collaborations with international industry such as IBM and Microsoft. These fellowships are offered for periods of one year, renewable for the duration of the project. During 2011, BSC-CNS hosted 112 student researchers associated to several research projects.

Mobility Programs BSC-CNS has always supported mobility programs. The objective is to provide access to advanced computing infrastructures to researchers worldwide in order to promote collaborative research involving scientists from different countries and provide training to scientists in high performance computing in order to solve scientific and technological problems. Visitors are also provided with financial support to cover their stay. BSC-CNS is involved in two major mobility programs:



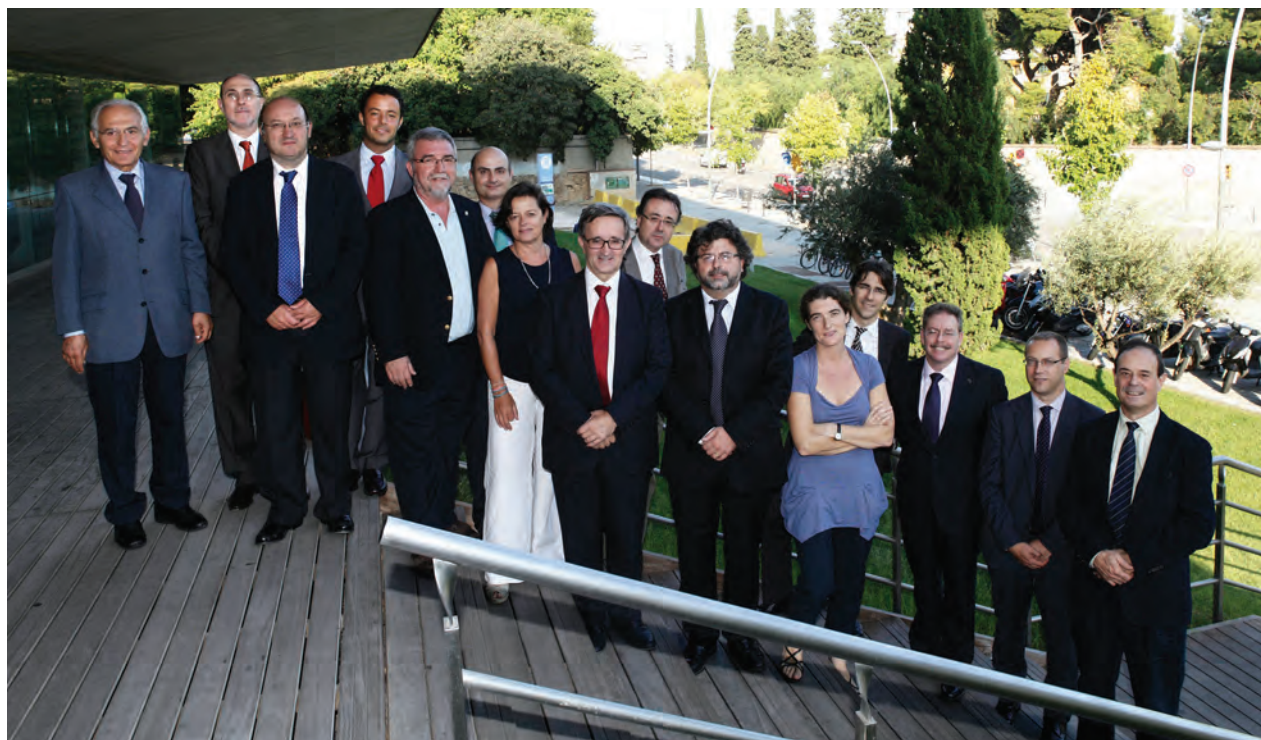
At the Spanish level, BSC-CNS participates in a national access program called ICTS, whose objective is to leverage the knowledge in supercomputing and eScience from the BSC-CNS. This program, which holds selection meetings every 4 months, allowed 3 researchers to access BSC-CNS facilities in 2011; their expenses were covered by the Spanish Ministry of Science and Innovation (MICINN).



At the international level, HPC-Europa2 is a consortium of seven leading High Performance Computing (HPC) infrastructures, including BSC-CNS. The program enables researchers working in any eligible country in Europe to visit a participating research institute to carry out a collaborative visit of up to 13 weeks duration and to gain access to some of the most powerful HPC facilities in Europe. During 2011 BSC-CNS hosted 36 of these visitors.



» BSC-CNS Governing Bodies



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Francesc Subirada, Associate Director, BSC

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Commission Secretaries:

Ramón Fernández Calvo, State lawyer

Javier Zuloaga, State lawyer

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Iolanda Font de Rubinat, Deputy Director General of Research, DEiC

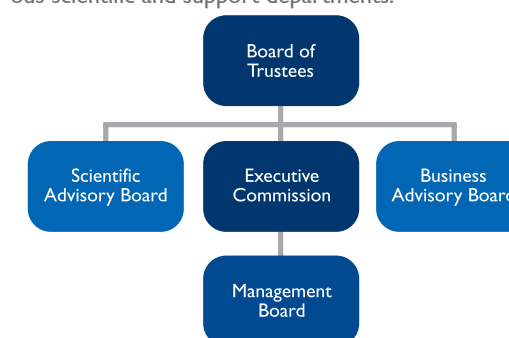
Representatives UPC

Ana Isabel Pérez, Vice Rector for Research

Xavier Gil, Vice Rector for Scientific Policy

Strong Governance

Overall governance of the BSC-CNS is provided by the Board of Trustees, formed by members of the three institutions that are partners of the BSC-CNS Consortium, and will be further supported by the Scientific and Business Advisory Boards (still in formation). Strategic direction is provided by the Executive Commission and this devolves to day-to-day management via the Management Board. Reporting to the Management Board are the various scientific and support departments.



Representatives BSC-CNS

Mateo Valero, Director, BSC

Francesc Subirada, Associate Director, BSC

Ernest Quingles, Manager, BSC

Commission Secretaries

Ramón Fernández Calvo, State lawyer

Javier Zuloaga, State lawyer

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Mateo Valero, Director

Management Board Vice-Chairman

Francesc Subirada, Associate Director

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Computer Sciences Associate Director

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Sergi Girona,
Operations Director

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Ramón Beivide, Universidad de Cantabria

Ramón López de Arenosa, Ministerio de Ciencia e Innovación

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Assistant: Andrés Aguilera, Universidad de Sevilla

Chemistry and Material Sciences Expert Panel

Coordinator: Elvira Guardia, Universitat Politècnica de Catalunya

Assistant: Mariona Sodupe, Universitat Autònoma de Barcelona

Physics and Engineering Expert Panel

Coordinator: Francisco Domínguez-Adame, Universidad Complutense de Madrid

Assistant: Francisco Castejón, CIEMAT

Astronomy, Space and Earth Sciences Expert Panel

Coordinator: Gustavo Yepes, Universidad Autónoma de Madrid

Assistant: Ramón Carbonell, CSIC-Institute Earth Sciences "Jaume Almera"

RES Users' Committee (CURES)

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Javier Jiménez Sendín, **Fernando Martín García**

Chemistry and Material Sciences (QCTM) representatives

Rubén Pérez, **Núria López**

Biomedicine and Health Sciences (BCV) representatives

Carme Rovira, **Francisco Javier Luque**

Astronomy, Space and Earth Sciences (AECT) representatives

Jordi Torra, **Miguel Ángel Aloy**

» BSC-CNS Staff and Collaborators during 2011

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Academic Programs Coordinator: Ulises Cortés

Director Assistant: Lourdes Cortada

Associate Director Assistant: Judith Camba

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Visitor: Nathaniel Azuelos

Visitor: Ricardo Bianchini

Visitor: Rudolf Eigenmann

Visitor: Speziale Ettore

Visitor: Valeria Quadros

Visitor: Yale Patt

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Accelerators For High Performance Computing
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Associate Researcher: Marisa Gil

Student Researcher: Javier Cabezas

Student Researcher: Marc Jordà

Student Researcher: Víctor García

Autonomic Systems and e-business Platforms

Autonomic System and e-Business Platforms Group
Manager: **Jordi Torres**

Senior Researcher: Vicenç Beltran

Researcher: Juan Luís Pérez

Researcher: Mario Macías

Research Support Engineer: Josep Subirats

Associate Researcher: David Carrera

Associate Researcher: Javier Alonso

Associate Researcher: Jordi Guitart

Associate Researcher: Yolanda Becerra

Student Researcher: Gemma Reig

Student Researcher: Iñigo Goiri

Student Researcher: Jordà Polo

Student Researcher: Josep Oriol Fito

Student Researcher: Zeus Gómez

Computer Architecture for Parallel Paradigms

Computer Architecture For Parallel Paradigms Group
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Computer Architecture For Parallel Paradigms Group
Manager: **Osman Unsal**

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Associate Junior Researcher: Oscar Palomar

Student Researcher: Adria Armejach

Student Researcher: Azamolsadat Seyedi

Student Researcher: Daniel Nemirosky

Student Researcher: Ferad Hasanov Zyulkyarov

Student Researcher: Gökçen Kestor

Student Researcher: Gulay Yalcin

Student Researcher: Isidro González

Student Researcher: Ivan Ratkovic

Student Researcher: Milan Stanic

Student Researcher: Milovan Duric

Student Researcher: Nebojsa Miletic

Student Researcher: Nehir Sonmez

Student Researcher: Nikola Bezanic

Student Researcher: Nikola Markovic

Student Researcher: Oriol Arcas

Student Researcher: Otto Fernando Pflücker

Student Researcher: Sasa Tomic

Student Researcher: Srdjan Stipic

Student Researcher: Timothy Hayes

Student Researcher: Vasileios Karakostas

Student Researcher: Vesna Smiljkovic

Student Researcher: Vladimir Gajinov

Extreme Computing

Extreme Computing Group Manager: **Vassil Nikolov Alexandrov**

HPC Professional Training And Postgraduate Studies
Coordinator: Evguenia Stoilova Alexandrova

Visitor: Janko Strassburg

Grid Computing and Clusters

Grid Computing Group Manager: **Rosa M. Badia**

Senior Researcher: Daniele Lezzi

Senior Researcher: Raül Sirvent

Researcher: Jorge Ejarque

Researcher: José María Pérez

Researcher: Marta García

Researcher: Enric Tejedor

Researcher: Pieter Bellens

Research Support Engineer: Javier Alvarez

Support Engineer: Francesc Lordan

Support Engineer: Roger Rafanell

Associate Researcher: Julita Corbalan

Student Researcher: Aislan Foina

Student Researcher: Jan Ciesko

Student Researcher: Judit Planas

Student Researcher: Lluís Martinell

Student Researcher: Maja Etinski

Student Researcher: Rahul Gayatri

Student Researcher: Tomasz Patejko

Student Researcher: Vinoth Krishnan Elangovan

Student Researcher: Vladimir Marjanovic

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Álex Ramírez

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Senior Researcher: Miquel Pericàs

Senior Researcher: Nikola Puzovic

Senior Researcher: Yoav Etsion

Associate Researcher: Carlos Villavieja

Associate Researcher: Friman Sánchez

Associate Researcher: Mauricio Alvarez

Associate Researcher: Paul Carpenter

Student Researcher: Alejandro Rico

Student Researcher: Branimir Dickov

Student Researcher: Felipe Cabarcas

Student Researcher: Karthikeyan Palavedu

Student Researcher: Milan Pavlovic

Student Researcher: Muhammad Shafiq

Student Researcher: Nikola Rajovic

Student Researcher: Tassadaq Hussain

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Unconventional Computer Architecture and Networks
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Resident Student: Ruken Zilan

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Senior Researcher: Jaime Abella

Senior Researcher: Roberto Gioiosa

Research Support Engineer: Mikel Fernández

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Associate Researcher: Miquel Moreto

Associate Researcher: Xavier Verdú

Associate Researcher: Emery Berger

Student Researcher: Alessandro Morari

Student Researcher: Bojan Maric

Student Researcher: José Carlos Ruiz

Student Researcher: Kamil Kedzierski

Student Researcher: Leonidas Kosmidis

Student Researcher: Marco Paolieri
Student Researcher: Milos Panic
Student Researcher: Muhammad Ismail Ahmed
Student Researcher: Petar Radojkovic
Student Researcher: Qixiao Liu
Student Researcher: Víctor Javier Jiménez
Student Researcher: Vivek Sabbineni
Student Researcher: Vladimir Cakarevic

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Senior Researcher: Gabor Janos Dozsa
Researcher: Roger Ferrer
Researcher: Xavier Teruel
Research Support Engineer: Sergi Mateo
Research Support Engineer: Víctor López
Associate Researcher: Carlos Alvarez
Associate Researcher: Daniel Jiménez
Associate Researcher: Juan José Costa
Associate Researcher: Marc González
Associate Researcher: Montserrat Farreras
Associate Research Support Engineer: Guillermo Miranda
Student Researcher: Ahimed Yazdanpanah Ahmadabadi
Student Researcher: Cecilia González
Student Researcher: Daniel Cabrera
Student Researcher: Diego Luis Caballero
Student Researcher: Ivan Tanasic
Student Researcher: Javier Bueno
Student Researcher: Lluç Alvarez
Student Researcher: Lluís Vilanova
Student Researcher: Michail Alvanos
Student Researcher: Nikola Vujic
Student Researcher: Oscar Amorós
Student Researcher: Ramon Bertran
Student Researcher: Sara Royuela

Performance Tools

Performance Tools Group Manager: **Judit Giménez**
Senior Researcher: José Carlos Sancho
Senior Researcher: Kevin Andrew Huck

Researcher: Eloy Martínez
Researcher: Francesc Xavier Pegenaute
Researcher: Germán Matías Llorc
Researcher: Harald Servat
Researcher: Juan González
Researcher: Pedro Antonio González
Student Researcher: Ana Jokanovic
Student Researcher: Vladimir Subotic

Storage Systems

Storage Systems Group Manager: **Antonio Cortés**
Researcher: Aul Hermann Lensing
Researcher: Ernest Artiaga
Researcher: Jacobo Giralt
Researcher: Jan Wiberg
Researcher: Jonathan Martí
Researcher: Juan González
Researcher: Matthias Werner Brugger
Researcher: Ramon Nou
Researcher: Thanos Makatos
Student Researcher: Albert Miranda

Earth Sciences Department

Earth Sciences Director: **José María Baldasano**
Research Support Engineer: Albert Soret
Technical Support Engineer: David Carrió
Technical Support Engineer: Francesc Martínez
Technical Support Engineer: Luca Telloli
Technical Support Engineer: Kim Serradell

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Air Quality Group Manager: **Santiago Gassó**
Senior Researcher: Gustavo Arévalo
Senior Researcher: Valentina Sicardi
Research Support Engineer: Joana Aina Ortiz
Research Support Engineer: Marc Guevara
Associate Researcher: Maria Goncalves
Associate Researcher: Pedro Jiménez
Visitor: Alejandra Acosta
Visitor: Donald Dabdub
Visitor: Joana Cardoso
Visitor: Sylvain Mailler

Student Researcher: Gina Ferrer
Student Researcher: Kasja Witlox
Student Researcher: M Teresa Pay

Metereological Modelling

Metereological Modelling Group Manager: **Oriol Jorba**
Resident Student: Alba Badia
Resident Student: Angel Alberto Rincón
HPC Visitor: Lucy Bricheno
HPC Visitor: Thomas Loridan
Student Researcher: Michele Spada

Mineral Dust

Associate Researcher: Carlos Pérez
Associate Researcher: Enric Terradellas
Research Support Engineer: Francesco Benincasa
Student Researcher: Karsten Haustein
Resident Student: Sara Basart

Life Sciences Department

Life Sciences Director: **Modesto Orozco**

Computational Genomics

Computational Genomics Group Manager: **David Torrents**
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Senior Researcher: Josep Maria Mercader
Senior Researcher: Lise Olivia Andrieux
Researcher: Xavier Pastor
Research Support Engineer: Montserrat Puiggrós
Research Support Engineer: Valentí Moncunill
Visitor: Laura Martínez
Student Researcher: Leyden Fernández
Student Researcher: Santiago González
Student Researcher: Silvia Bonas
Associate Resident Student: Elisa Durán

Electronic and Atomic Protein Modelling

Electronic and Atomic Protein Modelling Group Manager: **Víctor Guallar**
Senior Researcher: Armin Madadkar
Senior Researcher: Maria De Fatima Assunção
Senior Researcher: Martin Ivanov Kotev

Senior Researcher: Ryoji Takahashi
Researcher: Marcelo Puiatti
Researcher: Israel Cabeza
Researcher: Suwipa Saen
Research Support Engineer: Daniel Lecina
Research Support Engineer: Manuel Augusto Rivero
HPC Visitor: Didier Devaurs
Visitor: James Valdes
Visitor: Rose Afzali
Student Researcher: Diego Fernando Masone
Student Researcher: Frank Heinrich Wallrapp
Student Researcher: Max Von
Student Researcher: Sandra Acebes
Student Researcher: Seyed Ali Hoseini
Student Researcher: Víctor Alejandro Gil

INB-Computational Node 2

INB - Computational Group Manager: **Josep Lluís Gelpí**
Researcher: Dmitry Repchevsky
Researcher: Laia Codo
Research Support Engineer: Alexis Torrano
Research Support Engineer: Pau Andrio
Software Engineer: Romina Royo

Molecular Modelling and Bioinformatics

Life Sciences Department Director: **Modesto Orozco**
Senior Researcher: Josep Ramon Goñi
Research Support Engineer: Carles Fenollosa
Research Assistant: Nuria Villegas
Research Assistant: Santiago Villalba
Visitor: Alba Gutiérrez
Visitor: Eduardo Mayol
Visitor: Manuel Rueda

Protein Interactions and Docking

Protein Interactions and Docking Group Manager: **Juan Fernández**
Senior Researcher: Athi Narayanan
Senior Researcher: Iain Moal
Support Engineer: Carles Pons
Associate Researcher: Solène Grosdidier
HPC Visitor: Athanasios Papakyriakou
Visitor: Elodie Japaud
Visitor: Ida Fardi

Visitor: Jordi Triguero
Visitor: Mireia Rosell
Visitor: Montserrat Barbany
Student Researcher: Albert Solernou
Student Researcher: Brian Jiménez
Student Researcher: Chiara Pallara
Student Researcher: Laura Pérez
Student Researcher: Miguel Romero

Computer Applications in Science & Engineering Department

Computer Applications In Science And Engineering
Director: **José María Cela**
Senior Researcher: José De la Puente
Senior Researcher: Mauricio Gaspar Hanzich
Senior Researcher: Rogeli Grima
Senior Researcher: Volodymyr Puzyrov
Researcher: Albert Farrés
Researcher: Anne-Cécile Lesage
Researcher: Josep Fèlix Rubio
Researcher: Natalia Gutiérrez
Researcher: Tano Varadinov
HPC Visitor: Neil Ashton
Visitor: Benoit Ozell

High Performance Computational Mechanics

High Performance Computational Mechanics Group
Manager: **Mariano Vázquez**
Senior Researcher: Fernando Martín Cucchiatti
Senior Researcher: Xavier Rubio
Researcher: Georg Huhs
Researcher: Hadrien Calmet
Student Researcher: Alexis Torrano
Student Researcher: Oscar Francisco Peredo
Student Researcher: Pierre Lafortune
Student Researcher: Simone Marras
Student Researcher: Margarida Moragues
Student Researcher: Cristina Montañola
Student Researcher: Ruth Aris
HPC Visitor: Amarpal Singh

HPC Visitor: Denis Doorly
HPC Visitor: Veronique Peiffer
Visitor: Deepack Hanumanthappa
Visitor: Alberto Gambaruto
Visitor: Paula Villar
Visitor: Peter Wise
Visitor: Takuji Nakashima

Physical and Numerical Modelling

Physical and Numerical Modelling Group Manager:
Guillaume Houzeaux
Senior Researcher: Angel Heriberto Coppola
Senior Researcher: Arnau Folch
Researcher: Miquel Català
Researcher: Mohammed Jowkar
Researcher: Raúl De La Cruz
Student Researcher: Ane Beatriz Eguzkitza
Student Researcher: Chiara Scaini
Student Researcher: Cristobal Augusto Samaniego
Student Researcher: Jelena Koldan
Researcher: Xavier Saez
Research Support Engineer: Genís Aguilar
Research Support Engineer: Juan Esteban Rodríguez
Research Support Engineer: Miguel Ferrer
HPC Visitor: Alastair West
HPC Visitor: Roberto Sulpizio
Visitor: Eduard López

Operations Department

Operations Director: **Sergi Girona**

System Administration

Systems Group Manager: **Javier Bartolomé**
Helpdesk: Antonio Espinar
Helpdesk: Pedro Gómez
Helpdesk: Ferran Sellés
Linux/Unix Administrator PRACE: Guillermo Aguirre
Linux/Unix Administrator PRACE : Gabriele Carteni
Network Administrator: Albert Benet
Performance Technician: Alejandro Lucero

Performance Technician: Carles Fenoy
Security And Networks: Juan Carlos Sánchez
System Administration: David Ocaña
System Administration: Jordi Valls
System Administration: Sergi Moré
Visitor: Carlos Alejandro Rodríguez
Student Researcher: Damián Montaldo

User Support

User Support Group Manager: **David Vicente**
Support And Application Consultant PRACE:
Jorge Rodríguez
Technical Support: Xavier Abellán
User Support: Christian Simarro
User Support: Jorge Alberto Naranjo
Visualization Technician: Carlos Tripiñana
Web Graphic Designer: Jasmina Tomic
Webmaster: Silvina Rusinek
Webmaster: Nuria Montoya

Facility Management

Facility Management Group Manager: **Ahmet Senata**
Maintenance Assistant: Albert Riera
Maintenance Assistant: Oliver Herencia

Operations - RES Coordination

Technical Support RES Project: Montserrat González

Management Department

Management Director: **Ernest Quingles**

Business Administration

Administration, Finances and Human Resources Group
Manager: **Mercè Calvet**

Finances & Accounting

Accounting Manager: Ma Cristina Calonge
Accounting Assistant: Alba Delclòs
Finance Assistant: Judit Soldevila
Technical Support For Economic Management Projects:
Laura Viñas
Technical Support For Economic Management Projects:
Marina Utgés

General Services and Purchase

General Assistant: Laura Gutiérrez
General Assistant: Núria Sirvent
Information System Developer: Toni Matas
Purchasing Officer: Cristina Vargas
Purchasing Officer: Elena Miró
Purchasing Officer: Neus Jiménez
Student Researcher: Aurora Rodríguez
Student Researcher: Míriam Méndez
Student Researcher: Sara Mula
Student Researcher: Yousfan Del
Student Researcher: Alicia Giménez
Student Researcher: Yaiza Fernández

Human Resources

Human Resources Technician: Lara Cejudo
Human Resources Technician: Ana Isabel Martín
Human Resources Officer: Eva Esteban

Projects and Technology Transfer

Research Project Group Manager: **Eugene Griffiths**
EC Mobility Program Coordinator: Fermín Sánchez
Prace Research Manager: Carlos David Mérida
Prospect Administrator And Prace Business Analyst:
Marcin Ostasz
Research Project Manager: Anais González
Research Project Manager: Gina Michelle Alioto
Research Project Manager: Guadalupe Moreno
Research Project Manager: Pilar Callau
Research Project Manager: Javier Salazar
Research Project Manager: Marta Rosselló
Research Project Manager: Oriol Pineda
Student Researcher: Patricia Fernández

Marketing and Communication

Marketing Executive: Renata Giménez
Communications Officer: María José Barroso
Communications Officer: Sara Ibáñez
Dissemination Project Manager: Nagham Salman
Marenostrum Visitors Manager: Oriol Riu

The financial accounts for 2011 presented here were drawn up following the accounting principles laid out in the General Plan of Public Accounting. The operating budget of the BSC-CNS Consortium for the fiscal year 2011 was composed of ordinary income derived from contributions by its patrons, as well as project income derived from competitive funding sources and agreements reached with private organisations. This income was then employed to cover expenses, including costs of operations and fulfilment of all financial obligations.

» Income

The Consortium income of €14.339.608,67 recognised for fiscal year 2011 was derived from public administration contributions from the Ministry of Science and Innovation (MICINN), Generalitat de Catalunya (GdC) and European Commission (EC), as well as from agreements, contracts or other collaborative agreements with private organisations. Furthermore, the consolidated budget of the BSC-CNS included the assignment of internal resources carried over from the previous year's provisions.

INCOME	AMOUNT €
Ordinary Income	5.299.968,67
Ministerio de Ciencia e Innovación	4.288.320,00
Generalitat de Catalunya	1.011.648,67
Competitive Income	7.512.044,03
Ministerio de Ciencia e Innovación	1.776.586,16
Generalitat de Catalunya	153.356,50
European Commission	3.627.573,78
Private Companies	1.954.527,59
Other Income	7.256.176,97
Applied Previous Preserves	4.528.570,93
Strategic Investment	1.200.010,07
Overheads/Capital Transfers	1.527.595,97
TOTAL INCOME	20.068.189,67

Ordinary Income refers to the base operating budget provided by the Consortium Partners.

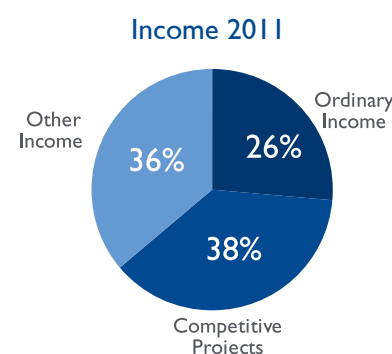
Competitive Income represents the funds derived from competitive project grants from various Ministries, the European Commission and R&D projects sponsored by private companies. Note that competitive project funds received in advance for future multi-year programs, that are progressively applied over the lifetime of each project, are not included as income in the current period.

Other Income includes strategic investments, overheads and capital transfers.

Strategic Investments are funds assigned by the Consortium Partners to finance key investments such as the construction of the new building to house the BSC-CNS and increases in supercomputing hardware.

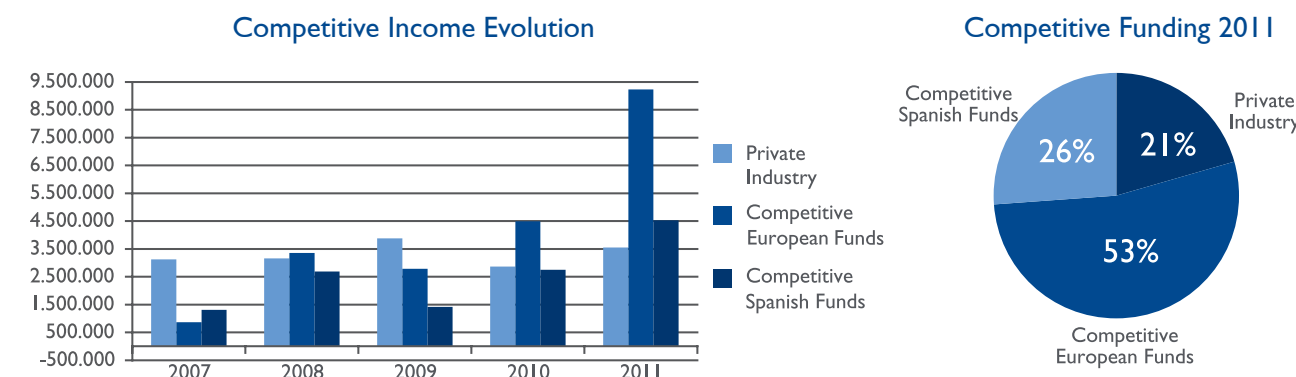
Overheads are incomes derived from ordinary projects, which according to the norms of the BSC/CNS are charged 10% to cover overhead expenses.

Capital Transfers are incomes derived from the yield on the capital accumulated from multiannual reserves for the execution of competitive projects and strategic investments, deposited in different bank accounts.



» Breakdown of Competitive Income

The charts below depict total competitive income received during the year, including advances of funds for multi-year projects. This is in contrast to the previous chart showing total income breakdown, where only income relating to the current fiscal year is included.



» Expenses

The expenses of the BSC-CNS Consortium in the fiscal year 2011 include all costs associated with personnel, running expenses and investments financed either by the ordinary budget or from project funding derived from competitive grants.

EXPENSES	AMOUNT €		
	Ordinary Budget	Projects Budget	Total
Personnel	4.143.178	4.623.622	8.766.800
Investments	6.124.353	756.389	6.880.742
Current Expenses	3.174.418	1.246.230	4.420.647
TOTAL EXPENSES	13.441.949	6.626.241	20.068.190

Personnel refer to salaries and associated charges directly related to the employment of staff contracted by BSC-CNS. It does not include salaries and associated charges of visitors or other collaborators who continued to be paid via their originating institution.

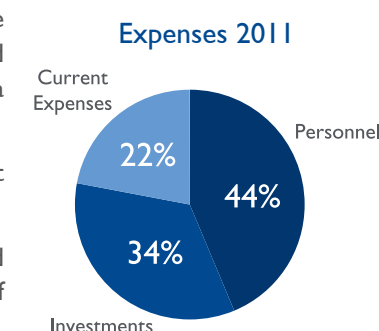
During 2011 there was significant growth in personnel funded by research project activities, with a 23% increase over the previous year.

Investments include all expenditures on computing and scientific equipment and infrastructure. They also include other key investments such as the construction of the new building to house BSC-CNS and strategic supercomputing hardware.

Current Expenses include office space rental, furniture, fixtures and fittings, office computer equipment, security services, maintenance and cleaning services, telephones and networking, legal services, marketing, insurances and power.

In 2011, BSC-CNS invited 15 public calls in order to accept 6 supply tenders, 8 services tenders and 1 works tender. The works tender was held for the launching of the first phase of construction of the new BSC-CNS building.

All of the acquisitions were made following the legal procedures established by the law regulating contracting in public administrations, and all contracts were open to public tenders. A total of 58 administration contracts were signed during the year. There was an increase of 38% over the previous year in purchasing activity.



» BSC-CNS - Center of Excellence Severo Ochoa



Mateo Valero, Director BSC-CNS and Principal Investigator of the Severo Ochoa Project

In 2011, BSC-CNS was one of only eight institutions to receive the Severo Ochoa award for excellence, an award given to Spanish research centres considered to rank internationally among the most competitive in their fields. This award confirmed BSC-CNS's reputation as one of the world's leading supercomputing centres. It will fund an ambitious research programme to design the supercomputing hardware, software and applications of the future, which are targeted toward the solving of significant social challenges in health and climate change.



Objectives of the programme

The "Severo Ochoa Center of Excellence" programme was launched by the Spanish Government with the aim of recognising, rewarding and promoting outstanding scientific research in Spain. It is a Specific Sub-Program for Support to strategic research programs to be developed by excellent centres and Institutions. The specific objectives of the programme are:

- ▶ To improve world-class research centres' capacity to organise and carry out research
- ▶ To improve their capacity to attract, recruit, train and retain human resources
- ▶ To further develop their relationships with other leading international centres, and
- ▶ To disseminate their research results to broader society



Design of the emblem of the "Severo Ochoa Excellence" award by the Ministry of Science and Innovation to the best research centers in Spain.

Proposal evaluation and selection of finalists

The Severo Ochoa evaluation committee was composed exclusively of internationally renowned scientists and led by three Nobel Prize winners. In the initial phase of evaluation, more than seventy centers were evaluated and the committee focused on scientific production and participation in research projects, in addition to the track record of the Scientific Director and the centre's Principal Investigators. In the second phase of evaluation, the committee reviewed the research and resource plan for the next four years.

When awarding the prize to the BSC-CNS, the committee highlighted its unique position as a centre offering supercomputing resources to the scientific community while performing frontier research in both the computer and data driven sciences (earth, life and engineering sciences), pushing frontiers that are vital to scientific and engineering progress as well as having great social importance.

The additional selected Spanish centres for excellence are:

- ▶ Centro Nacional de Investigaciones Cardiovasculares (CNIC)
- ▶ Centro Nacional de Investigaciones Oncológicas (CNIO)
- ▶ Graduate School of Economics (Barcelona GSE)
- ▶ Institute for Research in Biomedicine (IRB Barcelona)
- ▶ Instituto de Astrofísica de Canarias (IAC)
- ▶ Instituto de Ciencias Matemáticas (ICMAT)
- ▶ The Institute of Photonic Sciences (ICFO)



Francesc Subirada, Associate Director of BSC-CNS, receives the award from Ministra Garmendia

» The BSC-CNS Severo Ochoa Project

Supercomputers are used for modelling and simulation, and Exascale computing, which refers to machines which will be able to perform 1 million trillion calculations per second and that will employ up to 100 million processors working in parallel, is seen as a critical milestone for global progress in a multitude of scientific fields. However, attaining Exascale computing poses significant challenges, due to requirements on system hardware and software design, of which energy consumption is one of the main factors.

The BSC-CNS Severo Ochoa Project is made up of four main sub-projects. The first sub-project focuses on hardware and software technologies to facilitate the path to Exascale computing and data management by focusing on radical improvements in energy efficiency. The additional three scientific sub-projects employ supercomputing to solve grand societal challenges which include efficiently processing human genetic data in order to make personalised medicine a reality, forecasting and understanding climate change and modelling the functioning of human organs.

Each scientific sub-project requires strong collaboration between the computer sciences and the other scientific disciplines as well as the development of unique supercomputing tools which will be adapted to each discipline's respective needs. Specifically, multi-disciplinary teams within BSC-CNS will work together in order to create novel computer architectures, system software and applications. These teams will also collaborate with leading international centres in order to achieve pragmatic, effective solutions.



Josep Casanovas, Executive Manager of the BSC-CNS Severo Ochoa Project

BSC-CNS has employed a strong executive in order to ensure the Project's success. The Principal Investigator for the Project is the BSC-CNS Director, Mateo Valero, who named Prof. Josep Casanovas (full professor in Operation Research at the UPC BarcelonaTech, which specialises in simulation systems) executive manager of the Project. The scientific coordinator of the project is Prof. Eduard Ayguadé, Associate Director of the Computer Sciences Department of BSC-CNS, who played the leading role in the conception, planning and presentation of the project proposal.



Eduard Ayguadé, Scientific Coordinator of the project and Associate Director of the Computer Sciences Department of BSC-CNS

The Project aims to extend BSC-CNS's international leadership and influence on Exascale computing systems and applications design, and will also attract talented researchers and provide unique training and mobility opportunities for career development. Furthermore, the BSC-CNS Severo Ochoa Project will play a key role in achieving the strategic goals of the centre, bringing together in a cohesive way multiple strategic projects and initiatives.

One of the main objectives of BSC-CNS is to proactively transfer technology to industry, both as an objective in itself in terms of dissemination of scientific output, and also with the intention to generate industrial returns.

Increasing emphasis is being placed by BSC-CNS management on fomenting and facilitating interactions with industry at all levels, from direct R&D collaborations, to educational activities such as providing technical seminars, and staff exchanges with private industry R&D laboratories.

During 2011 a number of important new agreements were signed and existing collaborations strengthened and expanded. Some 125 private companies interacted with BSC-CNS through various research programs throughout the year.

» Iberdrola-BSC Research Collaboration



BSC-CNS and Iberdrola Renovables are collaborating to design mathematical models to improve the design of Iberdrola's wind farms. Led by the CASE Department, the project tackles the extremely challenging simulation of wind flows and wind turbine placement with the aim of significantly increasing the efficiency and power output of the farms.

» IBM-BSC Research Collaboration



The main objective of the bilateral IBM-BSC research project is to define the hardware and software components for the new generations of Petascale supercomputers, under the umbrella of a memorandum of understanding, led by Mateo Valero and Jesús Labarta. During 2011, the collaboration focused on the development of a software stack for leveraging the BG/Q architecture in Big Data problems. MapReduce has been adopted in a first step in order to perform a deep study of the performance of BG/Q running Big Data workloads. In future research the plan is to study more generic call-back frameworks (data-driven) beyond MapReduce providing bindings for high-level query languages. Additionally, graph computing programming models will also be explored on top of the BG/ASF architecture. Other topics have also been subject of joint research, including a) the development of resource management strategies for BigData applications in the Cloud, with special attention to Web workloads and extended Data Analytics programming models; b) power modeling and adaptive data prefetching techniques for the IBM POWER7 processor; and c) code transformations for irregular access patterns.

» Intel-BSC Exascale Laboratory



On November 2011 Intel Corporation and BSC-CNS signed a multi-year agreement to create the Intel and BSC Exascale Laboratory in Barcelona, located at the premises of BSC-CNS and focused on developing programming models and tools that will be needed to exploit extraordinary levels of parallelism in future Intel-architecture based supercomputers. When building Exascale systems consisting of millions of cores, getting all of them to work together for an extended period of time represents a major problem. Hence, completely new software concepts and methods will be required to bring power consumption to acceptable levels and to make the system fault tolerant. The Intel and BSC Exascale Laboratory will focus on highly scalable parallel run-time systems to support the enormous amount of parallelism. Future exascale supercomputers will be hugely complex and challenging to understand and to control. The new lab will try to solve many of these challenges in conducting R&D that will enable better software tools to analyse and predict performance and behaviour of highly complex exascale systems.

» Microsoft-BSC Research Centre



On 2nd November 2011, the BSC-Microsoft Research Centre (BSCMSRC), led by Osman Unsal and Adrián Cristal, celebrated its 5th birthday. The Centre was established to focus on the way in which multicore architectures and the software stack for the mobile and desktop market segments will be designed and interact over the next 10 years and beyond. On one side BSCMSRC researchers continued research activities on transactional memory (TM), including the development of sophisticated TM applications and benchmarks and the TMBox FPGA platform with 16 cores with support for TM. During 2011 novel proposals have been done: TM-cache design, a new prototype utilizing Simultaneous Multithreading (STM) and the Atomic Dataflow Model. On another side, BSCMSRC researchers have worked on the integration of the BSC's StarsS programming model with the Barrelfish Research OS, a new message-passing open-source Operating System, being developed by Microsoft Research and ETH, Zurich. Finally, BSCMSRC researchers are exploring the suitability of low-power vector processors for handheld and datacenter applications.

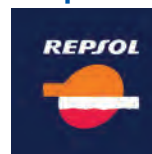
» NVIDIA-BSC/UPC Research Collaboration



BSC-CNS, in association with the Universitat Politècnica de Catalunya (UPC), was named by NVIDIA as a CUDA Center of Excellence at the International Conference for High Performance Computing, Networking, Storage and Analysis (SC11), held in Seattle (USA) in November 2011. The recognition means that BSC-CNS will employ GPU computational equipment and will be provided financing by NVIDIA to support the growing number of research and training programs relating to the technology.

The Center, lead by Prof. Nacho Navarro, recognises BSC-CNS's broad-based research success in leveraging the NVIDIA CUDA technology and GPU computing, both in major research initiatives such as Global Memory for Accelerators (GMAC) and in projects dealing with the optimisation of applications, such as Reverse Time Migration (RTM). For the next three years, BSC-CNS and UPC plan to launch a Training Program in Parallel Programming using CUDA architecture and the StarsS implementation developed at BSC-CNS. Other projects include optimising the management of execution resources in multi-GPU environments with GMAC, and to construct a new prototype of GPUs in cluster to explore the promising use of low energy consuming GPUs in platforms oriented for supercomputation. First applications will centre in 3D simulations of plasma on complex geometries, a cardiac simulator and visualisation of elastic waves in seismic images.

» Repsol-BSC Research Center



On 19th September 2011, the Repsol-BSC Research Center was officially inaugurated in a ceremony presided over by the Spanish Minister of Science and Innovation, Cristina Garmendia, the Generalitat of Catalunya's Minister for Economy and Knowledge, Andreu Mas-Colell, and the President of Repsol, Antoni Brufau.

The new Center, which will initially employ eleven fulltime researchers, will undertake various research projects to develop advanced technologies applicable to the exploration of hydrocarbons and other areas of interest to Repsol, such as modelling of subterranean and subsea reserves, fluid flows, etc. The establishment of the Center is the result of many years of successful collaboration between BSC-CNS and Repsol, a highlight of which was the now commercialised Kaleidoscope project which developed algorithms that enable Repsol to process subterranean seismic images up to 15 times faster than its competitors, and was voted one of the five most innovative projects in the global energy sector.

» Other Industry and Institutional Collaborations

In addition to the major collaborations detailed above, BSC-CNS is actively engaged with private industry and government on a range of applied projects. During 2011, BSC-CNS collaborated with over 125 private companies both within Spain and internationally, either in direct R&D collaborations or via European or nationally sponsored project consortia.

Of particular note are the development of operational air quality forecasting and assessment services for various regional governments throughout Spain, and the analysis of impacts on air quality for power generation and other industries;

- ▶ Servei Meteorològic de Catalunya (SMC): to generate regional climate scenarios at high resolution for Catalonia during the 21st century.
- ▶ Agencia de Medio Ambiente y Agua of Andalusia: to provide the Andalusia Government with an operational air quality forecasting and assessment service, which will allow the simulations of photochemical and particulate matter pollution with high spatial and temporal resolution for Andalusia: 1 km² and 1 hour.
- ▶ PRYSMA Calidad y Medioambiente S.A.: to perform an impact assessment on the air quality due to the change of fuel in a cement factory.
- ▶ IDOM Zaragoza: to perform an impact assessment on the air quality from the installation of a biomass plant.
- ▶ AEMET (The State Meteorological Agency): to implement, disseminate and validate the operational prediction of the North African dust transport in the Iberian Peninsula as well as to perform modelling, detection, follow-up and characterisation studies of atmospheric material.
- ▶ Spanish Ministry of the Environment: to develop and implement an operational high-resolution air quality forecasting system for Spain, providing end-users with an air quality forecasting and assessment service for Spain and Europe with higher detail for some hot spot areas.
- ▶ Government of the Canary Islands: to develop an information system about the air quality forecast and surveillance of the Canary Islands.

» PRACE - Partnership for Advanced Computing in Europe



Background

The Partnership for Advanced Computing in Europe (PRACE) is a pan-European Research Infrastructure for High Performance Computing (HPC) and forms the top level of the European HPC ecosystem. The infrastructure consists of several tier-0 supercomputers (including one at BSC-CNS) distributed across the continent, providing outstanding computing services to enable world-class research on world-class systems. The systems are installed at France, Germany, Italy and Spain. Through PRACE, European scientists and technologists in the 22 member countries are being provided with world-class supercomputers with capabilities comparable to those available in the USA and Japan. These leadership class systems will help the continent's scientists and engineers to remain internationally competitive.



BSC-CNS and PRACE



The BSC-CNS played a key role in the creation of the PRACE Research Infrastructure at all levels, with Sergi Girona serving as Chairman of the Board of Directors, significant technical contributions, and leadership of the organisational design. This included the selection of the best legal format, design of the governance structure, funding and usage models, and the peer review process, resulting in the PRACE statutes and initial agreement which were signed

in May 2010. From that date, PRACE has operated as a Belgium-based legal entity (AISBL-Association Internationale Sans But Lucratif) in parallel to the supporting European projects.

During 2011, BSC-CNS continued to play a leading role, hosting the All Hands Meeting for the conclusion of the First Implementation Phase Project (IIP) and the Kick-Off Meeting for the Second Implementation Phase Project (2IP).

Spanish participation in PRACE

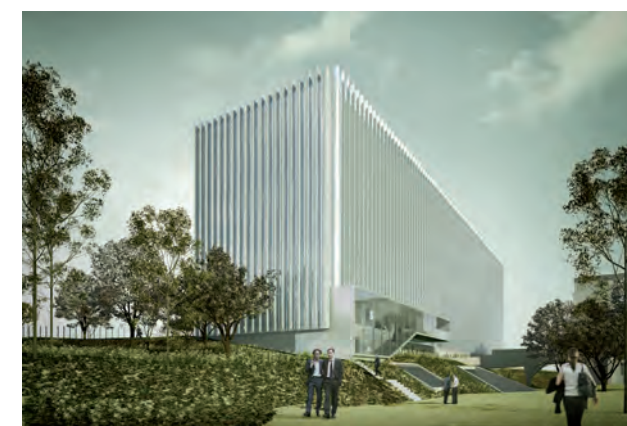
Although the PRACE network is still being established, Spanish scientists have already been very successful in both leading and participating in important research projects that have won time on the nodes that have been installed to date. This high level of participation is reflected in the election of Dr. Gustavo Yepes from the Universidad Autónoma de Madrid (Spain) as Vice Chair of the permanent Programme Committee of the User Forum at the first User Forum Meeting which was held in April 2011 in Brussels.

Some of the projects which ran on PRACE nodes in 2011 include:

- ▶ QCD Simulations for Flavor Physics in the Standard Model and Beyond, Prof. Vittorio Lubicz, 35 million CPU hours on JUGENE, with participation of Federico Mescia (UB) and Vicent Giménez Gómez (UV),
- ▶ Entrainment effects in rough-wall boundary layers, Javier Jiménez Sendín, UPM, 40 million CPU hours on JUGENE,
- ▶ Non diffusive transport in ITG plasma turbulence, Edilberto Sánchez, CIEMAT, 20 million CPU hours on JUGENE,
- ▶ Ab Initio Modeling of Solar Active Regions A Leading-Edge Solar Plasma Physics Experiment, Aake Nordlund, 60 million CPU hours on JUGENE, with participation of Fernando Moreno Insertis (IAC),
- ▶ Large Scale simulations of Ly-alpha and Ly-break galaxies in the high-z universe: Probing the epoch of reionization, Gustavo Yepes, UAM, 5 million CPU hours on CURIE FN,
- ▶ Extreme Earthquake Wave Propagation Modelling (E2WPM), Mike Ashworth, 20 million CPU hours on JUGENE, with participation of Eduardo Cabrera (UAB),
- ▶ The molecular bases of the transport cycle of APC antiporters, Modesto Orozco, BSC-CNS, 33.7 million CPU hours on JUGENE,
- ▶ Modeling gravitational wave signals from black hole binaries, Sascha Husa, UIB (Illes Balears), 14.7 million CPU hours on HERMIT, 2 million CPU hours on CURIE FN,
- ▶ Branch point motion in star polymers and their mixtures with linear chains, Ángel Moreno, CSIC, CFM, San Sebastián, 3 million CPU hours on CURIE FN,
- ▶ First principles design of a biocatalyst for water oxidation, Carme Rovira, PCB-UB, 37.5 million CPU hours on CURIE TN,
- ▶ Singlet physics - the missing link to precision lattice QCD, Karl Jansen, 19 million CPU hours on JUGENE, with participation of Gregorio Herdoiza, UAM,
- ▶ Light quark mass dependence of two-hadron energies in Lattice QCD, Assumpta Parreño, UB, 30 million CPU hours on CURIE TN.

In 2011, construction started on the new building to house all BSC-CNS staff, who are currently dispersed in several separate facilities belonging to the UPC and Consorci de la Zona Franca. The building, which will complete construction in 2013, is being constructed adjacent to the Capella Torre Girona which houses the MareNostrum supercomputer, and will be connected to it via a subterranean passage. In addition to enabling all BSC-CNS staff to be housed under one roof, it will also have a dedicated section to host a future supercomputer even more powerful than the MareNostrum.

Covering 12.965m2 with 3 levels below ground and 5 levels above ground, the building incorporates advanced features such as water recycling, automatic illumination to maximise use of natural light, and natural cooling to achieve a B-level energy efficiency rating.



Artist's impression of the New BSC-CNS Building



Sectional Plan of the New BSC-CNS Building Showing Functional Areas

The construction is planned in three phases. The first phase commenced in April 2011, following the site preparation work that was started in 2010, which required the demolition of two older buildings of the UPC.

This first phase has seen the laying of the foundations and construction of the subterranean levels up to ground level. This required excavation of large amounts of earth and removal from the site, construction of retaining and structural walls, placements of pillars and slabs and formation of access ramps.

The areas that have been structurally completed thus include the future parking and the space where the new supercomputer will be housed, due to be installed in 2012.

Images showing construction of phase one of the New BSC-CNS Building





Jesús Labarta and Eduard Ayguadé,
Directors of the Computer Sciences Department

The scientific mission of the Computer Sciences Department is to influence the way computing machines are built, programmed and used. This is done through the proposal and development of novel processor, memory and interconnect architectures, programming, performance analysis and execution environments, resource management layers, etc., bridging what computer technology offers and application requirements, usually in collaboration with manufacturers.

» Overview

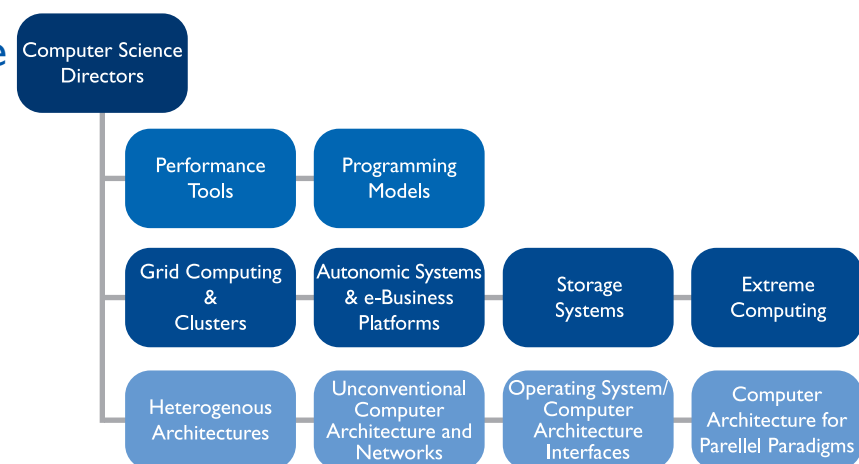
The Computer Sciences Department, led by Jesús Labarta and Eduard Ayguadé, is structured in 10 research groups. Although each group has its own specialised lines of research, the teams often come together to collaborate on projects that require vertical integration, such as the new Exascale EU projects Mont-Blanc and DEEP. This vertical interaction is considered critical to the quality and success of the research, as feedback between the different groups enables application programmers to influence the direction of future systems architecture while better knowledge of architectures improves the design and implementation of novel programming models, execution environments and applications.

» Unique Strength

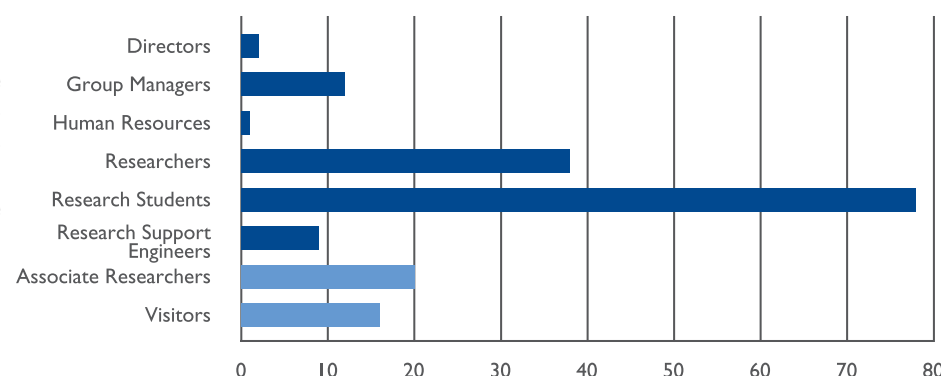
The combination of broad coverage of all facets of computer systems design and programming, along with in-depth expertise in each area, are somewhat unique amongst supercomputing centres. This unique strength of the Computer Sciences Department has attracted leading computing companies such as IBM, Intel, Microsoft or NVIDIA to invest during 2011 in collaborative systems design R&D projects.

» Organisational Structure

During 2011, some 140 staff and students, and a further 36 associated or visiting researchers, worked within the Department, organised in 10 research Groups; four focused on Computer Architecture (Parallel Paradigms, Unconventional Computer Architecture and Networks, Operating System/Computer Architecture Interfaces and Heterogeneous Architectures), two focussed on improving productivity when programming and optimising parallel applications on large scale parallel systems (Programming Models, including accelerators, and Performance Tools) and four focused on programming models and resource management middleware for large cluster and Cloud architectures (Storage Systems, Grid Computing and Clusters, Autonomic Systems and e-Business Platforms and Extreme Computing).



Computer Science Department Staff & Collaborators 2011



» Key Projects & Networks

During 2011, the Computer Sciences Department participated in the following EU projects::

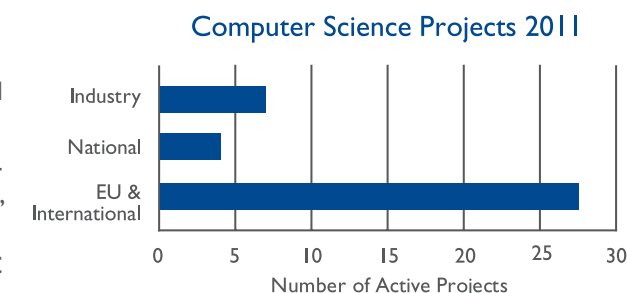
- ▶ 14 FP7 projects: DEEP, EnCORE, EUBrazilOpenBio, HOPSA-EU, IOLanes, Mont-Blanc, OPTIMIS, parMERASA, PROARTIS, ScalaLife, SIENA, TERAFLUX, TEXT, VENUS-C;
- ▶ 4 networks of excellence: HiPEAC, HPC-Europa, PlanetHPC and RISC;
- ▶ The SCALUS Marie Curie Initial Training network;
- ▶ The IESP (International Exascale Software Project) and EESI (European Exascale Software Initiative);
- ▶ The First and Second Implementation Phase in the PRACE EU FP7 project;
- ▶ The DEISA2 (Distributed European Infrastructure for Supercomputing Applications) consortium;
- ▶ EU COST IC804 action "Energy efficiency in large scale distributed systems";

and collaborations with:

- ▶ Intel Corporation with a multi-year agreement to create the Intel and BSC Exascale Laboratory in Barcelona;
- ▶ NVIDIA, who designated the BSC-CNS, in association with the Universitat Politècnica de Catalunya (UPC), as CUDA Center Of Excellence (CCOE);
- ▶ Microsoft Research through the BSC-Microsoft Research Center agreement;
- ▶ IBM Research through the ASF (Active Storage Fabric) SoW;
- ▶ The European Space Agency (ESA), with the "Multicore OS benchmark" project;
- ▶ Cisco Systems on the "Convergence of Cloud and Grid computing and IOT".

and two national projects:

- ▶ The Spanish Consolider program "Supercomputing and eScience", coordinating the Basic Research in Supercomputing workpackage;
- ▶ The Plan Avanza2 NUBA project.



Impacting the Future of Computing

In collaboration with market leaders such as IBM, Intel, Microsoft and NVIDIA, as well as other international computing centres and standardisation efforts, the researchers of the Computer Sciences Department are involved in a range of projects covering the full spectrum of next generation computer design, from novel processor and multicore (homogeneous and heterogeneous) architectures, architectural support to the software stack (e.g. runtime systems and OS), programming and execution models (e.g. OpenMP and StarSs), as well as support for the efficient programming and management of GRID and Cloud architectures. The results of their work are considered a reference worldwide.

» Scientific Output

The research results of the Department have been published in the proceedings of high quality conferences in the area, including International Conference on Parallel Architectures and Compilation Techniques (PACT), International Conference on Supercomputing (ICS), International Conference on Parallel Processing (ICPP), International Supercomputing Conference for High Performance Computing, Networking, Storage and Analysis (SC), MICRO conference, Symposium on Principles and Practice of Parallel Programming, International Parallel & Distributed Processing Symposium (IPDPS), International Symposium on Code Generation and Optimization (CGO), International Symposium on Performance Analysis of Systems and Software (ISPASS), Symposium On Applied Computing (SAC), International Conference on Computer Design (ICCD) and International Symposium on Software Reliability Engineering (ISSRE). In addition, other more consolidated research results have been published in prestigious journals in the area.

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Heterogeneous Architectures



Led by Alex Ramírez, this Group, in close interaction with the Programming Models Group, aims to design and evaluate the next generation of HPC systems based on heterogeneous components with a dual purpose: first, to develop the most energy efficient supercomputers, capable of achieving the 50 GFLOPS/Watt required by future Exaflop supercomputers; second, to focus the developments on the actual needs of the applications and the runtime system, and anticipate the needs of the runtime system for future architectures so that software can be ready when research trends become products. During 2011 the Group advanced ongoing projects (ENCORE and TERAFLUX) and participated in international Exascale efforts (PRACE, EESI, IESP, PlanetHPC, and Mont-Blanc) focusing on design and deployment of a new class of HPC systems built from energy-efficient components.

Computer Architecture for Parallel Paradigms

Led by Adrián Cristal and Osman Unsal, this Group does research on architectural support for novel programming models and execution environments for future multicore architectures, and forms the core of the BSC-Microsoft Research Centre (www.bscmsrc.eu) which focuses on lowering the programmability wall raised by multicore architectures; low-power vector processors, hardware support for object oriented programming, programming language runtimes and synchronisation. The Group also conducts research in the application of Transactional Memory for other emerging domains, such as reliability or dataflow execution. In 2011, the Group started a new research topic in exascale reliability, with particular emphasis on exploiting the StarsS programming model for resilience.



Operating System / Computer Architecture Interface

Led by Francisco J. Cazorla, the CAOS Group focuses on hard real-time systems and operating systems for HPC systems. Research in hard real-time systems is based in three key projects; parMERASA, started in 2011, architectures with random timing behaviour for hard-real time systems (PROARTIS) and a project with the European Space Agency (started in 2011). Research in operating systems for HPC is conducted in collaboration with IBM. The Group also participated in the HiPEAC and ARTIST networks of excellence, and performed research in fault-tolerant and energy-efficient hard real-time architectures, and CPU and energy accounting.



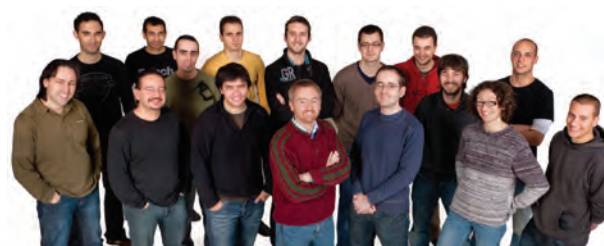
Unconventional Computer Architecture and Networks

Led by Mario Nemirovsky, the Group conducts research on massive multithreaded architectures focused on big data, latency sensitive and network processing architectures (e.g. Grid, Cloud, and Data Centers). With some 2.5 quintillion bytes of data created daily, and 90% of the existing data in the world created in the last two years, working with these massive amounts of data is a major computational challenge. Furthermore the rapidly increasing number of sensors and actuators is driving demand for latency sensitive applications, while networks and their applications, including data centers and high performance systems are becoming ever more pervasive. During 2011 the Group collaborated with Cisco Systems investigating the convergence of Cloud and Grid computing and Internet of Things (IoT).



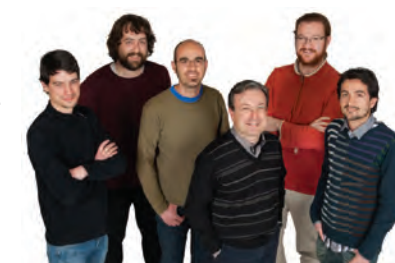
Programming Models

Led by Xavier Martorell, the Group explores new programming models and their efficient implementation for current and future architectures, ranging from multicore SMP architectures with support for accelerators (GPUs, FPGAs) to clusters of SMPs, and exascale systems. This exploration is supported with the development of powerful compiler (Mercurium) and runtime (Nanos++) prototypes. In 2011, the Group continued developing OmpSs, the result of joining the programming models OpenMP and StarSs, improved support for GPUs, FPGAs and clusters in OmpSs, and also worked on power modelling for multicore architectures and code transformations for processors with local memories. Several new EU projects were initiated (Mont-Blanc and DEEP) in addition to ongoing ones (EnCORE, TERAFLUX and TEXT). The Group coordinated the programming models cluster and applications taskforce in the HiPEAC2 Network of Excellence. The Group also played a key role in NVIDIA's designation of BSC-CNS as a CUDA Center Of Excellence (CCOE).



Performance Tools

Led by Judit Giménez, this Group is working on the design of tools to instrument, analyse and predict the behaviour of parallel applications on parallel systems. The main goal of the Group is to provide technology to understand the issues that determine the actual performance of a parallel application or that contribute to its bottlenecks. This is extremely important both in novel homogeneous and heterogeneous multi-core architectures as well as in highly scalable cluster systems. During 2011 the Group developed new functionalities on infrastructures, progressed open research lines (to increase the tools intelligence and detail) and participated in training sessions. The Group has been involved in HOPSA, ScalaLife, HPC-Europa2, Mont-Blanc, DEEP, PRACE and G8-ECS projects, as well with the new Intel-BSC Exascale Lab.



Grid Computing & Clusters

Led by Rosa M. Badia, this Group researches new programming and execution models, and resource management techniques for distributed computing. The team explores solutions in order to simplify application development, enable dynamic exploitation of parallelism at runtime and perform combined scheduling decisions at different levels. The Group focused on two projects: COMPSs/ServiceSs and SERA, and also participated in several EU projects (OPTIMIS, VENUS-C, SIENA, ScalaLife, IS-ENES, transPLANT and EU-Brazil OpenBio), and in the NUBA Spanish project. The Group also continued development of the StarSs programming model in cooperation with the Programming Models Group, specifically on the GPU and cluster versions of StarSs, hybrid MPI/SMPs (TEXT EU project) and support for array regions and transactional memory (TERAFLUX EU project) in SMPs.



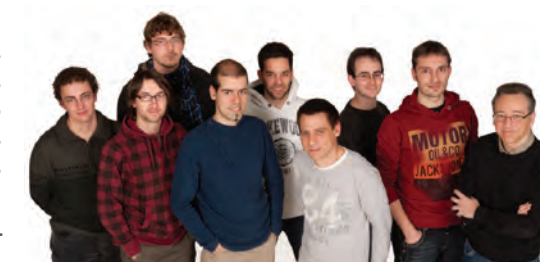
Autonomic Systems and eBusiness Platforms

Led by Jordi Torres, this Group performs high-level research in eBusiness applications and platforms executing on high-productivity multiprocessor architectures as well as distributed environments and new architectural proposals. The aim is to research autonomic and intelligent resource management for today's business applications, creating new components at middleware level that provide holistic solutions for new IT challenges: Cloud Computing, Big Data, Business Analytics, High Performance Computing or Sustainable Computing. During 2011 the group worked in two EU

projects (VENUS-C and OPTIMIS) and one national project (NUBA) in the area of Cloud Computing. Collaborations were launched with IBM on Active Storage Fabrics and with Microsoft Research on the support on Barrelfish to task-based programming models. The EU COST IC804 action "Energy efficiency in large scale distributed systems" was also further developed.

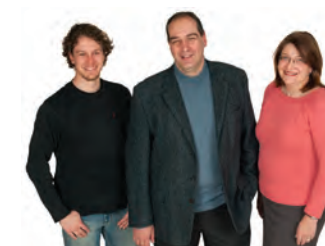
Storage Systems

Led by Toni Cortés, this Group explores appropriate solutions to the scalability of parallel storage systems in large installations (in which very large volumes of data need to be generated and accessed) and new file-system approaches to increase their performance and/or usability (better metadata management). In 2011 the Group focused on three areas: storage system scalability, new metadata management, and a testing environment. Within these areas, key efforts were the development of new data placement policies in large heterogeneous environments merging randomised and deterministic approaches (in cooperation with Universities of Paderborn and California and the SCALUS project), using the advantages of multicore system to improve I/O (IOLanes), and a new file system based on direct lookups instead of the traditional directory-by-directory lookup (SCALUS) and on virtualised metadata management.



Extreme Computing

Led by Vassil Alexandrov, this Group (created during 2011) focuses on solving problems with uncertainty on large scale computing systems. The Group's main expertise is in the area of Computational Science, Scalable Algorithms for advanced Computer Architectures, Monte Carlo methods and algorithms. In particular, scalable Monte Carlo algorithms are developed for Linear Algebra, Computational Finance, Environmental Models, Computational Biology, etc. In addition the research focuses on scalable and fault-tolerant algorithms for extreme scale (peta and exa scale) architectures. In June 2011 the Group assumed leadership of the EU Brazil OpenBio EU project and since September 2011 the technical program of RISC (A Network for Supporting the Coordination of Supercomputing Research Between Europe and Latin America) EU project.





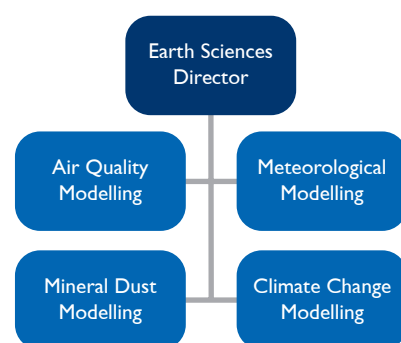
José María Baldasano,
Director of the
Earth Sciences
Department

The Earth Sciences Department of the BSC-CNS has the aim of modelling and understanding the behaviour of the Earth System, focusing its research activities on atmospheric processes and climate change modelling.

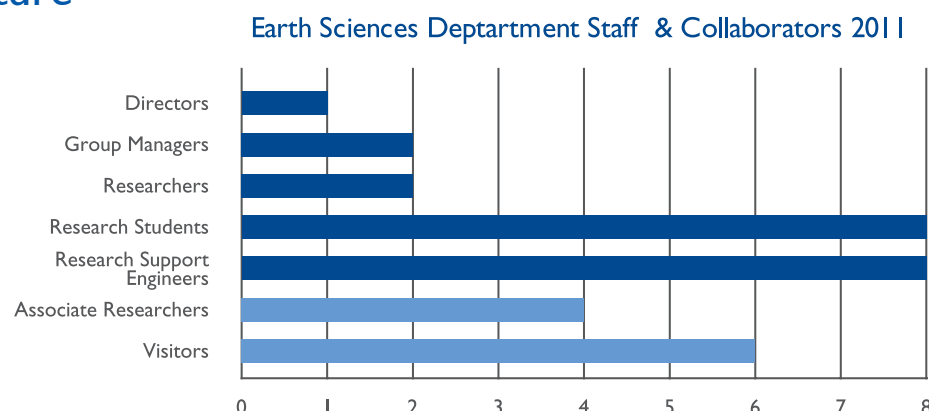
» Overview

The high performance capabilities of MareNostrum enable the Earth Sciences Department to increase the spatial and temporal resolution of earth systems, in order to improve knowledge of dynamic patterns of air pollutants in complex terrains and interactions and feedbacks of physico-chemical processes occurring in the atmosphere. Also possible are analyses with high-resolution global circulation models and downscaling to regional models. This coupling of global and regional climate models will contribute to a detailed description of the impacts of climate change. The main topics of research are: high-resolution air quality and meteorological modelling; global and regional mineral dust modelling; and global and regional climate modelling. Currently, the Group maintains daily high-resolution operational air quality forecasts for Europe and Spain (www.bsc.es/caliope) under the umbrella of the CALIOPE project funded by the Spanish Ministry of the Environment; and mineral dust forecasts for the Euro-Mediterranean region and East Asia (www.bsc.es/projects/earthscience/DREAM). The Department, also in collaboration with the World Meteorological Organization (WMO) and the Spanish Meteorological Agency (AEMET), have created the Regional Center for Sand and Dust Storm Warning System (SDS-WAS) covering Europe, northern Africa and the Middle East. Other research activities involve the diagnosis of the behaviour of Earth System Modelling (ESFM) codes in a supercomputer framework and the improvement of parallel versions of atmospheric models to increase their horizontal and temporal resolution.

» Organisational Structure

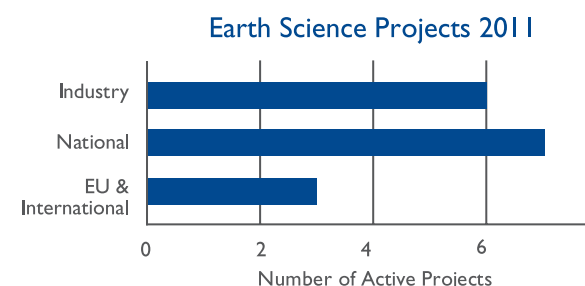


The Department is structured in four Groups that represent the main topics of Earth Sciences research: air quality modelling, mineral dust modelling, meteorological modelling and global and regional climate modelling. These Groups are interrelated and work in a cooperative form. They are led by a senior scientist and composed of a researcher, post-doctoral fellows and doctoral students. The technical support staff is shared by all the research Groups. During 2011 some 31 staff, collaborators and visitors worked with the Department.



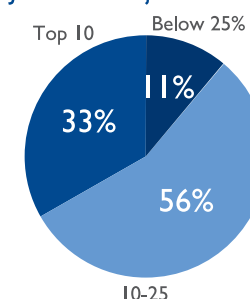
» Key Projects

- Continued the FIELD_AC (Fluxes, Interactions and Environment at the Land-Ocean Boundary. Downscaling, Assimilation and Coupling), FP7-Project of the Space Programme);
- Continued the IS-ENES (InfraStructure for the European Network for the Earth System Modelling), FP7-Project of the Capacities Programme;
- Continued participation in EC-Earth consortium (European Earth System model based on ECMWF). Currently, the EC-Earth consortium consists of 22 academic institutions and meteorological services from 10 countries in Europe funded under FP7;
- Continued the MACC-II (Monitoring Atmospheric Composition and Climate) FP7-project in collaboration with AEMET, to establish the core global and regional atmospheric environmental services to be delivered as a component of Europe's GMES initiative;
- Participated in the SyeC Consolider Program funded by MICINN;
- Continued the CICYT project: Coupling of a Fully Online Chemical Mechanism within the Atmospheric Global-Regional UMO Model funded by MICINN; in cooperation with NCEP, NOAA (USA);
- Initiated the CICYT project: Coupling of a fully online multi-component aerosol module within the atmospheric global-regional NMMB model, funded by MICINN;
- Participated in the CICYT project: Currents, waves and wind: Improving Risk Assessment through Assimilation in Numerical models of the Coastal Environment (COVARIANCE) funded by MICINN, in collaboration with LIM/UPC, CSIC and Servei Meteorològic de Catalunya;
- Continued the development of the CALIOPE Air Quality Forecasting System, extending coverage to Andalusia (funded by the Junta de Andalucía) and to Canarias (funded by the Canarias Government);
- Generation of climate projections for the 21st century in Catalonia, funded by METEOCAT;
- Participated in the COST Action ES1004 European framework for online integrated air quality and meteorology modelling (Eu-MetChem) to generate online integrated Atmospheric Chemical Transport and Meteorology modelling with two-way interactions between different atmospheric processes including chemistry (both gases and aerosols), clouds, radiation, boundary layer, emissions, meteorology and climate;
- Participated in the COST Action ES1002 European framework for Weather Intelligence for Renewable Energies (WIRE) to enhance the methodologies of forecasting wind and solar power production in the time domain of a few minutes up to several days;
- Participated in the European Network for Earth System Modelling (ENES);
- Participated in the European Aerosol Research Lidar Network: EARLINET, to validate and improve models that predict the future state of the atmosphere and its dependence on different scenarios;
- Participated in AERONET (Aerosol RObotic NETwork), an optical ground based aerosol monitoring network and data archive supported by NASA's Earth Observing System and expanded by federation with many non-NASA institutions;
- Hosted the Northern Africa-Middle East-Europe (NA-ME-E) Node of the SDS-WAS Regional Center. The SDS-WAS mission, supported by the WMO, is to enhance the ability of countries to deliver timely and quality sand and dust storm forecasts, observations, information and knowledge;
- Collaborated with the US National Centers for Environmental Prediction (NOAA/NCEP/EMC) within the framework of a Memorandum of Understanding to develop NMMB/BSC-CTM, international joint project proposals and researcher mobility.
- PRACE Project 2010PA0419 on CURIE
- Contributed to the Spanish network RETEMCA (Red Temática de Modelización de la Contaminación Atmosférica);
- Participated in several projects of technology transfer, such as modeling air quality of power plants.



» Scientific Output

Distribution of 2011 Published Articles by JCR-IF Rank journals in Area



The diffusion of research results obtained by the Earth Sciences Department has been significant. These results have been presented in a numerous ISI-JCR journals, European and international congresses and symposia organised during 2011, such as the Annual CMAS Conf., Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes; American Union Geophysical, European Geosciences Union General Assembly Meeting and other congresses organized by the European Meteorology Society (EMS), GLOREAM Conf., International Workshop on Air Quality Forecasting and Research. The number of ISI-JCR publications has increased considerably in 2011 (from 3 in 2007 to 8 in 2011). The JCR publications in 2011 have an average quality of 3,4 (Average JCR Science Edition Impact Factor) that suppose an augment with regard to 2008 (2,4); 2009 (2,9); 2010 (3,3) and were distributed over the subjects categories of "Meteorology & Atmospheric Sciences" and "Environmental Sciences".

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» Air Quality

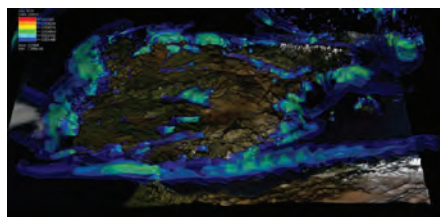


Figure 1 - Air quality modelling system (WRF-ARW/HERMES-EMEP/CMAQ/BSC-DREAM8b) forecast results

The Air Quality Group focuses its research on understanding the physico-chemical processes in the atmosphere that contribute to a decrease of air quality, and analyse the interactions between air pollutants and atmospheric processes, with the aim of obtaining a precise estimation of the air quality through high-resolution modelling, especially the relation between emissions, atmospheric transport, chemistry and deposition. For that purpose, an air quality modelling system with high spatial and temporal resolution (1 km – 4 km and 1 hour) is under development, implementation and evaluation under supercomputing infrastructures. It will consist of a set of models that will take into account emissions of anthropogenic and natural pollutants, meteorology and chemistry.

In 2011 the activities of the Group were mainly related to maintain and improve the dairy operational air quality forecast of the CALIOPE system, developed in the framework of the CALIOPE project, funded by the Spanish Ministry of the Environment and Rural and Marine Affairs. CALIOPE encompasses an operational high resolution air quality forecasting system, namely WRF-ARW/HERMES-EMEP/CMAQ/BSC-DREAM8b, being applied to Europe as a mother domain: 12 km 12 km, 1 h as well as to Spain as the nested domain: 4 km 4 km, 1 h, and with higher detail for some hot spot areas (<http://www.bsc.es/caliope>). Such high resolution of the modeling system is made possible by its implementation on the MareNostrum supercomputer hosted by the Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS). During 2011 enhancements of operational forecast system implementation were introduced. A near-real time forecast operational evaluation was implemented, by means of comparisons of the performance of the outputs of the model with online ground-based observations from different institutions: European Environment Agency; Generalitat de Catalunya, Gobierno de Cantabria, Junta de Andalucía, Gobierno de Canarias, Comunidad de Madrid, Ayuntamiento de Madrid, Govern d'Andorra and Govern de les Illes Balears. Also, in order to produce more accurate simulations, that is model results that fit satisfactorily the observations, it has been operationally applied a post-processing bias-adjustment technique based on Kalman filter.

Technology transfer activities were also undertaken with several companies and institutions (PRYSMA, IDOM, Gobierno de Canarias, AEMET, EGMASA-Junta de Andalucía, etc.), and the air quality environmental impact analysis of new power generation and industrial installations were analysed.

» Climate Modelling

In 2011 the activities of the Climate Modelling Group were mainly related to the EC-Earth project which forges weather forecasting and climate change studies into a single framework under the seamless prediction paradigm. The Group worked in global climate simulations using EC-Earth. Activities related to EC-EARTH included porting version 2.3 to MareNostrum and diagnosing its performance in MareNostrum. An historical run was performed with EC-EARTHv2.3 for 150 years, starting from 1860. Future simulations corresponding to two different radiative forcing scenarios under the Coupled Model Intercomparison Project Phase 5 (CMIP-5) were also run in MareNostrum (RCP4.5 and RCP8.5), covering from 2000 to 2100. Results are being currently postprocessed. A 3rd future scenario is under preparation in order to test the effects of multiplying by 4 CO₂ concentration from 2000 to 2100. Those scenarios results will be part of the CMIP5 report, which will provide future climate change information to be considered in the future IPCC-AR5 report (Fig. 2).

The group also has developed a downscaling exercise over Catalonia. Two different runs of the ECHAM5 global climate model have been used to provide the boundary and initial conditions to run WRF-ARW and MM5 regional models with high resolution (10 km) over Catalonia. Simulations from 1970 to 2000 are currently being analysed and will be compared with equivalent simulations using ERA40 reanalysis data. Future runs from 2010 to 2050 are in preparation for three different emissions scenarios, namely A1B, B1 and A2 IPCC emission scenarios. Results from this project, developed jointly with the Servei Meteorològic de Catalunya, will provide useful information for the assessment of impacts over Catalonia, and the development of strategies to mitigate climate change effects.

The group continues its contribution in the IS-ENES FP7 project, devoted to fostering the integration of the European climate and Earth system modelling community and the development of Earth System Models (ESM) for the understanding of climate change. Performance evaluation of ESMs were done on the MareNostrum supercomputing architecture. In collaboration with several European groups, a prototype of a grid distributed execution of an ESMs has been tested.

» Meteorological Modelling

The work done in 2011 focused on the further development and evaluation of the modeling system NMMB/BSC Chemical Transport Model (NMMB/BSC-CTM). NMMB/BSC-CTM is a fully integrated meteorological and air quality model for global to sub-synoptic scale applications. The group has finished the implementation of the gas-phase chemistry within the meteorological driver NMMB during 2011. The model development is a team effort among several research institutions

(National Centers for Environmental Prediction, NASA Goddard Institute for Space Studies and University of California, Irvine). Evaluation tasks focused on global and regional domain applications for 2004 year. The role of the stratospheric ozone handling on the troposphere chemistry is under study with the new model. Furthermore, the impact of the photoexcited NO₂ chemistry on global air quality has been assessed with NMMB/BSC-CTM (Fig 3). Complementing the development work of the gas-phase chemistry, the implementation of a multicomponent aerosol module within NMMB/BSC-CTM for global applications started in 2011. Preliminary results of the global distribution of sea-salt have been obtained during 2011.

Within the FIELD_AC project of the FP7 framework program, the group contributed to study the sensitivity of mesoscale meteorological models on coastal meteorology. Coupling of meteorological models with current and wave models were undertaken to advance in the modelling of coastal phenomena in collaboration with partners of the project. Additionally, the group advances in the exploration of new numerical techniques to better exploit massively parallel architectures for meteorological applications. The dynamical core tested provides reliable results for dry-atmosphere test cases and the study of moist atmosphere ideal cases provides promising results.

Finally, research on clean energy resources is also carried on. A solar irradiance forecasting system for Spain by means of numerical weather prediction and statistical post-processing techniques has been analysed. An annual evaluation of the system was performed and four different post-processing methods to improve the skills of the system were applied.

» Mineral Dust Modelling

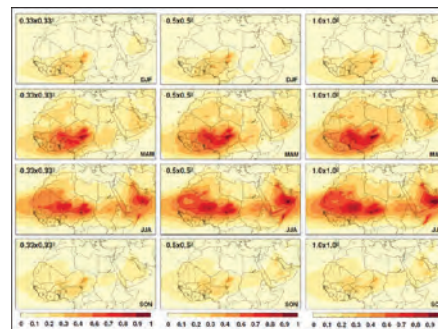


Figure 4 - Simulated seasonal model AOD for experiments 1, 9, and 10. Three spatial model resolutions between 0.33x0.33° and 1.0x1.0° are displayed from left to right

The Mineral Dust Group provides daily operational forecasts of mineral dust for North Africa, Middle East, Europe and East Asia based on the updated version of Dust Regional Atmospheric Model, BSC-DREAM8b. Also BSC-DREAM8b is offline coupled in an air quality forecasting system CALIOPE, and therefore CALIOPE is the unique operational forecasting air quality system over Europe including the contribution of Saharan dust on an hourly basis. In 2011 the Group continued with the development of the new generation atmospheric mineral dust model (NMMb-BSC/Dust) coupled on-line to the new generation unified atmospheric model NMMb of the National Centers for Environmental Prediction (NCEP). The new modelling system is intended to be a powerful tool for research and to provide efficient global and regional chemical weather forecasts at sub-synoptic and mesoscale resolutions on MareNostrum supercomputer (Figure 4) including a physically-based dust emission scheme taking into account the effects of saltation and sandblasting, soil moisture and viscous diffusion close to the ground. In this period, it is completed an extensive

evaluation and analysis of the model using a suite of observational data with specific focus on the regional scale. Also it is initiated the preparation of the model for operational dust forecasts in Northern Africa, Europe, and Middle East.

» SDS-WAS WMO Regional center

Activities in the framework of World Meteorological Organization WMO Regional Centre for Northern Africa, Middle East and Europe were also undertaken (Dust forecast, training courses, results diffusion, data management, web maintenance, etc.). The World Meteorological Organization (WMO) has launched the Sand and Dust Storm Warning and Assessment System (SDSWAS) that bridges the technological gap between research and operational services. Regional activities related to modelling, observations and applications are coordinated through the Asia/Central Pacific Regional Centre for SDSWAS at the China Meteorological Agency in Beijing, China. The Regional Centre for Northern Africa, Middle East and Europe is based at the BSC and the AE-Met (Spanish Weather Service) in partnership with other operational and research organisations (e.g. Meteo-France, UK Met Office, ECMWF, LISA, LSCE, IFT, EUMETSAT, CNR, AERONET/PHOTONS, Tunisian Met Service, University of Athens, University of Tel Aviv, Egyptian Meteorological Agency, METU and NMHSs).

Two training Courses on WMO SDS-WAS (satellite and ground observation and modelling of atmospheric dust) held in Antalya, Turkey. It has been organized and funded by the World Meteorological Organization (WMO), EUMETSAT and the Turkish State Meteorological Service (TSMS) with the collaboration of the Spanish State Meteorological Agency (AEMET) and the Barcelona Supercomputing Center (BSC-CNS). It has been coordinated by the Regional Center for Northern Africa, Middle East and Europe of the WMO SDS-WAS programme.

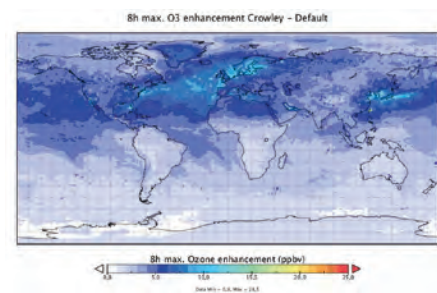


Figure 3 - Impact of the photoexcited NO₂ chemistry at global scale assessed with NMMB/BSC-CTM model



Figure 5 - Web-based portal for user access to regional research and forecast activities and services of the WMO Regional Centre for Northern Africa, Middle East and Europe



Modesto Orozco,
Director of the
Life Sciences
Department

The aim of the scientists in the Life Sciences Department is to understand the molecular biology and evolution of living organisms using theoretical models and simulation algorithms.

» Overview

The Department benefits greatly from its unique situation in a major supercomputer centre, and also exists within a large and active environment of research in experimental biology. Its research line is tightly integrated in a collaborative effort with the Institute for Research in Biomedicine (Joint IRB-BSC Research Program on Computational Biology) and also has strong collaborations with ICREA and the National Institute of Bioinformatics (INB). Major areas of research include Molecular Modelling, Structural Bioinformatics, Computational Genomics, Network Medicine, Subatomic Study of Protein Functions, and Protein-Protein Docking.

Developments of note in 2011 include the awarding to Life Sciences Director Modesto Orozco of an Advanced ERC grant, the launching of MedicaHead, an integrated platform for technology transfer which aims to join all the different methodological developments carried out by the groups in the department, and continued growth in personnel and scientific output.

» Joint IRB-BSC Program on Computational Biology

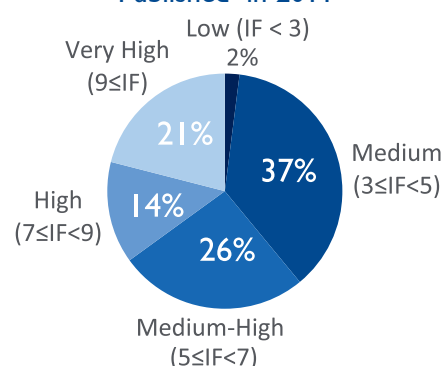


INSTITUTE
FOR RESEARCH
IN BIOMEDICINE

The Computational Biology Program was created as a joint venture between the BSC-CNS and the Institute for Research in Biomedicine (IRB Barcelona) with the mission to face the computational challenges in molecular biology. The Program, coordinated by Modesto Orozco, includes researchers from the Structural and Computational Biology Programme at IRB Barcelona and from the Life Science Department of the Barcelona Supercomputing Center. During the lifetime of the Program, scientists from IRB Barcelona will enjoy access to MareNostrum, the most powerful supercomputer in Europe, and other internal computational resources at the Barcelona Supercomputing Center. In return, BSC-CNS scientists will also have permanent access to services and facilities at the Institute for Research in Biomedicine. The Program, funded in equal parts by IRB Barcelona and BSC-CNS, established an external scientific committee, which oversees and evaluates the joint activities carried out by both institutions.

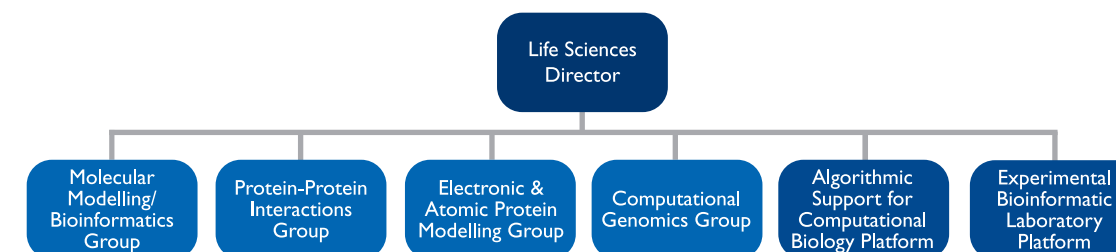
The Program pursues excellence in research in bioinformatics and computational biology. Its research lines range from atomistic studies on bio-macromolecules to the analysis of high-order cell regulatory mechanisms, sequence analysis, gene regulation and expression, systems biology, network medicine and drug design. With the Joint IRB-BSC Program publishing 50 journal papers during the year, achieving an institutional H-index of 72.

ISI Impact Factor of Articles
Published in 2011



» Organisational Structure

The structure of the Department and the technology platforms enables coverage of the entire field of computational biology, from atomistic detail to holistic views of the entire ecosystem. The Groups integrate different independent researchers, led by senior scientists, who work in different aspects of computational biology.



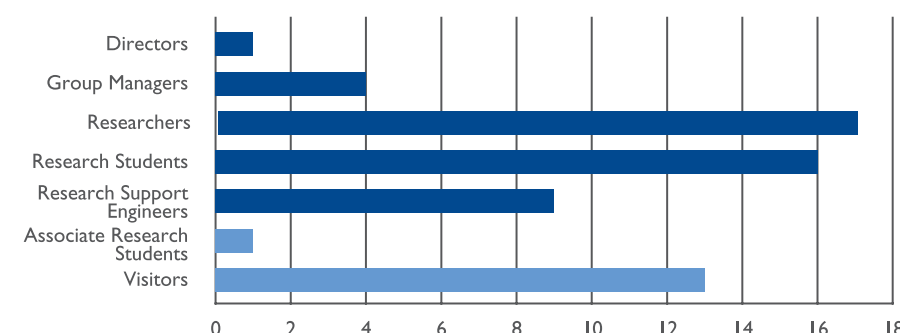
Structure of the Life Sciences Department of the BSC-CNS

The Department once again grew strongly during 2011 thanks to the success in gaining new projects, reaching 60 people during 2011.

The Department is composed of 4 research groups and 2 research platforms:

- ▶ BSC-CNS research groups Electronic and Atomic Protein Modeling (EAPM), Protein Interactions and Docking (PID) and Computational Genomics (CG),
- ▶ the Molecular Modeling and Bioinformatics (MMB) and the Experimental Bioinformatics Laboratory (EBL), jointly run by BSC-CNS and IRB,
- ▶ the Computational Node (CN) of the National Institute of Bioinformatics, jointly run by BSC-CNS and INB.

Life Sciences Department Staff & Collaborators 2011

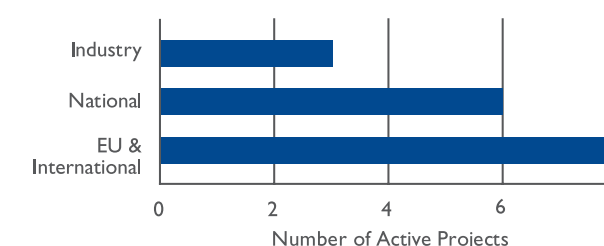


» EU & National Projects

Key activities during 2011 included participation in the following key BSC-CNS projects:

- ▶ Blueprint - A BLUEPRINT of haematopoietic epigenomes. Funded by FP7.
- ▶ EESI - European Exascale Software Initiative. Funded by FP7.
- ▶ ScalaLife - ScalaLife—Scalable Software Services for Life Science. Funded by FP7.
- ▶ TransPLANT - Trans-national Infrastructure for Plant Genomic Science. Funded by FP7.
- ▶ CONSOLIDER SYEC - Supercomputation and eScience. Consolider program, Spanish Government.
- ▶ ELIXIR - Construction and operation of a sustainable infrastructure for biological information in Europe to support life science research and its translation to medicine and the environment, the bio-industries and society. Funded by FP7.
- ▶ MITIN - Integration of the systems models of mitochondrial function and insulin signalling, and its application in the study of complex diseases. Funded by FP7.
- ▶ PELE - a la carte drug design tools. ERC Advanced Grant
- ▶ MEDICAHEAD - a platform to identify new medical treatments. VALOR project, Catalan Government.
- ▶ Biochemical Modelling. Funded by CICYT, Spanish Government.
- ▶ Protein Docking Challenges. Funded by CICYT, Spanish Government.

Life Science Projects 2011



» Scientific Output

The Life Sciences Department defines a unique environment that combines very active groups working in computational biology with top supercomputing and experimental resources. The research efforts can be classified into four main areas:

- ▶ Research in Target & Drug Discovery: Developing new tools for the pharmaceutical industry.
- ▶ Research in Genomics & System Biology: Understanding the origin of diseases and infection mechanisms.
- ▶ Research in BioSupercomputing: Improving the use and access of supercomputing and database resources in Life Sciences.
- ▶ Basic Research in BioPhysics: Discovering the mechanisms of biological systems at the molecular scale.

Organised Events:

- ▶ ICREA Network Medicine conference (<http://mmb.irbbarcelona.org/netmed2011>) sponsored by ICREA, Biocat, Genoma España, the Spanish government and the Catalan government. More than 150 international scientists attended, with presentations from 20 top keynote speakers.
- ▶ AMBER European hands-on workshop (<http://mmb.irbbarcelona.org/amber2011/>) co-organized by AMBER and the Joint program and sponsored by NVIDIA. Focused on Drug Discovery and GPU portability, the workshop was very successful with the 60 seats filled out in a few days, and a waiting list of over 100 computational biologists.

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Molecular Modelling and Bioinformatics (MMB) Group

The Group's long term objective is to understand the behavior of living organisms by means of theoretical models, whose roots are anchored in the basic principles of physics and chemistry. With this general aim the Group works with different methodologies, from mining of biological databases to classical dynamics and quantum chemistry calculations. The use of this wide range of methodologies allows the exploration of a wide range of problems, from drug design to genome analysis. Special emphasis is made in connecting basic interactions with global properties of biological systems.



Electronic and Atomic Protein Modeling (EAPM) Group

The Electronic and Atomic Protein Modeling Laboratory in the Life Science department at the Barcelona Supercomputer center is devoted to the development of computational algorithms to advance in the understanding of protein's biochemistry and biophysics. For these purposes, the Group applies and develops two different set of techniques: classical and quantum simulations.



Protein Interaction and Docking (PID) Group

The Group's main research focus is the study of protein interactions at the molecular level. Proteins do not act alone but through the formation of specific complexes with other proteins and biomolecules. Understanding the process of protein association is important not only to increase basic knowledge of essential life processes at molecular and cellular level, but also for biomedical and therapeutic applications. The key challenge undertaken by the Group is the development of new computer tools for the modeling of protein interactions, and the large-scale application with the help of high-performance computing resources.



Computational Genomics (CG) Group

The aim of the Computational Genomics Group is to investigate different processes of the biology of genomes and to contribute to the understanding of how the sequence and the structure of these macromolecules determine their basic functions. The Group's research lines are, on one side, centered into deciphering the code and the mechanisms that control when and where genes are expressing their function in the cell. The Group has developed tools and strategies for the identification and classification of gene regulatory regions to study their function, their evolution and their role in the adaptation of organisms to their environment. The Group is also interested in finding how modifications and alterations of the sequence are

directly responsible or confer susceptibility to certain diseases. This is done through the application of systems biology approaches and sequence analysis strategies involving large DNA sequencing efforts to understand the causes and the evolution of complex pathological processes, such as type 2 diabetes, anemia, and even the immunological rejection of transplanted liver. Simultaneously, the Group invests time in developing tools for the analysis of the cancer genome in the context of the Cancer Genome Project to identify somatic mutations, with particular interest on those affecting regulatory regions. Finally, the Computational Genomics Group devotes collaborative efforts within high impact projects related to the assembly and the primary analysis of genomes and metagenomes.

INB-BSC-CNS

The National Institute of Bioinformatics is a research platform funded by the Instituto de Salud Carlos III with the aim of giving support to Bioinformatics groups related to Spanish Genomic and Proteomics projects. The Institute has a nodal structure distributed among the most important bioinformatics research groups in Spain. Barcelona Supercomputing Center's Life Sciences program hosts the Computational Bioinformatics node of INB (INB-GN6). The special purpose of the computational node, with the help of BSC computational resources and expertise, is to provide access to biological databases, both generic and related to supported projects, and to develop web services and applications covering a broad range of analysis software.



Experimental Bioinformatics Laboratory (EBL) Platform

The Experimental Bioinformatics Lab (EBL) is part of the collaborative research program between the Institute of Research in Biomedicine (IRB Barcelona) and the Barcelona Supercomputing Center (BSC). The EBL is devoted to experimentally verify in silico models performed by computational scientists in the areas of systems biology (protein-protein interaction networks) and genome regulation. Experimental functional genomics techniques (e.g. high-throughput yeast-two-hybrid screening or genome-wide nucleosome position mapping) in combination with biochemical and cell biology methods are implemented.



José Maria
Cela, Director
of the CASE
Department

The aim of the Computer Applications in Science and Engineering (CASE) Department is to develop new computational strategies to simulate complex problems specifically adapted to run efficiently on modern supercomputers. Collaborative projects with industry and scientific groups are the main motivation underlying all development carried out in CASE.

» Overview

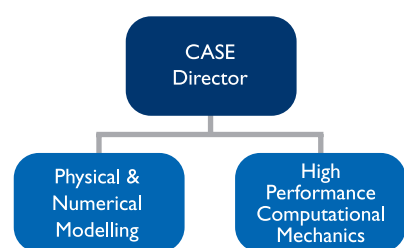
The applications developed by the CASE department are truly multidisciplinary, requiring a deep level of expertise in many fields. In order to

successfully develop these applications, the skills of the CASE team in numerical methods and parallel programming must be complemented by experts in the appropriate areas. The Department therefore develops collaborations with other scientific groups in all areas of science and technology. Examples of institutions with strong research links with CASE include CIEMAT, CSIC, IAC, ICFO, IMDEA and different universities. This is complemented with strong links with Industrial partners in need of advanced simulations of complex technology problems, such as REPSOL or Iberdrola. The main research field of CASE is High Performance Computational Mechanics, which requires a deep background in Computer Science, Physics and Numerical Methods. Major research areas are Computational Fluid Dynamics and Solid Mechanics, Ab-initio DFT and TD-DFT molecular dynamics, Seismic Imaging and Parallel Programming. Major application areas are Aerospace, High Energy Physics (plasma core and edge transport, plasma wall interaction), Biomechanics (Cardiovascular and Respiratory systems), Geophysics and Atmospheric flows. Recently, CASE has also opened a new line in large scale social simulation.

To achieve its objectives, the CASE team develops and co-develops four main high performance codes, which are used in national/international projects and are the core of the collaborations and contracts with companies:

- ▶ Alya: HPCM system. Fluid mechanics, Solid mechanics, Electric propagation, Combustion, etc.
- ▶ FAI3D: Volcanic ash transport. Used in production in South American Volcanic Ash Advisory Centres (VAAC)
- ▶ BSIT (Barcelona Seismic Imaging Tools): Acoustic/Elastic waves, Forward Modelling, RTM, FWI. Promoted by Repsol.
- ▶ SIESTA: Ab-initio molecular dynamics. CASE is a co-developer of this code.

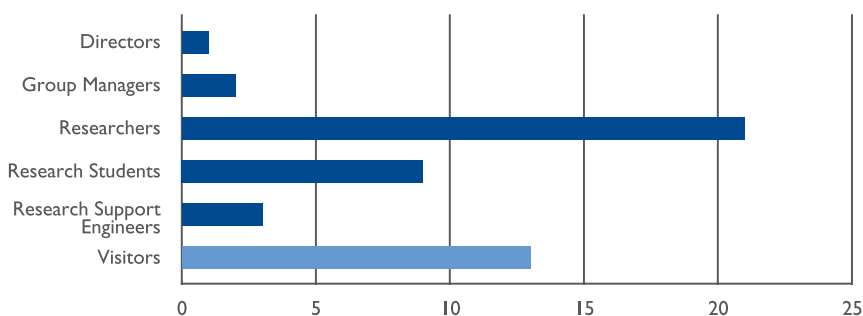
» Organisational Structure



The CASE Department is led by José María Cela. The research lines fall naturally in two main Groups; Physical & Numerical Modelling (PNM) and High Performance Computational Mechanics (HPCM). Each Group consists of around 15 people, comprising several senior scientists, post and pre-doctoral students and visiting scientists. PNM research lines are horizontal and HPCM lines are vertical, in the sense that the PNM Group is in charge of developing the core components which are then assembled and modified as required by the HPCM Group into applications tailor-made to meet specific project needs. Due to the multidisciplinary character of CASE research activities, both groups are involved in all projects.



CASE Department Staff & Collaborators 2011



» Key Projects

In 2011, the CASE Department carried out work under the scope of the following projects:

EU funded projects

- ▶ PRACE IIP: Partnership for Advanced Computing in Europe.
- ▶ ETSF: Generating a software infrastructure for the spectroscopy community.
- ▶ W2PLASTICS: Magnetic Sorting and Ultrasound Sensor Technologies for Production of High Purity Secondary Polyolefins from Waste.
- ▶ DEISA: Leading work packages 5 and 9 on "Enabling of Applications".
- ▶ C2CA: Recycling of Concrete to Cement and Aggregates, modeling combustion, compressible flows, radiation and solid N-body impact.
- ▶ COPA-GT: A Marie Curie training project for turbine operation in aerospace and energy production plants.
- ▶ NEMO: A Marie Curie training project for the next generation of European volcanologists.
- ▶ INNFACTO2011: Wind model based on the open source CFD code OpenFoam and applied supercomputing techniques.
- ▶ Scalable Parallel Simulation for Policy Analysis, to create HPC tools for the analysis of migration processes.
- ▶ MontBlanc: porting of EUTERPE code to MontBlanc Architecture.

Enterprise funded projects:

- ▶ REPSOL-BSC Research Center: a joint research unit to develop state of the art tools in seismic imaging, including Full Waveform Inversion, RTM with elastic waves and controlled source electromagnetic methods.
- ▶ Iberdrola: Optimisation of wind farms both on-shore and off-shore.
- ▶ Confidential Partner: Race yacht design

Nationally funded projects:

- ▶ Supercomputación y e-Ciencia (CONSOLIDER): Coordination of the project, to develop a set of scientific Grand Challenges for Petaflop supercomputers and design the architecture of those machines.
- ▶ Simulpast. Simulating the past to understand human behaviour (CONSOLIDER), to develop an innovative and interdisciplinary methodological framework to model and simulate ancient societies and their relationship with environmental transformations.
- ▶ ATMOST (Plan Nacional), to model ashes and contaminant dispersion in the atmosphere.
- ▶ MIVAL3D (Generalitat de Catalunya), to simulate the cardiac mytral valve.

» Scientific Output

Except for work that is private and confidential and can not be published, research results of the CASE Department were presented in congresses and conference lectures as well as a number of scientific publications, including: ParCFD2011, DDM20, SC2011, the International Conference on Computational & Mathematical Biomedical Engineering, FE11, USNCCM11.

In 2011, the CASE Department organised the 23rd. International Conference in Parallel Computational Fluid Dynamics ParCFD2011.

Case Projects 2011



International and national collaboration projects in biomechanics:

- ▶ Airflow in the Human Respiratory System, with Imperial College London to simulate the complete human respiratory system, including the air surrounding the face, partially supported by HPC-Europa.
- ▶ Computational Cardiac Mechanics: Coupled electromechanical simulation of the heart, including the mytral valve, to develop a simulator of the cardiac function considering the electrical activation potential and its coupling to the mechanical pumping action. Collaboration with UAB, Htal. St. Pau, Htal. Clinic, Htal. Bellvitge, T-Systems, PULSO, UPC, Univ. Lleida, IMDEA Materiales and the University of Cape Town.
- ▶ Mechano-biology with Uni. Zaragoza (Spain).
- ▶ Skeletal muscles with Uni. Illinois (USA).

Other collaborations:

- ▶ Solid Mechanics: with IMDEA (Spain) to develop a HP solid mechanics module, including X-FEM for fracture simulations.
- ▶ Turbulence: Application of turbulence models to high Reynolds number flows, with EDF (France), Univ. Manchester (UK), STFC, Daresbury (UK).
- ▶ Numerical simulation of the human large airways, with Imperial College (UK).
- ▶ Participation in "Musealización didáctica de espacios patrimoniales a partir de aplicaciones reactivas con contenidos multiplataforma, telefonía móvil y superficies táctiles", with DIDPATRI (Univ. Barcelona).
- ▶ Collaboration with IPHES (Spain) to develop a dynamic population simulator for hominid groups based on agents on a supercomputing infrastructure.
- ▶ Participation in "Arqueología y memoria de la aviación republicana (1938-1939)", funded by Ministerio de Presidencia, to apply new research methodologies to understanding the role of aviation during the Spanish Civil War.
- ▶ Partnership in Scientific Visualization VU@BSC, with inVisu (Canada).
- ▶ Car aerodynamics: DES models for car aerodynamics, with Uni. Hiroshima (Japan)
- ▶ EUTERPE code, with Max Planck IPP and CIEMAT, to port the code to new hardware platforms.

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CASE department consists of two formal groups: Physical and Numerical Modelling and High Performance Computational Mechanics. However, due to the industrial impact of the Kaleidoscope project and the work carried out by its associated team, the Seismic Imaging “group” deserves a separate and detailed description.

Physical and Numerical Modelling (PNM)

Computational Mechanics

The PNM Group researches basic themes, such as numerical modelling of physical phenomena, stabilisation techniques, algorithms and solution strategies, parallelisation strategies, coupled problems with domain decomposition methods, optimisation algorithms and error estimation techniques. In addition, PNM researchers investigate pre-process, post-process, data management and visualisation topics. The research lines within PNM cover the full range of techniques required to simulate a physical problem, usually governed by partial or ordinary differential equations. The main areas of investigation are:

- Mathematical modelling of a given physical process.
- Numerical modelling of the mathematical equations - space and time discretisation: high order time integration schemes; variational multi-scale; finite element; domain decomposition (Chimera, non-overlapping meshes); turbulence models; PIC methods; spectral methods; particle tracking and collisions, etc.
- Numerical algorithms to solve the discrete equations efficiently, or to couple a set of algorithms to solve complex physical problems: explicit and implicit schemes, monolithic and fractional algorithms, preconditioners and multigrid.
- Efficient implementation in a computational mechanics code: distributed/shared memory parallelisation with MPI/OpenMP, code optimisation; architecture dependent implementation (VMX, Cell).
- Code performance analysis and optimisation.
- Visualisation: in 2010, a tight collaboration with a post-process Canadian company inVisu was initiated. The objective is to manage (I/O) simulation results in an efficient way and to post-process them in a parallel environment. Parallel I/O libraries were also implemented.

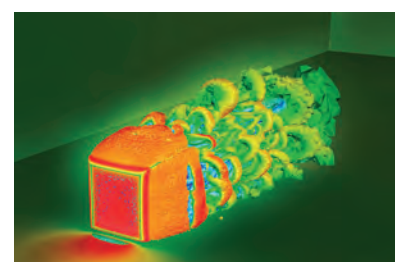
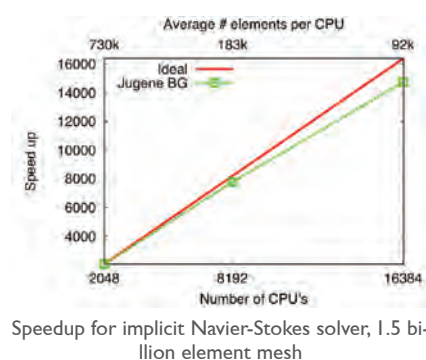
Due to the installation of new large scale supercomputers in Europe this year (Curie in France, Jugene in Germany), the Group dedicated a lot of resources to upgrade the high performance computational mechanics (HPCM) code Alya. Among the developments:

- Pre and post-process: Mesh multiplication (Parallel, uniform and on-the-fly mesh refinement and generation on the fly of up to 10 billion element meshes), enhanced scalability (Almost linear speedup obtained for more than 16000 CPUs), new postprocess format and HDF5 format (Postprocess strategy in Alya has been redesigned and collaboration with INVISU (Canada) to do on-the-fly visualization), chimera method in HPCM (Application to turbulent flows with free surface and solid mechanics).
- Solvers: Schur complement solver for symmetric scalar equations, sparse direct solver and preconditioner; a parallel version of SIESTA code with better load balancing and sparse iterative eigensolvers.
- Physical modeling: Mechano-biological model (Collaboration with Uni. Zaragoza), turbulence models (Models specially designed for wind farm applications (Iberdrola)), DES models, a large-strain solid mechanics simulation for anisotropic cardiac tissue, and lagrangian particle tracking for W2Plastics and C2CA projects.
- Numerical modeling: ALE method for mesh motion, Low-Mach model for C2CA project, free surface parallel solver for sailing boats, rigid body-fluid coupling, electro-mechanical coupling, fluid-structure coupling, and variational multiscale methods for compressible flows.

Computational Social Sciences

Since 2009, the Group has worked on the design of applications specially designed for use in social sciences and policy analysis areas. The Group is developing a new simulator capable of executing Agent-Based Models of human societies in a HPC environment, in order to explore:

- Emergence of behavioral patterns in human societies, understood as complex systems.
- Interaction between societies and their relationship with environment and landscape.
- Impact of change in human groups and population dynamics (both ancient and present).
- Design of artificial societies as models to understand human behavior.
- Methodological and theoretical foundations of social simulation.



DES simulation of car aerodynamics

- Volcanos ash transport.
- These topics are analysed from a multidisciplinary approach, as CASE joins efforts with research groups belonging to different disciplines, with diverse perspectives of social interaction (i.e. Archaeology, Demography, Economy, Heritage, History and Sociology).

High Performance Computational Mechanics (HPCM)

The HPCM Group conducts application research and development in different science and technology domains where simulations are needed: aerospace, bio-mechanics, solid state physics, high energy physics, geophysics, environment, meteorology, etc.

The activities of the HPCM Group are driven by direct interaction with users and industry. Usually the core problem requires modelling of physical processes which then must be solved by intensive numerical calculation. The principal application fields that have been developed to date with Alya, Fall3D, BSIT and SIESTA are:

- Alya applications: Biomechanics (hemodynamics, respiratory system air flow, cardiac simulations), building, energy and environment (mesoscale, urban environments, wind farms, plastics recycling), and vehicle dynamics (cars, racing yachts, high speed trains).
- Fall3D applications: Atmosphere science (Volcanic ash transport).
- BSIT applications: Geophysics (seismic imaging and oil reservoir simulations).
- SIESTA Applications: Ab-initio DFT and TDDFT molecular dynamic simulations.
- Other applications such as plasma physics

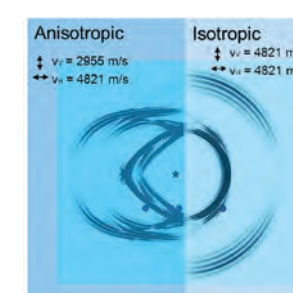
Within these fields, in 2011, some of the applications developed by the HPCM Group were:

- A large-strain solid mechanics simulation for anisotropic cardiac tissue. Collaboration with Hosp. Sant PAU, Univ. Autònoma de Barcelona.
- DES simulation of car aerodynamics. Collaboration with Univ. Hiroshima.
- High accuracy racing yacht hydrodynamics. Confidential contract.
- Simulation and optimization of a plastics recycling setup. W2Plastics project.
- Airflow simulations of the human large airways during normal breathing cycles. HPCEuropa2 project, collaboration with Imperial College (UK).
- An RTM seismic imaging facility on GPUs. Repsol contract.
- Wind farm simulation using RANS models. Iberdrola contract.
- Dynamic atmospheric mesoscale simulation.
- Ash transport: el Hierro (Spain), Puyehue (Patagonia), Eyjafjallajökull (Iceland).



Cardiac model

REPSOL-BSC Research Center



Elastic Wave propagation in anisotropic media

New hydrocarbon discoveries suggest that large reservoirs might lie in the Atlantic shelves of America and Africa, hidden under saline or basaltic bodies. In order to localise and retrieve these hydrocarbons, new imaging methods to explore these sub-salt areas are being developed, which will require supercomputers with a peak performance in the order of 10 Petaflops, requiring innovative computer architectures.

The research focuses on the use of elastic and electromagnetic wave modelling and inversion to develop new imaging algorithms, and in the practical implementation of those algorithms on different computer architectures.

In recent years state-of-the-art seismic imaging tools were developed (Kaleidoscope project) and received international recognition and awards. These tools used acoustic wave equations, requiring computers of 100 TFlops peak performance, however improved solutions require the use of elastic waves, multiplying computational needs 50-fold.

The research is focused on solving 4 grand challenges in hydrocarbon exploration:

- Use elastic wave equation for modelling large onshore exploration surveys.
- Develop a full waveform inversion algorithm based on elastic waves.
- Develop a geophysical inversion method for electromagnetic waves.
- Couple the elastic and the electromagnetic inversion procedures to obtain a novel reservoir characterisation tool.



Sergi Girona,
Operations
Department
Director

The key mission of the Operations Department is to ensure the continued availability and accessibility of RES systems 24 hours a day, 7 days a week and to provide support to all the users of the RES. Further core objectives are to manage upgrades to the MareNostrum and other RES nodes; facilitate access to RES facilities, including online electronic applications, remote access, and porting of code; manage the environmental aspect of the BSC-CNS installations; manage the technical aspects of integration of the MareNostrum in the DEISA and European HPC network grids; and ensure that RES staff receive appropriate training and skills development in order to be able to professionally carry out their duties in an environment of constant technological change and advancement.

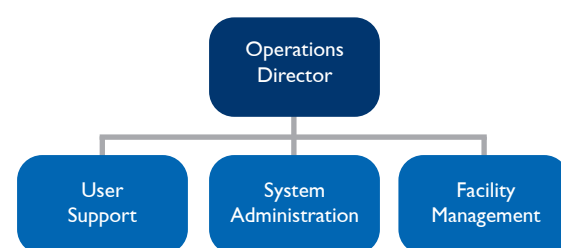
» Overview

The Operations Department, led by Sergi Girona, ensures the continued daily functioning of the RES supercomputers and remote access by users both within Spain and internationally. In addition to all the routine maintenance and operations tasks, the Department staff are also heavily involved in planning and designing new systems and support facilities. Furthermore, the entire Department participates in European projects such as PRACE, EESI, DEISA2, HPC-Europa and HPCWorld.

The constant upgrading and utilisation of cutting edge technology implies that staff within the Department, liaison staff at the RES nodes and scientific users all face continuous change in systems and procedures. The management of these changes and their dissemination to all who may be affected by them are also regular activities of the Department.

Construction of the new BSC-CNS building advanced significantly in 2011, and the corresponding engineering for hosting a large supercomputer was also progressed. With a computer room of 900 square meters and 800 square meters for infrastructures (including air conditioning, water pipes, pumps, etc.) the new facility will be cutting-edge. The new space, along with updates of the technology in the Chapel, will permit the capacities of BSC-CNS to be greatly extended.

» Organisational Structure



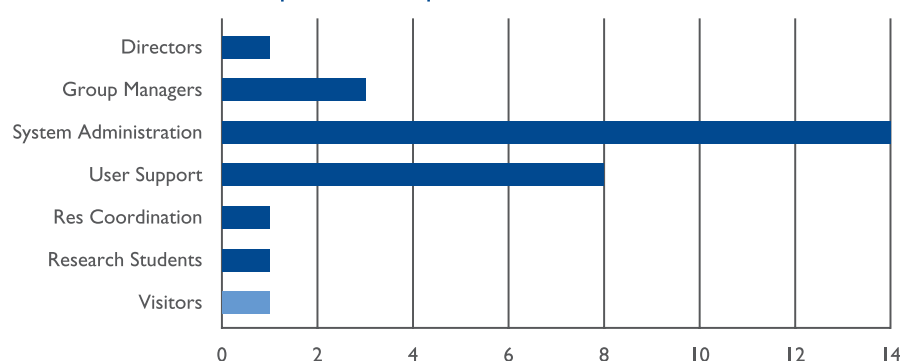
The Operations Department is structured in three groups: System Administration, User Support, and Facility Management.

Systems Administration supervises the daily operations of two key resources: the MareNostrum Supercomputer and the Spanish Supercomputing Network (RES), bearing responsibility for system administration, security, resource management, networking and helpdesk. This group also takes care of running all the other IT equipment installed at the BSC-CNS and related facilities.

User Support is responsible for direct user support providing detailed knowledge of programming models, libraries, performance tools and applications, and is also responsible for management of the BSC website, and the management and support of 3D visualisation equipment.

Facility Management is responsible for the safe and efficient working condition of key BSC-CNS facilities, such as the MareNostrum supercomputer and ancillary power, data and environmental systems.

Operations Department Staff & Collaborators 2011



» Key Projects

The Operations Department was involved in the following projects during 2011:

- ▶ **RES (Red Española de Supercomputación):** The Spanish Supercomputing Network offers coordinated HPC services to the Spanish scientific community. The Operations Department is responsible for the coordination of the network, including all support and administration services.
- ▶ **DEISA2:** the Distributed European Infrastructure for Supercomputing Applications is a consortium of leading national Supercomputing centres that aims to foster pan-European world-leading computational science research. The Operations Department is involved in most of the work packages, and coordinates the participation of the BSC-CNS in the project.
- ▶ **PRACE IIP:** In the PRACE First Implementation Phase, the Operations Department is involved in WP6, WP7 and WP8, and coordinates the participation of the BSC-CNS in the project.
- ▶ **PRACE 2IP:** In the PRACE Second Implementation Phase, the Operations Department is involved in WP2, WP7 and WP10, and coordinates the participation of the BSC-CNS in the project.
- ▶ **HPC-EUROPA-2:** In the Pan-European Research Infrastructure on High Performance Computing, the Operations team is involved in work packages NA2 and JRA2, and coordinates the participation of the BSC-CNS in the project.
- ▶ **HPC-WORLD:** HPCW is a consortium of 6 key-players in High Performance Computing, all around the world, 5 Supercomputing Centers (CINECA, BSC-CNS, FZJ, SDSC and BlueFern) plus GENCI, the French national agency in charge of HPC coordination.
- ▶ **EESI:** The objective of this Support Action, co-funded by the European Commission, is to build a European vision and roadmap to address the challenges of the new generation of massively parallel systems composed of millions of heterogeneous cores which will provide multi-Petaflop performances in the next few years and Exaflop performances in 2020.
- ▶ **EUDAT:** The EUDAT project aims to contribute to the production of a Collaborative Data Infrastructure (CDI). The project's target is to provide a pan-European solution to the challenge of data proliferation in Europe's scientific and research communities.

» System Administration

The System Administration Group is responsible for general operation, upgrades and maintenance of the MareNostrum and other BSC-CNS systems, as well as providing technical support to the operators of the other RES nodes. The Group also undertakes numerous special projects for continuous improvement of BSC-CNS systems and services and provides technical support to key research projects.



BSC HPC Data Services

During 2011 the Operations Department moved into production the new MareNostrum storage system, a 1.9 PB GPFS infrastructure with an aggregated performance of 15 GB/s system. Apart from being used by the different HPC clusters as the central production filesystem, 8 servers with 10 Gbit connectivity will be used exclusively for providing data services to internal and external users.

Some of the Data services that are provided: Mass transfer of data from/to the Internet via several technologies (Grid-FTP, BBP, SCP/SFTP, FTP+SSL, ...), Batch System for data migration from/to HSM and other local storages, NFS and CIFS exports for mounting internal workstations, Interactive access via SSH from the Internet.

More data services will be deployed during 2012, especially with the participation of BSC-CNS in the EUDAT project.

MinoTauro, the most efficient HPC system in Europe in 2011

During 2011 the Operations Department established the tender and implemented a new HPC cluster called MinoTauro, which is the most efficient HPC cluster in Europe and 7th of the World as stated in the Green500 list with a value of 1266 MFLOPS/Watt. On the other hand, MinoTauro is classified in position 114 of Top500 Supercomputers with a value of 103.2 TFlops, being the fastest supercomputer in Spain.

MinoTauro is a cluster composed of 128 Bull b505 compute nodes, with a total of:

- ▶ 1536 Intel Cores at 2.53 GHz
- ▶ 256 NVIDIA M2090 Cards
- ▶ 3 TB of main memory

Each node has an SSD internal drive with 250GB for operating system and execution out-of-core. MinoTauro has a non-blocking IB-QDR (40 Gbits per link) network for MPI traffic and 14 links of 10 Gbit Ethernet Network to connect to the central GPFS BSC Storage.



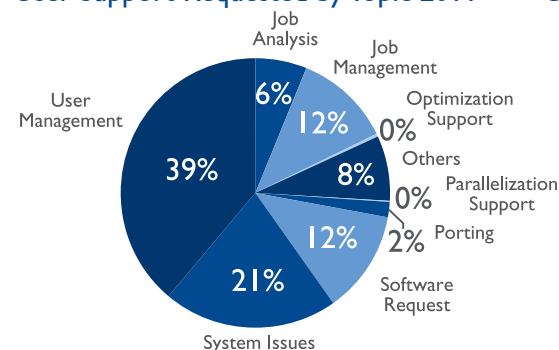
» User Support



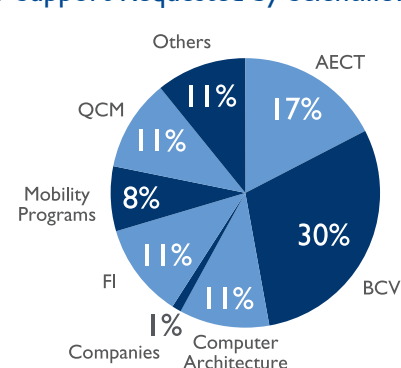
The User Support Group provides assistance with all aspects of scientific computing, this assistance includes general user support, code optimization and parallel model building support and porting serial and parallel codes for supercomputers such MareNostrum. The group is also involved in the creation of scripts for ease of use as well as assistance with software packages and tutorials on specialized topics or programs. In addition the support group is also in charge of the SC virtual reality and 3D visualization system, the BSC-CNS official website, the Intranet and the graphical design activities.

Some 4297 support requests were received in 2011 as presented in the figures below, split by support request area and by topic.

User Support Requested by Topic 2011



User Support Requested by Scientific Area 2011



Highlighted Projects

EUDAT



The User Support group is coordinating the participation of BSC-CNS in EUDAT, one of the largest projects in Europe with the mission to create a Collaborative Data Infrastructure (CDI) to provide a pan-European solution to the challenge of data proliferation in Europe's scientific and research communities. EUDAT comprises 25 European partners, including data centers, technology providers, and research communities and funding agencies from 13 countries. The project was launched on the 1st of October 2011, and is co-funded by the European Commission's Framework Program 7.

BSC-CNS is a key contributor, acting as WP leader and actively involved in the core tasks of the project.

New CMS for the BSC-CNS website

During 2011, the BSC-CNS website was migrated from a proprietary software to an Open Source CMS (Drupal). This CMS was chosen for its features and performance, experience gained in various projects over several years, and the opportunities to learn from and contribute to the huge existing user community. The migration of the web involved transferring a large number and variety of contents and the development and customization of new and existing Dru-

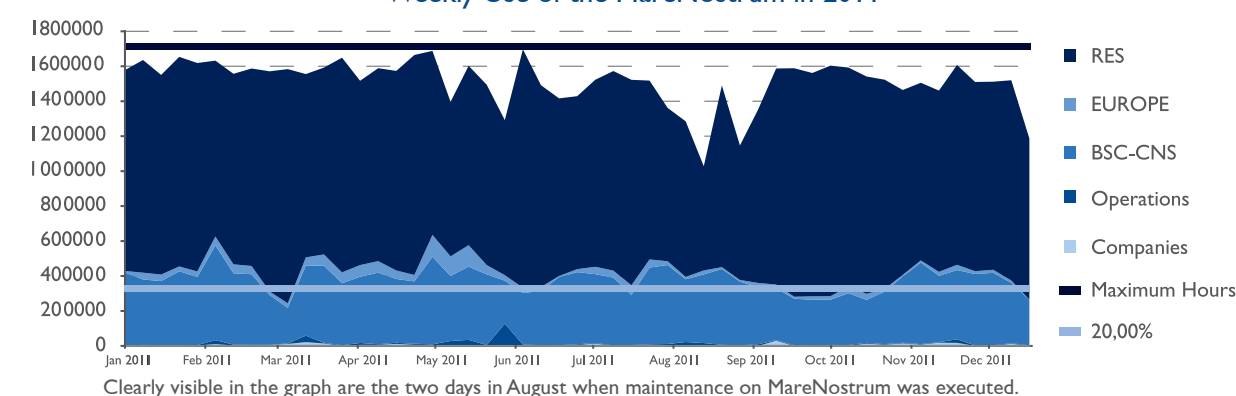
pal modules such as a LDAP and CAS modules, including interface enhancements to both end users and publishers, a new bibliographic system which allows working with scientific standard systems and formats such as BibText Records, among others, a fine grain control of user access permissions, the usage of semantic URLs, customised personal user pages, the display of audiovisual content, and especially, the flexibility to make changes and incorporate new features.

MareNostrum Performance 2011

MareNostrum was in full production the whole year, except for maintenance periods. Using the operative part of the year as the basis for calculations, the observed system utilisation was approximately 87%. In addition to BSC-CNS internal groups, more than 294 external groups accessed the MareNostrum system.

Utilisation is defined by the formula:
$$\left(\frac{\text{total}_{\text{cpu_hours}}}{\text{total}_{\text{hours}}} \right) \times 100$$

Weekly Use of the MareNostrum in 2011



» Facility Management

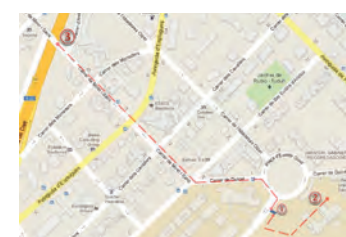
The mission of Facility Management (FM) is to keep the BSC-CNS facilities under its purview in a safe and efficient working condition.

The department provides support and recommendations for building and infrastructure expansions and renovations:

- ▶ FM participates in project, proposal and project management stages of new investments.
- ▶ FM maintains major building systems, performs required maintenance and supervises vendors for all architectural, mechanical and electrical requirements of its facilities.
- ▶ FM defines and places purchase requests for fixed asset materials.
- ▶ FM receives proposals and authorises payments for electrical and other utility needs of its facilities.
- ▶ FM coordinates and tracks service calls for repairs.



MareNostrum III



25 kV Underground Line & Switching substation.

In order to provide more powerful computation to researchers, in 2011 BSC-CNS decided to expand existing infrastructure.

In accordance with the new power requirements, construction works of a new medium voltage distribution line with the capacity of 2.500 kW were initiated. Switching substation 1 and the installation of medium voltage cables between the substation and the pre-existing transformer center (Bunker) 2 were completed.

Electrical Installations: Required IT Power: 1.400 kW Only one of the three existing transformers will be replaced with a 2000 KVA distribution transformer. Main and some sub switchgear systems will be replaced with new switchgear systems.

AC Installations: Total cooling capacity required for the new system will be 1400 kW.

Two new chillers will be installed. Each chiller will have 500kW cooling capacity and they will be integrated in to existing system of 5 chillers. The water temperature from the chillers will be 9-16 °C (variable).



The chillers.



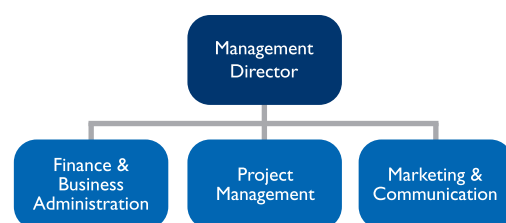
Ernest Quingles, Management Department Director

The key mission of the Management Department is to optimise coordination of the activities of the BSC-CNS and provide consolidated planning and management of support services to better meet the future challenges facing the centre. Other core objectives include reliable and timely financial reporting, human resources management, and building awareness of the BSC-CNS, its mission, activities and its services. The department also assists other departments in identifying, applying and managing competitive projects, initiating and developing systems and processes to increase the efficiency and effectiveness of staff and the quality of work, and developing electronic management tools.

» Overview

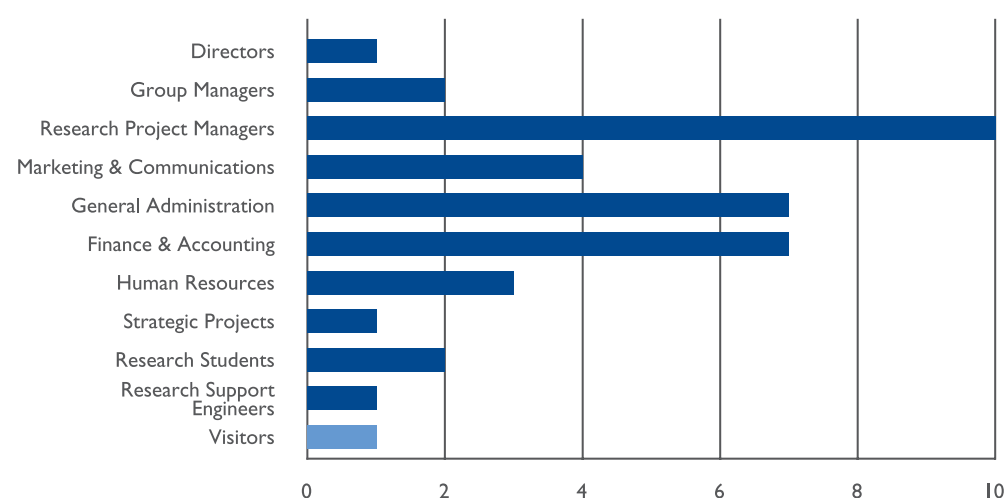
The Management Department, led by Ernest Quingles, aims to provide administrative and management services to all the other departments. It is responsible for the administration of finances, projects, human resources, communication and office management. Due to the continued growth of the BSC-CNS and constantly changing needs due to the range of activities carried out by the centre, the Management Department maintains a somewhat flexible internal structure, with work teams being formed to tackle different issues.

» Organisational Structure



The Management Department is structured in different units: Finance & Business Administration provides three key services: Human Resources, Finance and Accounting, and General Administration Support. The Project Management Unit is responsible for managing projects and technologies, identifying opportunities, initiating and managing project proposals funded by public scientific calls as well as by industry sponsored research contracts. The Marketing & Communication Unit is responsible for all activities related to the corporate image such as communication (media), events management, public visits to the MareNostrum supercomputer, dissemination of activities and results to academia and industry and promoting science in society.

Management Department Staff & Collaborators 2011



» Finance and Business Administration

The Business Administration area, led by Mercè Calvet, manages the Human Resources, Administrative and Financial services of the Center.

Finance & Accounting

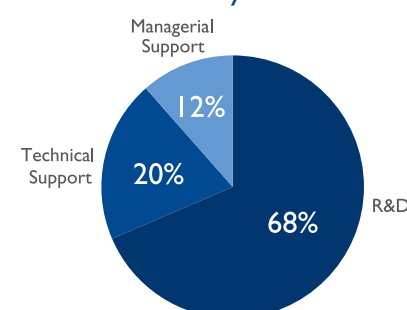
The Finance & Accounting Group is responsible for the financial resources management of the BSC-CNS (expenses, budgets, audits, bank relations, suppliers, receiving payments and budget deviations). The Group also prepares the financial reporting for project audits, working closely with the Project Management Group, and the Marketing & Communication Group in preparing budgets. In 2011 the SAP BI Tool implementation was finished and has been consolidated 100% as a Management central information system with better reporting capabilities. Also, it has been developed the new online queries system through the internet that is fed by data from the economic management system SAP Business I, and aims to facilitate Access to information on the state of the Center's Projects and the state of the Personnel Travels.



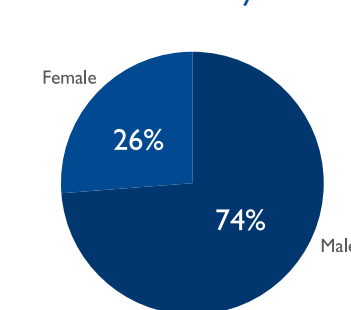
Human Resources

The Human Resources Group is responsible for managing selection processes, hiring and training, job descriptions, labour relations and collective bargaining, planning careers and internal promotion, and preventing work-related accidents. In 2011 the group work continued on a professional development system for all BSC-CNS staff. We have changed the workflows and we have incorporated annual objectives for each department with an individual evaluation system in order to recognize staff that make efforts to contribute to the BSC's progress and development of personal and professional skills. During this year the group has also designed an Employee Portal BSC's intranet, enabling some of personnel management services with online access systems.

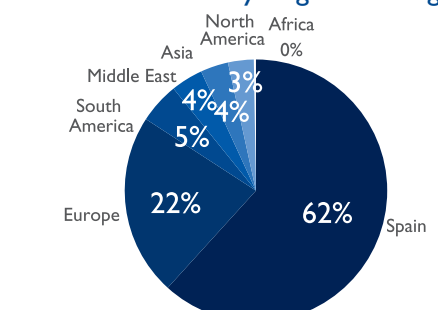
2011 Personnel by Function



2011 Personnel by Gender



2011 Personnel by Region of Origin

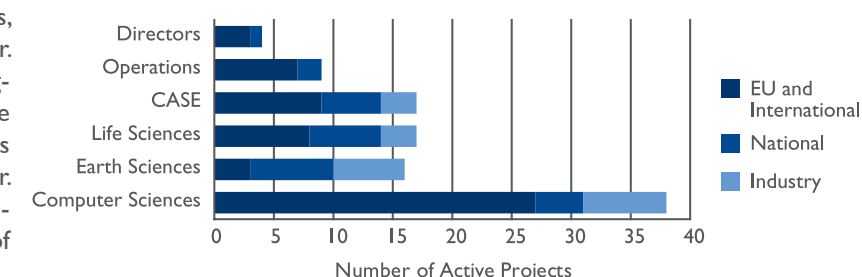


General Administration Support

The General Administration Group is responsible for activities such as organisation of official meetings, including those of the Access Committee, the Executive Commission, the Board of Trustees and other events. The Group manages travel services, space allocation, supply orders and execution of public tender processes, as well as providing general administrative support and reception services, such as receiving visiting researchers, official representatives and invited speakers.

In 2011, the BSC-CNS invited 15 public calls in order to accept 6 supply tenders, 8 services tenders and 1 works tender. The total administration contracts signed during the year has been of 58. The increase in the purchase's unit activities has been 38% over the previous year. The works tender was held for the launching of the 1st phase's construction of the new building of the BSC-CNS.

BSC-CNS Projects 2011



» Project Management

BSC-CNS's Project Management Office (PMO) is responsible for the management of publicly funded projects and collaborations with private industry. The PMO is also responsible for the detection and communication of new funding opportunities and for coordinating the submission of project proposals.

In 2011, BSC-CNS participated in 83 active projects, funded by national agencies, the European Commission and private industry. In addition to administering active projects, the Project Management Group assisted BSC-CNS researchers in submitting a large number of new project proposals during 2011 to help ensure continued funding for the BSC-CNS research activities.

» Marketing & Communication

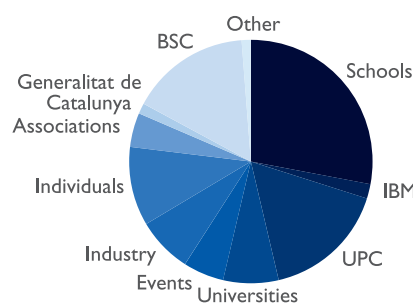
The Marketing and Communication Area is in charge of increasing awareness of the centre and disseminating information about research activities both in the scientific and industrial communities, as well as society in general.



Visitors

During the course of 2011, the BSC-CNS received a total of 7694 visitors from national and international centres, including universities, research centres, industry and non-profit organisations. Visitors to the MareNostrum are given a tour of the supercomputer and view a specially prepared video describing the technology used in the centre and the applications resulting from research that uses the supercomputing capacity of the MareNostrum and other RES nodes. The visits are sometimes tailored depending on the target audience. Two Open Days were organized; an entire week in January and in collaboration with the City Council on Saturday 22nd October 2011. This is another mechanism to disseminate BSC-CNS research results as well as familiarising the general public with supercomputing.

Visits to the MareNostrum 2011



BSC-CNS in the Media

During 2011 the BSC-CNS was mentioned 701 times in national and international newspapers and magazines, an increase of 700% over 2010. Most coverage was received in the print media, with online press in second place, followed by TV, radio and lastly wires.

In total, BSC-CNS sent out 21 press releases in Spanish, Catalan and English. A press conference to announce the joint Repsol – BSC research center was organised in September and was led by the Science and Innovation Minister of the Spanish Government, Cristina Garmedia; the Economy and Knowledge Minister of the Generalitat de Catalunya, Andreu Mas-Colell; the Chairman of Repsol, Antoni Brufau; the BSC-CNS Associate Director, Francesc Subirada, and Francisco Ortigosa, Geophysics Director at Repsol.

The press team regularly update the press dossiers of BSC-CNS, its joint centers, and the RES in English, Catalan and Spanish, and support the production of various press releases of European Projects (MONT-BLANC, EUDAT, PRACE, etc.).

Participation in Key Events, Seminars and Workshops

In 2011, BSC-CNS hosted and organized the following events:

- ▶ AMBER Workshop, 3-6 May 2011
- ▶ 23rd. International Conference on Parallel Computational Fluid Dynamics (PARCFD 2011), 16th – 20th May 2011
- ▶ HPC Europa TAM, 8 - 10th June 2011
- ▶ PUMPS summer school, 18 - 22 July 2011
- ▶ Seminario Uso Industrial de la Computación de Altas Prestaciones en España, 17 October 2011
- ▶ Barcelona Multicore Workshop, 1 - 4 November 2011
- ▶ EESI Final conference, 10 - 11 November 2011
- ▶ ICREA conference on Network Medicine Approaches to Human Disease: from Computers to the Clinic, 21 - 23th November 2011

» Computer Sciences 2011 Publications

Journals

- » Alejandro Duran, Eduard Ayguadé, Rosa M. Badia, Jesús Labarta, Luis Martinell, Xavier Martorell, Judit Planas, "OmpSs: A PROPOSAL FOR PROGRAMMING HETEROGENEOUS MULTI-CORE ARCHITECTURES", *Parallel Processing Letters*, 21, 2, 173-193, 2011-03-01
- » Azam Seyedi, Adrià Armejach, Adrián Cristal, Osman Unsal, Ibrahim Hur, Mateo Valero, "Circuit Design of a Dual-Versioning L1 Data Cache", *Integration The VLSI Journal*, 2011
- » B. Varghese, G. T. McKee, Vassil Alexandrov, "Can Agent Intelligence be used to Achieve Fault Tolerant Parallel Computing Systems?", *Parallel Processing Letters*, 21, 4, 379-396, 2011
- » Frimán Sánchez, Felipe Cabarcas, Alex Ramirez, Mateo Valero, "Scalable multicore architectures for long DNA sequence comparison", *Concurrency and Computation Practice and Experience*, 23, 17, 2011
- » Íñigo Goiri, Jordi Guitart, Jordi Torres, Ricardo Bianchini, Kien Le, Thu D. Nguyen, "Towards Sustainable Solutions for European Cloud Computing", *UPGRADE journal*, Vol. XII (4), 59-66, 2011-10-01
- » Iqbal, W., Dailey, M. N., David Carrera, Janecek, P., "Adaptive resource provisioning for read intensive multi-tier applications in the cloud", *Future Generation Computer Systems*, 27, 871-879, 2011
- » J. González, Judit Giménez, M. Casas, M. Moretó, Alex Ramirez, Jesús Labarta, Mateo Valero, "Simulating Whole Supercomputer Applications", *IEEE Micro*, 31, 2011-06-01
- » Paul Carpenter, Alex Ramirez, Eduard Ayguadé, "The Abstract Streaming Machine: Compile-Time Performance Modelling of Stream Programs on Heterogeneous Multiprocessors", *Transactions on HiPEAC*, 5, 3, 2011
- » Pieter Bellens, Josep M. Pérez, Rosa M. Badia, Jesús Labarta, "Making the Best of Temporal Locality: Just-in-Time Renaming and Lazy Write-Back on the Cell/B.E.", *International Journal of High Performance Computing Applications*, 25, 2, 2011
- » Ramon Bertran, Yolanda Becerra, David Carrera, Vicenç Beltran, Marc González, Xavier Martorell, Nacho Navarro, Jordi Torres, Eduard Ayguadé, "Energy accounting for shared virtualized environments under DVFS using PMC-based power models", *Future Generation Computer Systems*, 28, 2, 457 - 468, 2011
- » Ramon Nou, Ferran Julià, Kevin Hogan, Jordi Torres, "Path to achieving a self-managed grid middleware", *Future Generation Computer Systems*, 27, 1019, 2011
- » Roger Ferrer, Judit Planas, Pieter Bellens, Alejandro Duran, Marc González, Xavier Martorell, Rosa M. Badia, Eduard Ayguadé, Jesús Labarta, "Optimizing the Exploitation of Multicore Processors and GPUs with OpenMP and OpenCL", *Lecture Notes in Computer Science*, 6548/2011, 215-229, 2011-12-01
- » V. Jiménez, Francisco Cazorla, Roberto Gioiosa, E. Kursun, C. Isci, C. A. Buyuktosunoglu, Pradip Bose, Mateo Valero, "A Case for Energy-Aware Accounting and Billing in Large-Scale Computing Facilities Cost Metrics and Design Implications.", *IEEE Micro*, May-June 2011
- » V. Jiménez, Francisco Cazorla, Roberto Gioiosa, Mateo Valero, Carlos Boneti, E. Kursun, C. Cher, C. Isci, Alper Buyuktosunoglu, Pradip Bose, "Characterizing Power and Temperature Behavior of POWER6-Based System. (invited paper)", *IEEE Journal of Emerging and Selected Topics in Circuits and Systems*, 2011-09-01
- » Vassil Alexandrov, C. Gonzalez Martel, J. Strassburg, "Monte Carlo Scalable Algorithms for Computational Finance", *Procedia Computer Science*, 4, 1708-1715, 2011

Book Chapters

- » Jesús Labarta, "Trace-Based Tools", in *Performance Tuning of Cientific Applications*. CRC Press., 2011-01-03
- » Khandakar Ahmed, Vassil Alexandrov, "Identity and Access Management in Cloud Computing", in *Cloud Computing for Enterprise Architectures*, Mahmood Zaigham and Hill Richard (Eds.), XVI, Part 2, 115-133, 2011

International Conferences

- » Adrià Armejach, Azam Seyedi, J. Rubén Titos Gil, Ibrahim Hur, Osman Unsal, Adrián Cristal, Mateo Valero, "Using a Reconfigurable L1 Data Cache for Efficient Version Management in Hardware Transactional Memory", *Parallel Architectures and Compilation Techniques (PACT)*, 360-370, 2011-10-01
- » Aislan G Foia, Judit Planas, Rosa M. Badia, Francisco Javier Ramirez-Fernandez, "P-Means, a Parallel Clustering Algorithm for a Heterogeneous Multi-Processor Environment", *Proceedings of the HPCS 2011*, 2011
- » Alberto Miranda, S. Effert, Y. Kang, L. Miller, A. Brinkmann, Toni Cortés, "Reliable and Randomized Data Distribution Strategies for Large Scale Storage Systems", *18th Annual International Conference on High Performance Computing (HiPC 2011)*, 2011-12-19
- » Alejandro Rico, Alejandro Duran, Felipe Cabarcas, Yoav Etsion, Alex Ramirez, Mateo Valero, "Trace-driven simulation of multithreaded applications", *2011 IEEE International Symposium on Performance Analysis of Systems and Software*, 87--96, 2011
- » Alessandro Morari, Roberto Gioiosa, Robert Wisniewski, Francisco Cazorla, Mateo Valero, "A Quantitative Analysis of OS Noise", *2011 IEEE International Parallel & Distributed Processing Symposium (IPDPS)*, 2011-05-16
- » Alvarez, Lluc, Ramon Bertran, González, Marc, Xavier Martorell, Nacho Navarro, Eduard Ayguadé, "Design space exploration for aggressive core replication schemes in CMPs", *Proceedings of the 20th international symposium on High performance distributed computing*, 269-270, 2011-06-15
- » Angelos Bilas, Toni Cortes, Ricardo-Jiménez Peris, Bilha Mendelson, "Storage I/O in Modern Servers and Data-centric Applications: Efficiency and Scalability Challenges", *HiPEAC Conference*, 2011
- » Anika Schiller, Goodehard Sutmann, Luis Martinell, Pieter Bellens, Rosa M. Badia, "Multiparticle Collision Dynamics on the Cell Broadband Engine using CellSs", *Proc. of the Second International Conference on Parallel, Distributed, Grid and Cloud Computing for Engineering*, 2011
- » A. Vega, F. Cabarcas, A. Ramirez and M. Valero, "Breaking the Bandwidth Wall in Chip Multiprocessors". *Samos 2011: International Conference on Embedded Computer Systems; Architecture, Modelling and Simulation. SAMOS 11*. Samos, Greece. July 18-21, 2011.
- » Azam Seyedi, Adrià Armejach, Adrián Cristal, Osman Unsal, Ibrahim Hur, Mateo Valero, "Circuit Design of a Dual-Versioning L1 Data Cache for Optimistic Concurrency", *21st Great Lakes Symposium on Very Large Scale Integration (GLSVLSI'11)*, 2011-05-01

- » Bojan Maric,Jaume Abella,Francisco Cazorla,Mateo Valero,“Hybrid High-Performance Low-Power and Ultra-Low Energy Reliable Caches”, International Conference on Computing Frontiers (CF), 12:1-12:2, 2011-05-03
- » Carlos Villavieja,Vasileios Karakostas,Lluís Vilanova,Yoav Etsion,Alex Ramirez,Avi Mendelson,Nacho Navarro,Adrián Cristal,Osman Unsal,“DiDi: Mitigating The Performance Impact of TLB Shootdowns Using A Shared TLB Directory”, Parallel Architectures and Compilation Techniques (PACT), 2011-09-01
- » Carlos Villavieja,Yoav Etsion,Alex Ramirez,Nacho Navarro,“FELI: HW/SW support for On-Chip Distributed Shared Memory in Multicores”, Euro-Par, 2011
- » Catalin Ciobanu,Xavier Martorell,Georgi K. Kuzmanov,Alex Ramirez,Georgi Gaydadjiev,“Scalability Evaluation of a Polymorphic Register File: A CG Case Study”,Architecture of Computing Systems - ARCS 2011, 13-25, 2011-02-28
- » Cecilia González,Mikel Fernández,Daniel Jiménez,Carlos Álvarez,Xavier Martorell,“Automatic generation of application-specific hardware accelerators on OpenSPARC”, International Symposium on Code Generation and Optimization (CGO 2011), 2011-04-30
- » Daniele Lezzi,Roger Rafanell,Abel Carrion,Ignacio Blanquer,Rosa M. Badia,Vicente Hernandez,“Enabling e-Science applications on the Cloud with COMPSs”, International Euro-Par Conference 2011,Aug 2011
- » Enric Tejedor,Francesc Lordan,Rosa M. Badia,“Exploiting Inherent Task-Based Parallelism in Object-Oriented Programming”, Proceedings of the 12th IEEE/ACM International Conference on Grid Computing, Lyon, France, 74-81, 2011-09-01
- » Enric Tejedor,Jorge Ejarque,Francesc Lordan,Roger Rafanell,Javier Álvarez,Daniele Lezzi,Raul Sirvent,Rosa M. Badia,“A Cloud-unaware Programming Model for Easy Development of Composite Services”, Third IEEE International Conference on Cloud Computing Technology and Science, 375-382, 2011
- » Enric Tejedor,Montse Farreras,David Grove,Rosa M. Badia,George Almasi,Jesús Labarta,“ClusterSs: a Task-based Programming Model for Clusters”, Proceedings of the 20th International ACM Symposium on High Performance Distributed Computing, San Jose, California, USA, 267-268, 2011-06-01
- » Fries,A.,Castañeda,J.,Isasi,Y.,Taboada,G.L.,Portell,J.,Raul Sirvent,“An efficient framework for Java data processing systems in HPC environments”, Proceedings of SPIE, 8183, 2011
- » Fries,A.,Portell,J.,Isasi,Y.,Castañeda,J.,Raul Sirvent,Taboada,G.L.,“MPI-based Solution for Efficient Data Access in Java HPC”, INFOCOMP 2011, The First International Conference on Advanced Communications and Computation, 149-154, 2011-10-23
- » German Llort,Marc Casas,Harald Servat,Kevin Huck,Judit Giménez,Jesús Labarta,“Trace Spectral Analysis toward Dynamic Levels of Detail”, 17th IEEE International Conference on Parallel and Distributed Systems, ICPADS 2011, Tainan, Taiwan, 332 - 339, 2011-12-10
- » Gökçen Kestor,Roberto Gioiosa,T. Harris,Adrián Cristal,Osman Unsal,Mateo Valero,I. Hur,“STM2: A Parallel STM for High Performance Simultaneous Multi-Threading Systems”, The 20th IEEE International Conference on Parallel Architectures and Compilation Techniques (PACT), 2011-10-01
- » Gökçen Kestor,Vasileios Karakostas,Osman Unsal,Adrián Cristal,Ibrahim Hur,Mateo Valero,“RMS-TM: A Comprehensive Benchmark Suite for Transactional Memory Systems”, International Conference on Performance Engineering (ICPE 2011), 2011-03-01
- » G. Kestor,V. Karakostas, O. Unsal,A. Cristal, I. Hur and M.Valero. “A New Benchmark Suite for Transactional Memory”. 2nd Joint WOSP/SIPEW. ACM ICPE, International Conference on Performance Engineering. Karlshere, Germany, March, 14-16, 2011. Best Paper Award.
- » Gulay Yalcin,Osman Unsal,Adrián Cristal,Ibrahim Hur,Mateo Valero,“SymptomTM: Symptom Based Error Detection and Recovery Using Hardware Transactional Memory”, Parallel Architectures and Compilation Techniques (PACT), 199-200, 2011-10-01
- » Gulay Yalcin,Osman Unsal,Adrián Cristal,Mateo Valero,“FIMSIM: A fault injection infrastructure for microarchitectural simulators”, 29th International Conference on Computer Design (ICCD), 431-432, 2011-10-01
- » Harald Servat,Germán Llort,Judit Giménez,Kevin A. Huck,Jesús Labarta,“Unveiling Internal Evolution of Parallel Application Computation Phases”, ICPP, 155-164, 2011-09-15
- » Harald Servat,Germán Llort,Judit Giménez,Kevin Huck,Jesús Labarta,“Folding: detailed analysis with coarse sampling”, Tools for High Performance Computing 2011. Proceedings of the 5th International Workshop on Parallel Tools for High Performance Computing, 2011-09-20
- » Íñigo Goiri,Kien Le,Jordi Guitart,Jordi Torres,Ricardo Bianchini,“Intelligent Placement of Datacenters for Internet Services”, 31th International Conference on Distributed Computing Systems (ICDCS'11), 131-142, 2011-06-20
- » Íñigo Goiri,Kien Le,Ryan Beauchea,Thu D. Nguyen,Md. E. Haque,Jordi Guitart,Jordi Torres,Ricardo Bianchini,“GreenSlot: Scheduling Energy Consumption in Green Datacenters”, 24th ACM/IEEE International Supercomputing Conference for High Performance Computing, Networking, Storage and Analysis (SC'11), 2011-11-12
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- » Eduardo Quiñones, Jaume Abella, Francisco Cazorla, Mateo Valero, “Exploiting Intra-Task Slack Time of Load Operations for DVFS in Hard Real-Time Multi-core Systems”, In Work in Progress (WiP), under the the 24nd Euromicro Conference on Real-Time Systems (ECRTS 2011), 2011
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- » Proactive Software Rejuvenation solution for web environments on virtualized platforms. Javier Alonso. February 2011. Advisors Jordi Torres and Ricard Gavaldà.
- » Understanding and Reducing Contention in Generalized Fat Tree Networks for High Performance Computing. Germán Rodríguez. April 2011. Advisors Jesús Labarta and Ramón Beivide.
- » Reusing cached schedules in an out-of-order processor with in-order issue logic. Oscar Palomar. May 2011. Advisors Toni Juan and Juan J. Navarro.
- » Multifaceted Resource Management on Virtualized Providers. Iñigo Goiri. June 2011. Advisors Jordi Guitart and Jordi Torres.

- » Friman Sánchez. Exploiting Multiple Levels of Parallelism in Bioinformatics Applications. June 2011. Advisors Alex Ramirez and Mateo Valero.
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- » Parallel Video Decoding. Mauricio Álvarez. September 2011. Advisors Alex Ramirez and Mateo Valero.
- » Castell: a Heterogeneous CMP Architecture Scalable to Hundreds of Processors. Felipe Cabarcas. September 2011. Advisors Alex Ramirez and Mateo Valero.
- » Running Stream-like Programs on Heterogeneous Multi-core Systems. Paul Carpenter. October 2011. Advisors Eduard Ayguadé and Alex Ramirez.
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- » Baldasano, J. M., “Dust Transport Forecast Models and Early Warning System”, International Training Course on Meteorological Services, Sand and Dust Storm (SDS) Forecast and Early Warning System and Erosion Preventing Techniques and Controlling Methods and Forestry, 2011-02-23
- » Baldasano, J. M., “El Comportamiento Ético en el Actual Cambio Climático Antropogénico”, VII Congreso Mundial de Bioética, 2011-09-20
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- » Baldasano, J. M., “Noves Evidências sobre el Canvi Climàtic”, Aula de Humanidades, 2011-05-24
- » Baldasano, J. M., “Podem mesurar i modelitzar la qualitat de l'aire?. Fiabilitat i perspectiva de millora”, Jornada CECCP-RACC: “Qualitat de l'aire i transport viari a l'àrea de Barcelona, 2011-05-02

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- » Baldasano, J. M., V. Sicardi, María Teresa Pay, Gustavo Arévalo, Santiago Gassó, “To what extent bias-correction techniques improve the air quality forecast over Spain within the CALIOPE”, 3rd International Workshop on Air Quality Forecasting Research (IWAQFR), 2011-11-30
- » D. Arnold, D. Morton, I. Schicker, Oriol Jorba, K. Harrison, J. Zabloudil, G. Newby, P. Seibert, “WRF benchmark for regional applications”, 12th Annual WRF Users' Workshop, 12, 1-5, 2011-06-20
- » Maria Gonçalves, W. L. Chang, D. Dabdub, Oriol Jorba, Baldasano, J. M., “The Impact of HONO Sources in the Air Quality of the Iberian Peninsula”, GLOREAM-EURASAP 2011 Workshop on global and regional atmospheric modelling, 2011-01-26
- » Oriol Jorba, C. Pérez, K. Hausteijn, Z. Janjic, Baldasano, J. M., D. Dabdub, A. Badia, Michele Spada, “Online air quality developments undertaken within the NMMB multiscale model at the Barcelona Supercomputing Center”, 3rd International Workshop on Air Quality Forecasting Research (IWAQFR), 2011-11-30
- » Simone Marras, Mariano Vázquez, Oriol Jorba, Guillaume Houzeaux, Arnau Folch, Romain Aubry, “Solving Nonhydrostatic Dynamics with a variational multiscale Galerkin solver: Tests and parallel performance”, IPAM-UCLA Workshop, 2011-06-06

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- » Regional and Urban Evaluation of an Air Quality Modelling System in the European and Spanish Domains, María Teresa Pay, November 2011. Advisors José Mª Baldasano and Pedro Jiménez.

» Life Sciences 2011 Publications

Journals

- » A. Stein, Manuel Rueda, Panjkovich, Alejandro, Modesto Orozco, P. Aloy, “A systematic study of the energetics involved in structural changes upon association and connectivity in protein-protein interaction networks”, In second revision, 2011-02-22
- » Ayuso-Tejedor, S., García-Fandiño, R., Orozco, M., Sancho, J., Bernadó, P., “Structural analysis of an equilibrium folding intermediate in the apoflavodoxin native ensemble by small X-ray scattering”, Journal of molecular biology, 406(4) pp.604-619, 2011-03-04
- » Carles Pons, Glaser, Fabian, J. Fernández-Recio, “Prediction of protein-binding areas by small-world residue networks and application to docking”, BMC bioinformatics, 12, 378, 2011
- » Carles Pons, Talavera, David, de la Cruz, Xavier, Modesto Orozco, J. Fernández-Recio, “Scoring by intermolecular pairwise propensities of exposed residues (SIPPER): a new efficient potential for protein-protein docking”, J. Chem. Inf. Model., 51, 2, 370-7, 2011 Feb 28
- » Cossins, Benjamin P, Jacobson, Matthew P, Guallar, Victor, “A new view of the bacterial cytosol environment.”, PLoS computational biology, 7, 6, e1002066, 2011 Jun
- » D'Abramo, Marco, Modesto Orozco, Amadei, Andrea, “Effects of local electric fields on the redox free energy of single stranded DNA.”, Chemical communications (Cambridge, England), 47, 9, 2646-8, 2011 Mar 7
- » Daskalakis, Vangelis, Farantos, Stavros C, Guallar, Victor, Varotsis, Constantinos, “Regulation of electron and proton transfer by the protein matrix of cytochrome c oxidase.”, The journal of physical chemistry. B, 115, 13, 3648-55, 2011 Apr 7
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- » Flores, Oscar, Modesto Orozco, “nucleR: a package for non-parametric nucleosome positioning.”, Bioinformatics (Oxford, England), 27, 15, 2149-50, 2011 Aug 1
- » Francisco Javier Luque, Dehez, C. Chipot, Modesto Orozco, “Polarization effects in molecular interactions”, 2011-02-03
- » Helft, Laura, Reddy, Vignyan, Chen, Xiyang, Koller, Teresa, Federici, Luca, J. Fernández-Recio, Gupta, Rishabh, Bent, Andrew, “LRR conservation mapping to predict functional sites within protein leucine-rich repeat domains.”, PLoS one, 6, 7, e21614, 2011
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- » J. Fernández-Recio, “Prediction of protein binding sites and hot spots”, WIREs Comput. Mol. Sci., 1, 680-698, 2011
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- » Modesto Orozco, L Orellana, A Hospital, A.N Naganathan, A Emperador, Carrillo, Oliver, Josep L Gelpí, “Coarse Grained Representation of Protein Flexibility. Foundations, successes and shortcomings”, Computational Chemistry Methods in Structural Biology. In press., 2011-02-22

International Conferences

- » Aloy, P. “A network biology approach to human disease”. Systems Biology: Networks. Cold Spring Habor Laboratory, US. March 2011.
- » Aloy, P. “A network biology approach to human disease”. Systems Biology of Human Disease Conference. Harvard Medical School, Boston, US. June 2011.
- » Aloy, P. “A network biology approach to human disease”. EMBO Conference on Protein Interactions and Dynamics. Heidelberg, DE Oct 2010.
- » Aloy, P. “A network biology approach to human disease”. Invited Lecture. Southampton University, UK. October 2011.
- » Aloy, P. “A network biology approach to complex human diseases”. Invited Lecture. Sanger Institute. Hinxton, UK June 2011.
- » Badiola, N., Alcalde, V., Soler-López, M. and Aloy, P. “Unveiling the role of PDCD4 in Alzheimer’s disease”, Network medicine approaches to human disease. Barcelona, 21-23rd November 2011
- » D Repchevsky, “BioNemus. SAWSDL web-services.” Elixir Workshop, Amsterdam. February 21-23 2011
- » Durán, E., Djebali, S., Guigó, R, Torrents, D., Soler-lópez, M. and Orozco, M. “Unraveling of the hidden DNA structural/physical code provides novel insights on promoter location”, Quantitative methods in gene regulation. London, 22-23th September 2011
- » Deniz, Ö., Battistini, F, Flores, O., Soler-López, M. and Orozco, M. “The Chromatin Dynamics of Budding Yeast: Nucleosome Positioning During Cell Cycle”, Joint BIOCHEMICAL SOCIETY and WELLCOME TRUST Conference: From beads on a string to the pearls of regulation: the structure and dynamics of chromatin, Cambridge UK, 3-5th August 2011
- » Deniz, Ö., Battistini, F, Flores, O., Soler-López, M. and Orozco, M. “The Chromatin Dynamics of Budding Yeast”, GORDON Research Conference: Chromosome Dynamics, West Dover VT, 10-15th July 2011
- » Josep L Gelpí, “Data Management in Massive Genomic Projects”, IV International Symposium on Biomedical Informatics in Europe, Pazo de Lestrove, A Coruña. 2011
- » Josep L Gelpí, “HPC approaches to bioinformatics”, The 10th Annual Meeting on High Performance Computing and Infrastructure in Norway, 2011
- » Josep L Gelpí, “MoDEL Molecular Dynamics Extended Library”, nDDB Meeting - Grenoble - France, 2011-01-12
- » Josep L Gelpí, “Infraestructura de Web-Services y Supercomputación.” Tutoriales Formativos en Biomedicina Computacional. INB - COMBIOMED. Pazo de Lestrove (Coruña) 8 June 2011.
- » Fernández-Recio, J. “Protein-protein docking for multi-resolution modeling: integrating theoretical and experimental data.” Stanford-Sweden Multi-resolution Molecular Simulation Workshop. Uppsala (Sweden) 2011
- » Orozco, M. “DNA from atom to chromosome”. Annual series of invited conferences at the Institute for Personalized Medicine. Barcelona 2011.
- » Orozco, M. “The journey of a computational chemist along DNA”. International meeting of the World Association of Theoretically Oriented Chemist (WATOC). Santiago de Compostela. 2011.
- » Orozco, M. “DNA, from quantum chemistry to bioinformatics”. Telluride Meeting on RNA. Telluride. Colorado. USA
- » Orozco, M. The impact of methylation on the physical properties of DNA”. “Coarse-Grain Mechanics of DNA”. CECAM Conference. Lausanne, Switzerland. 2011.
- » Orozco, M. “On Silico Navigation in the DNA world”. Modeling Interactions in Biomolecules V. Kutná Hora, Czech Republic. 2011
- » Orozco, M. “New approaches to represent protein dynamics”. CPMD Meeting. Barcelona 2011.
- » Orozco, M. “Protein dynamics in the post-genome era”. CECAM workshop “Combining experimental and computational techniques to study protein behaviour”. Lugano, Italy 2011-11-03
- » Orozco, M. “EESI Final Exascale Conference”. E-Sciences in Exascale computers Meeting. Barcelona 2011
- » Orozco, M. “Pushing the frontiers of molecular dynamics simulations”. Biomed Conference on Protein Dynamics. Barcelona 2011.
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- » Pons, C., Fernández-Recio, J. “Integration of low-resolution data into all-atom protein docking.” 6th Congress of the Federation of the Israel Societies for Experimental Biology. Eilat (Israel) 2011
- » Salvatella, X. 2nd workshop from molecular and structural biology to disease therapy, Rosario, Argentina, October 2011.
- » Salvatella, X. Interbio NMR workshop, Oeiras, Portugal, September 2011.
- » Salvatella, X. Interbio symposium on frontiers of protein research, Oeiras, Portugal, May 2011.
- » Soler-López, M. “An advanced experimental approach for computational biologists to validate predicted protein-protein interactions”, EMBO Practical Course on Modern Biophysical Methods for protein-ligand interactions, Oulu, Finland, 17-21th October 2011
- » Soler-López, M., Zanzoni, A., Lluís, R., Stelzl, U. and Aloy, P. “Network modelling suggests new mechanistic details underlying Alzheimer’s disease”, RECOMB: DREAM Annual Conferences, Barcelona, 14-19th October 2011
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- » Victor Guallar, “Induced Fit Modeling with Monte Carlo Techniques: PELE (Protein Energy Landscape Exploratio”. 11th Structure-based Drug Design (SBDD). June 8-10th 2011, Boston (USA)

- » Victor Guallar, Victor Gil, Israel Cabeza de Vaca and Ali Hosseini, “PELE (Protein Energy landscape Exploration?)” Invited seminar at Novartis. June 14th 2011, Boston (USA)

- » Victor Guallar, Frank Wallrapp and Fatima Lucas, “QM and MM Methods: Obtaining an Electronic and Atomic View of Nature”, Chemistry Seminar at the University of California at Berkeley. June 20th 2011, Berkeley (USA)

- » Victor Guallar, Frank Wallrapp and Fatima Lucas, “QM/MM e-pathway in cytochrome C Oxidase”, Seminar at the Biophysical department. Albert Einstein School of Medicine. June 3rd. 2011. New York (USA)

- » Victor Guallar, “QM and MM methods: obtaining an atomic and electronic view of Nature”, Structural and Computational Biology Programme (IRB) and Department of Structural Biology (IBMB) Seminar, may 4th, Barcelona (Spain)

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- » Fleishman, Sarel J, Whitehead, Timothy A, Strauch, Eva-Maria, Corn, Jacob E, Qin, Sanbo, Zhou, Huan-Xiang, Mitchell, Julie C, Demerdash, Omar N A, Takeda-Shitaka, Mayuko, Terashi, Genki, Moal, Iain H, Li, Xiaofan, Bates, Paul A, Zacharias, Martin, Park, Hahnbeom, Ko, Jun-su, Lee, Hasup, Seok, Chaok, Bourquard, Thomas, Bernauer, Julie, Poupon, Anne, Azé, Jérôme, “Community-wide assessment of protein-interface modeling suggests improvements to design methodology.”, Journal of molecular biology, 414, 2, 289-302, 2011 Nov 25

- » Josep L Gelpí, “Infraestructura de Web Services y Supercomputación”, Tutoriales Formativos en Biomedicina Computacional.: Lestrove (Coruña) (ESPANYA), 2011

- » Josep L Gelpí, “Uso de Herramientas Bioinformáticas y Bases de datos biológicas con soporte de la supercomputación”, OMICS aplicada a la Medicina Clínica, Barcelona, 2011

Theses

- » Computational modeling applications: protein-protein docking, hot-spots prediction and allosteric effects, Solene Grosdidier, April 2011. Advisor Juan Fernandez-Recio.
- » Energy landscape of protein-protein interactions by computational docking: New orientational sampling tools and coarse grained modelling, Albert Solernou, February 2011. Advisor Juan Fernandez-Recio.
- » Structural prediction of protein complexes by computational docking with pyDock: Optimization and new developments for large-scale application, Carles Pons, July 2011. Advisor Juan Fernandez-Recio.
- » Mixed quantum and classical simulation techniques for mapping electron transfer in proteins, Frank Wallrapp, April 2011. Advisor Victor Guallar.

» Computer Applications in Science & Engineering (CASE) 2011 Publications Journals

- » A. Soba, E. Bea, Guillaume Houzeaux, Hadrien Calmet, José Ma. Cela, “Real space density functional theory and time depending density functional theory using finite/infinite element methods”, Comput. Phys. Comm., 2011
- » Anne-Cecile Lesage, Josep de la Puente, José Ma. Cela, Mauricio Araya-Polo, Gladys Gonzalez, “Comparison of irregular cartesian finite difference methods for acoustic RTM”, SEG Technical Program Expanded Abstracts, 30, 2845-2849, 2011
- » B. Eguzkitza, Guillaume Houzeaux, R. Aubry, Mariano Vázquez, “A Parallel coupling strategy for the Chimera and Domain Decomposition methods in Computational Mechanics”, Computers & Fluids, Submitted, 2011
- » C. Bonadonna, Arnau Folch, S. Loughlin, H. Puempel, “Future Developments in Modeling and Monitoring of Volcanic Ash Clouds”, EOS, 2011
- » D.J. Doorly, Guillaume Houzeaux, D.J. Taylor, Hadrien Calmet, Mariano Vázquez, “Numerical simulation of air flow in the large airways”, Submitted to Computers & Fluids, 2011
- » Guillaume Houzeaux, R. de la Cruz, Herbert Owen, Mariano Vázquez, “Parallel uniform mesh multiplication applied to a Navier-Stokes solver”, Submitted to Computers & Fluids, 2011
- » Guillaume Houzeaux, Romain Aubry, Mariano Vázquez, “Extension of fractional step techniques for incompressible flows: The preconditioned Orthomin(1) for the pressure Schur complement”, Computers & Fluids, 44, 297-313, 2011
- » H. Talebi, C. Samaniego, E. Samaniego, T. Rabczuk, “On the numerical stability and mass-lumping schemes for explicit enriched meshfree methods”, IJNME, 2011
- » Herbert Owen, Ramon Codina, “A free surface finite element model for low Froude number mould filling problems on fixed meshes”, International Journal for Numerical Methods in Fluids, 66, 833-851, 2011
- » Herbert Owen, Ramon Codina, “A third-order velocity correction scheme obtained at the discrete level”, International Journal for Numerical Methods in Fluids, In Press, 2011
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- » Mauricio Hanzich, P. Hernández, F. Giné, F. Solsona, J.L. Lérída, “On/Off-Line Prediction Applied to Job Scheduling on Non-Dedicated NOWs”, Journal of Computer Science and Technology, 26 (1), 99-116, Jan 2011
- » Rainald Lohner, Fernando Mut, Juan Cebral, Romain Aubry, Guillaume Houzeaux, “Deflated Preconditioned Conjugate Gradient Solvers for the Pressure-Poisson Equation: Extensions and Improvements”, Int. J. Numer. Meth. Engn., 87, 2-14, 2011
- » Xavi Rubio-Campillo, José Ma. Cela, Francesc Xavier Hernández, “The development of new infantry tactics during early XVIIIth century: a compu-

ter simulation approach to modern military history”, Journal of Simulation, submitted, 2011

- » Xavier Sáez,Alejandro Soba,Edilberto Sánchez,Ralf Kleiber,Francisco Castejón,José Ma. Cela,“Improvements of the particle-in-cell code EUTERPE for petascale machines”, Computer Physics Communications, 182, 2047 - 2051, 2011

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- » Raúl de la Cruz,Hadrien Calmet,Guillaume Houzeaux,“Implementing a XDMF/HDF5 Parallel File System in Alya”,Whitepaper of PRACE-IIP project, 2011

International Conferences

- » A. Soba,E. Bea,Guillaume Houzeaux,“Resolución de la ecuación de Khon-Sham mediante discretización del espacio real con elementos finitos e infinitos”,AFA, 2011
- » Adrian Jackson,Fiona Reid,Joachim Hein,Alejandro Soba,Xavier Sáez,“High Performance I/O”, Proceedings of the 19th Euromicro Conference on Parallel, Distributed and Network-based Processing (PDP), 349-356, 2011
- » Adrian Jackson,Fiona Reid,Stephen Booth,Joachim Hein,Jan Westerholm,Ats Aspnäs,Miquel Català,Alejandro Soba,“Parallel Optimisation Strategies for Fusion Codes”, Proceedings of the 19th Euromicro Conference on Parallel, Distributed and Network-based Processing (PDP), 357-364, 2011
- » Beatriz Eguzkitza,Guillaume Houzeaux,Mariano Vázquez,“An Implicit and Parallel Chimera Method”, 20th International Conference on Domain Decomposition Methods, 7-11 Feb.
- » Beatriz Eguzkitza,Guillaume Houzeaux,Romain Aubry,Oscar Peredo,Herbert Owen,Mariano Vázquez,“An Implicit and Parallel Chimera Type Domain Decomposition Method”, PARCFD2011, 16-21 May 2011
- » Bin Hu,F. Di Maio,P.C. Rem,Guillaume Houzeaux,Hadrien Calmet,Herbert Owen,“Development of inverse magnetic density separation of polyolefin mixtures”, Proceedings of the 26th International Conference on Solid Waste Technology and Management, 968-976, March 27-30
- » C. Samaniego,Guillaume Houzeaux,Mariano Vázquez,“A Parallel Fluid-Particle Solver”, 11th U.S. National Congress on Computational Mechanics, 25-28 July
- » Cristina Montañola-Sales,S. Onggo,J. Casanovas-Garcia,“Agent-based simulation validation: A case study in demographic simulation”, Proceedings of the 3rd International Conference on Advances in System Simulation (SIMUL11), 109-115, 2011-10-26
- » Cristóbal Samaniego,Guillaume Houzeaux,Mariano Vázquez,“A Parallel Fluid-Particle Solver”, Congresso de Métodos Numéricos em Engenharia - CMNE 2011, 14-17 June 2011
- » Christian Pelties,Josep de la Puente,Jean-Paul Ampuero,Gilbert Brietzke,Martin Kaser,“Dynamic Rupture Simulation with a High-order Discontinuous Galerkin Method on Unstructured Tetrahedral Meshes”, 2011 SCEC Annual Meeting, B-053, 2011
- » D.J. Doorly,D. Taylor,Guillaume Houzeaux,C. Rennier,N. Tolley,Mariano Vázquez,“Computational Modelling of Airflow in the Respiratory Tract”, PARCFD2011, 16-21 May 2011
- » Felix Rubio,Mauricio Hanzich,Ruth Aris,Mariano Vázquez,Guillaume Houzeaux,“Parallel Computational Electrophysiology in NVIDIA GPUs”, 2st International Conference on Mathematical and Computational Biomedical Engineering, 30 Mar. - 1 Apr.
- » Guillaume Houzeaux,Mariano Vázquez,Raúl de la Cruz,“A Parallel Incompressible Navier-Stokes Solver”, 16th International Conference on Finite Elements in Flow Problems (FEF 2011), March 23-25
- » Guillaume Houzeaux,Mariano Vázquez,Raúl de la Cruz,“A parallel Navier-Stokes incompressible flow solver”, PARCFD2011, 16-21 May 2011
- » Herbert Owen,Guillaume Houzeaux,Cristóbal Samaniego,Mariano Vázquez,“Recent ship hydrodynamics developments in the parallel two fluid flow solver Alya”, PARCFD2011, 16-21 May 2011
- » Jelena Koldan,Vladimir Puzrev,José Ma. Cela,Josep de la Puente,Francisco Ortigosa,Xiong Li,Yaoguo Li,Xiaohong Meng,“A parallel finite-element method for 3-D marine controlled-source electromagnetic forward modeling”, Global Meeting Abstracts, 15, 12-12, 2011
- » L. Margetts,S. McDonald,L.M. Lever,Hadrien Calmet,Guillaume Houzeaux,P.M. Mummery,“Predictive modelling of flow through porous microstructures”, PARCFD2011, 16-21 May 2011
- » Lubica Valentova,Frantisek Galovic,Josep de la Puente,“Inversion of Love wave traveltimes in Czech Republic using adjoint method”, Geophysical Research Abstracts, EGU2011-6858, 2011
- » Mariano Vázquez,P. Lafortune,Ruth Aris,Guillaume Houzeaux,A. Jerusalem,“High Performance Computational Electromechanical Model of the Heart”, Second African Conference on Computational Mechanics - AfriCOMPI1, Jan. 5-8, 2011
- » P. Lafortune,Ruth Aris,Mariano Vázquez,Guillaume Houzeaux,A. Jerusalem,“Large Scale Electro Mechanical cardiac Simulations”, 2nd International Conference on Mathematical and Computational Biomedical Engineering, 30 Mar. - 1 Apr.
- » Pierre Lafortune,Ruth Aris,Mariano Vázquez,Guillaume Houzeaux,Antoine Jérusalem,“Large Scale Electro Mechanical cardiac Simulations”, 2st International Conference on Mathematical and Computational Biomedical Engineering, 30 Mar. - 1 Apr.
- » Raúl de la Cruz,Mauricio Araya-Polo,“Towards a Multi-Level Cache Performance Model for 3D Stencil Computation”, Proceedings of the International Conference on Computational Science, ICCS 2011, 4, 2146-2155, 2011
- » Romain Aubry,Guillaume Houzeaux,Mariano Vázquez,“Extensions of a surface remeshing approach”, 49th AIAA Aerospace Sciences Meeting, 4-7 Jan.
- » Romain Aubry,Guillaume Houzeaux,Mariano Vázquez,“Some useful strategies for unstructured edge-based solvers on shared memory machines”, 49th AIAA Aerospace Sciences Meeting, 4-7 Jan.
- » Thomas Franz,Jeroen Kortsmits,Renee Miller,Mazin S. Sirry,Jesse R. Macadangdang,Karen Kadner,B. Daya Reddy,Sebastian Skatulla,Peter Zilla,Kevin Colville,Mariano Vázquez,Ruth Aris,Pierre Lafortune,Neil Davies,“High Performance Computational Mechanics and Electro-elasticity Towards Improved Understanding of Myocardial Infarction Therapies Based on Biomaterial Injectates”, ISC’11, 19-23 June 2011
- » Xavier Sáez,Alejandro Soba,Edilberto Sánchez,José Ma. Cela,Francisco Castejón,“Particle-In-Cell algorithms for Plasma simulations on heterogeneous architectures”, Proceedings of the 19th Euromicro Conference on Parallel, Distributed and Network-based Processing (PDP), 385-389, 2011

National Conferences

- » Arnau Folch,Guillaume Houzeaux,Mariano Vázquez,“Simulació amb superordinadors del transport de contaminants”, X Fòrum TIG SIG 2011, 15-16 March 2011





During 2011 the RES continued offering high value services to the Spanish and international scientific communities, organising training sessions and seminars to improve the dissemination of scientific results obtained by RES users, and to improve the knowledge base of both technicians and researchers. The demand for RES services exceeded by 35% the time available for allocation. More than 255 projects utilised RES resources in 2011, increasing the total number of projects supported since the creation of the RES to more than 1850, confirming again the importance and need of access to supercomputing facilities in Spain.

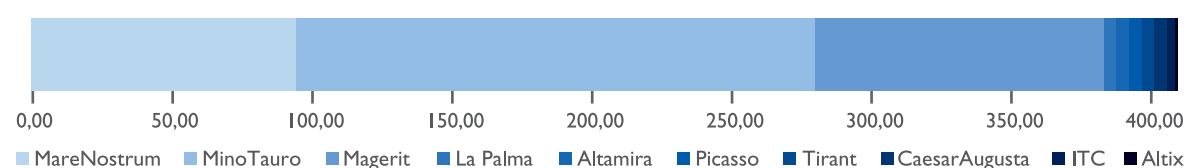


Nodes of the Spanish Supercomputing Network (RES)

» RES main goals, resources and members

The Spanish Ministry of Science & Innovation (MICINN) created the Spanish Supercomputing Network (Red Española de Supercomputación - RES) in July 2006 as a response to the need of the Spanish scientific community for increased capacity and access to intensive calculation resources, considering the supercomputing resources as a decisive asset for the scientific and technological development of the country.

RES Processing Power in TFLOP/s



The RES consists of a distributed virtual infrastructure of supercomputers located in different sites, each of which contributes to the total processing power available to users of different R&D groups in Spain. Generally, each node reserves 20% of capacity for use by researchers at the host institute, and the other 80% is made available to the RES. The exceptions are the nodes located at the ITC and CesViMa, which own their infrastructure, that offer 20% of computing power to the RES. Whatever its origin, all the computing capacity offered to RES is made available to the general scientific community via public calls evaluated by a single Access Committee.

During 2011, the total processing capacity of the RES has increased significantly, due to the upgrade of Magerit at CesViMa and the installation of MinoTauro at BSC. CesViMa offers 20% of Magerit capacity to RES and BSC offers up to 80% of MinoTauro Capacity to RES. The operation of the RES is coordinated by the Operations Department of the BSC-CNS, which includes support for global maintenance and upgrades, training of users and technicians, facilitation of access and all aspects related to user support.

» Access protocol and allocations in the RES during 2011

All the nodes of RES are accessible for use by Spanish and international scientists via electronic application following a single Access Protocol being evaluated by a single Access Committee.

The allocation of access to RES supercomputer facilities is based on criteria of efficacy, efficiency and transparency, mediated by a double filter system, with potential projects first being evaluated by the ANEP (National Agency of Evaluation and Prospective), followed by an evaluation by the Access Committee, composed of a Core Team and four Expert Panels formed by prestigious scientists external to the BSC-CNS. The four Expert Panels are defined according to the classification established by the Spanish Foundation of Science and Technology (FECYT).

The Expert Panels

- ▶ Astronomy, Space and Earth Sciences
 - ▶ Life and Health Sciences
 - ▶ Mathematics, Physics and Engineering
 - ▶ Chemistry and Materials Science and Technology
- Each of the above areas has a committee composed of a group leader, who acts as a chairing coordinator, an assistant, and eight experts in the area.

Access Committee Core Team 2011

- ▶ Ramón López de Arenosa, Ministerio de Educación y Ciencia
- ▶ Victoria Ley Vega de Seoane, ANEP
- ▶ Ramón Beivide, Universidad de Cantabria
- ▶ Eduard Ayguadé, BSC-CNS.

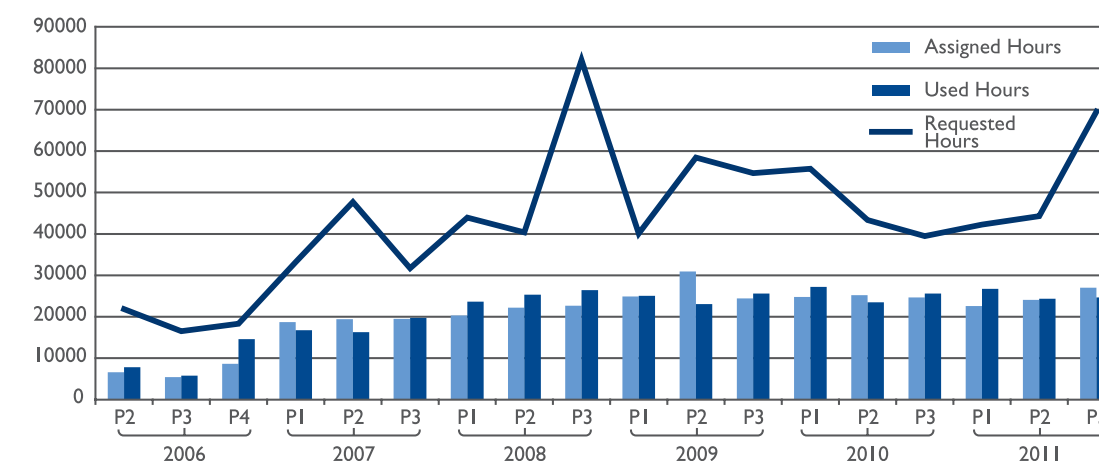
The Access Committee allocates to both Spanish and international researchers more than 26 million computational work hours every 4 months. In addition to internal research groups, more than 255 research projects made use of the RES system in 2011. It is important to note that many scientific projects often request several periods of access during the year (since they last 4 months) in order to perform different work activities. As specified in the Access Protocol, each request is treated separately and must pass the evaluation procedure of the Access Committee. Consequently, the number of activities reported for the RES is greater than the number of projects registered for the year.

» Access Requests 2011

Once the Access Committee has published its four monthly list of successful applicants and the number of computing hours that each one has been awarded and allocated, the Operations Department of BSC-CNS takes over the logistical processes of scheduling the users, preparing their software for loading and running the software, and ensuring the users have access to the data of the results and statistics on the performance of their code, to facilitate future code improvements.

The graph below shows the evolution of requested, assigned and used hours over the last 6 years.

Number of RES hours



The resource consumption was calculated 3 months before the end of the assignments corresponding to 2011

In the six years since RES commenced operation, the alliance of supercomputing centers has provided more than 416 million hours. Over the same period, the hours requested were 783 million, indicating that the demand was double the available resources that RES can provide to the scientific community, a clear indicator of the usefulness of supercomputing systems to scientific research.

» RES Users' Committee

The CURES (Committee of the Users of the Spanish Supercomputing Network) was established in 2010 to provide advice and feedback to management and technicians on the current state and future delivery of the resources and services provided by the RES.

CURES aims to promote the effective use of the High Performance Computing facilities of the RES by sharing information on experiences in using the different systems, suggesting new research and technology directions in scientific computing, and voicing user concerns. To this end CURES undertakes various communication activities, such as holding regular meetings, establishing shared databases, and posting information on relevant webpages.

The members of the CURES elect amongst themselves the Chair and Vice-Chair, who act as representatives on behalf of the whole committee. Each member is elected for a maximum of 2 years and half the members of the Committee should be renewed every year. In the case of Chair and Vice-Chair, are replaced alternately with the Vice-Chair assuming the Chair's role, thereby assuring continuity.

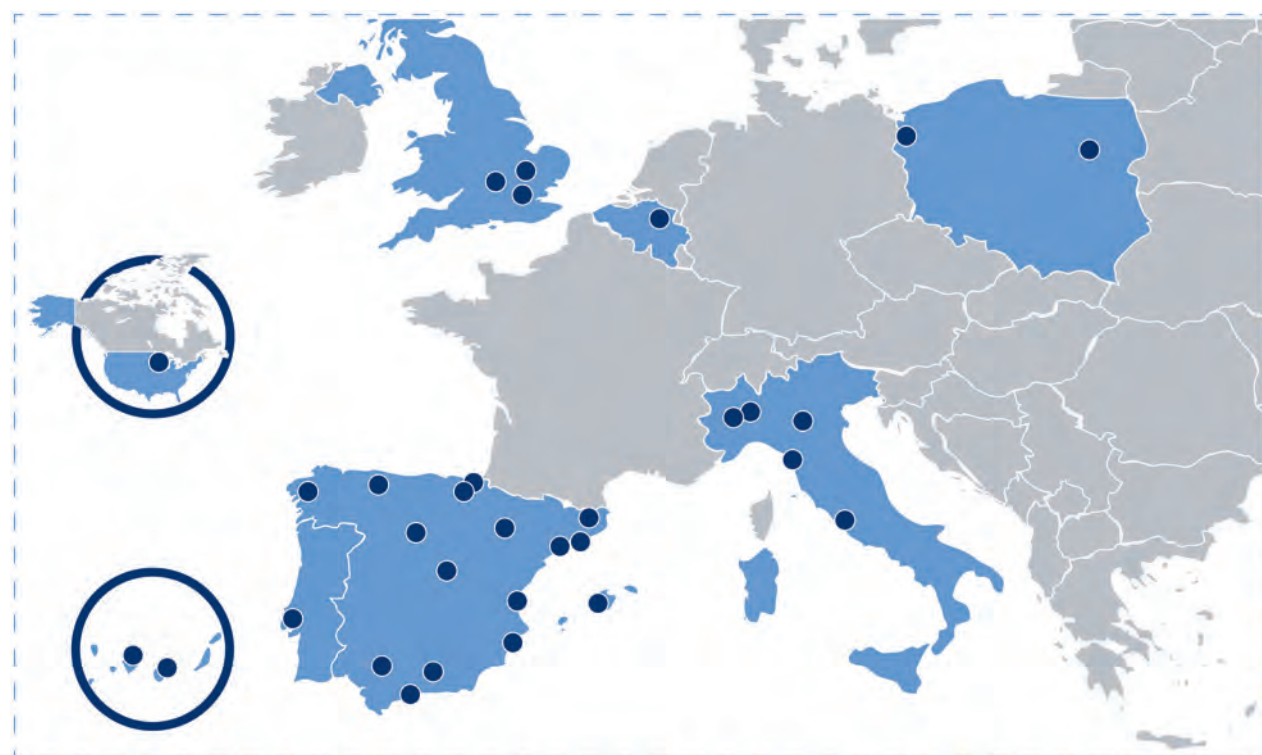
The CURES members

- ▶ Carme Rovira, UB
- ▶ Jordi Torra, UB
- ▶ Fernando Martín García, UAM
- ▶ Francisco Javier Luque, PCB
- ▶ Javier Jiménez Sendín, UPM
- ▶ Miguel Ángel Aloy, UV
- ▶ Núria López, ICIQ
- ▶ Rubén Pérez, UAM

» Broad Impact on Scientific Research

The awareness of the RES and the services it offers has spread quickly since 2006. More than 255 activities took advantage of the RES infrastructure in 2011, led by the most prominent researchers from institutions in over 30 cities in Spain, Europe and overseas.

The different research activities carried out on RES supercomputers during 2011 cover a huge range of scientific fields, including the use of next generation sequencing, development of new drugs, effects of turbulence in aviation, and black hole dynamics, among others. The results of these studies were disseminated in seminars and conferences all over the world, and also led to published articles in the some of the most prestigious scientific journals.



Cities of Origin of RES Users, 2011

The importance of the RES lies in the fact that these results would have been impossible to obtain in such short timeframes using traditional computers, that would take many years to complete such intensive calculations.

In addition to traditional channels of dissemination, the RES teams organised general and field-specific seminars to spread scientific findings, and also held training sessions to inform current and potential users on the available tools and the key issues to be considered during the execution of a project to maximise the benefit and efficiency of using the RES facilities. Additionally, in-depth technical training sessions were held for the teams that manage each RES node and any scientific users interested in the subject.

Another key objective for the RES, besides the training and dissemination of science, is to inform sectors of the scientific community who traditionally have not used supercomputers for their studies, on the advantages of accessing RES facilities and how to go about obtaining access.

» 5th RES User Conference

Every year, a user conference is held to disseminate the results obtained using the RES supercomputing facilities by different research groups in each of the four scientific areas. It also offers a forum for discussions between users, the RES Users Committee (CURES), the Access Committee and the RES management regarding the operation of the RES. Topics include the access procedure and requirements, the evaluation procedure, the support provided or any topic that is considered interesting for any of the parties involved.

In 2011, the 5th Users Conference took place the 26th October in Valencia and in addition to dealing with the above mentioned issues, developments at the RES node in Valencia were highlighted and the PRACE (Partnership for Advanced Computing in Europe) initiative was introduced, in order to ensure that the Spanish scientific community is kept informed of the different resources that will become available in the near future.

More information is available at <http://www.bsc.es/RES/quinta-jornada-usuarios-2011>.

» Scientific Seminars



Attendees to the NGS seminar

Next Generation Sequencing Seminar The seminar of Next Generation Sequencing was held the 17th and 18th March, 2011 in Málaga and was organised by BSC-CNS in collaboration with UMA (Málaga University). More than 70 people attended requiring the use of an additional room, demonstrating the high demand for such a seminar in Spain and the quality of the scientific discussion provided.

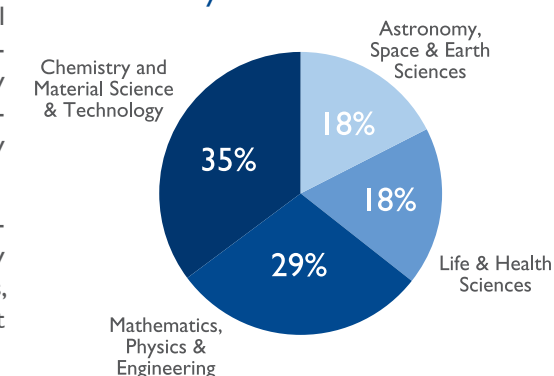
The objective of this seminar was to show researchers the computational problems involved in the analysis of readings taken with new sequencing technologies, as well as some of the solutions already available. Two major problems (the sheer volume of data and the shortness of the sequences) were addressed in detail, with demonstrations of the use of NGS for the quantification of gene expression, the quality of the results, the assembly

sequences, visualisation and storage. Renowned scientists and researchers shared with the attendants their findings from various projects and studies. Find further information at www.bsc.es/res/NGS-seminar.

Supercomputing for Lattice QCD The RES co-organised the 5th Iberian Grid Infrastructure Conference and organised a session aimed at users of supercomputing services to solve problems related with the quantum chromodynamics (QCD) theory of quarks and gluons, a lattice gauge theory formulated on a grid (or lattice) of points in space and time.

This very specific target group helped to focus explanations by RES technicians of the tools and working methods that will provide the most efficient use of resources for typical problems faced in this discipline. Find further information at www.ibergrid.eu/2011.

RES Hours Used in 2011 by Scientific Field



5th RES User Conference ad



Presentation of the RES in Ibergrid 2011

cosmology and robotics, among others. This provided the participants with a broad overview of topics of interest in working and professional fields which they wish to join. Further information at <http://benasque.org/2011/ fronterascompu>.

Computing Frontiers The seminar was organised in cooperation with the University of Zaragoza, the Science Center of Benasque Pedro Pascual and the RES. It was held from 22th to 27th July 2011 and was aimed primarily at college students and young researchers, to offer them an overview of various issues related to computing R&D in Spain.

The speakers were leading researchers working in both public research organisations and companies. They provided an indepth, transversal and multidisciplinary computing experience, covering topics such as biocomputing, nanoscience, safety and prevention,

» RES Users Trainings in 2011

RES Insular Sessions Two sessions were held in the Canary Islands the 27th and 28th September 2011, one in Las Palmas de Gran Canaria and another in La Laguna. These were organised by the RES, the ITC (Canary Islands Technologic Institute) and the IAC (Astrophysics Institute of the Canary Islands) with the main objective being to illustrate the usefulness of applying supercomputing resources to scientific research by presenting the outcome of different scientific activities developed in the RES by prestigious researchers. The technical teams of ITC, IAC and BSC-CNS also introduced themes and tools to enable users to use the computing resources in a more effective and efficient way. Find further information in www.bsc.es/res/jornadas-canarias-2011.



Insular session held in Gran Canaria

Programming models The RES, in cooperation with the University of Valencia and BSC-CNS, held the second edition of the Programming models seminar on 27th October 2011, in Valencia. It was conducted by experts from the Computer Science Department of BSC-CNS and aimed to provide an introduction to programming models such as GRIDSs, COMPSs, MPI, SMPs and STARs to scientific and technical developers in order to improve the code of the applications they run in supercomputers such as those that form the RES. Find further information at www.bsc.es/RES/programming-models-2011.

Requesting access to RES and PRACE On 13th December 2011, a RES and PRACE Access meeting was held in Barcelona for users, at which BSC-CNS provided information and answered questions on how to request access to supercomputing resources available through the RES and the European project PRACE. Find further information at www.bsc.es/RES/requesting-access-2011.

» RES Technical Seminars in 2011

Cluster management software and introduction to infiniband technology The RES organised the Technical Training Cluster management software and introduction to Infiniband on the 3rd and 4th May 2011, in Barcelona. The seminar was quite specialised and aimed at all the RES nodes technical teams, all staff part of an HPC center, and also any university staff or administrators of a cluster mainly focused in providing supercomputing services. The more than 50 attendants proved the high level of interest in such technologies.

Thanks must be offered to the participant companies that offered the training: Bull Technologies, IBM, Hewlett Packard, Mellanox Technologies and Bright Computing, who presented the main features and monitoring services for each cluster management software. A basic introduction to the operation and advantages of Infiniband technology was also provided. Find further information at www.bsc.es/RES/clusters-and-infiniband-seminar.



Attendees to the Cluster Management and Infiniband seminar

Visualisation and Real Virtuality The RES, in cooperation with CeSViMa and the University of Zaragoza, organised the technical training titled Virtualisation and Real Virtuality on 14th and 15th December 2011. For researchers and companies that access RES resources and develop their research, a good way of displaying results in order to both facilitate improvements in knowledge and experience, and to make the topics more understandable for the general public, is to utilise the Visualization and Real Virtuality construction of models to display results.

The workshop aimed to provide information to technicians at the different nodes regarding the 3D device recently made available to the RES community and also provide an opportunity to learn from the visualisation projects already developed by researchers, as well as identifying the needs of the scientific community. Find further information at www.bsc.es/res/NGS-seminar.

SLURM Workshop On 15th December 2011, the RES, in cooperation with CeSViMa organised a half-day workshop to allow all RES technicians to discuss problems and the current situation of the scheduling and resource management software. The meeting was conducted by the Performance Engineer at BSC-CNS and helped to share the knowledge amongst all the teams as well as to initiate discussion on possible future needs and related software.



Attendees to the Visualization and RV seminar

» BSC-CNS & RES Open House Week in 2011



Advertisement on the 5th Anniversary Open House

The RES and the BSC-CNS organised an Open House Week from the 24th to the 28th January 2011 in order to disseminate the science developed since the creation of the RES, to inform the scientific community of the new available 3D visualization equipment and to attract new students to the supercomputing field as well as to scientific degrees.

During the 5 days, more than 400 people visited the MareNostrum facility and attended a series of interesting talks conducted by experts. The Open House Week was extensively reviewed in the national and local media.

» Overview



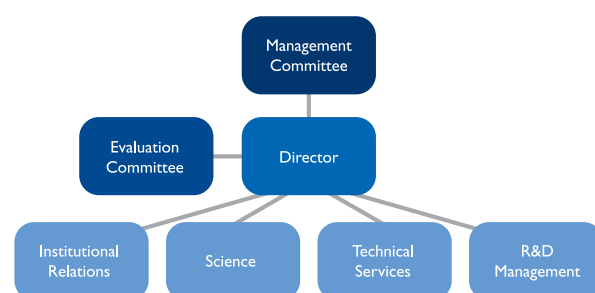
The MAGERIT Supercomputer

CeSViMa (Supercomputing and Visualization Center of Madrid, in Spanish “Centro de Supercomputación y Visualización de Madrid”) is located in the Excellent IT and Technology Transfer Montegancedo Campus, one of the sites of the Technical University of Madrid Science & Technology Park. CeSViMa, which is member of the Spanish Supercomputing Network (RES), Spanish e-Science Network and Madrid Laboratories and Infrastructures Network, focuses on three main objectives: High Performance Computing, Advanced Interactive Visualisation and Massive Storage.

Magerit (the ancient recorded name of Madrid) is the name of CeSViMa's supercomputer. The second version of Magerit supercomputer is a cluster of 245 nodes PS702, that provides close to 4000 CPUs and 200 TB of storage inter-connected by a very high bandwidth switch. The nodes are interconnected with a high bandwidth and low latency infiniband network.

On May 2011, when this setup was installed, Magerit became the most powerful and the most environmentally friendly supercomputer of Spain (position 136 in the TOP500 list of June 2011 and position 18 in the Green500 list of June 2011).

» Organisational Structure



CeSViMa Team as of January 2011. From left to right: Borja Chocarro, Rubén Galeano, Oscar Lozano, Oscar Cubo, Andrés Marín, Fernando Limón, Vicente Martín, María S. Pérez-Hernández, José María Peña, Pilar Flores and Jorge Guerra.

» Technical and Scientific Highlights 2011

Magerit supercomputer was upgraded in May 2011. This upgrade consisted of the replacement of all nodes (JS20 and JS21) with the latest blade technology (PS702) and the old interconnection network (myrinet) with a more suitable network (infiniband). With this configuration Magerit's computational power increased by a factor of 5 while incurring only half of the associated costs.

CeSViMa's operations team started scheduling the upgrade during late 2010 and the first months of 2011. This facilitated a very fast installation (it lasted barely one month) and services were not interrupted. The upgrade was finished a couple of months before the third RES period. This period used exclusively 20% of the new system which is the share assigned to the RES (5 times more resources). For a list of key scientific outputs during 2011, please consult the online version of this report.

» Key Projects 2011

- Transversal project: High Performance Computing Europe
- Alberto Abánades Velasco: CRP on Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems (ADS)
- Carolina Ahnert Iglesias: Métodos avanzados multiescala núcleo-celdas en geometrías tridimensionales y multigrupos para el cálculo de reactores de agua ligera
- Emilio Artacho: Exploring new avenues towards high-performance room temperature spintronics
- Ignasi Belda: Avaluation of different approaches for the generation of de novo molecules using statistical methods

- Rodolfo Bermejo Bermejo: Desarrollo de un modelo regional de clima con acoplamiento atmósfera-océano y la optimización del código para su ejecución en clusters masivamente paralelos. CLG2006-1264-C04-02/CLI
- Mercedes Boronat: Metal supported nano-particles over carbon based nanostructure catalysts for oxygen and hydrogen activation
- Vitor Cardoso: High energy collisions of black holes
- Gonzalo Fernando Colmenarejo Sánchez: Modelado estadístico de propiedades y actividades de moléculas con aplicación farmacológica
- Santiago Cuesta López: Modelling shock wave propagation in advanced materials and nanostructures

tures; Shock loading and wave propagation in advanced nano-structured materials

- Cecile Dreiss: Investigation of the oligomerization mechanistics of the Prion protein
- Javier Fernández Sanz: Catalysis modeling: cerium oxide nanoparticles supported on titania
- Franca Fraternali: Study of the self-assembly of Influenza Haemagglutinin fusion peptides in a model membrane
- Antonio García Dopico: Desarrollo de un modelo regional de clima con acoplamiento atmósfera-océano y optimización del código para computadores masivamente paralelos
- Juan José García Ripoll: QUITEMAD: QUINFOG
- Miguel González Pérez: Molecular dynamics study of ligands binding into the active site of human and yeast dipeptidyl-peptidase III
- José Javier Honrubia Checa: Ignición rápida de blancos de fusión inercial
- Javier Jiménez Sendín: Simulación de burbujas transicionales de separación en turbinas de baja presión
- Nikos Karayiannis: Modeling of Synthetic and Biological Molecules Through a Hierarchical Multiscale Approach
- Manuel Laso Carbajo: Multiscale Modeling of Nanostructured Interfaces for Biological Sensors (MNIBS)
- Felipe J. Llanes Estrada: Insensitivity to symmetry breaking in the very excited spectrum
- Vicente Lorenzo: Determination of the Stress-optical coefficient and plateau modulus from atomistic simulations of polyethylene melts
- F. Javier Luque: Exploring the mechanism of truncated hemoglobin N by molecular simulations
- Marco César Maicas Ramos: Caracterización de nanoestructuras magnéticas obtenidas por pulverización catódica y nanolitografía de haz de electrones
- Víctor Manuel Maojo García: Método de integración de fuentes de datos heterogéneas, públicas y privadas, orientado a la recopilación
- Vicente Martín Ayuso: Cálculos mecanocuánticos en sistemas mesoscópicos; QUITEMAD: GICC-UPM
- Miguel Ángel Martín-Delgado Alcántara: Decoherence Effects in Topological Quantum-Computing Models; QUITEMAD: Cryptography, Computation and Simulation
- Javier Martínez de Salazar Bascuñana: Dinámica,

compatibilidad molecular y nanoestructuras de poliolefinas de nueva generación

- Michele Parinello: Thermodynamic and mechanical properties of hybrid framework materials. When theory meet experiment
- José María Peña Sánchez: Algoritmos genéticos masivamente paralelos: Aplicaciones a problemas de ingeniería; Blue Brain Project
- David Pérez García: QUITEMAD: MIC
- Rubén Pérez Pérez: Carbon nanostructures and hydrogen production and storage by first-principles calculations and scanning probe techniques; Microscopios de proximidad: Transporte, reactividad y Manipulación en Nanoestructuras; Transporte en Nanoestructuras y Microscopios de Proximidad
- Manel Perucho Pla: Relativistic Outflows: Dynamics and Feedback in Galactic Evolution.
- José Ranilla Pastor: Search for Commutative Semifields of order 128
- Víctor Robles Forcada: Procesos de optimización para la obtención de conocimiento en bioinformática
- M^a Encarnación Rodríguez Hurtado: Sistema integral de modelización de la calidad del aire en la Península Ibérica (SIMCA)
- Jaime Rubio: Understanding protein-protein interactions: towards the design of inhibitors for the Bcl-2 protein family
- Ángel Rubio Secades: Optical and Charge Transfer Properties of Hybrid Organic-Dye/Oxide Nanostructure and Interface Systems for Solar Cells Application (ETSF activity)
- Roberto San José García: Sistema operacional de predicción de la calidad del aire para el continente europeo (MM5-CMAQ-EMIMO): Servicios de información regional
- Vassilis Theofilis: Aero-Acústica computacional y experimental para predicción y control de ruido (ACE-PCOR)
- Eusebio Valero Sánchez: Aero-Acústica computacional y experimental para predicción y control de ruido (ACE-PCOR)
- Pedro Velarde Mayol: Hiper
- Matthieu Verstraete: Electron phonon and anharmonic effects in Antimony under pressure
- Perla Wahnón Benarroch: Design and Characterization of Advanced Photovoltaic Materials with High Efficiency; Diseño, Síntesis y Caracterización de Materiales Fotovoltaicos Avanzados de Alta Eficiencia; Nuevos materiales fotovoltaicos de banda intermedia

» Overview



The LaPalma Supercomputer

The LaPalma supercomputer, one of the eight nodes belonging to the RES and financed by the Ministry of Science and Innovation (MICINN), is located in the “Centro de Astrofísica de La Palma (CALP)”, in Breña Baja. The LaPalma supercomputer, along with four other “brother nodes”, is formed from older processors derived from the MareNostrum which were relocated during its last upgrade, and the node is coordinated from the BSC-CNS. The installation of the supercomputer at LaPalma was a strategic step whose objective is to boost the observation activities in the Observatorio del Roque de Los Muchachos - above all through the incorporation of the Gran Telescope CANARIAS (GTC) - and in this way reinforce the telecommunication development on the island.

» Organisational Structure

There is a time assignment commission for managing the 20% of computational resources of LaPalma. This commission consists of members from different divisions of IAC.

For the administration and management of the supercomputer node, the Instituto de Astrofísica de Canarias (IAC) makes available its IT support team and has employed one engineer dedicated full-time to fulfill these functions.

The LaPalma Supercomputer Systems & Support Team: Carlos Martín Galán (Senior Engineer), Responsible Technician and the Manager of the Group. Antonio Díaz Chinaa (Senior Engineer), System Administrator. Justo Luna López (Engineer), System Administrator. Ubay Dorta Guerra (Engineer), System Administrator and User Support. Ángel de Vicente Garrido (Engineer), User Support. Victor Plasencia Darias (Operator), User Support.



LaPalma team (left to right): (back) Carlos Martín, Ubay Dorta, Justo Luna, Victor Plasencia, (front) Ángel de Vicente and Antonio Díaz.

» Technical and Scientific Highlights 2011

LaPalma's maximum processing capacity is 4,5 TFLOP/s (4.5 trillion floating points operations per second). Operations performed by LaPalma in one second would take more than 112,500 years for a person with a simple calculator. LaPalma, installed in a controlled environment room of 32 square metres, has one terabyte of principal memory (approximately equal to the memory of more than one million home PCs) and a further 14 TB of hard-disc data storage (equivalent to some 10 million books).

The various IAC installations on the islands and LaPalma communicate via a link of 10Gbps, of which the supercomputer can use up to 4Gbps.

From March 2011 to December 2011 LaPalma provided roughly 580k hours of CPU time for IAC researchers. The projects developed consumed 99% of available time.

For a list of key scientific outputs during 2011, please consult the online version of this report.

» Key Projects 2011

Propagation of magnetoacoustic waves in magnetic structures (P.I.: Elena Khomenko) Local helioseismology of solar active regions will be able to provide information about sub-surface magnetic fields to be used by magnetic dynamo models, in order for which the physics of waves in magnetised regions has to be well understood. Forward numerical simulations have become a preferred approach in recent years to attack the complex non-linear physics of waves in non-trivial magnetic field configurations. The project aims to understand: (i) Mechanisms of excitation of waves in sunspots. (ii) Physics of umbral flashes and running penumbral waves. (iii) Identify

wave types dominating helioseismological velocity signals detected in active regions. (iv) Analyse consequences of the strong magnetic field of sunspots onto helioseismology measurements and determination of sub-photospheric structure of solar active regions.

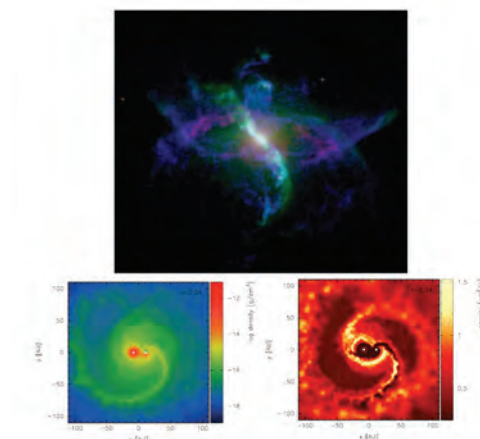
Stellar Spectral Synthesis Calculations in the H-band (P.I.: Carlos Allende) This project is involved in APOGEE, a massive spectroscopic survey of 1e5 stars in the H-band (1.5-1.7 μm) part of the Sloan Digital Sky Survey III (SDSS-III www.sdss3.org). One of the tasks is to develop ASPCAP, the Apogee Stellar Parameter and

Chemical Abundance Pipeline, a data analysis software to extract the astrophysical information in the spectra. ASPCAP uses a FORTRAN90 code to find the stellar model that best matches the observations. ASPCAP is based on interpolation in a library of model spectra. The computing time requested is for two tasks: 1) the calculation of the library itself, and 2) to perform Montecarlo simulations to test and understand the performance of ASPCAP.

Galaxy transformations through interactions, mergers and accretion (P.I.: Marc Balcells Comas) Galaxies with masses above $\log(M) = 11$ (in units of the Solar mass) already existed when the Universe was just 4 billion years old (redshift 2) and were extremely dense as compared to today's massive elliptical galaxies of the same mass. Acknowledging that massive galaxies suffer tens of accretions of smaller galaxies during their cosmic lives, this project aims to study whether the mass and the mechanical energy injected by these accretion events lead to a growth rate that explains the observations. The method is to re-simulate at high resolution merger histories of massive galaxies extracted from fully cosmological simulations, and analyze the evolution of the size and the internal velocity dispersion after each accretion. A parallel supercomputer is essential given the number of particles and number of mergers to be run.

Solar magneto-convection simulations and spectral synthesis for accurate chemical abundance determinations (P.I.: Damian Fabian) The research project uses solar magnetohydrodynamic simulations obtained with the parallel MHD code by A. Nordlund (Nordlund 1982, Stein & Nordlund 1989), coupled with the code LILIA (Socas-Navarro 2001), to derive synthetic absorption profiles and Stokes parameters. This allows the study of the formation of important spectral lines detected in the solar spectrum and to compare them with results from other theoretical studies and from observations. By taking into account the effect of magnetic fields, the project aims to derive a better-than-ever determination of the amount of different chemical elements in the Sun. This ground-breaking achievement can unravel crucial clues about the solar atmosphere, and (at least partly) contribute to solving some of the discrepancies still surrounding the field.

Smoothed Particle Hydrodynamic Simulations of the symbiotic binary, R Aquarii (P.I.: Romano Corradi) Jets are a common phenomenon in astrophysics. Highly collimated jets are produced in young and old stars, interacting binaries with white dwarfs, neutron stars or black holes, and on scales of galaxies, AGNs, radio galaxies, quasars, or the nuclei of recently merged galaxies (e.g. Cen A). Jets play an important role in the evolution of these systems by carrying mass, energy, and momentum, and probably serve a role similar to a relief valve where energy densities are uncontrollable. Launching jets from magnetized accretion disks



[Top] Image of the combined [OII], [OIII] and [OIII] emission images taken with the 2.6m Nordic Optical telescope in 2007. [Bottom] Density [left] and dust [right] cross-sections in the orbital (xy) plane of a binary model consisting of a pulsating Mira (left star) and an accreting white dwarf (right star). The orbital period in this case is 70 years.

is the most popular explanation. However, the physical processes by which the jets are launched and collimated operate on size scales of the source's accretion zone. Unfortunately, most jets are so distant that it is not possible to resolve the immediate environment of the outflow sources. In addition, many jet systems, especially in star forming regions or in the nuclei of galaxies, contain large amounts of dust that veils the outflows within opaque cocoons. In this respect, the highly evolved symbiotic star R Aquarii (R Aqr) displays what is perhaps the most propitious system to study, because it is one of the closest stellar jets (200 pc) and is bright, active and with relatively low extinction. In addition, the nature of the central engine of R Aqr, a white dwarf accreting from the wind of a Mira pulsating with a period of 387 days, is known, and the spectroscopic orbit (with a 44 year period) of the binary system has been derived by “M. Gromadzki and J. Mikolajewska. The spectroscopic orbit and the geometry of R Aquarii. *A&A*, 495:931–936, 2009.” For this reason, the project entails a comprehensive study of R Aqr. In particular, given its short distance and large expansion flows, the programme of multi-epoch imaging over several years reveals the evolution of the R Aqr outflows in real-time, producing privileged information that is generally not available in Astrophysics. The project aims to support this accurate observational study with a detailed modelling of the system, taking advantage of the fully-tested Smoothed Particle Hydrodynamics (SPH) code developed by S. Mohamed. Adopting the known binary and stellar parameters of the system, the simulation will enable investigation of the mass transfer processes from the red giant to the white dwarf in such a wide binary system, and to determine the mass accretion rate and hence the formation of the accretion disc which is supposed to be at the origin of the jet. This is the first time that such a detailed comparison between observations and models is attempted.

» Overview



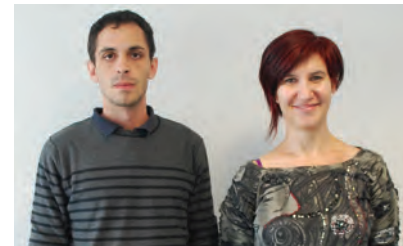
The Atlante Supercomputer

Atlante supercomputer joined the RES on February 16th 2009, becoming its 8th member and the 2nd member from the Canary Islands. It is managed by Instituto Tecnológico de Canarias (ITC), a public company of the Canary Islands Regional Government, that promotes the industrial development of the region, fostering research, development and innovation in emerging technological fields, in close collaboration with companies and research institutions.

The Atlante node is located at the Science and Technology Park of the University of Las Palmas de Gran Canaria [1]. The cluster is formed by 84 IBM JS21 blade servers with dual core PowerPC 970MP processors and 8GB RAM (336 CPUs in total), reaching 3.36 TFLOP/s. Atlante uses a Myrinet-2000 interconnection network and offers 8TB of storage disk.

» Organisational Structure

The technical staff of Atlante comprises two engineers from ITC (Yeray Gutiérrez Cedrés and María Belén Esteban Sánchez), who are responsible for system management and user support, and a group manager (Juan José Ascanio Amigó). A local Access Committee allocates the 80% of local CPU time amongst users from Canary Islands's Government, private companies and R&D groups, while the remaining processing time is provided to the RES network.



The Atlante Supercomputer Team:
Mª Belén Esteban Sánchez (right, User Support)
Yeray Gutiérrez Cedrés (left, System Administrator)

» Technical and Scientific Highlights 2011

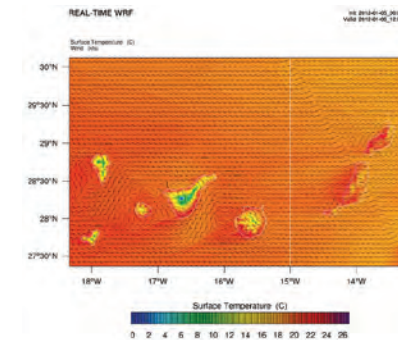
In 2011 Atlante node executed applications corresponding to Canary islands's Companies and Researchers with more than 2 million hours of CPU time, related to the following projects. For a list of key scientific outputs during 2011, please consult the online version of this report.

» Key Projects 2011

Photovoltaic Systems Simulator (Simulation of Photovoltaic Energy in Gran Canaria) The project deals with meteorological data processing to estimate the amount of energy that Photovoltaic Systems allocated in Canary Islands would be able to generate according to the expected weather conditions, which are estimated using Numerical Weather Prediction models (MM5) executed by the Atlante supercomputer. The Photovoltaic Systems Simulator was run in Atlante for the whole of 2011, and its estimations are used for the power load dispatch center operations.



Simulation of Photovoltaic Energy in Gran Canaria

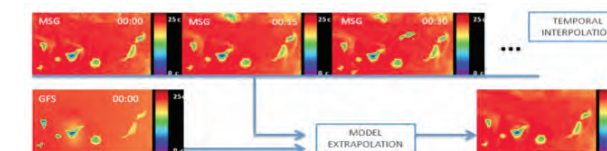


Development Of An Energy Forecast System With Applications In Photovoltaic Plants By Using Numerical Models

The technical complexity of energy systems and the increasing tendency of introducing renewable energies into these systems, makes it essential to use forecasting techniques to try to predict solar radiation. This makes it possible to organize and optimise all the net's resources. Therefore, the aim of this project is to develop a system which can predict the correct amount of solar energy which is going to reach the Earth's surface at the Canary Islands. The numerical model used was the Weather Research and Forecast model (WRF), executed in Atlante.

Meteosat Second Generation Surface Temperature Assimilation For Wrf Model Over Canary Islands Domain

One of the problems introducing electricity generated by renewable-based generation units is that the amount of energy generated depends on the weather conditions. In order to balance generation/demand and also guarantee the stability of the electrical system, the electrical network manager needs to know the clean generation forecast. The developmental tendency and primary method to deal with this problem involves predicting wind and/or solar radiation fields using numerical Weather Prediction Model (NWP). In this study Weather Research and Forecasting (WRF-ARV) model was used. The objective of this study is improve the initial ST conditions introducing values from TIR channels, calculated by MSG satellite, in order to obtain more accurate results using WRF model for solar shortwave flux at surface field.



Adaptive Evolutionary Travel Route System (Aetros)

The Adaptive Evolutionary Travel Route System (AETROS) model was designed to solve the travel route assignment problem in a new, dynamic way. Urban traffic present highly changing scenarios where statistic based optimisation approaches cannot cope with unforeseeable situations. AETROS is designed to be constantly

adapting to the current situation and drivers are not assigned a fixed origin-destination route. Instead, as they approach an intersection they will receive the latest optimal option for their destination.

Dragon Airborne Power Dragon Airborne Power (formerly Persan Engineering) is actively pursuing the development of high-altitude wind power systems, which calls for the computing-intensive simulation of the external aerodynamic flow and energy-capturing process on a proposed airborne turbine model using the finite-volume discretization of the Navier-Stokes equations. To this end, the Code Saturne flow solver was extensively used on Atlante, leading to the assesment of power levels, lift/drag/moment coefficients and stability derivatives needed to design a working prototype in the short term future.

Simulation Studies And Design Of Materials And Nanomaterials Under Extreme Conditions

One of the most fundamental goals in high pressure research is to mimic processes and phenomena similar to those occurring in the interior of the Earth and other planetary objects, and to understand physical and chemical properties that appear in exotic phase after phase transitions under extreme conditions. This project aims to develop an ab initio study of the structural, electronic and dynamical properties under extreme conditions, combined with different extreme conditions experimental techniques performed in synchrotron and neutron sources.

SLAM The problem of Simultaneous Localization and Mapping (SLAM) addresses the issue of a mobile robot moving through an environment of which no map is available a priori. The goal of SLAM is to reconstruct a map of the world and the path taken by the robot, being a key prerequisite to truly autonomous robots. The work focuses in multi-sensor fusion to improve the quality of the robot pose estimation as well as the map of the surrounding environment. Currently, we are also in the process of integrating inertial motion information to aid the state estimation. More specifically, we want these techniques to perform in real time, in which the quality of the map might be penalized, but enable us for active perception. Still, high computational task are required to obtain a ground truth, for which we process collected data offline in batch mode.

Efficient Computation Of Voronoi Neighbors

Some algorithms in Patter Recognition and Machine Learning as neighborhood-based classification and dataset condensation can be improved with the use of Voronoi tessellation. We study the use of a cooperative framework where multiple Cores in host and multiple GPUs cooperate to compute the Voronoi adjacency relationship in multidimensional Machine Learning datasets.

» Overview



The ALTAMIRA Supercomputer

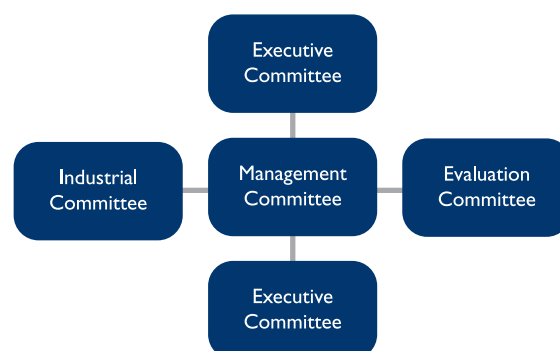
The ALTAMIRA node of the RES at the University of Cantabria is located in the Juan Jorda Building and is jointly managed by the IFCA Distributed Computing Team and the Computer Architecture Group (ATC) of the University of Cantabria.

IFCA (Instituto de Física de Cantabria) is a joint center of the University of Cantabria and CSIC with research lines in astrophysics, high energy physics and distributed computing, and participates in several national and European computing projects.

The main research areas of the Computer Architecture Group (ATC) of the University of Cantabria are the analysis, design, and evaluation of parallel computers, covering their principal aspects from programming to the lower hardware levels.

» Organisational Structure

The Altamira node has dedicated technical support, with oversight by the scientific computing divisions of both IFCA and ATC. Also involved in system administration and user support of the node are the managers of the computing research lines of IFCA and ATC.



Luis Cabellos and Miguel Ángel Núñez

» Technical and Scientific Highlights 2011

In 2011 the Altamira node executed applications corresponding to local users at the University of Cantabria with more than 570.000 hours of CPU.

For a list of key scientific outputs during 2011, please consult the online version of this report.

» Key Projects 2011

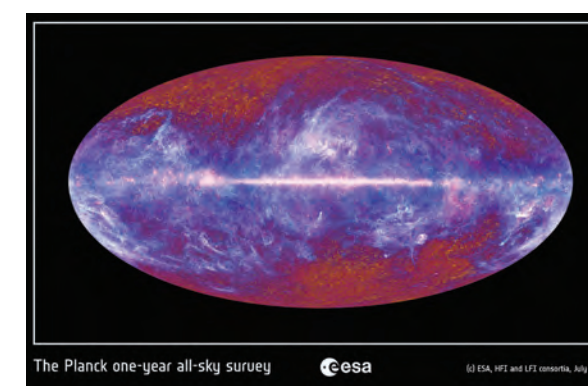
Efficient density-functional calculations with atomic orbitals on nanosized ferroelectric nanostructures Led by Javier Junquera, a study of the behaviour of ferroelectric capacitors utilising the SIESTA program. The SIESTA program has been optimised for use in supercomputers by the BSC-CNS and its operation was trialed in the Altamira supercomputer. This activity has led to the authors publishing a number of articles and being invited to conferences in the field.

Light scattering by micro-nano particles located on substrates Projects led by Pablo Alvella Echave and Fernando Moreno Gracia. Studies in the detection of defects in the microstructures of substrates used in the diffusion of light using different advanced numerical methods: Discrete Dipole Approximation (DDA), Extended discrete dipole approximation (E-DDA), Extinction's theorem (ET), amongst others. The Altamira supercomputer was needed to advance from 2D calculations to 3D calculations and thereby enable the study of further situations. The project is financed by a National Research Plan.



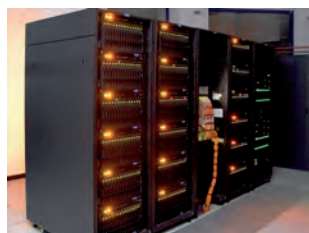
Ab initio investigation of the origin of the antiferrodistortive rotations in oxides Led by Pablo García Fernández, a study of the origin of AFD distortions in a variety of oxides with perovskite structure and different properties from a chemical, electrical and magnetic point of view using first-principles calculations.

Testing Gaussianity of Planck data Led by Enrique Martínez, the Group of Cosmic Microwave Background (CMB) of the Physics Institute of Cantabria undertook a number of different analysis projects, including the analysis of CMB data from two space missions, WMAP (NASA) and Planck (ESA), and preparing the data analysis and reduction of the new instrument Quijote. The project, financed by a National Research Plan, is carrying out data analysis for contribution to the Planck mission and also studying the contamination present in these data.



Projects of the Computer Architecture Group of University of Cantabria Altamira has running simulations to study interconnection networks for large parallel systems and for on-chip multiprocessor systems with the objective of proposing new topologies and architectures. Several research activities are using production codes taken from BSC-CNS as benchmarks to evaluate different architectural proposals.

» Overview

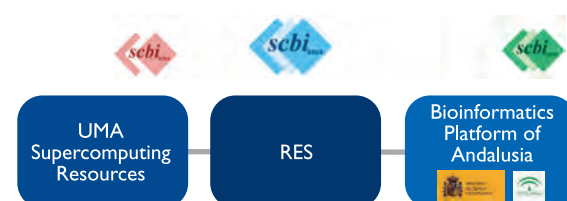


The Picasso Supercomputer

The Pablo Picasso node of the RES is located in the Bio-Innovation Building of the University of Málaga (UM) at the Technological Park of Andalusia (PTA), close to the city of Málaga. The computer is managed by the SCBI (Supercomputing and Bioinformatics Centre) of the UM, which runs several computational infrastructures supporting research activities within the University and in the Andalusian region, including the 512 CPU PowerPC-based cluster belonging to the RES, a 128 CPU Itanium-based SMMP and a 80 CPU x86-based cluster belonging to the UM. All these resources share computer room, cooling, power and fire extinguishing systems.

Other resources of note include a virtualisation infrastructure belonging to the Bioinformatics Platform of Andalusia, which hosts all its servers and desktop systems as virtual machines running on a cluster of VMWare ESX servers.

» Organisational Structure



SCBI team at Málaga (left to right):
Dario Guerrero Fernández (sysadmin)
Guillermo Pérez Trabado (manager)
Rafael Larrosa Jiménez (sysadmin)

The SCBI draws on 13 years of experience of the Computational Laboratory of the UM in running production supercomputers to support scientific research in several fields. It also incorporates a recently created research infrastructure, the Bioinformatics Platform of Andalusia, whose mission is to provide computational resources and commercial software licenses, and to transfer knowledge and experience on bioinformatics research to the scientific community in Andalusia.

The SCBI is an independent service with its own staff dedicated to administration of machines and user support, but also giving higher level support to researchers in the development of computational solutions for problems in several areas, especially biological research.

There is also strong cooperation with the Computer Architecture Department of the UM whose main research areas are analysis, design, and evaluation of high performance architectures, from the application level to the lower hardware levels.

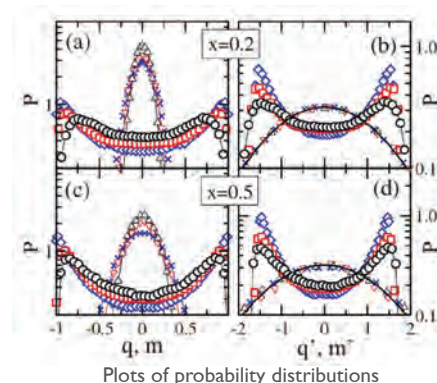
» Technical and Scientific Highlights 2011

In 2011 PABLO was consolidated as a useful resource for researches, providing service to several new users that have still not published but with promising research going forward. For a list of key scientific outputs during 2011 please consult the online version of this report.

» Key Projects 2011

Statistical physics, Department of Applied Physics of the University of Málaga Phase diagram of systems of interacting dipoles. The Group develops models and numerical simulations to study the collective behavior of many-particles systems. The behaviour of ensembles of magnetic nanoparticles and molecular magnets are investigated, exploring the physical limits of information storage in magnetic devices.

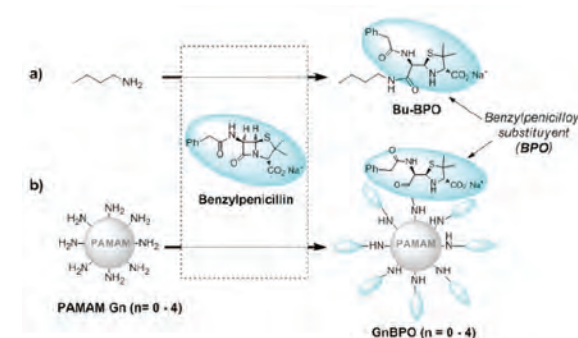
Plot I shows the results for the distributions of m and q at low temperature. Due to the central limit theorem and since the correlation lengths are finite in the paramagnetic phase, $P(m)$ and $P(q)$ are expected to be normal distributions.



Plots of probability distributions

Biomimetic Dendrimers and Photonic Its research is focused on the development of new molecular and supramolecular chemical entities, at nano and micro-scale, and their applications in biological medias of medical interest. Particular attention on the design and engineering at molecular level of nanostructured organic compounds and photonic devices is attained. Our research deals on the frontiers of nano-chemistry and biomedicine.

In the figure at the left it can be seen that in the context of penicillin allergy, the formation of the antigenic determinant structures is based on the electrophilic properties of the β -lactam ring against nucleophilic reagents such as alcohols, thiols and amines. A simple approach to establish what happens with the hapten molecule after reaction with natural high molecular weight nucleophiles such as proteins was carried out with a low-molecular-weight nucleophile (Scheme 1(a)). After controlling the resulting structure of the antigenic determinant, synthetic dendrimers were employed to mimic carrier proteins in order to evaluate multivalent defined structures with a monodisperse structure.



"Reaction schemes of benzylpenicillin with nitrogen nucleophiles such as (a) butylamine and (b) PAMAM dendrimers."

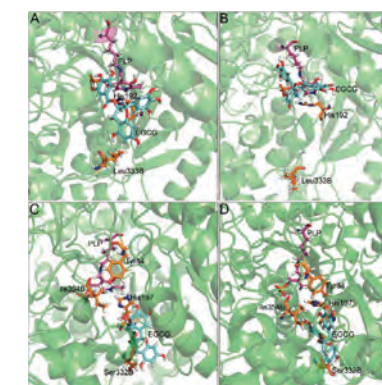
Molecular Modelling in rare diseases During 2011 the group did several researches on molecular dynamics, one of them has been published in the Journal of Chemical Information and Modelling, in it has been found the optimal EGCG inhibitor binding to histidine carboxylase and DOPA decarboxylase. Once the binding zones has been found with computational docking techniques, the structures were stabilized and refined.

In the image at the right, there are shown binding modes of EGCG to HDC and DDC as a first step for designing new polyphenol-based HDC/DDC-specific inhibitors.

Also, dynamic molecular simulations of systems composed by a receptor binded to G proteins, embebed in a membrane are being done, and results are expected soon.

Physical oceanography The Physical Oceanography Group of the University of Málaga is researching water exchange through straits.

Straits connecting semi-enclosed seas with the open ocean are key sites to determine the basin-scale properties as they are topographic constraints for the ventila-



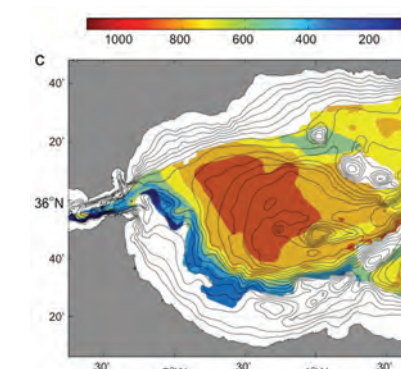
Details of the beginning and end of the MD simulations in DDC and HDC active sites, respectively

tion of deep/bottom waters. The different forces driving the exchange and its variability are investigated within this research line, which is funded by the Spanish Government (Ministerio de Ciencia e Innovación) under the INGRES projects.

Depth of the isotherm surface 12.85°C (in meters).

The figure at the right shows that farther away from the Strait entrance area the circulation appears to be quite independent of the strait status (open or closed) indicating that the gyre is mainly responsible for the banking of WMDW against the African slope. On the other hand, the shallowness of the isotherm in front of the strait in the open-strait run is attributable to the Bernoulli suction, whose effect is only noticeable around this area.

Radiation protection on medical physics The Radiation Protection in Medical Physics group carry out Monte Carlo simulations of X-ray radiation doses in voxelised phantoms, neutron induced activity assessment in a PET cyclotron facility, ambient doses due to activation products and neutron doses in voxelised phantoms. They have assessed the relevance of the neutron activation of the concrete vault of the PET cyclotron at CIMES, Universidad de Málaga, by predicting specific activities of the main activation products in the vault and their variation profiles as a function of penetration depth into concrete at present and after 10 years of cyclotron operation.



Depth of the isotherm surface 12.85°C (in meters).

» Overview

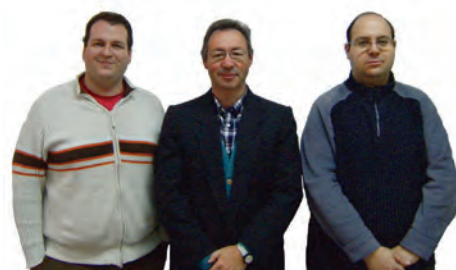


The TIRANT Supercomputer

The RES node located at the University of Valencia was inaugurated in January 2008. The supercomputer is called Tirant, in reference to the main character of the “Tirant lo blanc” novel, written in the Catalan language in 1490 by Joanot Martorell. The node is installed in a data centre specially designed to host it and is managed by technicians of the Servei d'Informàtica de la Universitat de València (SIUV). The SIUV has a long tradition in managing supercomputers: since 1978, the service has been central to the university's efforts in the field of scientific computation. The SIUV also hosts the RedIris PoP of the Valencian region, the network infrastructure of the university, the central database, the university web page, e-mail services, application services and other computer services.

» Organisational Structure

Tirant is managed by technicians from SIUV, an IT Group led by its Director. Two technicians are responsible for the system management (dealing with hardware problems, installation and configuration of software) and user support (compiling scientific programs, managing the system queue, solving user problems). The access committee is responsible for assigning CPU hours to Tirant users by evaluating new projects.

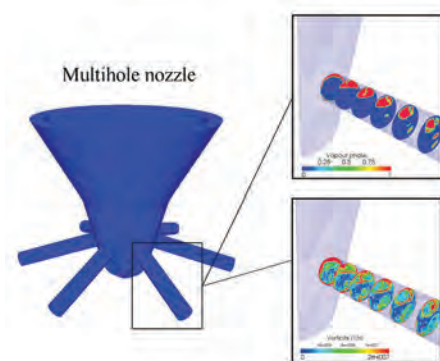


From the left: Alejandro Soriano - System Analyst, Jose María González - Operator and Josep Vicent Sala - System Analyst

» Technical and Scientific Highlights 2011

In 2011, Tirant offered 3,24 million CPU hours of which some 1,3 million hours was made available to the scientific community of the Valencia region, including researchers at the host University. The rest was made available to RES users. For a list of key scientific outputs during 2011, please consult the online version of this report.

» Key Projects 2011



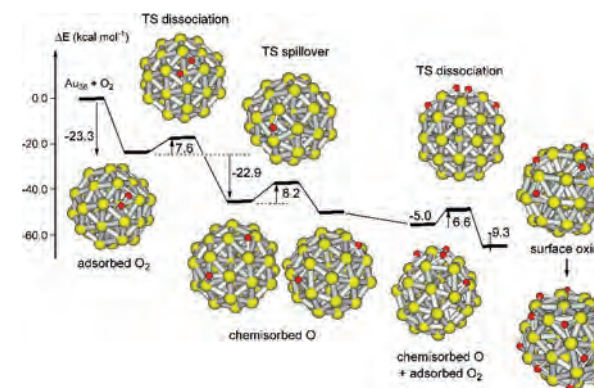
Martínez et al. Cavitation phenomena in Diesel injector nozzles

Study of the cavitation phenomena in Diesel injector nozzles It is well known that the details of the internal flow in diesel injection nozzles have a strong influence on spray development and the combustion process, and therefore on the efficiency and pollutant emissions of diesel engines. Thanks to the computing power of the RES node Tirant, Large Eddies Simulations have been performed by the group led by Francisco Javier Salvador, advancing knowledge of the cavitation phenomenon by

simulating a very complex phenomenon due to the extremely small dimensions of the discharge orifices of the nozzles (diameters of 0.2 μm and length about 1 mm), the high gradients of velocity and pressure and the bi-phasic nature of the flow.

Oxidized gold nanoparticles as catalysts for oxidation reactions Gold nanoparticles supported on inert materials are able to dissociate O_2 if their diameter is smaller than ~ 2 nm. In this project, led by Mercedes Boronat, the adsorption and dissociation of an increasing amount of O_2 molecules on a Au_{38} nanoparticle of ~ 1 nm diameter was theoretically studied, and the most reactive gold sites were identified. The stability and electronic properties of the resulting oxide-covered nanoparticles, as well as their catalytic activity in several oxidation reactions, such as CO oxidation, ethanol dehydrogenation and ethylene epoxidation were also studied by means of DFT calculations.

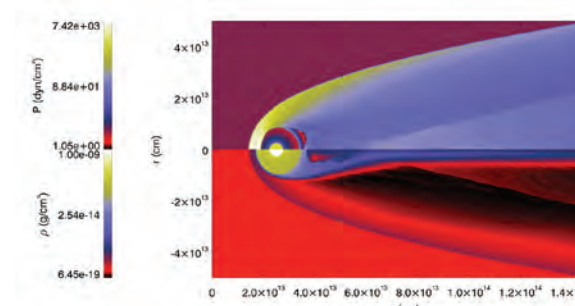
Bidimensional materials and alternatives to graphene. Ab initio calculations beyond density functional theory Led by Alejandro Molina, the group performed calculations of phonons of heterostructures composed of MoS_2 , graphene and BN . Calculations were



Boronat et al. Calculated energy profile for the formation of an oxide monolayer on a gold NP

also performed on the interaction between the graphene and its substrate, using the GW method to evaluate the electron-phonon interaction.

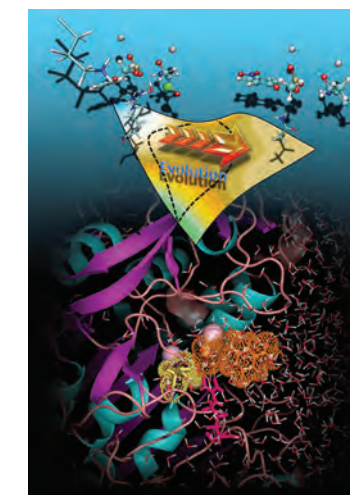
Verification of covering arrays Covering Arrays (CAs) are combinatorial objects that, with a small number of cases, cover a certain level of interaction of a set of parameters. The group led by Himer Avila developed an algorithm for CA verification and its implementation in sequential and parallel computing. To illustrate the scalability of the parallel algorithm they use the cases when $t = \{2, 3, 4\}$, $k = \{64, 128, 256, 512\}$ and processors = $\{4, 8, 12, 16\}$.



Perucho et al. Interaction between a jet and an inhomogeneous cloud

Relativistic Jets in Astrophysics During 2011, the group of Manel Perucho undertook small-size simulations aimed at specific studies of the interaction between relativistic extragalactic jets, and clouds of cold and dense gas that could penetrate into those jets. This interaction is very interesting from two points of view: On the one hand, there is the potential dynamic importance due to the mass-load of slow material into the jet, which could be significantly decelerated by these kinds of processes, as is expected to occur in the slow and decollimated FRI jets between parsec and kiloparsec scales. On the other hand, there is the radiative result of this interaction, because of the strong shocks generated inside the jet.

Thermal conductivity on semiconductor nanowires The group led by Andrés Cantarero performed AB initio calculations of the electronic band structure of indium phosphide. This is a semiconductor grown in the zincblende structure in bulk materials. However, in the form of nanowires the wurtzite phase is more stable. The group used the Becke-Johnson modified exchange potential and the linear augmented plane wave method to solve the band structure. The crystal structure has been optimised and the difference with the zincblende phase was discussed.



Tuñón et al. JACS cover picture

A theoretical study of enzymatic DNA methylation: towards rational design of new drugs During 2011, the group lead by Ignacio Tuñón made a theoretical study of the alkaline hydrolysis of a phosphodiester (methyl p-nitrophenyl phosphate or MpNPP) in the active site of Escherichia coli alkaline phosphatase (AP), a monoesterase that also presents promiscuous activity as a diesterase. The analysis of the simulations, carried out by means of molecular dynamics (MD) simulations with hybrid quantum mechanics/molecular mechanics (QM/MM) potentials, shows that the reaction takes place through a DNA or dissociative mechanism, the same mechanism employed by AP in the hydrolysis of monoesters.

Numerical RANS method using a OpenFoam code for internal flow in diesel injectors The activities in this study are related to simulating the internal flow of diesel injectors, the main field of research of the group of Oscar Venegas. The study focused on some interesting variables, such as the RANS method. Thanks to the many libraries available in OpenFOAM, several models developed for solving Reynolds-averaged N-S equations were employed in order to evaluate the accuracy of each model and their applicability for this particular physical phenomenon.

» Overview



The CAESARAUGUSTA Supercomputer

Located at the Faculty of Science of the University of Zaragoza, the CAESARAUGUSTA supercomputer was one of the initial seven founding nodes of the RES (Spanish Supercomputing Network). It is managed by the HPC group of the Institute for Biocomputation and Physics of Complex Systems (BIFI).

BIFI is a research institute that promotes interdisciplinarity to develop competitive research in computation applied to physics of complex systems and biological systems. Despite its youth, the Institute has already developed intensive research activity in several fields of computation: cluster, grid computing, cloud computing, GPUs, dedicated computers (FPGAs) and volunteer computing.

» Organisational Structure

CAESARAUGUSTA is maintained by technical staff of the Computation Area at BIFI. This includes hardware and software administration as well as first level user support, all of which are coordinated with the BSC-CNS operations department.

There is also a local Access Committee which manages the 20% of the CPU time which is at the disposal of the University of Zaragoza. This time is assigned by the Committee after evaluating the applications received for each four-month period (coinciding with RES schedule). During 2011, the members of the local Access Committee were:

- ▶ Pablo Ibáñez Marín. Professor at Departamento de Informática e Ingeniería de Sistemas and member of Grupo de Arquitectura de Computadores UZ (gaZ).
- ▶ Luis Rández García. Professor at Departamento de Matemática Aplicada and member of Instituto Universitario de Matemáticas y Aplicaciones UZ (IUMA).
- ▶ Alfonso Tarancón Lafita. Professor at Departamento de Física Teórica and Director at Instituto de Biocomputación y Física de Sistemas Complejos UZ (BIFI).

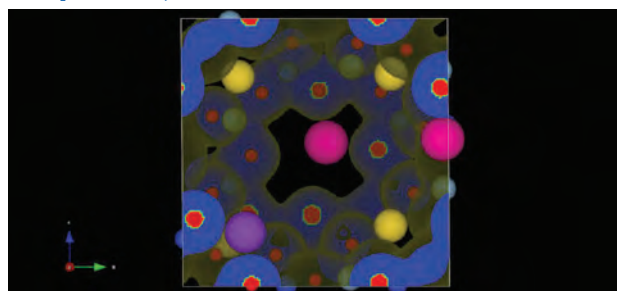


CAESARAUGUSTA Operations Team (from left to right): Javier Alcázar Luque (BIFI's sysadmin), Arturo Giner (BIFI's sysadmin), Guillermo Losilla (BIFI's HPC group manager), Alfonso Tarancón (BIFI's Director)

» Technical and Scientific Highlights 2011

In 2011 CAESARAUGUSTA's local Access Committee granted a total of 16 local projects, running 256.000 hours of CPU time. These activities have produced numerous scientific results and publications. For a list of key scientific outputs during 2011, please consult the online version of this report.

» Key Projects 2011



Calculated electron density of K12-A at the most stable configuration

Ab-initio simulation of reaction mechanisms on microwave-heated catalytic microreactors Led by Jesús Santamaría (Institute of Nanoscience of Aragon, University of Zaragoza). Microwaves (300 MHz to 300 GHz) can quickly, internally and specifically heat dielectric substances. An optimization of industrial catalytic synthesis seems possible for reactions containing microwave

absorbers. The project uses Density Functional Theory to study the movements of the cations in Linde Type A Na12, K12 and Na4Ca4 zeolites under microwave radiation and seeks for each composition different relaxation processes caused by the jump of the most unbalanced cations to diverse meta-stable sites inside the Al-O-Si framework. The kinetics of the ionic migration, dielectric heating, will be described according to transition state theory. It is expected that the order of magnitude of the theoretical rates for the jumps agree with the measured frequencies at the maximum dielectric loss. The theoretical scheme will enable the project to establish a predictive model for the description of the dielectric behaviour due to ionic mobility in dehydrated zeolites.

Critical properties of the Anisotropic Heisenberg Spin-Glasses in three dimensions Led by Víctor Martín Mayor (BIFI, Theoretical Physics Department

UCM), the project seeks to perform a finite size scaling study of the three-dimensional Heisenberg spin glass in the presence of weak random anisotropic interactions, up to sizes $L=32$. Anisotropies have a major impact on the phase transition. The chiral-glass susceptibility does not diverge, due to a large anomalous dimension. It follows that the anisotropic spin-glass belongs to a Universality Class different from the isotropic model, which questions the applicability of the chirality scenario.

The problem is computationally hard in two respects. First, in order to get meaningful results, thousands of instances of the problem (named samples) need to be simulated independently. Second, in order to reach thermal equilibrium, each sample needs to be simulated for a very long time. This project was feasible only thanks to the large computing power offered by the RES.

Excited States of the Green Fluorescent Protein Chromophore: Performance of Ab Initio and Semi-Empirical Methods Led by José Luis Alonso (BIFI, Theoretical Physics Department UZ). The complex photophysical properties of fluorescent proteins give rise to a wide field of applications as markers in molecular biology. Understanding these properties is essential for rational genetic engineering of new fluorescent proteins. Here, theoretical models are required to support the interpretation of structural and spectroscopic experimental data. This requires the accurate and reliable prediction of excited-state features of the chromophore and its interactions with the protein matrix. The project compares calculations of absorption and emission energies of semi-empirical (OM2/MRCI, ZINDO/S, and TD-DFTB) and ab initio (SORCI, CC2, and TDDFT) approaches for the HBDI chromophore in vacuo and wild-type green fluorescent rotein (GFP) using QM/MM models. Various factors are discussed, including the influence of electrostatic fields, the chromophore geometry, the size of the QM region, and methodological aspects, in particular charge-transfer states in TDDFT and the applicability of real-space TDDFT codes. The project also revisits previous opposing theoretical studies and benchmark gas-phase measurements.

A stepwise algorithm for combining diagnostic tests to predict binary response Led by Gerardo Sanz (Departamento de Métodos Estadísticos. UZ). Discrimination is an important feature of a predictive model in medicine, it reflects how to distinguish between the different states of a disease. In this context, a major issue, is to analyze the performance of different algorithms to build better predictive models in oncology. Through the use of high performance computing resources, the working group has continued the development of the project to build models that achieve a greater ability to discriminate between different disease states. In addition, for this purpose, non parametric approaches have been implemented in R programming language. We also have

examined different measures to identify new markers that are statistically significant in prostate cancer recurrence. The use of these measures can be effective to build Risk Scores that combine markers in order to improve the predictiveness of models. Moreover, we have worked with the URONCOR group using the RECAP (Registro español de cancer de próstata) database to build nomograms to predict prostate cancer recurrence and metastasis for patients treated with radiotherapy.

Numerical Simulation of Unsteady Free Surface Flows Led by Pilar García (Grupo Hidráulica Computacional, UZ). Computational Hydraulics is concerned with the study of free surface flow dynamics using numerical solutions of non-linear equations that are assumed to govern the involved physical processes. Computers are the essential tools for this activity. The fluid movement is governed by fundamental conservation laws that can be expressed in mathematical terms in the form of partial differential equations. Computational Hydraulics, belonging to Computational Fluid Dynamics (CFD), consists of replacing equations by numbers so that they provide information on the spatial and temporal evolution of the flow field. In general, this involves thousands or millions of data that are impossible to handle without a suitable computer use. The numerical modelling of free surface flows developed by this research team has led to efficient, robust and accurate simulation software tools. They are based on numerical methods for systems of conservation laws, whose initial scope was located in the context of simple geometries. The research team has extended the numerical schemes making feasible the application to realistic cases found in engineering applications, where the importance of the source terms in the equations, especially related with the bathymetry of the bed in river flows, requires special numerical treatments.

Thermodynamic glass transition in a spin glass without time-reversal symmetry Led by Alfonso Tarancón (BIFI, UZ). Spin glasses are a longstanding model for the sluggish dynamics that appears at the glass transition. However, spin glasses differ from structural glasses for a crucial feature: they enjoy a time reversal symmetry. This symmetry can be broken by applying an external magnetic field, but embarrassingly little is known about the critical behaviour of a spin glass in a field. In this context, the space dimension is crucial. Simulations are easier to interpret in a large number of dimensions, but one must work below the upper critical dimension (i.e., in $d < 6$) in order for results to have relevance for experiments. The project shows conclusive evidence for the presence of a phase transition in a four-dimensional spin glass in a field. Two ingredients were crucial for this achievement. On the one hand, massive numerical simulations were carried out on the Janus special-purpose computer. On the other hand, a new and powerful finite-size scaling method was introduced.

» The MareNostrum Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe, Gustavo Yepes, Universidad Autónoma de Madrid



A projected image of the most massive galaxy cluster from the MULTIDARK simulation. The image represents the gas density color coded according to their temperature (red color corresponds to a gas temperature of more than 10 million degrees Kelvin.) The yellow dots represent the stellar content of the galaxies. In this particular example, there are two massive galaxies sitting at the center of the clusters and in the process of merging.

Abstract The MareNostrum Numerical Cosmology Project (<http://astro.ft.uam.es/marenostrum>) is an international collaboration to carry out grand challenge cosmological simulations of the formation of galaxies, groups and clusters of galaxies and the large scale structures in the universe. The scientific objective is to understand the physical processes that were involved in the formation and evolution of these objects from initial conditions that are compatible with the early epochs of the Universe derived from the observations of the Cosmic Microwave Background radiation. The project uses state-of-the-art numerical codes based on different techniques, SPH (GADGET, GASOLINE) and AMR (ART, RAMSES). All of them are fully MPI parallelised.

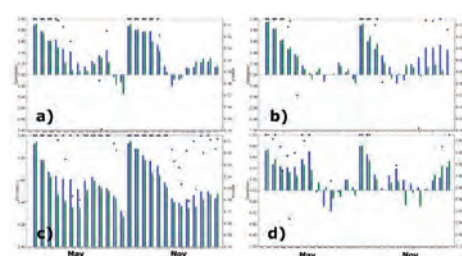
Results The simulation database created serves for many different studies on the formation and evolution of cosmic structures in the universe. Current work focuses on 3 main topics: The formation of our Local Universe (CLUES), Large Scale simulations of galaxy clusters (MUSIC), and the High-z Universe. The results led to more than 15 articles being published in international journals in 2011. These numerical data constitute a virtual laboratory to test hypotheses about the nature of the different components of the universe. The goal is to make them publicly available using web-based interfaces such as the CLUES project (<http://www.clues-project.org>) or the MULTIDARK database (<http://www.multidark.org>).

Publications **Comparison of an X-ray selected sample of massive lensing clusters with the MareNostrum Universe LCDM simulation**, Meneghetti M., et.al, 2011, Volume 530, id.A17 eprint arXiv:1103.0044.; **Haloos gone MAD: The Halo-Finder Comparison Project**, Knebe A., M., et.al 2011, MNRAS, Volume 415, Issue 3, pp. 2293-2318.; **Disentangling the dark matter halo from the stellar halo**, Libeskind, N. et.al, MNRAS, 2011, V418, pp 336-345 (arXiv:1107.4366).; **Large scale environmental bias of the QSO line of sight proximity effect**, Partl A. M., et.al, MNRAS, 2011, Volume 415, Issue 4, pp. 3851-3864.; **Renegade subhaloes in the Local Group**, Knebe A., et.al, 2011, Monthly Notices of the Royal Astronomical Society: Letters, V417, L56-L60.; **The dark matter assembly of the Local Group in constrained cosmological simulations of a Lambda cold dark matter universe**, Forero-Romero J. E., et.al, 2011, Monthly Notices of the Royal Astronomical Society, V417, pp 1434-1443.; **CLUES on Fermi-LAT prospects for the extragalactic detection of mnuSSM gravitino Dark Matter**, Gomez-Vargas G. A., et.al, JCAP; inpress 2011, (arXiv:1110.330).; **Baryon and Sunyaev-Zeldovich effect properties of MareNostrum and MultiDark simulated clusters (MUSIC)**, Sembolini F., et.al, 2011, ASP Conf Series. arXiv:1111.3764.

» Assessment of the limit of initial-condition useful skill in interannual climate prediction, Francisco J. Doblas-Reyes, IC3

Abstract The goal is to investigate whether seasonal and annual mean atmospheric climate variables are predictable in the forecast range one-to-five years, which is beyond the generally accepted limit of predictability forced by surface tropical temperatures. Understanding the mechanisms that destroy the information contained in the initial conditions of the climate system as the forecast progresses will help extend the predictability limit for longrange operational climate forecasts. The EC-EARTH Earth System Model will be used in a set of ensemble interannual forecasts initialized with the best analyses of the climate system available. The focus will be on the European and Mediterranean area, as well as strongly climate-sensitive areas such as South America and Africa.

Results The Climate Forecasting Unit (CFU) of the Institut Català de Ciències del Clima (IC3) undertakes research on the development and assessment of dynamical and statistical methods for the prediction of global and regional climate on time scales ranging from a few weeks to several years, running the EC-Earth climate model (<http://eearth.knmi.nl>) on MareNostrum as well as several other supercomputing platforms. In a first for such an experiment in Spain, five-member re-forecasts using the longest possible forecast dataset were performed with EC-Earth v2.2 over the period 1976-2005 and compared with the eleven-member ECMWF's operational seasonal forecast System 3, the gold standard in climate prediction. As seen in the Figure, both System 3 and EC-Earth display an ability to predict the tropical Atlantic average SSTs several months in advance, enabling predictions of the frequency of tropical cyclones. EC-Earth shows a slightly higher correlation for the boreal summer and autumn in the Atlantic3 and meridional mode indices. EC-Earth has proven to be a competitive climate forecast system, with the goal of future work to improve the model components responsible for untapped predictability, which will allow the formulation of useful, reliable climate predictions.



Ensemble-mean correlation for the a) Atlantic3, b) tropical Atlantic meridional mode, c) average tropical Atlantic and d) Indian ocean dipole SST indices of the EC-Earth (blue) and System 3 (green) re-forecasts as a function of the start date and forecast time. The two sets of 13 pairs of bars in each panel correspond to the results for the 13 forecast months of the May and November start dates. The right axis marks the p-value of the correlation, which is shown by the dots on the vertical of the coloured bars. When no dot is shown, the p-value is larger than 0.10. Re-forecasts for the period 1976-2005 have been used. The reference is taken from ERA-40/Int.

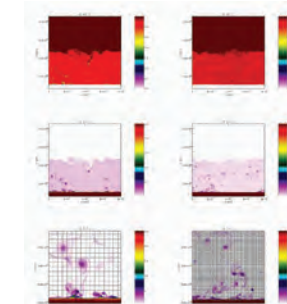
Publications **Sensitivity of decadal predictions to the initial atmospheric and oceanic perturbations**, Du, H., et.al, 2012, Climate Dyn., doi:10.1007/s00382-011-1285-9.; **On the assessment of near-surface global temperature and North Atlantic**, García-Serrano, J. et.al, 2012, Climate Dyn., under review.; **Decadal prediction of the West African monsoon**, García-Serrano, J., et.al, 2012, J. Geophys. Res., submitted.; **North Pacific major warm events in 1963 and 1968**, Guémas, V., et.al, 2012, J. Climate, submitted.

» Multidimensional simulation of stellar explosions: classical novae and type I X-ray bursts, Jordi José, UPC BarcelonaTech

Abstract Classical novae are stellar explosions in binary systems with an energy release that is only surpassed by supernovae and gamma-ray bursts. They repeatedly eject $10^{-4} - 10^{-5}$ solar masses of nucleosynthetically enriched gas into the interstellar medium, recurring on intervals in the range $10 - 10^5$ yr. These events are considered the main sources of Galactic ^{15}N , ^{17}O , and ^{13}C , and contribute to the abundances of other species, such as ^7Li and ^{26}Al . However, the origin of the large enhancements and inhomogeneous distribution of these species, as observed in the ejecta, has remained unexplained for half a century.

Results In phase one of the Project, the role of Kelvin-Helmholtz instabilities as a possible natural mechanism for self-enrichment of accreted nova envelopes with core material was explored by means of the multidimensional code FLASH. A series of 9 numerical simulations were performed to test the possible influence of the initial perturbation (duration, strength, location, and size), the resolution adopted, or the size of the computational domain on the results. It was shown that results do not depend substantially on the specific choice of these parameters. In phase two, the first successful 3D simulation of mixing at the core-envelope interface during CO nova outbursts was performed, showing that buoyant fingering drives vortices from the Kelvin-Helmholtz instability, which inevitably enriches the accreted envelope with material from the outer white-dwarf core. Such mixing also naturally produces large-scale chemical inhomogeneities. Both the metallicity enhancement and the intrinsic dispersions in abundances are consistent with observations. The study has been extended to the modelling of other nova types (including ONe, recurrent and primordial novae) as well as to similar explosive scenarios, such as type I X-ray bursts.

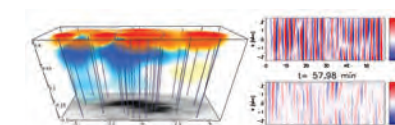
Publications **Kelvin-Helmholtz instabilities as the source of inhomogeneous mixing in nova explosions**, Casanova, J., et.al, 2011, Nature, 478, 490-492.; **Classical and Recurrent Nova Models**, José, J., et.al, 2011, in Binary Paths to Type Ia Supernovae Explosions, Di Stefano, R. et.al, in press.; **Recent advances in the modelling of classical novae and type I X-ray bursts**, José, J., et.al, 2011, Journal of Physics - Conf. Series, in press.; **Mixing in Classical Novae: A 2-D Sensitivity Study**, Casanova, J., et.al, 2011, Astron. & Astrophys., 527, A5 (7 pages).; **On mixing at the core-envelope interface during classical nova outbursts**, Casanova, J., et.al, 2011, Proc. Science, PoS(NIC XI) 204 (5 pages).; **Nuclear Astrophysics: the Unfinished Quest for the Origin of the Elements**, José, J., Iliadis, C., 2011, Rep. Progr. Phys., 74, 096901 (48 pages).



Snapshots of the ^1H (upper panels) and ^{12}C (middle panels) mass fractions at different times, corresponding to a 2D sensitivity study. Structures such as vortex are better resolved in the finer resolution model displayed in the lower right panel. All 2D runs have been performed with MareNostrum.

» Magneto-convection and wave simulations of solar and stellar atmospheres Elena Khomenko, Instituto de Astrofísica de Canarias

Abstract The project has two different objectives; to perform 3D magnetohydrodynamic (MHD) simulations of the Sun and stars with the final goal of producing magnetohydrodynamic simulations of stellar atmospheres and deriving synthetic spectra for accurate abundance analysis, including the influence of magnetic fields, and of three-dimensional and non-local thermodynamic equilibrium effects, and to perform magnetohydrodynamic simulations of waves including the realistic physics of strong-magnetic field structures on the Sun, like sunspots and magnetic flux tubes in order to understand the role of waves in the magnetic coupling of different solar layers and to advance new developments in helioseismology of magneto-atmospheres.

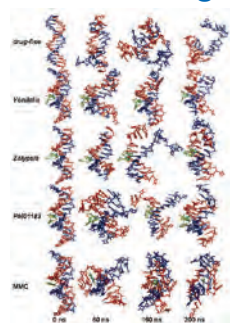


Wave field in numerical simulations of an observed sunspot umbra

Results The project modeled the wave pattern of real observed solar magnetic features: a sunspot and a complex pore region, both simulations driven by the observed velocity field. Being extremely time-consuming and scientifically challenging, this is the first time such kind of simulations were performed in three spatial dimensions. They reproduce the observed power spectra in the photosphere and chromosphere of the magnetic features, allowing the evaluation of the energy contribution of magneto-acoustic waves into the heating of solar chromosphere. Magnetic field effects on deriving abundances of chemical elements from spectral observations were evaluated and a large sample of spectral lines of neutral iron in 3D MHD models calculated. Two main factors were identified that cause the change in equivalent widths, the Zeeman broadening and the modification of the temperature stratification, act in different amounts and in opposite directions. The overall effects are non-negligible and should be taken into account when discussing precise values of the chemical abundances.

Publications **Magnetoacoustic Wave Energy from Numerical Simulations of an Observed Sunspot Umbra**, Felipe, T., et.al, The Astrophysical Journal, Volume 735, Issue 1, article id. 65, 2011.; **Magneto-acoustic waves in sunspots from observations and numerical simulations**, Felipe, T. et.al, J. Phys.: Conf. Ser. 271 012040, 2011

» Molecular dynamics simulations of DNA melting in the presence and absence of some antitumour drugs covalently bonded in the minor groove, Federico Gago, Universidad de Alcalá



Representative snapshots showing the time evolution of the DNA duplexes during the MD simulations in the absence of any bonded drug (top) and in the presence of Yondelis®, Zalypsis® or PM01183 covalently bonded to the blue strand, or MMC (bottom) covalently bonded to both blue and red strands. Drug carbon atoms are coloured in green.

Abstract Disruption of double-stranded (ds) DNA and local formation of single-stranded (ss) regions are necessary for normal DNA replication, transcription and repair. These vital processes can be affected by antitumour drugs including the prototypical interstrand crosslinker mitomycin C (MMC) and monofunctional DNA-binders such as the ecteinascidins. Monoadducts involving these latter drugs, which bind covalently to the exocyclic N2 of a guanine in the DNA minor groove have been shown to increase substantially the melting temperature of selected DNA oligonucleotides. To study their effects on the DNA melting process, a 15-mer dsDNA was simulated at 400 K and 0.1 M NaCl to favour strand separation both in the presence and in the absence of drugs covalently bonded within the minor groove to one or two strands. The differences in the kinetics and intensity of the disassociation process were analysed.

Results The results provide an atomistic view of the process of DNA melting in the presence and absence of several bonded anti-tumour drugs, and they are found to be in agreement with the large stabilisation that single Yondelis®, Zalypsis® and PM01183® monoadducts are shown to impose on the DNA double helix. On the contrary, the prototypical interstrand crosslinker mitomycin C prevents strand separation because of the fact that it forms a covalent bond with each DNA strand, but its effect on duplex stabilisation does not appear to extend beyond the CpG step to which it is covalently attached. Therefore, this is another example of how theory and experiment can be successfully merged to help us improve our understanding in atomic detail of how antitumour drugs act on such a vital macromolecule as DNA.

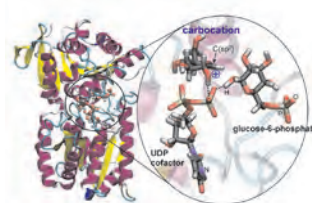
Publications Bueren-Calabuig JA, et.al, **Temperature-induced melting of double-stranded DNA in the absence and presence of covalently bonded antitumour drugs: insight from molecular dynamics simulations**. Nucl. Acids Res. (2011) Oct;39(18):8248-57. doi: 10.1093/nar/gkr512.

» Elucidating the catalytic mechanism of retaining glycosyltransferases, Carme Rovira, Parc Científic de Barcelona

Abstract One of the most important reactions in the metabolism of carbohydrates is the formation of the glycosidic bond, i.e. the covalent linkage between simple monosaccharides (monomers) to build polysaccharides such as glucogen, starch or cellulose (polymers). Glycosyltransferases (GTs) are the enzymes responsible for the formation of the glycosidic bond. These enzymes can operate with retention or inversion of the configuration of the anomeric carbon of the glycosidic bond they form. The mechanism of inverting GTs is well known, but the mechanism of retaining GTs has remained one of the most puzzling aspects in the field of glycobiology. By means of ab initio metadynamics dynamics we investigate how the glycosyl transfer reaction takes place in the active site of the GT enzyme trehalose-6-phosphate synthase (OtsA).

Results To explain the net retention of configuration in the glycosyl transfer reaction some authors had proposed an extremely unusual and controversial mechanism (named "front-face") in which the reaction takes place on a single "face" of the sugar. The process, with two covalent bonds forming and breaking in the same region of space, is expected to be very costly from an energetic point of view, being therefore highly unlikely. By means of ab initio metadynamics, this study demonstrated that the front-face mechanism is indeed feasible. However, the synthesis of the glycosidic bond does not take place in a concerted (one-step) way but in multiple steps which involve very small energetic barriers. A main feature of the reaction is the formation of a positively-charged species (a carbocation) with an extremely short half-life (a few picoseconds) that moves quickly from the donor to the acceptor sugar (see Figure). GTs are responsible for the structure of many carbohydrates and knowledge of their mechanism of action will help to modify their function, improving the synthesis of known carbohydrates and new structures, and contributing to the design of inhibitors for GTs involved in infectious diseases.

Publications A. Ardèvol, et. al, **The molecular mechanism of enzymatic glycosyl transfer with retention of configuration: evidence for a short-lived oxocarbenium ion-like species**, Angewandte Chemie Intl. Edition. 50, 10897-10901 (2011). Editorially rated as "Very Important Paper" (top 5% of the journal). C. Rovira, et.al, **Dulces misterios de la naturaleza**, Investigación y Ciencia. 423, 12-14 (2011).



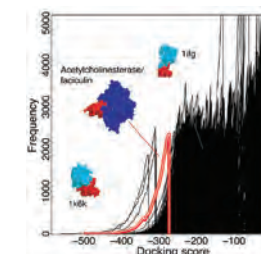
Computed structure of the short-lived carbocation intermediate in the interior of the enzyme trehalose-phosphate synthase. This enzyme contributes to the synthesis of trehalose, a natural disaccharide used as food ingredient for its good preservative properties.

» Prediction of interaction partners using protein docking, Alfonso Valencia, CNIO

Abstract Protein-protein interactions play a central role in the functioning of cells from regulation of processes to forming large molecular machines that perform essential roles such as transcription and translation. Therefore deciphering the interactome for a given species is the goal of many experimental and computational efforts in Systems Biology. Separately the prediction of the structure of protein complexes by computational docking methods is generally applied to pairs of proteins that are known to interact. Despite the relationship between these two fields, to date docking programs have not been used to predict interaction partners and it has been widely thought that docking programs were not accurate enough to do this. The goal of this project is to assess if protein docking methods can be used to predict PPIs.

Results In 2011 we developed a proof of principle demonstrating the ability to use protein docking to predict protein interactions. For a set of complexes we compared the docking scores of the known interactors with the docking of one of the interactors with a large set of random proteins. For nearly two-thirds of proteins we find that the docking scores for the real interactors is better than at least 80% of the random dockings and they are distinguishable from the random results. This result shows that docking programs can be used to predict PPIs and we are now investigating the development of new methods in this area.

Publications Wass, M. N., et. al, **Towards the prediction of protein interaction partners using physical docking**, Molecular systems biology, 7, 469 (2011).



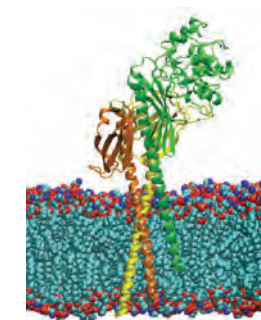
Protein docking results for Acetylcholinesterase with fasciculin2. The docking results for this complex (red/white line) is at better docking scores than docking of fasciculin2 with the random set of proteins (black lines).

» Simulation studies of peptide-based gene delivery vectors, Syma Khalid, Systems and Synthetic Biology Modelling Group, University of Southampton

Abstract Peptide-based gene delivery vectors can be engineered such that all of the properties required for efficient function can be built into a single peptide. This project aims to undertake a systematic simulation study to uncover molecular details of the complexes formed by such vectors. Understanding the role played by lipid-peptide interactions in a systematic and reproducible manner will aid in rationally designing peptides that are more efficient at crossing membranes and penetrating into cells.

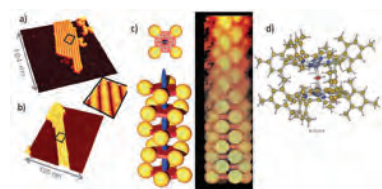
Results The project studied the influence of the membrane composition on the dynamics and interactions of antimicrobial peptides (AMPs), in order to understand the recognition processes as such peptides assemble at the bilayer surface, with particular focus on cell-penetrating properties of peptides. The project simulated multiple copies of peptides in membranes of various, biologically realistic lipid compositions. The simulations reveal details of the peptide-membrane recognition process and the conformational dynamics as they interact with the membrane. Initial observations on the stability of peptide aggregates are revealing an interesting dependency upon membrane composition over the course of long-timescale simulations, which is of direct relevance to the design of peptide vectors for specific cell types. Importantly, this lipid dependent behaviour was observed across multiple simulations.

Publications Syma Khalid, et. al, **Melittin vs E.coli: Insights from Molecular Dynamics Simulations**, Biophysical Journal, 100, 3, 497a, February 2011.; Syma Khalid, et. al, **Simple cell, complex envelope: modelling the heterogeneous membrane of E. coli**, European Biophysics Journal with Biophysics Letters, 40, 1, 199, August 2011.; Cisneros DA, et. al, **Minor pseudopilin self-assembly primes type II secretion pseudopilus elongation**, EMBO J. 2011 Dec 9. doi: 10.1038/emboj.2011.454. [Epub ahead of print]



Simulation studies of the pseudopilin complex.

» Self-assembly of molecules on surfaces, Manuel Alcamí Pertejo, Universidad Autonoma de Madrid



a) STM images of the nanorods of ZnTMP formed on different surfaces a) Au(111) b) Cu(100). c) Schematic diagram showing the proposed structure for the nanorods. d) Structure obtained in the simulations.

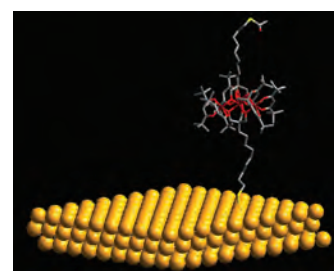
Abstract The main objective is to study the self-assembly of molecules on surfaces. First-principle simulations are used to characterize the supramolecular structures formed on the surfaces, to compare them with the observed patterns in STM experiments and to understand the factors governing the self-assembly process. This is of significant interest since self-assembly of molecules with large acceptor or a donor capabilities is expected to increase the efficiency of organic solar cells.

Results Self-assembly of molecules on surfaces was studied: electron donors as porphyrins and phthalocyanines or acceptors as tetrathiafulvalene (TTF). One of the most interesting results is that zinc meso-tetrakis(4-sulfonatophenyl)porphyrin (ZnTMP) form very large nanorods (up to hundreds of nm) when deposited in Cu(100) or Au(111). Theory predicts that these structures can only be obtained in the presence of molecules like water, that bridge the central Zn atoms. The study also obtained a very accurate description of a graphene layer deposited on Ru(0001), which presented ripples making it an excellent playground for the self-assembly of molecules. Self-Assembled Monolayers (SAM) of thiolates were studied by using both static and dynamical calculations. Finally the weak interactions between He and the surface of fullerenes were studied and used to explain recent experiments on C60H_n complexes. As accurate descriptions of the surfaces require very large unit cells (i.e. more than 400 atoms in Graphene/Ru(0001)), the dynamical calculations were only possible using large computing resources.

Publications D. Stradi, et al, **A Density Functional Theory study of the Manganese-Phthalocyanine**, *Theor. Chem. Acc.* 128, 497-503 (2011); P.N. Abufager, et. al, **Theoretical study of the structure of self-assembled monolayers of short alkylthiolates on Au(111) and Ag(111): the role of induced substrate reconstruction and chain-chain interactions**, *Phys. Chem. Chem. Phys.* 13, 9353-9362 (2011); D. Stradi, et. al, **Role of dispersion forces in the structure of graphene monolayers over Ru surfaces**, *Phys. Rev. Lett.* 106, 186102 (2011); M. Trelka, et. al, **Surface assembly of porphyrin nanorods with one-dimensional zinc-oxygen spinal cords**, *Crys. Eng. Comm.* 13, 5591-5595 (2011); Y. Wang, et. al, **Formation of self-assembled chains of tetrathiafulvalene on Cu(100) surface**, *J. Phys. Chem. A* 115, 13080-13087 (2011); C. Leidlmair et al, **Structures, energetics and dynamics of helium adsorbed on isolated fullerene ions**, *Phys. Rev. Lett.* 108, 076101 (2011).

» Single-Molecule Magnets: Magnetism on Surfaces and Quantum Transport, Eliseo Ruiz, Universitat de Barcelona

Abstract Some polynuclear transition metal complexes, known as single molecule magnets (SMM), show a slow relaxation of the magnetisation and, as a result, each individual molecule behaves as a magnet. Hence, SMMs have been proposed either as potential materials for information storage at the molecular level or as qubits in quantum computers, due to their quantum-controlled spin flip. In the field of storage information, the Holy Grail is an SMM with a high enough spin inversion barrier to avoid both the thermal spin flip and quantum tunnelling effects. The synthesis of new SMMs is usually a serendipitous search for large energy barriers (large total spin and large and negative magnetic anisotropy). However, theoretical methods using density functional methods enable the understanding and rationalisation of experimental data and the identification of new synthetic targets.



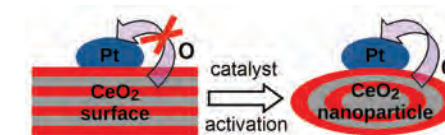
Fe₄ single-molecule magnet with stand-up coordination with a gold surface.

Results The use of single molecules to store information will improve by at least two orders of magnitude the capacity of the actual hard disks. The key point is to design system with a sufficiently large magnetic anisotropy to allow using them at high temperatures. The control of the magnetic anisotropy is very important and its magnitude is very difficult to predict. Hence, the use of computational methods that allow the calculation the magnetic anisotropy, such as using density functional theory including spin-orbit effect (or CASSCF methods) are a great help for experimental chemists to choose the best synthetic targets and also to control if their properties change when the molecules are deposited on a surface. Transport properties through magnetic molecules can be calculated using DFT methods combined with non-equilibrium Green functions. These kind of spintronic devices can introduce an additional parameter to the usual electronic circuits - the spin of the carriers. Some systems, such as Fe^{II} spin-crossover complexes, can play the role of spin filters that allow only the conduction of electrons with spin down.

Publications Ayako Hosoi, et al, **A Molecular Pair of [GdNi₃] Tetrahedra Bridged by Water Molecules**, *Chem. Eur. J.* 2011, 17, 8264 – 8268; Gang Wu, et. al, **S=22 Mn₁₀ Supertetrahedral Building-Block to Design Extended Magnetic Networks**, *Inorg. Chem.* 2011, 50, 8580–8587; Daniel Aravena, et. al, **The Dilemma of Cr^{III}Ni^{II} Exchange Interactions: Ferromagnetism versus Antiferromagnetism**, *Chem. Eur. J.* 2011, 17, 8841 – 8849; Ana I. S. Neves, et. al, **Ni₂,3-thiophenedithiolate Anions in New Architectures: An In-Line Mixed-Valence Ni Dithiolene (Ni₄S₁₂) Cluster**, *Eur. J. Inorg. Chem.* 2011, 4807–4815; Eliseo Ruiz, **Exchange Coupling Constants using Density Functional Theory: Long-Range Corrected Functionals**, *J. Comput. Chem.* 2011, 32, 1998–2004; Daniel Aravena, et. al, **Coherent Transport through Spin-Crossover Single Molecules**, *J. Am. Chem. Soc.* 2012, 134, 777.

» Reactivity Control in Catalysis by Nanostructuring: Modelling Platinum/Ceria Nanostructures, Konstantin M. Neyman, Universitat de Barcelona / ICREA

Abstract Sustainable energy production is now one of the greatest challenges. In response to the society's needs and ecological concerns, it is essential to find new, cheap and environmentally friendly energy conversion and storage systems. Finding appropriate catalysts to aid in energy production is currently a key research bottleneck. Metal-support interactions can remarkably improve catalysts. The origin of such interactions usually remains a mystery at the atomic level. The project deals with two interactions proposed to take place on technologically important Pt/ceria catalysts: electron transfer from Pt to ceria (CeO₂) and O transfer from ceria to Pt. The aim is to clarify if (and why) the electron transfer occurs on various ceria surfaces, whereas the partial oxidation of Pt is a nano-effect only inherent to nanostructured ceria.

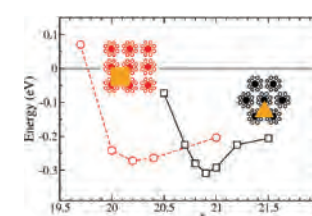


Ceria dioxide in the form of nanoparticles, unlike extended surface terraces, provides oxygen atoms that are mobile enough to catalytically activate platinum supported on them.

Results Interactions of metal particles with oxide supports can radically enhance the performance of supported catalysts. At the microscopic level, the details of such metal-oxide interactions usually remain obscure. This combined electronic structure modelling and experimental study identifies two types of oxidative metal-oxide interaction on well-defined models of technologically important Pt/ceria (Pt/CeO₂) catalysts: 1) electron transfer from the Pt nanoparticle to the ceria support, and 2) oxygen transfer from ceria to Pt. The electron transfer is favourable on ceria supports, irrespective of their morphology. Remarkably, the oxygen transfer is shown to require the presence of nanostructured ceria in close contact with Pt and, thus, is inherently a nanoscale effect. These findings enable us to detail the formation mechanism of the catalytically indispensable Pt–O species on ceria and to elucidate the extraordinary structure–activity dependence of ceria-based catalysts in general.

Publications Georgi N. Vayssilov, et. al, **Density functional modeling of the interactions of platinum clusters with CeO₂ nanoparticles of different size**, *J. Phys. Chem. C* 115 (2011) 16081-16086; Albert Bruix, et. al, **Effects of deposited Pt particles on the reducibility of CeO₂(111)**, *Phys. Chem. Chem. Phys.* 13 (2011) 11384-11392; Georgi N. Vayssilov, et. al, **Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles**, *Nature Materials* 10 (2011) 310-315.

» Assembly of large molecular complexes on metals from DFT, Valerio Bellini, CNR-Nano-S3



Interaction energy / molecule in the case of a square (red) or hexagonal (black) arrangement of the Cr₇Ni-butane molecules as a function of the molecule-molecule distance.

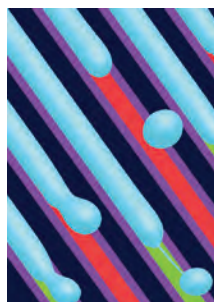
Abstract A key challenge in recent years has been the search for methods to graft, in a controlled way, molecular magnets onto the surface of materials, and assemble them in an ordered way. Complex assemblies can be obtained on surfaces by using simple molecular bricks in UHV conditions. Interest is now focused on large molecules that exhibit special functionalities as single units. Molecular nanomagnets have recently shown great potential for the storage and processing of information at molecular level and in some, suitable features for qubit encoding. This project aims to simulate, by density-functional methods, the adsorption and assembly of large polynuclear magnetic complexes on metal surfaces, whose behavior depends critically on the eventual functionalisation as evidenced in recent experiments.

Results Adsorption properties were characterised of two different derivatives of the Cr₇Ni antiferromagnetic ring, which differ in the fact that one derivative is functionalised with a thiol group anchored on the alkyl chain placed in the middle of the ring, and the other is left unfunctionalised, on a Au(111) surface slab composed of 4 Au layers. The CP2K simulation package was used for the calculations.

The results show: 1) Although only interacting via van der Waals forces with the surface, the adsorption energy of the Cr₇Ni-butane derivative is sizable, around 2.6 eV; the chemical binding of the Cr₇Ni-thiobutane derivative leads to a larger absorption energy estimated to be around 4.5 eV. 2) In the case of the Cr₇Ni-butane derivative, the molecule does not feel any sizable potential barrier when moving across the surface, while the chemical binding of the S atom in the Cr₇Ni-thiobutane derivative energetically hinders any movements of the molecule. 3) Simulation of molecule-molecule interactions (see Figure) shows that the preferred two-dimensional packing of the Cr₇Ni rings is hexagonal. These theoretical results explain with success the different experimental data obtained by the Modena group.

Publications A. Ghirri, et al, **Self-assembled monolayer of Cr₇Ni molecular nanomagnets by sublimation**, *ACS Nano* 5, 7090 (2011); V. Bellini, et. al, **Propagation of spin information at supra-molecular scale through hetero-aromatic linkers**, *Phys. Rev. Lett.* 106, 227205 (2011)

» Multiscale modeling of active fluids: selfpropellers and molecular motors, Ignacio Pagonabarraga, University of Barcelona



Wetting-controlled emission of droplets from force fluid filaments on a structured solid substrate. Liquid microfilaments are forced along chemically treated stripes bounded by a strongly hydrophobic substrate. The displaced gas intrudes under the leading edge of the filament promoting the formation of a liquid neck.

Abstract Soft matter can be forced either externally, reacting to inhomogeneous environments, or converting chemical energy through metabolic processes to provide internal mechanisms of selfpropulsion in active soft materials. This project focuses on the collective dynamics of soft materials and how patterns emerge. The project exploits a coarse grained approach to face the multiscale nature of these systems with appropriate coupling to the embedding solvent. The project focuses on the collective dynamics of microrobots and Janus colloids, model microorganisms and molecular motors and confined fluid mixtures. Understanding the spontaneous self assembly of these systems opens the possibility to manipulate fluid flow and mass transfer at the microscale and under confinement. The results of the project will clarify which possibilities offers the dynamic coupling through the solvent to achieve such goals.

Results Lattice Boltzmann, a flexible, mesoscale method to model the dynamics of complex fluids, was used to address the dynamics of both intrinsically and externally forced systems. In the former situation, the project analyzed the instability of forced fluid filaments displacing on heterogeneous substrates. It was shown that the differential wetting properties of the solid substrate lead to a new mechanism for controlled drop emission at small scales. The project also studied the kinetics of self propelled colloids immersed in a solvent and characterized the emergence of long range aggregates that displace preferentially along a forcing, gravitational field and identified the generation of streamers. The results show that both intrinsically driven and strongly forced suspensions display a significant increase in their collective fluctuations. Such an increase enhances the dynamic correlation in the collective motion of colloidal and active suspensions and plays a central role in the observed emerging patterns and self-organized structures.

Publications R. Ledesma-Aguilar, et. al, **Controlled drop emission by wetting properties in driven liquid filaments**, Nature Materials 10, 367 (2011); G. Giupponi, et. al, **Colloidal electrophoresis for strong and weak ion diffusivity**, Phys. Rev. Lett. 106, 248304 (2011); G. Giupponi et. al, **Determination of the zeta potential for highly charged colloidal suspensions**, Phil. Trans. Roy. Soc. London A 369, 2546 (2011); R. Ledesma-Aguilar, et. al, **Growth saturation in unstable three-dimensional thin films due to transverse hydrophilic-hydrophobic striped substrates** Soft Matter 7, 6051 (2011); P. Magaretti, et. al, **Running faster together: large hydrodynamic coupling of molecular stepping Motors**, submitted.

» Interface engineering in multifunctional oxides, Jorge Iñiguez, Institut de Ciència de Materials de Barcelona (ICMAB-CSIC)

Abstract The aim is to study a family of nano-structured oxides with great potential for the engineering of electronic effects, considering super-lattices that combine nickelates with other transition-metal oxides, and running quantum simulations to check whether the chemical heterogeneity at the interfaces allows control of their charge and spin state. This would open the door to many interesting effects: For example, the project will try to produce heterostructures in which insulating interfaces separate metallic layers, to thus form confined electron gases, or induce large magnetoelectric effects. Note that, on top of their fundamental appeal, effects of this type attract great interest in the field of oxide-based electronics and spintronics. Experimental collaborators will try to realize the most promising theoretical predictions.

Results The study of nickelate super-lattices was very successful, finding that strong interface-driven effects are obtained in short-period superlattices made of LaNiO₃ and LaMnO₃: The interfacial Ni and Mn cations adopt an electronic configuration that resembles the one occurring in the La₂NiMnO₆ double-perovskite compound, and their spins couple ferromagnetically. Moreover, such an interface effect induces in the (otherwise non-magnetic) LaNiO₃ layers a magnetic order that resembles a spin-density wave, and we argue that such an ordering is responsible for the exchange bias recently discovered in these systems by experimental colleagues at the University of Geneva (Switzerland). During the development of this project, a continuous feedback loop between experiment and simulation was established, which was key to its success. The use of RES resources was critical due to the large number of heavy calculations.

Publications **Exchange bias in LaNiO₃/LaMnO₃ superlattices**, Marta Gibert, et. al, Nature Materials 11, 195 (2012).

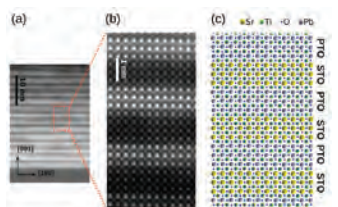
» Strain tuning of ferroelectric-antiferrodistortive coupling in PbTiO₃/SrTiO₃ superlattices, Javier Junquera, Universidad de Cantabria

Abstract The interest in ultra-short period PbTiO₃/SrTiO₃ (PTO/STO) superlattices has been fueled in recent years mostly due to the appearance of an improper ferroelectric (FE) polarization from the coupling of two rotational antiferrodistortive (AFD) modes of the oxygen octahedra cages. Using first-principles simulations, based on the density functional theory as implemented in the SIESTA code, the phase diagram of the PTO/STO superlattices was explored to gain further insight about the coupling between the FE, AFD and the strain degrees of freedom in monodomain phases, and to find

new paths to engineer functional properties in this system. The second step focused on the formation of polarization domains and the structure of domain walls in PTO/STO superlattices, considering the influence of the lateral domain size, orientation and energy of domain walls, and the influence of AFD instabilities. These are challenging simulations because they require accurate computations on systems with up to almost 1000 atoms in the simulation box.

Results The main results are: In the monodomain phase the presence of the paraelectric SrTiO₃ layer imposes an electrostatic penalty on the out of plane polarization of the PbTiO₃, favouring the rotation of the polarization out of the normal direction and giving rise to an enhanced piezoelectric response at very low strain values. An enhanced FE-AFD coupling is observed at the PTO/STO interface that cannot be accounted by typical steric effects, but is explained by a covalent model. The dependence of the FE-AFD coupling with respect to the periodicity of the superlattice reveals that this effect is dominant for the shortest periodicity (1|1) and contributes to stabilize the FE instability. This contribution, however, decreases in magnitude rapidly with the periodicity and changes sign (thus contributing to destabilize the FE distortion) for periodicities larger than (3|3). Results on polydomain phases reveal structures departing from the 180° domains typically assumed, forming vortices at domain walls. Also found was a progressive transition, as a function of the periodicity of the superlattice, from a strongly electrostatic coupled regime (where the ground-state is a monodomain configuration with a constant out-of-plane component of the polarization preserved throughout the structure), to a weakly coupled regime (where the polarization is confined within the PbTiO₃ layers forming domains). The results are in good agreement with x-ray diffraction, transmission electron microscopy, and ultra-high resolution electron energy loss spectroscopy experimental measurements.

Publications P. Aguado-Puente, et. al, **Interplay of Couplings between Antiferrodistortive, Ferroelectric, and Strain Degrees of Freedom in Monodomain PbTiO₃/SrTiO₃ Superlattices**, Phys. Rev. Lett. 107, 217601 (2011); P. Aguado Puente. PhD Thesis. Universidad de Cantabria (2011)



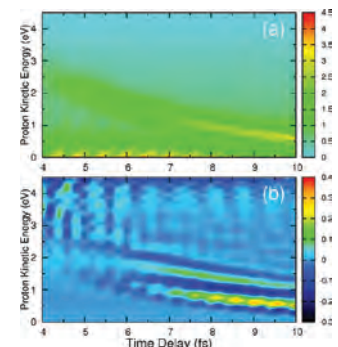
High-resolution transmission electron microscopy (TEM) image of a PTO/STO superlattice experimentally grown and the simulation box theoretically computed, showing how realistic our simulations are (overlap in size with experiment).

» Probing molecular nuclear and electron dynamics through ionization induced by attosecond xuv pulses and free electron lasers, Fernando Martín, Universidad Autónoma de Madrid

Abstract Attosecond laser technology allows one to explore the ultrafast electronic and nuclear dynamics induced by electromagnetic radiation. A full theoretical description of the dynamics of molecules subject to ultrashort laser pulses remains a challenge due to the computational difficulty to include all electronic and vibrational degrees of freedom. A time dependent ab initio treatment was developed that overcomes this difficulty, and utilized to perform: i) a systematic study on the influence of laser parameters on autoionisation processes, ii) attosecond pump-probe numerical experiments on molecules, iii) a study on single and double ionization of molecules induced by strong fields as well as by single and trains of ultrashort laser pulses, and iv) a study of Young's double-slit interference and diffraction at high photon energies. The work has been carried out in parallel with experiments.

Results Ab-initio time-dependent calculations were performed for a full-dimensional description of the interaction of the H₂ molecule with ultrashort laser pulses. The main results were: I) The existence of interferences between different autoionising states in the dissociative photoionisation of randomly oriented H₂ molecules, with large amplitude oscillations in the photoelectron asymmetry parameter as a function of electron energy, in full agreement with experimental results; II) The time evolution of autoionising states was studied using an attosecond pulse train (APT) pump - IR probe set up. It was found that the coupling with the IR field leads to an enhancement of the dissociative ionization channel; III) The use of UV-pump-UV-probe schemes to trace the evolution of nuclear wave packets (NWP) in excited molecular states was investigated by analysing the asymmetry of the electron angular distributions, providing a clearer tracing of the NWP than the analysis of the proton kinetic energy distribution; IV) Two-center interference effects and diffraction in homo- and heteronuclear diatomic molecules as well as in small polyatomic molecules were studied using a newly developed theoretical method. For diatomic molecules, it was found that the interferences are of the same type as those observed in the famous Young's double-slit experiment. In polyatomic molecules, electrons ejected from the central atom are efficiently diffracted by the peripheral atoms, thus providing interesting structural information.

Publications T. J. Reddish, et. al, **Observation of interference between two distinct autoionizing states in dissociative photoionization of H₂**, Phys. Rev. Lett. 108, 023004 (2012); F. Kelkensberg, et. al, **Attosecond control in photoionization of hydrogen molecules**, Phys. Rev. Lett. 107 043002 (2011); A. González-Castrillo, et. al, **Clocking ultrafast wave packet dynamics in molecules through UV-induced symmetry**, Phys. Rev. Lett. 108 063009 (2012); S. E. Canton, et. al, **Direct observation of Cohen-Fano interferences in vibrationally resolved valence-shell photoionization spectra of H₂, N₂ and CO**, Proc. Natl. Ac. of Sciences 108 7302 (2011);



Dissociative single ionization probability and asymmetry parameter for dissociative ionization of H₂ using a UV pump - UV probe scheme with two identical pulses at different time-delays, as a function of time-delay and proton kinetic energy.

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- » Assessing the impact of long-term large scale climate variability on regional climate simulations - Francisco Alvarez-Garcia, Universidad de Alcala
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- » Catalysis modeling: cerium oxide nanoparticles supported on titania (cont) - Javier Fdez Sanz, Universidad de Sevilla
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