

EXCELENCIA  
SEVERO  
OCHOA



Barcelona Supercomputing Center ~ Red Española de Supercomputación



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2012 Annual Report

2012 Annual Report





The 2012 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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» 2012 Review



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

Although 2012 was a very challenging year in Spain due to the on-going economic crisis, we are very pleased to report that BSC-CNS has nevertheless continued to improve services and grow its scientific production, as a result of its diversified activities, multiple funding streams and above all, excellent scientific and technical performance.

**Mission**

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

During the second half of 2012, the main supercomputer at BSC-CNS underwent a major upgrade. The new MareNostrum III will comprise, in its final configuration, 48,896 Intel Sandy Bridge processors in 3,056 nodes, with 96,6 TB of main memory and 84 Xeon Phi processors. The first phase, installed in 2012, gave an initial performance of 0,7 PFlops which will rise to 1, IPFlops as all system components are brought online in early 2013. MareNostrum III is one of only six nodes in four countries that together form the pan-European PRACE Tier-0 network, which provides world-class supercomputing services to European scientists, and as such 70% of its capacity is dedicated to PRACE. A further 24% of MareNostrum III capacity, along with capacities provided by other nodes in the Spanish Supercomputing Network (RES), is available for public access via the Spanish (RES) Access Protocol, thus guaranteeing Spanish scientists access to first class supercomputing services. The final 6% capacity is reserved for use by BSC-CNS scientists.

Designing, installing and commissioning one of the world's most powerful supercomputers is a major achievement and the Directors wish to thank all involved in the project, especially the Operations team, led by Sergi Girona, for their hard work under challenging logistic and funding restrictions.

In conjunction with the installation of MareNostrum III, some of the old MareNostrum II processors were salvaged and transferred to the RES nodes at the University of Valencia and the Astrophysics Institute of Canarias. In addition, the nodes at the Technological Institute of Canarias, the University of Cantabria, the University of Zaragoza, and the University of Málaga were also upgraded significantly during 2012.

**Powerful Computing**

BSC-CNS is the National Supercomputing Facility in Spain and manages the MareNostrum III and MinoTauro supercomputers. Upon installation, MareNostrum III was ranked 36<sup>th</sup> in the world (November 2012 Top500 List), while Minotauro was ranked 114<sup>th</sup> (Dec 2011 Top500 List), and the most efficient HPC cluster in Europe, ranked 7<sup>th</sup> in the world (Green500 list).

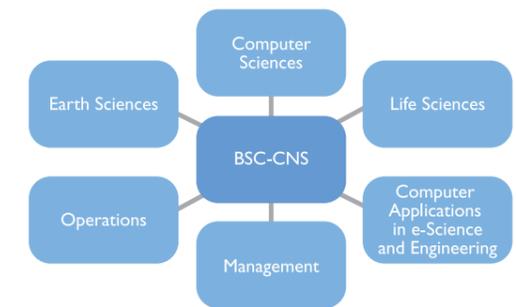
Another project which advanced strongly in 2012, thanks to significant financial support from Repsol Foundation, was the new BSC-CNS building which is located adjacent to the chapel that hosts the MareNostrum III. All the below-ground levels of the building have now been completed, including a specially designed space to hold a future supercomputer. This building will eventually house all BSC-CNS staff who are currently spread out amongst various sites in the UPC campus.

The Severo Ochoa project, which aims to design supercomputing hardware, software and applications targeted at solving significant social challenges in health and climate change, got into full swing in 2012, with the hiring of key staff and formation of numerous multidisciplinary working groups. This integration into working teams of people from different departments, with different backgrounds and skills, is particularly pleasing and it is hoped that Severo Ochoa will serve as a kernel to promote further integration in many other BSC-CNS activities.

**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, Computer Applications in Science & Engineering (CASE), Operations 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.



The Computer Science department also focused on internal integration between different research groups during 2012. Major European Exascale EU projects such as Mont-Blanc, to develop energy efficient exascale supercomputing architectures, and DEEP, to develop novel exascale systems for grand-challenge applications, and Mateo Valero's Advanced ERC grant RoMoL: Riding on Moore's law, which aims to develop a totally new way of conceiving computers with parallel architectures, are engendering extensive vertical integration, with feedback between the different groups enabling 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.

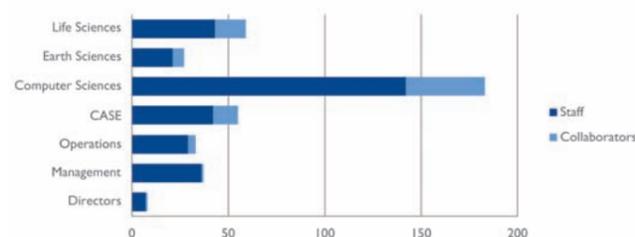
In addition to the two major exascale projects mentioned above, the Computer Science department participated in a further 19 European projects, the 2nd phase of PRACE implementation, two networks of excellence and the European Technology Platform for HPC (ETP4HPC), contributing to the draft of the European Strategic Research Agenda towards Exascale computing. The Department further consolidated its extensive collaborations with major industry multinationals, including Intel, NVIDIA, Microsoft, IBM and Xilinx, and key international and national HPC initiatives, with partners such as the European Space Agency (ESA), and the G8-ECS (Enabling Climate Simulations at Extreme Scale) initiative, amongst others. Impacts of published research results were once again very pleasing, with strong participation in the high quality conferences in the field, including PACT, ASPLOS, ICPP, Supercomputing (SC), MICRO, IPDPS, DATE, CF, HiPC, IISWC, GRID and CCGrid, and publications in prestigious journals including IEEE Transactions on Computers, IEEE Transactions on Parallel and Distributed Systems, ACM Transactions on Embedded Computing Systems, ACM Transactions on Architecture and Code Optimization, Concurrency and Computation: Practice and Experience and Bioinformatics.

The Life Sciences department also continues to grow and excel. The Joint Program with IRBB is functioning very well and in 2012 extended to incorporate a group from the Institute for Predictive and Personalized Medicine of Cancer (IMPCC). Scientific production and impact was very pleasing with publications in 2012 in leading journals such as Nature, Nature Genetics, Nature Nanotechnology, Accounts in Chemical Research, J. Am. Chem. Soc and PNAS, the submission of two new patents, and the highly successful organisation of international meetings such as BioNMR2012, the EMBO Workshop in Computational biology, and the DESMOND European hands-on workshop. The Department also participated in many important European projects such as the Human Brain Project, the International Cancer Genome Consortium, the European Exascale Software Initiative, the Human Epigenome (BluePrint), and Plant Genomics (TransPlant), amongst others.

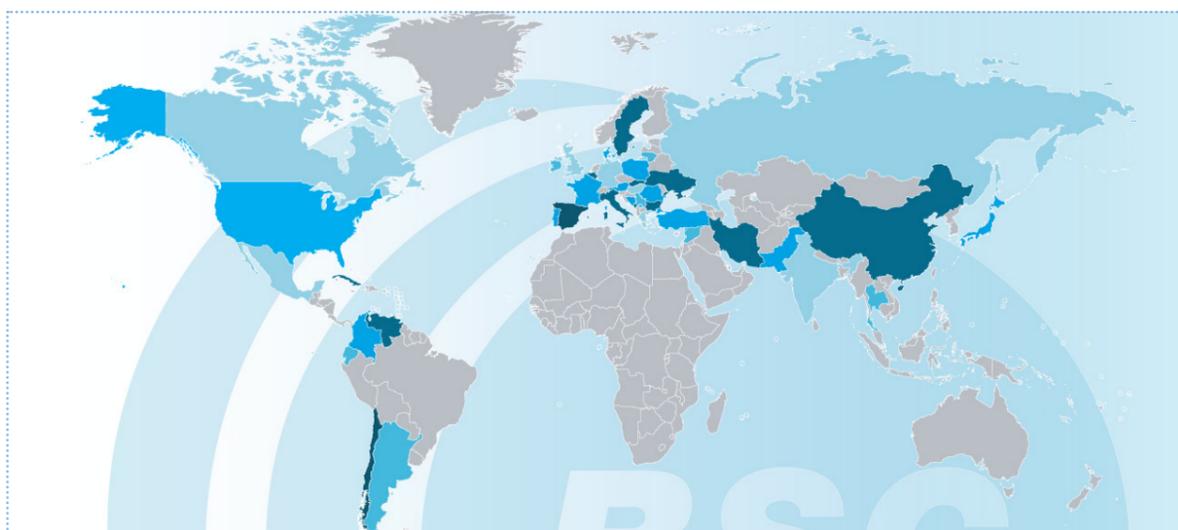
In Earth Sciences there was also a strong increase in project activity and scientific production. Of particular note are the increasingly sophisticated and detailed air quality models developed and run by the Department which have expanded to new areas: the CALIOPE project, funded by the Spanish Ministry of the Environment, which maintains daily high-resolution operational air quality forecasts for Europe and Spain, was extended during 2012, in collaboration with local governments, to Andalucía and the Canary Islands; the Department continues to host the Northern Africa-Middle East-Europe (NA-ME-E) Node of the SDS-WAS Regional Center, to deliver timely and quality sand and dust storm forecasts; and continued development of key models on chemical transport, aerosols, mineral dust, and air quality, and their integration at mesoscale and with wave and other models. The impact of published papers was once again very high with 19% of papers in the top 10% of the field and a further 75% of papers in the top 25% of the field.

Meanwhile, CASE continues to expand the range and scope of the applications to which its codes are applied. The Department now develops or co-develops five main high performance codes, which are at the core of international projects and collaborations with companies: Alya for modelling of biological and mechanical systems, such as the human heart, respiratory system or yacht designs; FAIL3D, to model volcano ash transport, used in South American Volcanic Ash Advisory Centres (VAAC); BSIT, Barcelona Seismic Imaging Tools, promoted by Repsol for subsea seismic analysis; SIESTA, for ab-initio molecular dynamics; and Pandora, an agent-based modelling framework for social simulation. Collaboration with industry continues to grow, with the department participating in five major industry-funded projects during 2012.

BSC-CNS People 2012



In addition to the national recognition of Severo Ochoa, BSC-CNS has consolidated its international reputation as a centre of excellence with world-class infrastructure. This is clearly seen in its ability to continue attracting the best and brightest young researchers from across the globe, despite the difficult economic situation in Spain. During 2012, some 402 people performed research or provided support at the centre. Over 38% of staff are of foreign nationality, with over 40 countries represented including: Argentina, Austria, Belgium, Bosnia, Bulgaria, Canada, Colombia, Chile, China, Cuba, Denmark, Ecuador, France, Germany, Greece, Hungary, India, Iran, Ireland, Italy, Japan, Lithuania, Mexico, Montenegro, Pakistan, Poland, Portugal, Romania, Russia, Serbia, Slovakia, Sweden, Syria, Thailand, Turkey, Ukraine, United Kingdom, USA, Venezuela and Spain.



World Map of Countries of Origin

Despite the lengthy shutdowns of MareNostrum and some of the other RES nodes for upgrades, over 200 external projects from all over Spain, and even some from Europe, utilised some 65 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 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 105 journals and book chapter publications, and some 140 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.

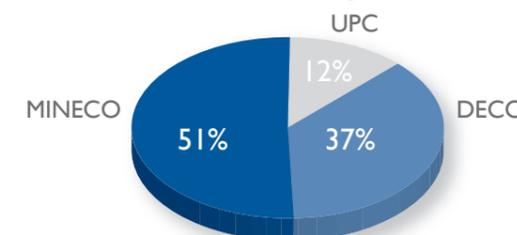
The income of BSC-CNS in 2012 was €30.6 M, of which €21.5 M corresponded to ordinary budget and strategic investments funded by the patrons of BSC-CNS, the Spanish and Catalan Governments; and €9.1 M from competitive projects. Of particular note, almost €3.1 M of funding was derived from projects with private companies.

BSC-CNS continued to grow its portfolio of competitive R&D projects, both via the FP7 program of the European Union and also via major collaborations with a number of multinational companies, including not only the major IT companies (IBM, Intel, Microsoft and NVIDIA), but also other industries such as Repsol and Iberdrola. In 2012, BSC-CNS participated in 47 competitively funded EU projects, 17 collaborative projects with industry, 2 training projects, and 15 national projects. The new Horizon 2020 program to launch in 2014 presents new challenges for BSC-CNS, but preparations commenced already in 2012 to lay the groundwork for future project calls and BSC-CNS has strong ambitions to take leading roles in many of the most important European HPC projects.

### Patrons of the BSC-CNS

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

BSC-CNS Patronage



Spanish science is passing through a very difficult phase. Despite this, BSC-CNS has weathered the storm well, even managing modest growth in personnel and a major upgrade of core facilities. This is not trivial, and is due to the determination of BSC-CNS management to maintain the hard-won reputation of BSC-CNS as a key global centre of reference in High Performance Computing and e-Science. Management in turn have been strongly supported by the staff, students, collaborators and visiting researchers who truly 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, MINECO, DECO and UPC for their continued strong support, and to the European Commission, Repsol and other funding agencies and private companies who sponsored research and development activities during 2012.

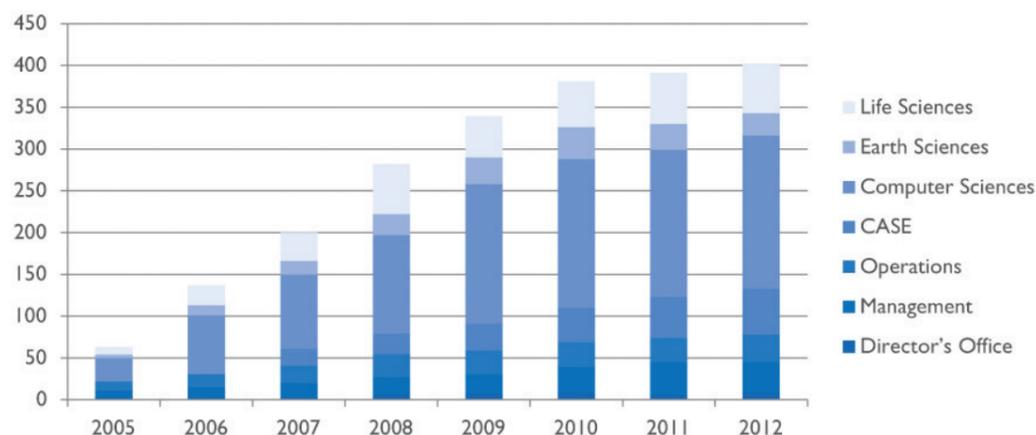
Mateo Valero, Director

Francesc Subirada, Associate Director

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

As at 31<sup>st</sup> December 2012, the core staff of BSC-CNS included 100 permanent positions, 151 dedicated to specific projects and 70 scholarship students. These numbers were significantly augmented by additional staff who participated in BSC-CNS via a number of programs. Total personnel who worked at BSC-CNS throughout the year increased slightly from 391 during 2011 to 402 during 2012, 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 2012, 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 2012, BSC-CNS hosted 100 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 BSC-CNS. This program, which holds selection meetings every 4 months, allowed 6 researchers to access BSC-CNS facilities in 2012; their expenses were covered by the Spanish Ministry of Economy and Competitiveness (MINECO).



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 2012 BSC-CNS hosted 74 of these visitors. The expenses for their stays were covered by the European Research Infrastructure Program.



## » BSC-CNS Governing Bodies



Members of the BSC-CNS Executive Committee

## BSC-CNS Staff and Collaborators during 2012

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**José Ignacio Doncel**, Deputy Director General of Planning for Technological and Scientific Infrastructures

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**Iolanda Font de Rubinat**, Deputy Director General for Research

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#### Representatives BSC-CNS

**Mateo Valero**, Director  
**Francesc Subirada**, Associate Director

**Ernest Quingles**, Manager

#### Commission Secretaries:

**Ramón Fernández Calvo**, State lawyer  
**Noelia Calmache**, State lawyer

### Members of the BSC-CNS Executive Committee

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**M<sup>a</sup> Luisa Poncela**, Director General for Innovation and Competitivity, MINECO

#### Vice President

**Josep Ma Martorell**, Director General for Research, DECO

#### Representative MINECO

**José Ignacio Doncel**, Deputy Director General of Planning for Technological and Scientific Infrastructures

#### Representative DECO

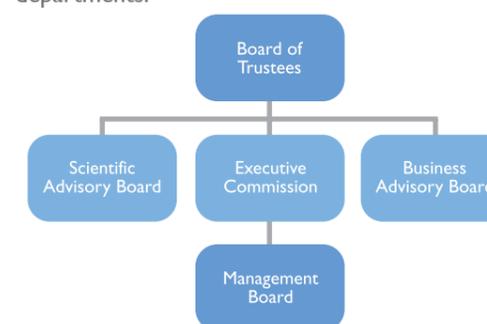
**Iolanda Font de Rubinat**, Deputy Director General for Research

#### Representatives UPC

**Ana Isabel Pérez**, Vice Rector for Research  
**Xavier Gil**, Vice Rector for Scientific Policy

## Strong Governance

Overall governance of BSC-CNS is provided by the Board of Trustees, formed by members of the three institutions that are partners of BSC-CNS, 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

**Francesc Subirada**, Associate Director

**Ernest Quingles**, Manager

### Commission Secretaries

**Ramón Fernández Calvo**, State lawyer

**Noelia Calmache**, State lawyer

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**Dr. Paul Messina**, Director of Science, Argonne Leadership Computing Facility - USA

**Prof. Manuel Peitsch**, Chairman of Board of Directors, Swiss Institute of Bioinformatics

**Prof. Leonard Barrie**, Vice-President of Research, The Cyprus Institute (Cyl)

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### Management Board Vice-Chairman

**Francesc Subirada**, Associate Director

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**Modesto Orozco**, Life Sciences Director

**Sergi Girona**, Operations Director

**José María Cela**, Computer Applications in Science and Engineering Director

**Ernest Quingles**, Management Director

## Access Committee

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**Ramón Bevide**, Universidad de Cantabria

**Ramón López de Arenosa**, Ministerio de Ciencia e Innovación

**Eduard Ayguadé**, Barcelona Supercomputing Center-Centro Nacional de Supercomputación

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Coordinator: **Patrick Aloy**, Institut de Recerca Biomèdica

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

## BSC-CNS Staff and Collaborators during 2012

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Coordinator: **Gustavo Yepes**, Universidad Autónoma de Madrid

Assistant: **Ramón Carbonell**, CSIC-Institute Earth Sciences “Jaume Almera”

### RES Users' Committee (CURES)

### Physics and Engineering (FI) representatives

**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**

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Director Assistant: Lourdes Cortada

Associate Director Assistant: Judith Camba

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Professional HPC Training: Evguenia Stoilova Alexandrova

Academic Programs Coordinator: Ulises Cortés

Visitor: Antonio Aloisio

### Computer Sciences Department

Computer Science Department Director: **Jesús Labarta**

Computer Science Department Associate Director:

**Eduard Ayguadé**

Visitor: Julio Ramón Bevide

### Accelerators for High Performance Computing

Accelerators For High Performance Computing Group

Manager: **Nacho Navarro**

Junior Researcher: Javier Cabezas

Doctoral Student: Aswinkumar Sridharan

Doctoral Student: Ivan Tanasic

Doctoral Student: Marc Jordà

Doctoral Student: Víctor García

Associate Researcher: Marisa Gil

HPC Visitor: Andrius Pa ukste

### Autonomic Systems and e-business Platforms

Autonomic System and e-Business Platforms Group

Manager: **Jordi Torres**

Junior Developer: Álvaro Villalba

Junior Developer: Cesare Cugnasco

Junior Developer: Juan Luis Pérez

Junior Researcher: Mario Macías

Doctoral Student: Gemma Reig

Doctoral Student: Jordà Polo

Doctoral Student: Zeus Gómez

Trainee Developer: Josep Subirats

Trainee Developer: Roger Hernández

Associate Researcher: David Carrera

Associate Researcher: Jordi Guitart

Associate Researcher: Ricard Gavaldà

Associate Researcher: Yolanda Becerra

### Computer Architecture for Parallel Paradigms

Computer Architecture For Parallel Paradigms Group

Manager: **Adrián Cristal**

Computer Architecture For Parallel Paradigms Group

Manager: **Osman Unsal**

Postdoctoral Researcher: Nehir Sonmez

Postdoctoral Researcher: Sasa Tomic

Doctoral Student: Adrià Armejach

Doctoral Student: Azam Seyedi

Doctoral Student: Daniel Nemirovsky

Doctoral Student: Gokcen Kestor

Doctoral Student: Gulay Yalcin

Doctoral Student: Ivan Ratkovic

Doctoral Student: Milan Stanic

Doctoral Student: Milovan Duric

Doctoral Student: Nikola Markovic

Doctoral Student: Omer Subasi

Doctoral Student: Oriol Arcas

Doctoral Student: Srdjan Stipic

Doctoral Student: Timothy Hayes

Doctoral Student: Vasileios Karakostas

Doctoral Student: Vesna Smiljkovic

Doctoral Student: Vladimir Gajinov

Associate Researcher: Francisco Javier Arias

Associate Researcher: Óscar Palomar

### Extreme Computing

Extreme Computing Group Manager: **Vassil Alexandrov**

**Alexandrov**

Doctoral Student: Janko Strassburg

Visitor: Aneta Karaivanova

Visitor: Florian Urmetzer

Visitor: Krassimir Georgiev

### Grid Computing and Clusters

Grid Computing Group Manager: **Rosa Maria Badia**

Senior Researcher: Daniele Lezzi

Senior Researcher: Raül Sirvent

Junior Developer: Carlos Díaz

Postdoctoral Researcher: Pieter Bellens

Junior Researcher: Enric Tejedor

Junior Researcher: Jorge Ejarque

Junior Researcher: José María Pérez

Doctoral Student: Jan Ciesko

Doctoral Student: Judit Planas

Doctoral Student: Maja Etinski

Doctoral Student: Marta García

Doctoral Student: Rahul Kumar Gayatri

Doctoral Student: Tomasz Patejko

Doctoral Student: Vinoth Krishnan Elangovan

Trainee Developer: Francesc Lordan

Trainee Developer: Javier Álvarez

Trainee Developer: Roger Rafanell

Associate Researcher: Julita Corbalán

Visitor: Elisabeth Larsson

Visitor: Fabrizio Marozzo

Visitor: Kenneth Skovhede

Visitor: Martin Tillenius

### Heterogeneous Architectures

Heterogeneous Architectures Group Manager: **Àlex Ramírez**

**Ramírez**

Senior Researcher: Isaac Gelado

Senior Researcher: Miguel Pericàs

Junior Developer: James David Vipond

Postdoctoral Researcher: Nikola Puzovic

Doctoral Student: Alejandro Rico

Doctoral Student: Branimir Dickov

Doctoral Student: Karthikeyan Palavedu

Doctoral Student: Milan Pavlovic

Doctoral Student: Muhammad Shafiq

Doctoral Student: Nikola Rajovic

Doctoral Student: Oscar Domínguez

Doctoral Student: Thomas Grass

Doctoral Student: Ugljesa Milic

Trainee Student: Jorge Luis Florit

Associate Researcher: Carlos Villavieja

Associate Researcher: Friman Sánchez

Associate Researcher: Paul Matthew Carpenter

Visitor: Kiril Dichev

### Unconventional Computer Architecture and Networks

Unconventional Computer Architecture and Networks

Group Manager: **Mario Nemirovsky**

Visitor: Damián Roca

### Operating System / Computer Architecture Interface

Operating System Group Manager: **Francisco Javier Cazorla Operating**

**Cazorla Operating**

System Group Manager: Francisco Javier Cazorla

Senior Researcher: Eduardo Quiñones

Senior Researcher: Jaume Abella

Junior Developer: Mikel Fernández

Postdoctoral Researcher: Carles Hernández

Postdoctoral Researcher: Roberto Gioiosa

Doctoral Student: Bojan Maric

Doctoral Student: Gabriel Fernández

Doctoral Student: Javier Jalle

Doctoral Student: José Carlos Ruiz

Doctoral Student: Leonidas Kosmidis

Doctoral Student: Milos Panic

Doctoral Student: Mladen Slijepcevic

Doctoral Student: Petar Radojkovic

Doctoral Student: Qixiao Liu

Doctoral Student: Víctor Javier Jiménez

Doctoral Student: Vladimir Cakarevic

Associate Researcher: Alejandro Pajuelo

Associate Researcher: Javier Verdú

Associate Researcher: Miquel Moreto

HPC Visitor: Sascha Uhrig

Visitor: Emery Berger

Visitor: Stelios Manousopoulos

### Programming Models

Parallel Programming Models Group Manager: **Xavier Martorell**

**Martorell**

Senior Developer: Julian David Morillo

Senior Researcher: Àlex Duran

Senior Researcher: Gabor Janos Dozsa

Senior Researcher: Isaac Juan Rudomin

Senior Researcher: Vicenç Beltran

Junior Researcher: Javier Teruel

Junior Researcher: Roger Ferrer

Doctoral Student: Ahimed Yazdanpanah Ahmadabadi

Doctoral Student: Alejandro Fernández

Doctoral Student: Antonio Filgueras

Doctoral Student: Daniel Cabrera

Doctoral Student: Diego Caballero

Doctoral Student: Javier Bueno

Doctoral Student: Lluc Álvarez

Doctoral Student: Lluís Vilanova

Doctoral Student: Michail Alvanos

Doctoral Student: Nikola Vujic

Doctoral Student: Ramon Bertran

Doctoral Student: Sara Royuela

Doctoral Student: Tassadaq Hussain

Doctoral Student: Vladimir Marjanovic

Trainee Developer: Florentino Sainz

Trainee Developer: Sergi Mateo

Trainee Developer: Víctor López

Associate Researcher: Carlos Álvarez

Associate Researcher: Daniel Jiménez

Associate Researcher: Juan José Costa

Associate Researcher: Marc González

Associate Researcher: Montse Farreras

Developer In Training: Guillermo Miranda

HPC Visitor: Alessandro Cilardo

HPC Visitor: Fisnik Kraja

HPC Visitor: Mateo Comin

## BSC-CNS Staff and Collaborators during 2012

Visitor: Artur Martin Podobas  
Visitor: Ettore Speziale

### Performance Tools

Performance Tools Group Manager: **Judit Giménez**  
Senior Researcher: José Carlos Sancho  
Junior Developer: Eloy Martínez  
Junior Developer: Pedro Antonio González  
Postdoctoral Researcher: Claudia Andreina Rosas  
Junior Researcher: Francesc Xavier Pegenaut  
Junior Researcher: German Llorca  
Junior Researcher: Harald Servat  
Junior Researcher: Juan González  
Doctoral Student: Ana Jokanovic  
Doctoral Student: Vladimir Subotic  
HPC Visitor: Oleg Tsemaylo

### Storage Systems

Storage Systems Group Manager: **Antonio Cortés**  
Senior Researcher: Anna Queralt  
Senior Researcher: Ramon Nou  
Junior Researcher: Ernest Artiaga  
Junior Researcher: Jacobo Giralt  
Junior Researcher: Jan Wiberg  
Junior Researcher: Jonathan Martí  
Junior Researcher: Matthias Werner Brugger  
Junior Researcher: Paul Hermann Lensing  
Doctoral Student: Alberto Miranda  
Doctoral Student: Josep Oriol Fito  
Junior Developer: Juan González  
Junior Developer: Thanos Makatos  
Trainee Developer: Daniel Gasull  
Visitor: Isak Nuhic

### Earth Sciences Department

Earth Science Department Director: **José María Baldasano**  
Research Support Coordinator Technician: Kim Serradell  
Research Support Technician: Albert Soret  
Research Support Technician: David Carrió  
Research Support Technician: Francesc Martínez  
Research Support Technician: Luca Telloli  
Research Support Technician: Miguel Castrillo

### Air Quality

Air Quality Group Manager: **Santiago Gassó**  
Senior Researcher: Gustavo Arévalo  
Postdoctoral Researcher: María Teresa Pay  
Postdoctoral Researcher: Valentina Sicardi  
Research Support Technician: Marc Guevara  
Doctoral Student: Víctor Manuel Valverde  
Trainee Student: Gina Ferrer

### Mineral Dust

Postdoctoral Researcher: **Sara Basart**  
Research Support Technician: Francesco Benincasa  
Associate Researcher: Carlos Pérez  
Associate Researcher: Enric Terradellas  
HPC Visitor: Anna Pederzoli  
HPC Visitor: Eduard Chemyakin

### Atmospheric Modelling

Metereological Modelling Group Manager: **Oriol Jorba**  
Doctoral Student: Alba Badia  
Doctoral Student: Ángel Rincón  
Doctoral Student: Michele Spada  
Visitor: Marc Carreras

### Climate Change

Trainee Student: Lola Guerreiro  
Associate Researcher: Maria Gonçalves

### Life Sciences Department

Life Sciences Director: **Modesto Orozco**  
Visitor: Kenneth Merz

### Computational Genomics

Computational Genomics Group Manager: **David Torrents**  
Postdoctoral Researcher: Josep María Mercader  
Postdoctoral Researcher: Lisa Olivia Andrieux  
Research Support Technician: Marco Paulo Seco  
Doctoral Student: Leyden Fernández  
Doctoral Student: Santiago González  
Doctoral Student: Silvia Bonas  
Associate Researcher: Ana Rojas  
Visitor: Kasper Nielsen  
Visitor: Laura Martínez

### Electronic and Atomic Protein Modelling

Electronic and Atomic Protein Modelling Group Manager: **Víctor Guallar**  
Senior Researcher: Armin Madadkar  
Postdoctoral Researcher: Maria De Fatima Assunção  
Postdoctoral Researcher: Martin Ivanov Kotev  
Postdoctoral Researcher: Ryoji Takahashi  
Postdoctoral Researcher: Suwipa Saen  
Research Support Technician: Daniel Lecina  
Research Support Technician: Manuel Augusto Rivero  
Doctoral Student: Emanuele Monza  
Doctoral Student: Israel Cabeza  
Doctoral Student: Sandra Acebes  
Doctoral Student: Seyed Ali Hoseini  
Doctoral Student: Víctor Gil  
Doctoral Student: Xavier Oro  
Visitor: Alba Rincón  
Visitor: Andreu Tarraco  
Visitor: Rose Afzali

### INB-Computational Node 2

INB - Computational Group Manager: **Josep Lluís Gelpí**  
Research Support Technician: Anna Mantsoki  
Research Support Technician: Dmitry Reptchevski  
Research Support Technician: Laia Codo  
Research Support Technician: Montserrat Puiggrós  
Research Support Technician: Pau Andrió  
Research Support Technician: Romina Royo  
Research Support Technician: Stamatina Fragkogiani  
Research Support Technician: Valentí Moncunill

### Molecular Modelling and Bioinformatics

Life Sciences Department Director: **Modesto Orozco**  
Senior Researcher: Josep Ramon Goñi  
Postdoctoral Researcher: Robert Soliva  
Research Support Technician: Carles Fenollosa  
Research Support Technician: Núria Villegas  
Research Support Technician: Santiago Villalba  
Visitor: Alejandro Giraldo  
Visitor: Konstantinos Alexiou  
Visitor: Manuel Rueda

### Protein Interactions and Docking

Protein Interactions and Docking Group Manager: **Juan Fernández**  
Postdoctoral Researcher: Iain Moal  
Postdoctoral Researcher: Santiago Esteban  
Doctoral Student: Brian Jiménez  
Doctoral Student: Chiara Pallara  
Doctoral Student: Didier Barradas  
Doctoral Student: Laura Pérez  
Doctoral Student: Miguel Romero  
Associate Researcher: Solène Grosdidier  
Visitor: Elodie Japaud  
Visitor: Jordi Triguero  
Visitor: Mireia Rosell  
Visitor: Montserrat Barbany

### Computer Applications in Science & Engineering Department

Computer Applications In Science And Engineering Director: **José María Cela**  
Senior Developer: George Huhs  
Senior Developer: Rogeli Grima  
Senior Researcher: Jorge García  
Senior Researcher: Josep De la Puente  
Senior Researcher: Mauricio Hanzich  
Senior Researcher: Volodymyr Puzyrov  
Postdoctoral Researcher: Ángel Coppola  
Postdoctoral Researcher: Jean Antoine Kormann  
Postdoctoral Researcher: Maria Cristina Marinescu  
Postdoctoral Researcher: Xavier Rubio  
Doctoral Student: Cristina Montañola  
Doctoral Student: Pierre Lafortune  
Junior Developer: Hadrien Calmet

Junior Developer: Natalia Gutiérrez  
Junior Researcher: Albert Farrés  
Junior Researcher: Fèlix Rubio  
Junior Researcher: Xavier Saez  
Associate Researcher: Carles Serrat  
HPC Visitor: Alberto Gambaruto  
HPC Visitor: Alister Bates  
HPC Visitor: Etienne Boileau  
Visitor: Óscar Borrego  
Visitor: Pawel Lenarczyk

### High Performance Computational Mechanics

Physical and Numerical Modelling Group Manager: **Mariano Vázquez**  
Senior Developer: Antoni Artigues  
Postdoctoral Researcher: Fernando Martín Cucchiatti  
Postdoctoral Researcher: Jazmín Aguado  
Visualisation Technician: Guillermo Marín  
Doctoral Student: Alexis Torrano  
Doctoral Student: Margarida Moragues  
Doctoral Student: Ruth Aris  
HPC Visitor: Daniel Mira  
HPC Visitor: Esteban Ferrer  
HPC Visitor: Peter Wittek  
Visitor: Eugene Skouras

### Physical and Numerical Modelling

Physical and Numerical Modelling Group Manager: **Guillaume Houzeaux**  
Postdoctoral Researcher: Eva Casoni  
Junior Developer: Genis Aguilar  
Junior Developer: Juan Esteban Rodriguez  
Junior Developer: Miguel Ferrer  
Junior Developer: Mohammad Jowkar  
Doctoral Student: Augusto Samaniego  
Doctoral Student: Beatriz Eguzkiza  
Doctoral Student: Jelena Koldan  
Doctoral Student: Oscar Francisco Peredo  
Junior Researcher: Tano Varadinov  
HPC Visitor: Benjamin Uekermann  
Visitor: Florent Dizes

### Environmental Simulations

Environmental Simulations Group Manager: **Arnau Folch**  
Postdoctoral Researcher: Matias Oscar Ávila  
Junior Researcher: Raúl De la Cruz  
Doctoral Student: Chiara Scaini  
Doctoral Student: Simone Marras  
Visitor: Florencia Reckziegel

## BSC-CNS Staff and Collaborators during 2012

### Operations Department

Operations Director: **Sergi Girona**

### System Administration

Systems Group Manager: **Javier Bartolomé**

Helpdesk Technician: Antonio Espina r

Helpdesk Technician: Ferran Sellés

Helpdesk Technician: Pedro Gómez

Network Technician: Albert Benet

Performance Technician: Alejandro Lucero

Performance Technician: Carles Fenoy

Security and Network: Juan Carlos Sánchez

System Administration: David Ocaña

System Administration: Gabriele Carteni

System Administration: Guillermo Aguirre

System Administration: Jordi Valls

System Administration: Jorge Holgado

System Administration: Sergi Moré

Visitor: Alejandro Flores

Visitor: Feliu Sagols

Visitor: Francisco Ortiz

### User Support

User Support Group Manager: **David Vicente**

Support Applications Consultant: Christian Simarro

Support Applications Consultant: Jorge Rodríguez

Support Applications Consultant: Pablo Rodenas

User Support Consultant: Jorge Alberto Naranjo

User Support Consultant: Xavier Abellán

Visualisation Technician: Carlos Tripiana

Web Graphical Designer: Jasmina Tomic

Web Graphical Designer: Laura Bermúdez

Webmaster: Núria Montoya

Webmaster: Silvina Rusinek

### Facility Management

Facility Management Group Manager: **Ahmet Emin**

**Senata**

Maintenance Technician: **Albert Riera**

Facility Management Consultant Operations: **Ramon**

**Pallisa**

### 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: **M. Cristina Calonge**

Purchasing Officer: Cristina Vargas

Support Accounting Technician: Alba Delclòs

Support Accounting Technician: Judit Soldevila

Support Purchasing Officer: Neus Jiménez

Technical Support for Economic Management Project:

Laia Traveset

Technical Support for Economic Management Project:

Laura Viñas

Technical Support for Economic Management Project:

Marina Utgés

### General Services and Purchase

General Assistant: Laura Gutiérrez

General Assistant: Núria Sirvent

Trainee Student: Alicia Giménez

Trainee Student: Aurora Rodríguez

### Human Resources

HR Support Technician: Anna Martín

HR Technician: Lara Cejudo

Trainee Student: Carla Santamaria

Trainee Student: Marc Rabinal

### IT Support

Information System Developer: Toni Matas

### Projects and Technology Transfer

Project Management Office Manager: **Eugene Griffiths**

Business Analyst: Marcin Ostasz

Prace Project Manager: Carlos David Mérida

Project Manager: Francesca Arcara

Project Manager: Gina Michelle Alioto

Project Manager: Guadalupe Moreno

Project Manager: Javier Salazar

Project Manager: Marta Rosselló

Project Manager: Oriol Pineda

Project Manager: Pilar Callau

Project Support Technician: Eulalia Iglesias

### Marketing and Communication

Head Communications: **Gemma Ribas**

Communications Officer: María José Barroso

Communications Officer: Sara Ibáñez

Dissemination Project Officer: Nagham Salman

Marenostrum Visitors Manager: Oriol Riu

Marketing Officer: Renata Giménez

The Education and Training Team was created in 2012 with the appointment of Maria Ribera Sancho, responsible for Academic BSC-CNS Programs, and Nia Alexandrova for HPC Professional Training and Postgraduate Studies.

### » Mission

The mission of the team is to coordinate training activities and develop opportunities for collaboration with other leading HPC and SC centres in education, training and mobility.

### » Activities

There is a long standing tradition of BSC-CNS leadership at national and European level with excellent training opportunities. In line with the BSC-CNS strategy to establish the Centre as an educational centre of excellence providing training and professional skills for researchers and industry, as well as talent capture and retention at university level, various developments were initiated.

During 2012 the team focused on building training curricula based on cutting-edge scientific research and development of models, software tools and simulation environments for high-performance computing and application areas, targeting research communities and industry with supercomputing needs. Based on the PRACE Advanced Training Centre status and in cooperation with the rest of the PATC centres, the team is working to develop appropriate European HPC professional training curricula, available beyond the PRACE partnership. The courses delivered so far were very successful in attracting participants both from academia and industry.

The Professional Training Program is based on a set of core courses from the PATC curricula complemented by a myriad of ad-hoc courses that are provided on and off BSC-CNS premises by BSC-CNS researchers for a variety of audiences.

The close relationship that BSC-CNS has with UPC, and in particular with the Barcelona School of Informatics, creates a unique opportunity for trainees who wish to continue their studies to take a BSC-CNS led post-graduate program at Master or PhD level. Also, to facilitate talent capture and retention and support local universities in the development of postgraduate programs tuned to the needs of the HPC industry and supercomputing as research area, BSC-CNS is involved in the design and delivery of the HPC Stream of MIRI Master programs and other HPC related courses at Bachelor and Master level.

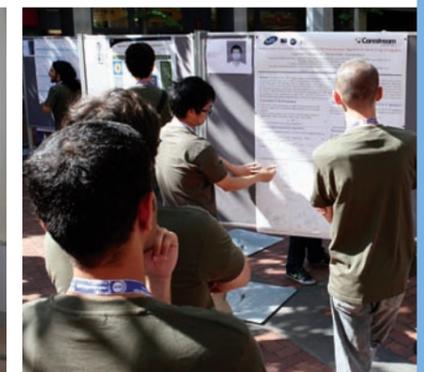
### » Involvement in Key Projects

**In 2012 the team was engaged in:**

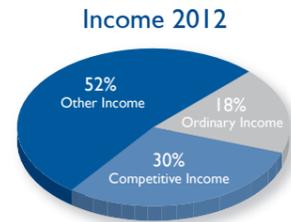
- ▶ PRACE 2IP and 3IP projects,
- ▶ Severo Ochoa project which Training and Mobility Work Package,
- ▶ ESSI project,
- ▶ RISC (A Network for Supporting the Coordination of Supercomputing Research Between Europe and Latin America),
- ▶ EU Brazil OpenBio project.

### » Presentations and Papers

- ▶ M. R. Sancho, N. Alexandrova "Education and Training at BSC", poster on the SC12 HPC Educators Program, Salt Lake City, USA, 11 – 15 November 2012
- ▶ N. Alexandrova, V. Alexandrov and Raul Ramirez "The Role of Computational Science and Emerging Technologies in the Natural Sciences Education at University Level", Procedia Computer Science, Elsevier, Volume 9, pp. 1789-1798, 2012.



The financial accounts for 2012 presented here were drawn up following the accounting principles laid out in the General Plan of Public Accounting. The operating budget of BSC-CNS for the fiscal year 2012 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

**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 BSC-CNS and increases in supercomputing hardware.

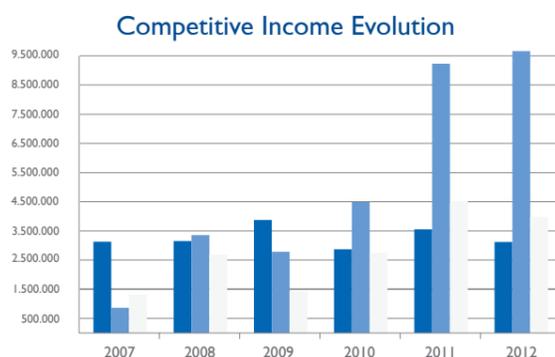
**Overheads** are incomes derived from ordinary projects, which according to the norms of BSC-CNS are charged 10% to cover overhead expenses.

**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.

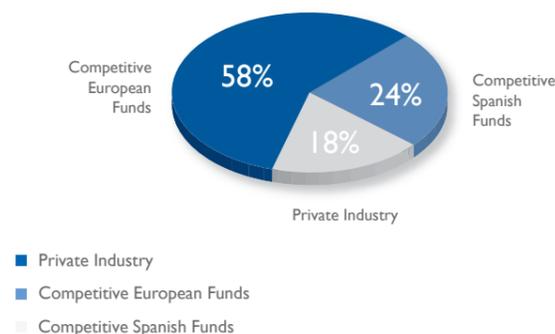
INCOME	AMOUNT €
Ordinary Income	5.494.140,00
Ministerio de Ciencia e Innovación	4.288.320,00
Generalitat de Catalunya	1.205.820,00
Competitive Income	9.111.389,38
Ministerio de Ciencia e Innovación	1.586.626,89
Generalitat de Catalunya	137.410,08
European Commission	4.268.645,78
Private Companies	3.118.706,63
Other Income	15.956.300,15
Applied Previous Reserves	11.883.855,00
Strategic Investment	1.986.719,13
Overheads/Capital transfers	2.085.726,02
<b>TOTAL INCOME</b>	<b>30.561.830</b>

» 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.



Competitive Funding 2012



» Expenses

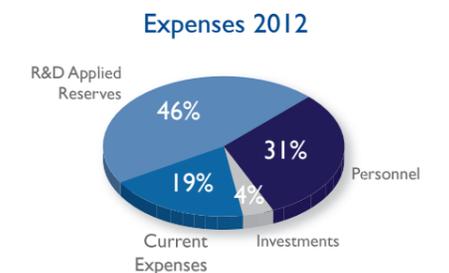
EXPENSES	AMOUNT €		
	Ordinary Budget	Projects Budget	Total
Personnel	4.125.655	5.232.805	9.358.461
Investments	100.251	1.074.283	1.174.534
Current Expenses	2.978.737	2.807.174	5.785.911
R&D Applied Reserves	14.242.924	0	14.242.924
<b>TOTAL EXPENSES</b>	<b>21.447.568</b>	<b>9.114.262</b>	<b>30.561.830</b>

**Personnel** refers 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.

**Investments** include general expenditures on computing and scientific equipment and infrastructure. Key investments such as the construction of the new building to house BSC-CNS and the MareNostrum supercomputer upgrade are registered as R&D Applied Reserves.

**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.

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 11 public tender contracts were signed during the year.



» BSC-CNS - Center of Excellence Severo Ochoa



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

BSC-CNS received the “Severo Ochoa Centres of Excellence” support and accreditation in the 2011 call, a programme of the Secretary of State for Research, Development and Innovation of the Ministry of Economy and Competitiveness that aims to promote excellence in scientific research in Spain. The award confirmed BSC-CNS’s reputation as one of the world’s leading centres applying and doing research on supercomputing technologies. The program commenced in January 2012 with an ambitious research programme: to design the supercomputing hardware, software and applications of the future, which are targeted towards the solving of significant social challenges in health and climate change.



In addition to improving the capacity of world-class research centres to organise and carry out research, the program also plans to consolidate best practices in support services, based on the recognition that efficient management of human resources, training and communication are key elements for promoting outstanding results in research.

» The BSC-CNS Severo Ochoa Project

The BSC-CNS Severo Ochoa research program takes as its starting point the fact that Exascale supercomputers will be crucial in tackling major societal problems in areas such as human health and the environment.

The increasing computational requirements of numerical simulations in these scientific fields, together with new requirements in terms of data management and storage, lead to so called Big Data challenges.

However, attaining Exascale and Big Data poses significant challenges, due to requirements on system hardware and software design, of which energy consumption is one of the main factors. The project aims to consolidate the BSC-CNS as a world leader in High Performance Computing research, including applications in three challenging scientific domains:

- ▶ **Personalised medicine (Life Sciences Department):** combining genomics, proteomics and transcriptomics analysis with computer simulation to create models capable of predicting certain diseases or the effects of drugs on patients before a pathology starts;
- ▶ **Multi-scale air quality climate modelling (Earth Sciences Department):** Developing a high-resolution modelling system for short- and long-term applications as well as new methodologies to run high-resolution models on exascale machines and methodologies to handle big amounts of data produced by complex high-resolution models;
- ▶ **Computational biomechanics-Alya Red (Computer Applications in Science and Engineering Department):** Developing the Cardiac Computational Model (CCM) through the implementation and validation of various advanced physiological models.

The circular graphic summarizes the BSC-CNS Severo Ochoa program, which is made up of four main scientific sub-projects: the proposal and development of novel models in three application domains mentioned above rotate around novel components in the hardware and software stacks to achieve the Exascale and Big Data.

The Computer Sciences Department focussed during 2012 on defining and/or implementing first prototypes of novel technologies to facilitate the implementation of the applications including:

- ▶ **the adaptation of the BSC-CNS's programming models COMPSs/OmpSs** for the data demands of workflow applications and energy-efficiency of the target architectures;

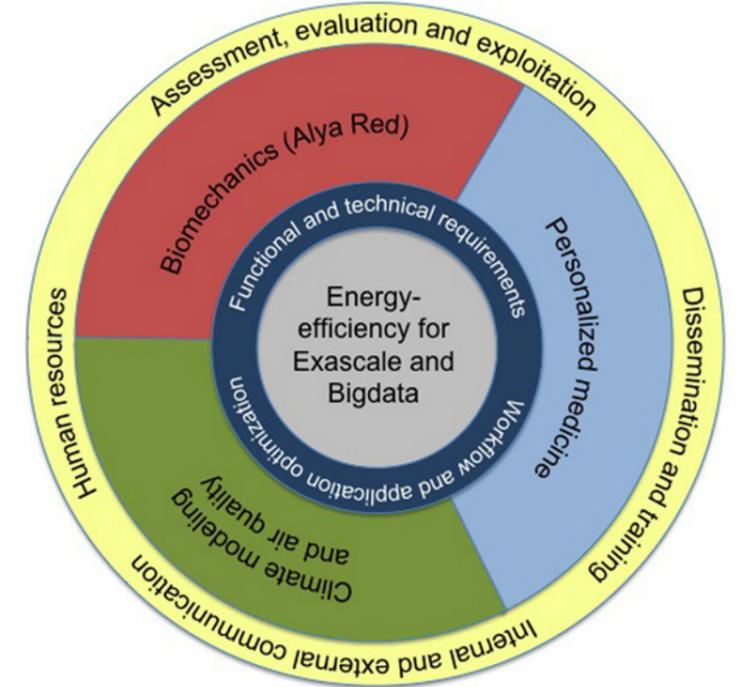
- ▶ **design of methodologies and technologies to support data organisation** in key/value non-relational databases;
- ▶ **proposal of a "persistent objects"-based (as opposed to files) storage platform** and its integration with the programming model and data organisation components;
- ▶ **design of new storage hierarchies and architectures** based on low-power components (synergies with Mont-Blanc EU project);
- ▶ **and design of Domain Specific Languages** (DSL for accelerator-based architectures).

The four scientific sub-projects benefit from the support provided by three additional support sub-projects: a clear Human Resources policy, efficient management and well-structured communications and training activities.

During the first year of the program, BSC-CNS designed an Education and Training Strategy, including the BSC-CNS PRACE Advanced Training Centre and the Severo Ochoa mobility programme which will include financial help for incoming and outgoing short stays.

Regarding human resources, work started on designing a strategy for obtaining the EU's Excellence in HR badge, including the recruitment, reception and integration plan; the performance management plan including the career plan and system of objectives, as well as the internal training plan.

Finally, the first steps in defining the BSC-CNS's Internal and External Communication Strategy were taken, highlighting the researchers' role in communicating research results and achievements and favouring the sharing of knowledge among departments and teams within the same department.



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



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



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 2012, more than 200 IT and senior executives from companies of different types and sizes visited BSC-CNS facilities, and were given presentations with examples of usage of HPC in their respective sectors. A total of 13 sectorial visits were organised. Some of the industrial sectors covered were: aeronautics, automotive, telecommunications, media, pharma, logistics, textile, and governmental IT related organisations. The existing collaborative R&D program agreements that BSC-CNS has with Repsol, Microsoft, Intel, IBM and Nvidia were extremely active, with significant progress and successful results obtained in multiple projects. During 2012 a new program agreement was signed with Fundación Botín, as well as other specific projects with different companies. All of them are described in the following list:

#### » IBM-BSC Research Collaboration



During 2012, the collaboration with IBM focused on three main directions: 1) Workload management of data analytics workloads composed of a set of MapReduce jobs running on top of a NoSQL back-end and transactional workloads producing data to be dumped to the NoSQL back-end, 2) High performance architectures for Big Data with particular attention to the IBM BlueGene Active Storage (BGAS) architecture and the Parallel In-Memory Database (PIMD) as the key/value store and 3) Power modeling and adaptive data prefetching techniques for the IBM POWER7 processor. A new 3-year collaboration framework was defined during 2012 with the aim of starting new joint research agreements during 2013.

#### » Intel-BSC Exascale Laboratory



The main objective of the Intel-BSC Exascale Laboratory, led by Jesús Labarta, is to conduct research activities on novel programming models and prediction tools that will be needed to exploit extraordinary levels of parallelism in future Intel-architecture based supercomputers, consisting of millions of cores. Bringing power consumption to acceptable levels and to make the system fault tolerant are two key issues investigated during 2012, and whose management needs to be transparently handled by highly scalable parallel run-time systems. Future exascale supercomputers will be hugely complex and challenging to understand and to control. During 2012, BSC-CNS performance analysis and prediction tools were extended to consider these future exascale systems.

#### » Microsoft-BSC Research Centre



The BSC-Microsoft Research Centre (BSCMSRC), led by Osman Unsal and Adrián Cristal, continued research activities on transactional memory (TM), including the development of sophisticated TM applications and benchmarks, the Atomic Dataflow Model combining TM and dataflow, architectural proposals to support TM and the TMBox FPGA platform with 16 cores with support for TM. BSCMSRC researchers also explored the suitability of low-power vector processors for mobile and data intensive workloads, including the design of their Instruction Set Architecture (ISA), new architectures and functional vector units. Finally, BSCMSRC researchers worked on the integration of the BSC-CNS StarsS programming model with the message-passing Barrelfish Research OS.

#### » NVIDIA-BSC/UPC Research Collaboration



The BSC-CNS CUDA Center of Excellence (CCoE), in association with the Universitat Politècnica de Catalunya (UPC) and led by Nacho Navarro, recognizes BSC-CNS's broad-based research success in leveraging the NVIDIA CUDA technology and GPU computing. As a CCoE, BSC-CNS and UPC currently offer a number of courses covering CUDA architecture and programming languages for parallel computing and organized the PUMPS summer school in Barcelona.

In addition, research is being conducted in different directions: 1) Use of low-power GPUs in platforms oriented to high-performance computing and the design of the CARMA kit; 2) Leveraging CUDA for productive programming in clusters of multi-GPU systems using OmpSs; 3) Optimisation of applications in different domains: Reverse Time Migra-

tion (with the CASE Department), electronic and atomic protein modeling (with the Life Sciences Department), merge sort in single node multi-GPU systems and iterative solvers for sparse linear systems; and 4) The development of software infrastructures to ease the development on GPU-based systems for different system topologies, TLB design space exploration, and mechanisms and policies for scheduling multiprogrammed workloads on GPUs.

#### » Fundación Botín



The Botín Foundation will help establish a technology business project presented by Life Sciences director Modesto Orozco as part of their programme "Mind the Gap". The project NOSTRUM DRUG DISCOVERY, to be carried out jointly by BSC-CNS and IRB Barcelona is a drug-design simulation platform which aims to reduce the need for clinical trials. The Botín Foundation has chosen to support the project due to its innovative nature and likelihood of commercial viability. The project received the approval of a prestigious international committee of experts in investment strategies for the biotechnology and biomedicine industries. The Foundation will invest in the project to set up a spin-off company over a two-year timeframe so that the company can attract venture capital funding and enable market commercialisation of its products. The goal of the "Mind the Gap" programme is to bring the worlds of science and business together to ensure that important research findings with commercial potential reach the market in the form of services or products that improve the health and well-being of society.

#### » Repsol-BSC Research Center



The Center is undertaking 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. During 2012, the Repsol-BSC Research Center was involved in the following research topics:

- ▶ **Exploration:** RTM, elastic forward modeling, full wave-form inversion, controlled source electromagnetic method.
- ▶ **Vreactor:** simulation of chemical reactions in biodiesels inside batch reactors, coupling with mixing blades, transfer of chemical species through the interfaces of immiscible liquids.
- ▶ **Repsolver phase I:** expert system for simplifying the user interface of multiphysics massively parallel simulations.

#### » 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 simulations of wind farms. The main objective is to significantly increase the efficiency and power of wind farms by developing numerical techniques to optimise placement of wind turbines.

#### » Xilinx-BSC Research Collaboration



During 2012, the joint collaboration with Xilinx continued, undertaking research on OmpSs support for FPGA accelerators. Researchers from the Computer Sciences department developed support for FPGA accelerators based on the Xilinx leading-edge technology.

#### » European Space Agency



The collaboration with the European Space Agency (ESA) is structured around two projects: 1) 'Architectural solutions for the timing predictability of next-generation multi-core processors', with the objective of enabling the Worst Case Execution Time analysis of time-critical space applications in a multi-core execution environment such as the New Generation Multi-Core Processor (NGMP); and 2) 'Multicore OS Benchmark', with the objective of evaluating the time-predictability behavior of multicore processor mentioned above and doing research on task scheduling aspects for multicores.

## » 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 2012, BSC-CNS collaborated with over 100 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 international public bodies, and the analysis of impacts on air quality for power generation and other industries;

- ▶ **Meteorological Service of Catalonia (SMC):** to generate regional climate scenarios at high resolution for Catalonia during the 21<sup>st</sup> century. 
- ▶ **Environment and Water Agency of Andalucía:** 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 km<sup>2</sup> and 1 hour. 
- ▶ **International Research Institute for Climate and Society:** to enable cooperative efforts between the IRI and BSC-CNS in areas connecting climate, atmospheric aerosols and health. 
- ▶ **National Oceanic and Atmospheric Administration - National Centers for Environmental Predictions and Environmental Modeling Center:** to develop a new chemical weather prediction system and chemical transport model intended to be a powerful tool for research and to provide experimental efficient global and regional chemical weather forecast. 
- ▶ **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 for 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 France, Germany, Italy and Spain, to provide outstanding computing services to enable world-class research. Through PRACE, European scientists and technologists are provided with world-class supercomputers with capabilities comparable to those available in the USA and Japan. These leadership class systems will help Europe remain internationally competitive. During 2012, four new Members have joined PRACE: Denmark, Israel, Slovenia and Belgium, demonstrating the high-level of interest in HPC and reinforcing PRACE as a major tool for research and industry in Europe.



### » BSC-CNS and PRACE

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 form, 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.



BSC-CNS continued to play a leading role during 2012, selected as one of six PRACE Advanced Training Centres (PATC), coordinating training and education activities enabling researchers to utilise the PRACE computational infrastructure. The long-term vision is that PATCs will be the key drivers of European HPC education. BSC-CNS was evaluated by participants as the best of the six PATCs in 2012.

The PRACE 3<sup>rd</sup> implementation phase (PRACE-3IP) began in 2012, with a budget of €26.6 M. BSC-CNS participates in all aspects and leads the work package on policies and procedures for legal and strategic support.

Within the framework of the PRACE Implementation Phases, BSC-CNS deployed a 16-node cluster of hybrid ARM + CUDA GPU nodes to serve as a software development vehicle, and prepare for the deployment of the first large-scale cluster using ARM processors to drive a high-end NVIDIA Tesla accelerator in 2013. BSC-CNS also led and coordinated activities in four key research areas: auto-tuned and automatic techniques to be applied in parallel programming models, scalable numerical algorithms, performance tools, and file systems. BSC-CNS also contributed significantly to work in engineering and material sciences, with outstanding improvements for Alya and SIESTA codes in a prototype solver, which was successfully tested on systems with tens of thousands of atoms, making new classes of physical problems accessible to first principle calculations.

### » Spanish participation in PRACE

- ▶ Extreme Star-Formation Modelling: From the Galactic Fountain to Single Stars in One Run, Prof. Paolo Padoan (ICREA-ICC), 16 million hours on SuperMUC
- ▶ Ab Initio Modelling of Solar Active Regions, Prof. Aake Nordlund, 45 million hours on JUGENE, with participation of Dr. Damian Fabbian and Dr. Fernando Moreno-Insertis (IAC)
- ▶ Numerical simulation of air flow in the human large airways, Dr. Guillaume Houzeaux (BSC), 20 million hours on FERMI
- ▶ First Lattice QCD study of B-physics with four flavours of dynamical quarks, Prof. Silvano Simula, 30 million hours in FERMI, with participation of Dr. Vicent Gimenez Gomez and Dr. Nuria Carrasco Vela (UV)
- ▶ The domain interplay in protein kinases: free energy calculations on the allosteric effect of the SH2 domain on kinase activation, Dr. Francesco L. Gervasio (CNIO), 25 million hours on SuperMUC
- ▶ HiResClim: High Resolution Climate Modelling, Dr. Colin Jones, 38 million hours in MareNostrum, with participation of Dr. Muhammad Asif, Dr. Domingo Manubens and Dr. Francisco Doblas-Reyes (IC3)
- ▶ Data analyses of the CURIE High-redshift simulations, Prof. Gustavo Yepes (UAM), 2.5 million hours on CURIE
- ▶ Modelling gravitational wave signals from black hole binaries, Prof. Sascha Husa (UIB), 37 million hours on SuperMUC
- ▶ LocalUniverse - Our Neighbourhood in the Universe: From the First Stars, Dr. Ilian Iliev, 26 million hours on SuperMUC, with participation of Prof. Gustavo Yepes, Dr. Alexander Knebe and Dr. Daniel Severino (UAM)
- ▶ Mocking the Universe: Large Volume Cosmological Simulations for Galaxy Surveys, Prof. Gustavo Yepes (UAM), 22 million hours on SuperMUC
- ▶ Linear-scaling ab initio study of surface defects in metal oxide and carbon nanostructures, Prof. Rubén Pérez (UAM), 16.25 million hours on CURIE
- ▶ MHILQCD - Multi-hadron interactions in Lattice QCD, Dr. Assumpta Parreño (UB), 27.1 million hours on MareNostrum
- ▶ MetaHMGB1 - Binding of the HMGB1 protein to platinated DNA: a metadynamics study, Prof. Paolo Carloni, 2.7 million hours on CURIE, with participation of Dr. Giulia Rossetti (BSC)
- ▶ The Folding and Functional Binding Landscape of a Protein Molten-Globule, Prof. Modesto Orozco (IRB), 33.8 million hours on MareNostrum

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 12.965m<sup>2</sup> 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

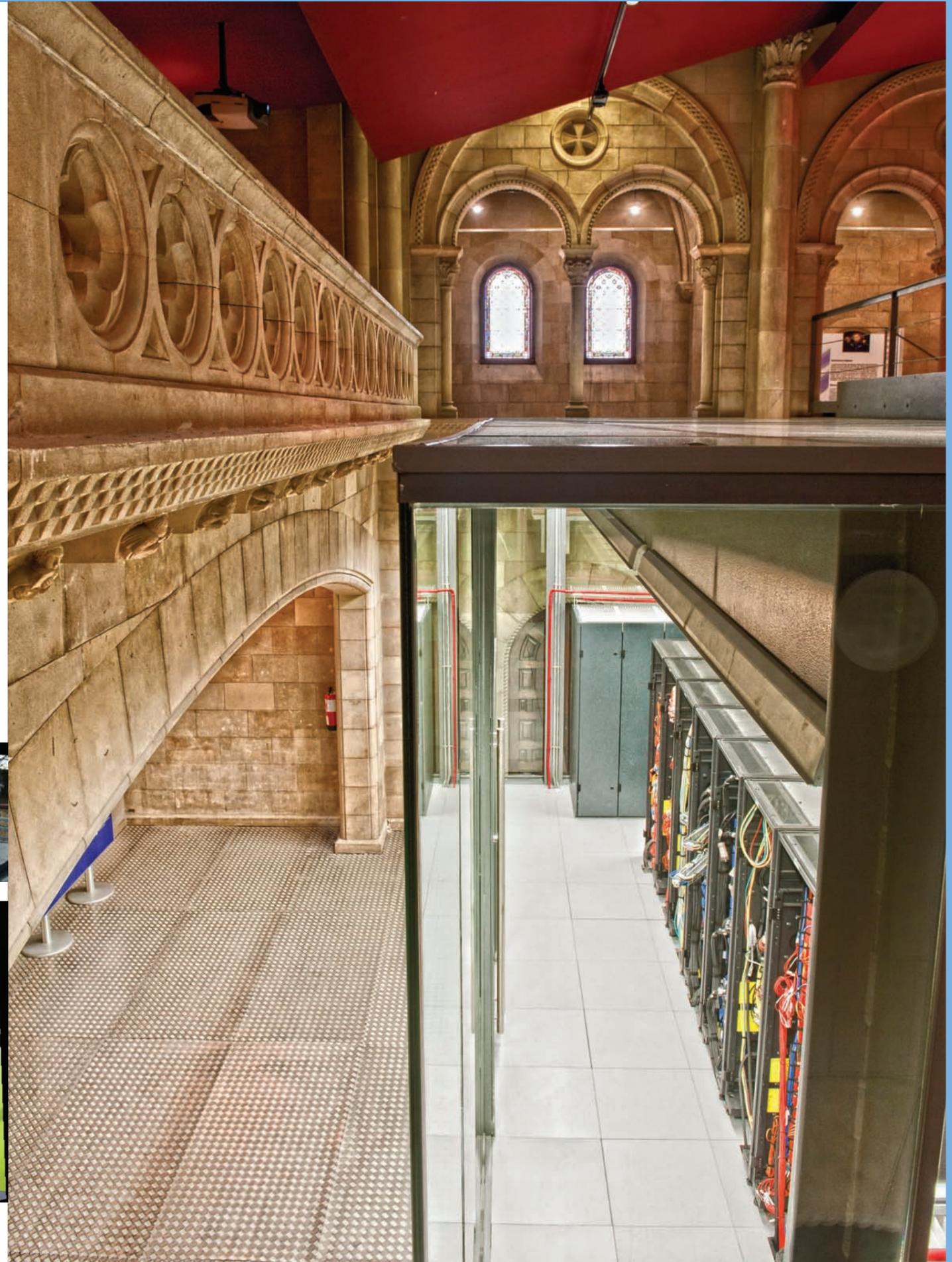
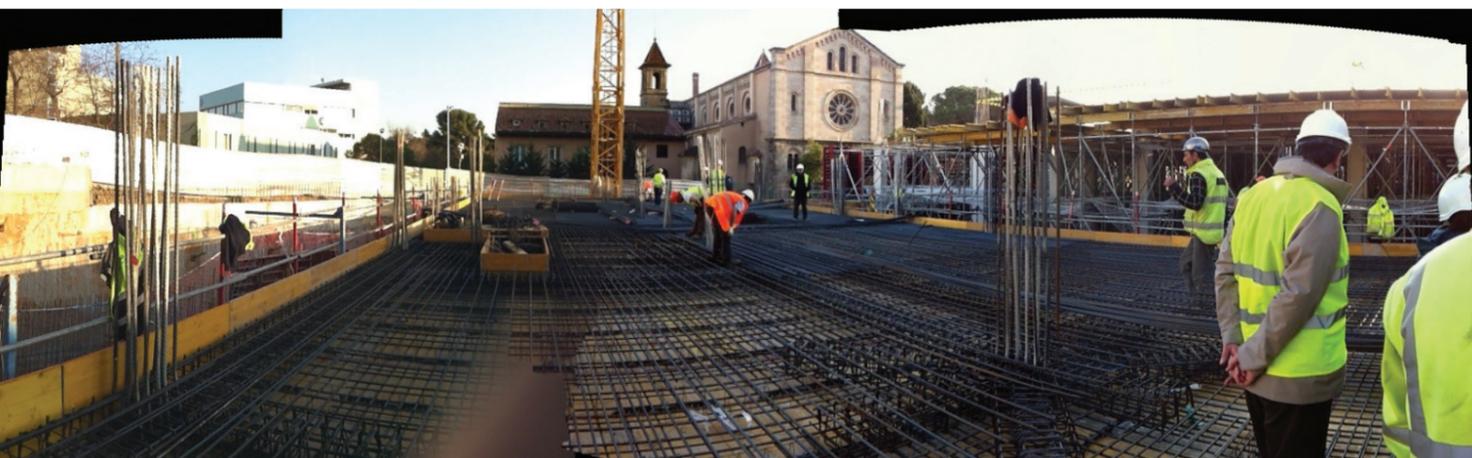


Sectional Plan of the New BSC-CNS Building Showing Functional Areas

The Phase I construction of the new building, awarded to the construction company Ferrovial, was completed in early February 2012. As planned, all excavations, retaining walls and floors up to ground level were completed. This section of the building includes the three subterranean floors that will house the future supercomputer and parking facilities.

On 22nd November 2012, BSC-CNS published the tender for Phase 2 of the building construction, with a maximum cost of €1.916.226. The tender closed on 28<sup>th</sup> December 2012, with construction planned to begin in the first half of 2013.

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 11 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 Exascale EU projects Mont-Blanc and DEEP and the recently awarded ERC grant RoMoL and the Severo Ochoa national project. 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 to invest during 2012 in collaborative systems design R&D projects.

### » Organisational Structure

During 2012, some 142 staff and students, and a further 41 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 focused on improving productivity when programming and optimising parallel applications on large scale parallel systems (Programming Models, including accelerators for HPC, 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).

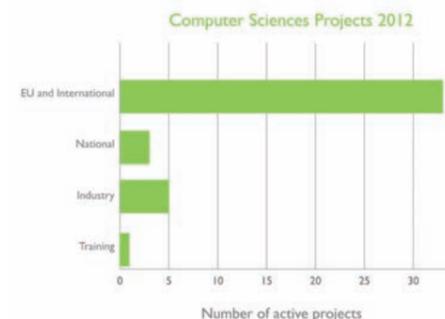
- ▶ The Second Implementation Phase in the PRACE EU FP7 project;
- ▶ 2 networks of excellence: HiPEAC-3 and RISC;
- ▶ The European Technology Platform for HPC (ETP4HPC), contributing to the draft of the European Strategic Research Agenda towards Exascale computing;
- ▶ The SCALUS Marie Curie Initial Training network and
- ▶ The EU COST IC804 action "Energy efficiency in large scale distributed systems";

#### -Collaborations with:

- ▶ Intel Corporation with a multi-year agreement Intel-BSC Exascale Lab, on topics related to programming models, performance prediction tools and algorithms;
- ▶ NVIDIA through the CUDA Center Of Excellence (CCoE), in association with the Universitat Politècnica de Catalunya (UPC-BarcelonaTECH); the centre was one of the 4 finalists in the 2012 CCoE awards;
- ▶ Microsoft Research through the BSC-Microsoft Research Centre agreement, on topics related to low-power architectures and architectural support for programming languages;
- ▶ IBM Research through the following Joint Study Agreements: "ASF (Active Storage Fabric)", "Power management", "Exploitation of the low-power/high-performance characteristics of POWER7 architectures" and "PGAS programming models";
- ▶ Xilinx Ireland to research on OmpSs support for FPGA accelerators;
- ▶ The European Space Agency (ESA), with the "Multicore OS benchmark" and "Architectural solutions for the timing predictability of next-generation multi-core processors" project;
- ▶ The G8-ECS (Enabling Climate Simulations at Extreme Scale) international collaboration initiative and;
- ▶ ORNL (USA) on the Extreme-scale Simulator (xSim) toolkit.

#### -Three national projects:

- ▶ The BSC-CNS Severo Ochoa program, contributing to the design of the hardware and software stacks for future Exascales and BigData applications;
- ▶ The Spanish Consolider program "Supercomputing and eScience", coordinating the Basic Research in Supercomputing workpackage;
- ▶ The Plan Avanza2 NUBA project.



### » Scientific Output

For additional information, please see the *Detailed Report of Research Activities 2012 for the Computer Sciences Department*, available in the online version of this report.

**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.

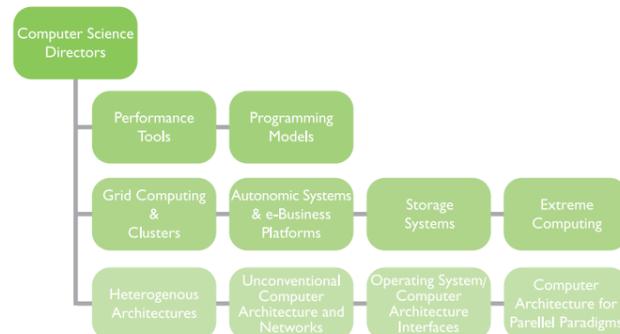
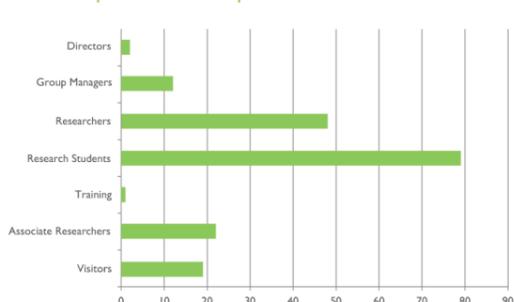
The research results of the Department were published in the proceedings of high quality conferences in the area, including International Conference on Parallel Architectures and Compilation Techniques (PACT), Architectural Support for Programming Languages and Operating Systems (ASPLOS), International Conference on Parallel Processing (ICPP), International Conference on High Performance Computing, Networking, Storage and Analysis (Supercomputing (SC)), International Symposium on Microarchitecture (MICRO), International Parallel & Distributed Processing Symposium (IPDPS), the Design, Automation, and Test in Europe (DATE) conference, International Conference on Computing Frontiers (CF), IEEE International Conference on High Performance Computing (HiPC), International Symposium on Workload Characterisation (IISWC), Great Lakes Symposium on VLSI, International Conference on Grid Computing (GRID) and International Symposium on Cluster, Cloud and Grid Computing (CCGrid).

In addition, other more consolidated research results have been published in prestigious journals in the area, including IEEE Transactions on Computers, IEEE Transactions on Parallel and Distributed Systems, ACM Transactions on Embedded Computing Systems, ACM Transactions on Architecture and Code Optimization, Concurrency and Computation: Practice and Experience and Bioinformatics.

#### Communication & Dissemination 2012

Publishing	
Journal Articles	30
Book Chapters	8
Conference Presentations	
International	52
National	1
Workshops	
Workshops	10
Education	
Thesis	9

Computer Science Department Staff & Collaborators 2012



### » Key Projects and Networks

During 2012, the Computer Sciences Department participated in:

#### -The following EU projects:

- ▶ 21 FP7 projects: AXLE, COMPOSE, DEEP, EnCORE, HOPSA-EU, IOlanes, IS-ENES, LIGHTNESS, Mont-Blanc, EUBrazil OpenBio, OPTIMIS, ParaDIME, parMERASA, PROARTIS, ScalaLife, SIENA, TERAFLUX, TEXT, TransPLANT, VENUS-C and ARTEMIS VeTeSS;



**Heterogeneous Architectures** Led by Álex Ramírez, this Group, in close interaction with the Programming Models Group, aims to design and evaluate the next generation of HPC systems capable of achieving the 50 GFLOPS/Watt required by future Exaflop supercomputers. The Group believes that embedded components, coming from the embedded and mobile device markets, will replace current HPC components coming from the PC and server markets, due to their larger unit count, lower unit price, rapid evolution, and higher energy efficiency. To that end, during 2012 the Group developed a series of prototypes to tackle system integration challenges and anticipate the needs of the runtime system for future architectures so that software can be ready when research trends become products.

**Computer Architecture for Parallel Paradigms**

Led by Adrián Cristal and Osman Unsal, this Group's main research areas cover architectural support for novel programming models and execution environments for future multicore architectures. The Group represents the core of the BSC-Microsoft Research Centre ([www.bscmsrc.eu](http://www.bscmsrc.eu)) which focuses its research on lowering the programmability wall raised by multicore architectures: research areas include low-power vector processors, transactional memory, programming language runtimes and synchronisation. During 2012, the Group started new research activities in reliability, non-volatile memories and hardware support for Big Data, and started two new FP7 research projects.



**Operating System / Computer Architecture Interface**

Led by Francisco J. Cazorla, the CAOS Group focuses its activities on hard real-time and high-performance systems. In the area of hard real-time systems the group worked on the PROARTIS and parMERSA EU projects and started working on the VeTeSS ARTEMIS project. The collaboration with the European Space Agency was also extended one more year. In the area of high-performance systems, the group collaborated with IBM on a bilateral research project. Other areas in which the CAOS group was involved include CPU accounting, energy accounting and hybrid systems for high-performance and ultra-low power operation.



**Unconventional Computer Architecture and Networks**

Led by Mario Nemirovsky, the Group is conducting research on massive multithreaded architectures focused on big data, latency sensitive and network processing architectures (e.g. Grid, Cloud, and Data Centres). Working with the massive amounts of data created today is the next major computational challenge. As the Internet of Things (IoT) becomes more pervasive, the number of sensors and actuators will increase and the need for latency sensitive applications will explode in the near future. Additionally, networks and their applications are fundamental parts of Internet from its core to its edge. Network and its applications play a critical role in today's data centres and high performance systems. Finally, as new materials became available in special grapheme, new architectures driven by the use of these materials are being studied. During 2012, the Group concentrated on studying these systems and defining new architectures to address these challenges.



**Programming Models**

Led by Xavier Martorell, the Group explores new programming models and their efficient implementation for current and future architectures. Research platforms range from manycore SMPs with support for accelerators (GPUs, MIC, FPGAs), to clusters of SMPs with accelerators, to exascale systems. The research is supported by two powerful tools: the Mercurium compiler, used to prototype new programming model approaches, and Nanos++, the runtime library supporting the variety of hardware resources under consideration. In 2012, the Group improved the support for GPU, the MIC, FPGA and clusters in OmpSs, continued the work on power modelling for multicore architectures and code transformations for processors with local memories. The public release of Tareador, a new tool to predict the performance of task decompositions, was developed and deployed to support teaching and training activities. During 2012, the Group continued the participation in the ongoing EU projects (EnCORE, Mont-Blanc, DEEP, TERAFLUX and TEXT), the HiPEAC-3 network of excellence and contracts with Intel and IBM. The Group also consolidated its collaboration with Xilinx Research Labs in Dublin, doing research on OmpSs for FPGA.



**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 2012, the activities of the Group focused on developing new functionalities on the infrastructures, progressing on the research lines targeting performance analytics, participation in projects and contracts and dissemination through publications and training.



**Grid Computing & Clusters**

Led by Rosa M. Badia, this Group is researching 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. In these directions, the efforts of the Group focused on further development of the COMPSs/ServiceSs programming model in order to enable the inclusion of web-services as elements of the applications, extensions to enable the deployment of the applications themselves as web-services, the development of a graphical IDE to help application developers, and the interoperability of the runtime back-end with different cloud middlewares.



**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 of this group is to research autonomic and intelligent resource management for today's business applications. The objective is to create new components at middleware level that provides holistic solutions for some of the new IT challenges in the industry: Cloud computing, Big Data, business analytics, high-performance computing or sustainable computing.



**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), new file-system approaches to increase their performance and/or usability (better metadata management), and new approaches to store and manage Big Data. In 2012, the Group focussed on increasing the performance and adaptability of parallel file systems, adding security functions to the Group's virtualised file system, and on developing a new storage abstraction based on self-contained objects.



**Extreme Computing** Led by Vassil Alexandrov, this Group 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. The Group continued with the leadership and work in the EU Brazil

OpenBio project and the leadership of the technical program of RISC (A Network for Supporting the Coordination of Supercomputing Research Between Europe and Latin America).



José María Baldasano, Director of the Earth Sciences Department

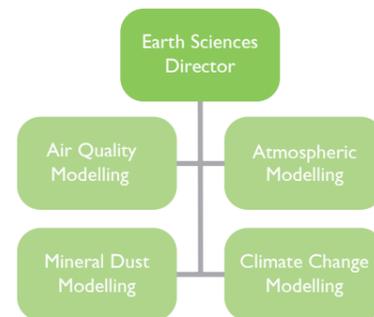
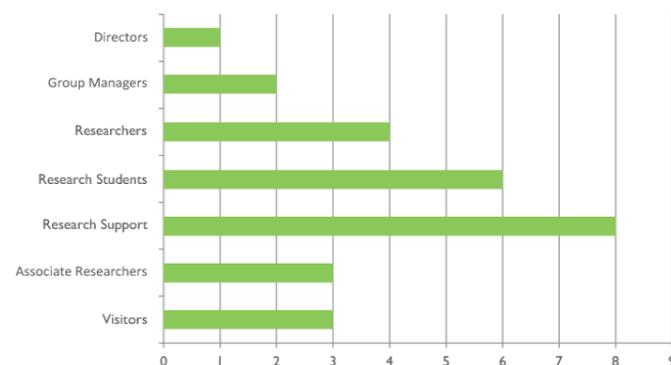
The Earth Sciences Department of BSC-CNS has the aim of modelling and understanding the behaviour of the Earth System, focusing its research activities on atmospheric processes and climate change modelling.

» 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 (<http://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 (<http://www.bsc.es/projects/earthscience/BSC-DREAM/>). The Department, also in collaboration with the World Meteorological Organization (WMO) and the Spanish Meteorological Agency (AEMET), have created the Regional Centre for Sand and Dust Storm Warning System (SDS-WAS) covering Europe, northern Africa and the Middle-East (<http://sds-was.aemet.es/>). 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.

Earth Sciences Department Staff & Collaborators 2012



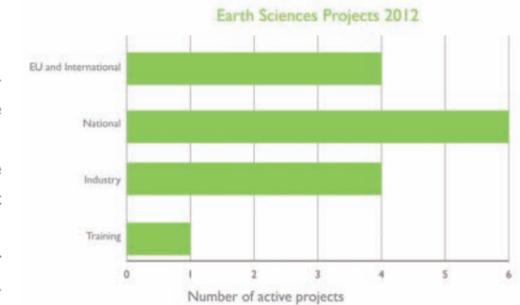
» Organisational Structure

The Department is structured in four Groups that represent the main topics of Earth Sciences research: air quality modelling, mineral dust modelling, atmospheric 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 2012 some 27 staff, collaborators and visitors worked with the Department.



» Key Projects

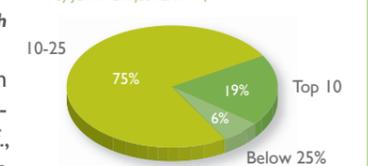
- ▶ Initiated the APPRAISAL project. Air Pollution Policies for Assessment of Integrated Strategies At regional and Local scales is an FP7-Project funded by the European Commission under the Environment programme;
- ▶ Continued the FIELD\_AC project. Fluxes, Interactions and Environment at the Land-Ocean Boundary. Downscaling, Assimilation and Coupling is an FP7-Project funded by the European Commission under the Space Programme;
- ▶ Concluded the IS-ENES project InfraStructure for the European Network for the Earth System Modelling is an FP7-Project, funded by the European Commission under the Capacities Programme, Integrating Activities;
- ▶ Continued the participation in European consortium for the development of EC-Earth: European Earth System model based on ECMWF modelling systems. Currently, the EC-Earth consortium consists of 22 academic institutions and meteorological services from 10 countries in Europe (FP7-Project, funded by the European Commission);
- ▶ 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, funded by the European Union;
- ▶ Led the Earth Science work package in the SyeC Consolider Program coordinated by the BSC-CNS and funding by the Spanish Science and Education Ministry (MEC);
- ▶ Concluded work on the CICYT project: Coupling of a Fully Online Chemical Mechanism within the Atmospheric Global-Regional UMO Model funded by MINECO; in cooperation with NCEP, NOAA (USA);
- ▶ Continued the CICYT project: Coupling of a fully online multi-component aerosol module within the atmospheric global-regional NMMB model funded by MINECO;
- ▶ Participated in the CICYT project: Currents, waves and wind: Improving Risk Assessment through Assimilation in Numerical models of the Coastal Environment (COVARIANCE) funded by MINECO, in collaboration with LIM/UPC, CSIC and Servei Meteorològic de Catalunya;
- ▶ Continued the extension of the CALIOPE project to the Autonomous Community of Andalusia, funded by the Junta de Andalucía;
- ▶ Continued the extension of the CALIOPE project to the Autonomous Community of Canarias, funded by the Canarias Government;
- ▶ Supported by the "Servei Meteorològic de Catalunya" of the Territory and Sustainability Department of Catalonia Government (Spain), generation of climate projections for the 21<sup>st</sup> century in Catalonia;
- ▶ Participated in the COST Action ES1004. European framework for online integrated air quality and meteorology modelling (EuMetChem) - is focusing on a new generation of online integrated Atmospheric Chemical Transport (ACT) and Meteorology (Numerical Weather Prediction and Climate) 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). The main objective of the Action is to enhance the methodologies of forecasting wind and solar power production in the time domain of a few minutes up to several days ahead;
- ▶ Participated in the European Network for Earth System Modelling (ENES);
- ▶ Participated in the European Aerosol Research Lidar Network: EARLINET. The dataset generated is used 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 is to enhance the ability of countries to deliver timely and quality sand and dust storm forecasts, observations, information and knowledge is supported by the WMO;
- ▶ Collaborated with The National Centres for Environmental Prediction (NOAA/NCEP/EMC) within the framework of a Memorandum of Understanding (MoU). Under this MoU is intended that both institutions will keep on collaboration for NMMB/BSC-CTM development, international joint projects proposal and researcher mobility's;
- ▶ Collaborated with the The Trustees of Columbia University in the City of New York for the International Research Institute for Climate and Society (IRI) within the framework of a Memorandum of Understanding (MoU). Under this MoU is intended that both institutions will keep on collaboration for areas connecting climate, atmospheric aerosols and health, as well as sharing of dust model data;
- ▶ The Earth Science group of BSC-CNS was officially recognised by the Government of Catalonia as a research group;
- ▶ Actively contributed as a member of the Spanish network RETEMCA (Red Temática de Modelización de la Contaminación Atmosférica).



» Scientific Output

For additional information, please see the *Detailed Report of Research Activities 2012 for the Earth Sciences Department*, available in the online version of this report. The diffusion of research results obtained by the Earth Sciences Department has been significant. These results have been presented in numerous ISI-JCR journals, European and international congresses and symposia organised during 2012, such as the Annual CMAS Conf., Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes; American

Distribution of 2012 Published Articles by JCR-IF rank journal in subject area



Communication & Dissemination 2012	
Publishing	
Journal Articles	12
Book Chapters	1
Conference Presentations	
International	36
National	6
Workshops	
Workshops	8
Education	
Thesis	3

Union Geophysical, European Geosciences Union General Assembly Meeting and other congresses organised by the European Meteorology Society (EMS), GLOREAM Conf., International Workshop on Air Quality Forecasting and Research. The number of ISI-JCR publications in 2012 increased compared to 2011 (from 8 in 2011 to 12 in 2012). The JCR publications in 2012 had an average quality of 3,3 (Average JCR Science Edition Impact Factor).

## » Research Groups

**Air Quality** 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 validation 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 2012 the activities of the Group were mainly related to maintaining and improving the daily 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/HERMESEMP/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 modelling system is made possible by its implementation on the MareNostrum supercomputer hosted by BSC-CNS. During 2012 some enhancements of operational CALIOPE forecast system were implemented, especially for air quality data management (forecast model and measurements), by establishing a database to centralise postprocessing and forecast evaluation. Extension of the application of the Kalman filter to Europe and Barcelona domains was done. Several improvements in the maps generation scripts were implemented for: weather, emissions and air quality. Also the emission inventory for Europe was updated. Technology transfer activities were also undertaken with several companies and institutions: Government of Canarias, AEMET, Junta de Andalucía, etc.

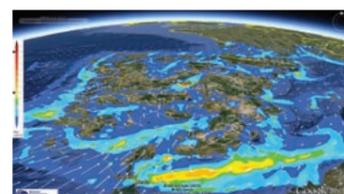


Figure 1 - Air quality modelling system (WRF-ARW/HERMES-EMEP/CMAQ/BSC-DREAM8b) NO2 forecast results

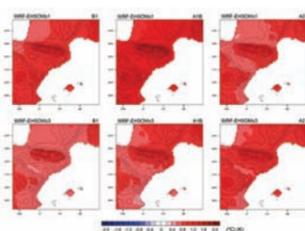


Figure 2 - Change in Annual Mean Temperature in the 2001-2050 period in respect to the 1971-2000 period for the North Western Mediterranean Basin as derived from the regionalisation exercise performed with WRF-ARW forced by ECHAM5/MPI-OM general circulation model according to three different emission scenarios: BI, A1B and A2 from the SRES2000 of the IPCC

**Climate Modelling** In 2012 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. In this framework, three different simulations were performed with EC-EARTHv2.3: an historical run, from year 1850 to 2005, and two future projections scenarios below different global forcings: the Representative Concentration Pathways 4.5 and 8.5, covering from 2000 to 2100. These simulations will take part in the Coupled Model Intercomparison Project Phase 5 (CMIP5) and therefore will be considered in the future IPCC-AR5 report. During 2012 the Group activities were mainly devoted to: (1) extract the necessary variables from the model outputs, according to the CMIP5 priorities, (2) transfer the data to the CMIP5 servers for their public availability, (3) preliminary assessment of the temperature and mean sea level pressure projected by the historical run and RCP simulations, by means of intercomparison of results with other groups projections and comparing the historical period with global observational databases.

In parallel, the group continued its activities of dynamic downscaling over the Western Mediterranean region, in collaboration with the Servei Meteorològic de Catalunya. Within this project present time climate conditions were obtained by means of the Regional Climate Model WRF-ARW, forced by the ERA40 reanalysis, for the 1971-2000 period. Future projections covered the 2001-2050 period and the A2, A1B and B1 emissions scenarios defined in the SRES report of the IPCC. 2012 activities were mainly devoted to the analysis and spread of results. Mean trends and variability for temperature and precipitation were analysed for the region. Present time conditions were extensively assessed against observations and an intercomparison with other climate downscaling projects was performed. Future trends analysis allowed deriving the expected changes of temperature and precipitation with a high degree of detail for the Catalonia region. This information was provided to the impacts community for its use in the planning of mitigation and adaptation strategies to climate change. Additionally, temperature and precipitation extremes are being analysed and different climate indexes assessed, both in present time and future projections. The group also continues contributing to 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. In collaboration with the Grid Computing group, the grid technologies have been explored for Earth System Models simulations.

**Atmospheric Modelling** The work done in 2012 continued the development and evaluation of the modelling system NMMB/BSC-Chemical Transport Model (NMMB/BSC-CTM). The new modelling system provides the capabilities to model global to local meteorological and chemistry conditions in a unified environment. Verification efforts of the system at global scale and over a European domain were undertaken. The group, coordinated with the Mineral Dust group, contributed to the ICAP (International Cooperative on Aerosol Prediction) model intercomparison initiative with experimental global forecasts of aerosols. A new multicomponent global aerosol module is under development within NMMB/BSC-CTM. In 2012, the sea-salt implementation was verified at both global and regional scales (Figure 3). Complementing all these efforts, the group, in collaboration with the University of California Irvine, started the coupling of a secondary aerosol module in NMMB/BSC-CTM. In the framework of the Severo-Ochoa excellence project, the group started collaboration works with the Computer Sciences Department to improve and extend the computing performance of the system NMMB/BSC-CTM, to be prepared for future exascale architectures. Within the FIELD-AC project of the FP7 framework program, the group continued the work on sensitivity studies of mesoscale meteorological models on wave models. 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. Finally, promising results were obtained in the exploration of new numerical techniques to better exploit massively parallel architectures for meteorological applications. A dynamical core based on the Alya system, developed at the Computer Applications in Science & Engineering Department, was extensively tested for dry and moist atmosphere ideal test cases.

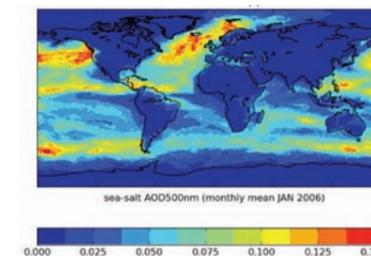


Figure 3 - January monthly mean Aerosol Optical Depth of sea-salt aerosol computed with NMMB/BSC-CTM model.

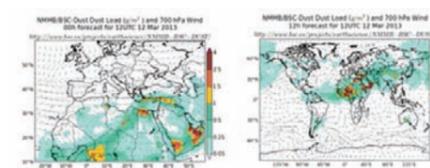


Figure 4 - Dust forecast of the NMMB/BSC-Dust model for 12th March 2013 at 12UTC for the regional (left panel) and global (right panel) domains. Extracted from: [www.bsc.es/projects/earthscience/NMMB-BSC-DUST/](http://www.bsc.es/projects/earthscience/NMMB-BSC-DUST/)

**Mineral Dust Modelling** 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 BSC-DREAM8b version 2. The model is participating in the Sand and Dust Storm Warning and Assessment and Advisory System (SDS WAS) Regional Centre for Northern Africa, Middle East and Europe. 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 2012 the group continued with the development of the NMMB-BSC/Dust model. This model is on-line coupled to the new generation unified atmospheric model NMMb of the National Centres for Environmental Prediction (NCEP). NMMB-BSC/Dust includes a physically-based dust emission scheme taking into account the effects of saltation and sandblasting, soil moisture and viscous diffusion close to the ground. 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 in the framework of the NMMB/BSC-CTM project. In this period, the NMMB/BSC-Dust model is in pre-operational status and provides operational dust forecast over North Africa- Middle East-Europe and global regions (Figure 4). The dust forecasts are daily published and evaluated (against ground-based and satellite observations) in the new website of the model (<http://www.bsc.es/projects/earthscience/NMMB-BSC-DUST/>). Furthermore, the NMMB/BSC-Dust model is participating in the International Cooperative on Aerosol Prediction (ICAP) model intercomparison initiative (<http://www.nrlmry.navy.mil/aerosol/icap.1087.php>) as well as in SDS WAS Regional Centre for Northern Africa, Middle East and Europe.

**SDS-WAS WMO Regional center** Activities in the framework of World Meteorological Organization (WMO) Sand and Dust Storm Warning and Assessment and Advisory System (SDS-WAS) Regional Centre for Northern Africa, Middle East and Europe (NA-ME-E), hosted by AEMET and BSC-CNS, were also undertaken. The web portal of the NA-ME-E Regional Centre (<http://sds-was.aemet.es>, Figure 5) provides National Meteorological and Hydrological Services with the necessary information to issue operational predictions and warning advisories related to the dust content in the atmosphere. In this period, new operational dust forecast systems (DREAM8-NMME-MACC, CHIMERE, NMMB/BSC-Dust, MetUM, GEOS-5 and NGAC) and observational datasets were included in the activities of NA-ME-E Regional Centre. In 2012, the Regional Centre organized and coordinated the "II Lectures on Atmospheric Mineral Dust" (<http://sds-was.aemet.es/events/ii-lectures-on-atmospheric-mineral-dust>), which was held in Barcelona in November. The centre participated in two training courses: Course on the use of satellite products for agrometeorological applications (held at the Agriculture, Hydrology, Meteorology (AGRHYMET) Regional Centre of Niamey, Niger, 19-23 November 2012) / The "Workshop on Meteorology, Sand and Dust Storm (SDS), Combating Desertification and Erosion" (held in Ankara, Turkey, 26-28 November 2012).



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 2012 include publications in leading journals with interdisciplinary impact such as Nature, Nature Genetics, Nature Nanotechnology, Accounts in Chemical Research, J.Am.Chem.Soc. or PNAS. Another highlight was the organisation of BioNMR2012 meeting (co-sponsored by RES, ELIXIR and the Spanish government and the Catalan government, the EMBO Workshop in Computational biology and the DESMOND European hands-on workshop. Also of note was the ICREA academy award received by Prof. Orozco, and the major opportunities that emerge from participation in European flagship projects, including the Human Brain Project, the International Cancer Genome Consortium, the European Exascale Software Initiative, the Human Epigenome (BluePrint), the Plant Genomics (TransPlant) and many others.

### » Joint IRB-BSC Program on Computational Biology

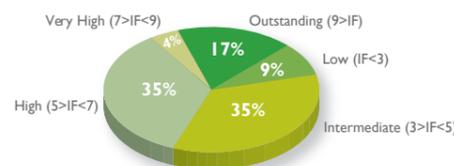


INSTITUTE FOR RESEARCH IN BIOMEDICINE

The Computational Biology Program was created as a joint venture between BSC-CNS and the Institute for Research in Biomedicine (IRB Barcelona) with the mission to address the computational challenges in molecular biology. The Program, coordinated by Modesto Orozco, includes researchers from the Structural and Computational Biology and the Chemistry and Molecular Pharmacology Programmes at IRB Barcelona, and from the Life Science Department of BSC-CNS. 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 BSC-CNS. In return, BSC-CNS scientists will also have permanent access to services and facilities at the IRB Barcelona. 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.

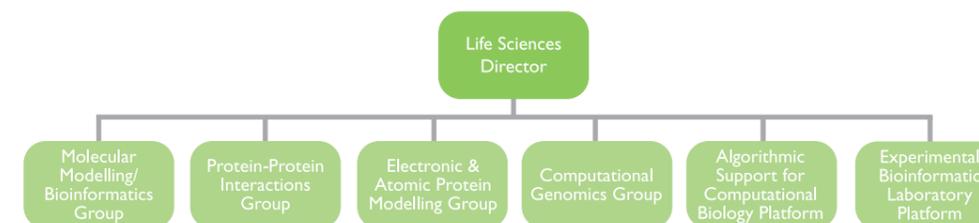
The Program, which in 2012 involved some 110 people, pursues excellence in research in bioinformatics and computational biology. Its research lines range from atomistic studies on bio-macromolecules to the analysis of high-order cell regulatory mechanisms, sequence analysis, gene regulation and expression, systems biology, network medicine and drug design. The Program published 60 journal papers during the year, achieving an institutional H-index of 72. Also of note, two principal investigators of the Program are currently holding Advanced ERC grants.

ISI Impact Factor of Articles Published in 2012



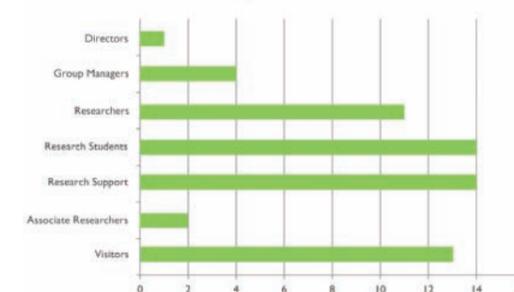
### » Organisational Structure

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



Structure of the Life Sciences Department of the BSC-CNS

Life Sciences Department Staff & Collaborators 2012



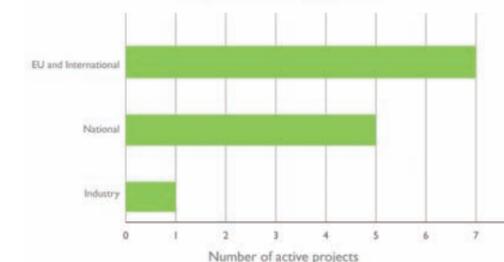
BSC-CNS research groups Electronic and Atomic Protein Modelling (EAPM), Protein Interactions and Docking (PID) and Computational Genomics (CG), the Molecular Modelling and Bioinformatics (MMB) and the Experimental Bioinformatics Laboratory (EBL), jointly run by BSC-CNS and IRB, the Computational Node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

### » EU & National Projects

Key activities during 2012 included participation in the following key BSC-CNS projects:

- ▶ PELE - a la carte drug design tools. ERC Advanced Grant. The project aims to provide, to the large community of scientists working in molecular target therapies, a fast and accurate tool capable of obtaining an atomic detailed mechanism of the protein-ligand induced fit, of its recognition process and of the ligand migration. In 2012 the project advanced towards the web-server simulation of PELE.
- ▶ Blueprint - A BLUEPRINT of haematopoietic epigenomes. Funded by FP7. This is a large-scale research project that aims to apply highly sophisticated functional genomics analysis on a clearly defined set of primarily human samples from healthy and diseased individuals and to provide at least 100 reference epigenomes to the scientific community.
- ▶ ICGC - International Cancer Genome Consortium. The Life Sciences department participates in the Spanish consortium for chronic lymphocytic leukemia, supporting the Genome and Exome analysis in 2012.
- ▶ TransPLANT - Trans-national Infrastructure for Plant Genomic Science. Funded by FP7. The project address these challenges of large and complex genomes of plants to develop a trans-national infrastructure for plant genomic science. During 2012 the work was focused on the development of a more efficient analysis framework.

Life Sciences Projects 2012



- ▶ ProCoGen - Promoting a functional and comparative understanding of the conifer genome- implementing applied aspects for more productive and adapted forests. Funded by FP7. The project studies how advances in next-generation DNA sequencing technologies could have an enormous impact on the rate of progress and achievements made by tree breeding programmes.
- ▶ MEDICAHEAD - a platform to identify new medical treatments. VALOR project, Catalan Government. The project completed the first prototype of the application in 2012.
- ▶ Biochemical Modelling. Funded by CICYT, Spanish Government.
- ▶ Protein Docking Challenges. Funded by CICYT, Spanish Government.



## » Scientific Output

For additional information, please see the *Detailed Report of the Joint BSC-IRB program 2012*, available in the online version of this report.

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.

Communication & Dissemination 2012	
Publishing	
Journal Articles	38
Conference Presentations	
International	25
National	3
Workshops	
Workshops	3
Education	
Theses Read	1

### Organised Events:

In 2012 the department's dissemination activities included the organisation of the BioNMR conference that attracted more than 100 international scientists. The conference, with 15 top keynote speakers, was mainly funded by the BioNMR European consortium and co-sponsored by RES, ELIXIR and by the Spanish and Catalan governments. In October the department organised the EMBO Workshop in Computational biology. EMBO workshops are regarded as amongst the highest quality events in Europe. This course was designed to explain advanced computational methods for analysis of high-throughput data in molecular biology. Also highly successful was the DESMOND European hands-on workshop co-organised by DE Shaw Labs, ScalaLife and the Joint program.

## » Research Groups



### Molecular Modelling and Bioinformatics (MMB) Group

The Group's long term objective is to understand the behaviour 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 placed on connecting basic interactions with global properties of biological systems.



### Electronic and Atomic Protein Modeling (EAPM) Group

The Electronic and Atomic Protein Modelling Laboratory in the Life Science department at BSC-CNS 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 modelling 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, centred 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, anaemia, 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. BSC-CNS Life Sciences program hosts the Computational Bioinformatics node of INB (INB-GN6). The special purpose of the computational node, with the help of BSC-CNS 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 IRB Barcelona and BSC-CNS. 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 María 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 multi-disciplinary, requiring a deep level of expertise in many fields. In order to successfully develop these applications, the skills of the CASE team

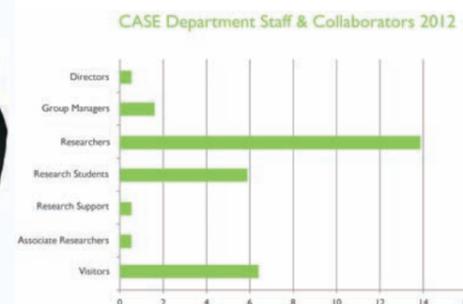
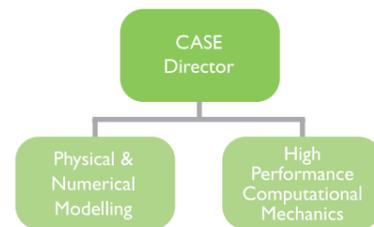
in numerical methods and parallel programming must be complemented by experts in the appropriate areas. The Department therefore develops collaborations with other scientific groups in all areas of science and technology. Examples of institutions with strong research links with CASE include CIEMAT, CSIC, 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 five 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.
- ▶ FAIL3D: Volcanos 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.
- ▶ Pandora: An HPC Agent-Based Modelling framework for social simulation.

» 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.



» Key Projects

In 2012, the CASE Department carried out work under the scope of the following projects:

EU funded projects:

- ▶ PRACE 2IP-3IP: Partnership for Advanced Computing in Europe.
- ▶ ETSF: Generating a software infrastructure for support of the spectroscopy community.
- ▶ W2PLASTICS: Magnetic Sorting and Ultrasound Sensor Technologies for Production of High Purity Secondary Polyolefins from Waste. Turbulent flow in complex geometries; particle tracking and collisions.
- ▶ C2CA: Recycling of Concrete to Cement and Aggregates. The Department models combustion, compressible flows, radiation and solid N-body impact.
- ▶ COPA-GT: A Marie Curie training project for Turbines operation in Aerospace and energy production plants with research in compressible flows, combustion, aeroelasticity and optimisation algorithms.
- ▶ 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. This project aims to create high-performance computing tools useful in the analysis of migration processes.
- ▶ MontBlanc: The Department ports to the MontBlanc Architecture the EUTERPE code.
- ▶ PRACE Access call project. Numerical simulation of air flow in the human large airways. 22M CPU hours on Fermi supercomputer, Italy.

Enterprise funded projects:

- ▶ Respol-BSC reserach center: RTM, elastic forward modelling, full wave-form inversion, controlled source electromagnetic method (in Alya code)
- ▶ Vreactor: simulation of chemical reactions in biodiesels inside batch reactors, coupling with mixing blades, transfer of chemical species through the interfaces of immiscible liquids (in Alya code).
- ▶ Respolver phase I: expert system for simplifying the user interface of multiphysics massively parallel simulations.
- ▶ Iberdrola: Optimisation of wind farms both on-shore and off-shore (in Alya code).
- ▶ Confidential Partner: Race yacht design (in Alya code).

Nationally funded projects:

- ▶ Supercomputación y e-Ciencia (CONSOLIDER): Coordination of the project, whose aim is to develop a set of scientific Grand Challenges for Petaflop supercomputers and design the architecture of those machines. Some of the applications were also developed with the collaboration of CASE researchers.
- ▶ Simulpast. Simulating the past to understand human behaviour (CONSOLIDER): The aim of the project is to develop an innovative and interdisciplinary methodological framework to model and simulate ancient societies and their relationship with environmental transformations.
- ▶ ATMOST (Plan Nacional): This project started in 2009 and aims to model ashes and contaminant dispersion in the atmosphere.
- ▶ MIVAL3D (Generalitat de Catalunya): The objective is to simulate the cardiac mytral valve.
- ▶ S4E (Plan Nacional): Supercomputing for Energy. Three specific topics are considered: hydrocarbon exploration, wind energy and marine energy. These topics were selected for mainly two reasons:

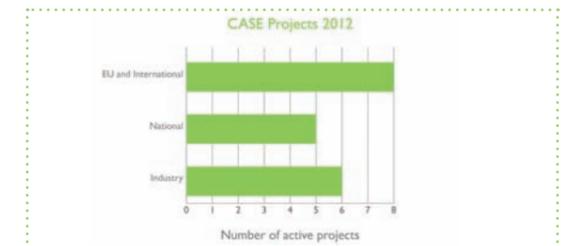
First, they are represented by key industries in Spain. Second, the CASE Department of BSC-CNS gained an extensive research experience in these topics during the last five years.

The CASE department also develops international/national collaboration projects in the area of biomechanics:

- ▶ Airflow in the Human Respiratory System: In collaboration with both the Aeronautics and Bioengineering Departments at Imperial College London (Denis Doorly, Alister Bates and collaborators). A simulation of the complete human respiratory system, including the air surrounding the face, was carried out. This project is being partially supported by HPC-Europa European project.
- ▶ Airflow in large and small airways. Collaboration with the Aeronautics and Bioengineering Departments at Imperial College London and Dr. Shahrouz Aliabadi and his research team including Dr. Bela Soni from Jackson State University.
- ▶ Computational Cardiac Mechanics: Coupled electromechanical simulation of the heart, including the mytral valve. The project objective is 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.
- ▶ Skeletal muscles: with John Georgiadis and Armen Garibans (Univ. of Illinois, USA).

Other collaborations:

- ▶ Solid Mechanics: CASE is collaborating with Antoine Jerusalem (Oxford University) and Guillermo Viguera (IMDEA, Spain) in the development of a HP solid mechanics module, including X-FEM for fracture simulations.
- ▶ Turbulence: Application of turbulence models to high Reynolds number flows: Collaboration with EDF (France), Univ. Manchester (UK), Science & Technology Facilities Council, Daresbury (UK).
- ▶ Participation in "Adaptation of historical spaces to teaching museums via reactive applications with multiplatform, mobile telephony and tactile surface contents", from DIDPATRI research group (University of Barcelona). The aim of this project is the development of new technology designed for the new generation of museums.
- ▶ Collaboration with Jordi Agustí (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)". This project, funded by the "Ministerio de Presidencia", aims to apply new research methodologies to the understanding of the role of aviation during the Spanish Civil War.
- ▶ Euterpe code: Collaboration with Max Planck IPP and CIEMAT to port the EUTERPE code to new hardware platforms.



## » Scientific Output

For additional information, please see the *Detailed Report of Research Activities 2012 for the CASE Department*, available in the online version of this report.

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: 2012 IEEE 4th International Conference on Cloud Computing Technology and Science, AGU Fall Meeting 2012, EGU General Assembly 2012, International Journal for Numerical Methods in Biomedical Engineering, Journal of Volcanology and Geothermal Research, International Journal of Modeling and Optimization, and others.

Communication & Dissemination 2012	
Publishing	
Journal Articles	22
Book Chapters	1
Conference Presentations	
International	16

» **Research Groups** 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.
- ▶ Code performance analysis and optimisation.
- ▶ DES simulation of car aerodynamics
- ▶ RANS turbulence models. Models specially designed for wind farm applications (Iberdrola).
- ▶ A large-strain solid mechanics simulation for anisotropic cardiac tissue.
- ▶ Lagrangian particle tracking. Drag and Saffman forces, Brownian motion.
- ▶ Numerical modelling
- ▶ ALE method for mesh motion.
- ▶ Low-Mach model for C2CA project.
- ▶ Chemical transport through interfaces.
- ▶ Rigid body-fluid coupling.
- ▶ Fluid-structure coupling. Overlapping of MPI communications.
- ▶ Variational multiscale methods for compressible flows.

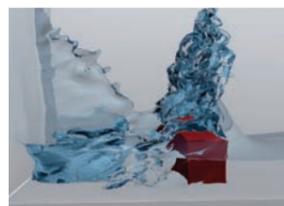
Due to the installation of new large scale supercomputers in Europe during the last years (Curie in France, Jugene in Germany, Fermi in Italy), the Group has been dedicating a lot of resources to upgrade the high performance computational mechanics (HPCM) code developed at the department, Alya. Some of these developments have been carried out in the context of PRACE2IP and PRACE3IP project. Among the developments:

### Pre and post-process

- ▶ Mesh Multiplication. Parallel, uniform and on-the-fly mesh refinement. Generation on the fly of up to 10 billion element meshes. A surface correction technique was also implemented to account for curvature of the original geometry.
- ▶ New postprocess format and HDF5 format. Postprocess strategy in Alya has been redesigned.
- ▶ Paraview plugins to visualize particle paths, based on Hive and Hadoop.
- ▶ Chimera method in HPCM. Application to turbulent flows, free surface flows and solid mechanics.

### Solvers

- ▶ Sparse direct solver.
- ▶ Implementation of the Neumann preconditioner.
- ▶ A parallel version of SIESTA code with better load balancing and sparse iterative eigensolvers.
- ▶ Speedup tests were carried out on the main European supercomputers on up to 22528 CPUs: Lindgren - Cray XE6 - Sweden, Jugene - Blue Gene/P - Germany and Curie - BullX - France.



Dam break: free surface flow

**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 behavioural 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 behaviour.
- ▶ Methodological and theoretical foundations of social simulation.

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.
- ▶ Vehicle dynamics: cars, racing yachts, high speed trains.
- ▶ Simulation of chemical reactions in biodiesels inside batch reactors, coupling with mixing blades, transfer of chemical species
- ▶ through the interfaces of immiscible liquids.
- ▶ **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:** Plasma physics.

Within these fields, in 2012, 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).

**REPSOL-BSC Research Center** 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. Moreover, new algorithmic problems should be investigated for the proper simulation of elastic wave phenomena. The capability of working with elastic waves, furthermore, opens the possibility of a real full waveform inversion procedure, potentially the most accurate tool for inverting the reservoir's properties to date. As a consequence, elastic wave modelling will lead us to retrieve ever more accurate models of the Earth's subsurface. In addition, the group aims to investigate the inversion of electromagnetic waves to obtain images of the subsurface's resistivity, which is directly associated with the different reservoir's fluid contents (water, hydrocarbons). Finally, a joint elastic and electromagnetic inversion could further constrain the properties of the hydrocarbon reservoirs beyond the capabilities of seismic or electromagnetic methods alone. 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 continuous 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 HPC World.

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.

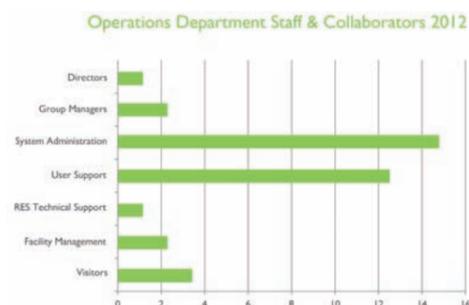
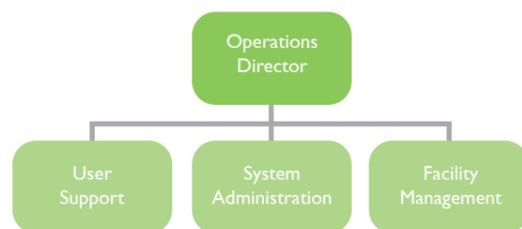
Construction of the new BSC-CNS building advanced significantly in 2012, as did the corresponding engineering for hosting a large supercomputer. With a computer room of 900 square meters and 800 square meters for infrastructures (including air conditioning, water pipes, pumps, etc.) the new facility will be cutting-edge. The new space, along with technology updates in the Chapel, will permit the computing capacities of BSC-CNS to be greatly extended in the future.

### » 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-CNS 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.



### » Key Projects

The Operations Department was involved in the following projects during 2012:

- ▶ 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.

- ▶ 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.
- ▶ iCORDI: The iCORDI project focuses on coordinating a series of cross-infrastructure experiments on global interoperability with a selected group of projects and 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.



### MareNostrum upgrade

During 2012 the Operations department performed the upgrade of MareNostrum II to MareNostrum III; the first part of the year was dedicated to the tender preparation and evaluation, and the planning of all the tasks related to the upgrade.

MareNostrum II, which had been in production since 2006, was powered off in September 2012 and its components were distributed amongst different RES nodes to upgrade their own respective supercomputers. Using MareNostrum II components, a 256-node cluster was also installed at another BSC-CNS data centre to provide computational resources during the upgrade process.

Once the facility installation was completed, the tasks for MareNostrum III hardware and software installation were initiated. This process completed around 2nd January 2013 when the new supercomputer entered production as the new PRACE Tier-0 machine.

The new MareNostrum III supercomputer will provide an increase in computing capability of ten times compared to the old MareNostrum II, with an increase of only 30% in terms of power consumption; these are the main technical characteristics:

- ▶ 3056 Compute nodes with a total of almost 50.000 cores
- ▶ 94 TB of main memory (32 GB per node)
- ▶ Peak Computing performance of 1 PFlop/s
- ▶ Infiniband network FDR-10 full-fat tree providing 40 Gbit/s per each node

**Active Archive** Along with the new MareNostrum III, a new data infrastructure will be installed during the first-months of 2013, which will provide 4.1 Petabytes of storage for scientific data, based on GPFS technology. Apart from providing raw storage, this facility will also host and allocate data services for BSC-CNS researchers, RES users and European projects like EUDAT and PRACE.

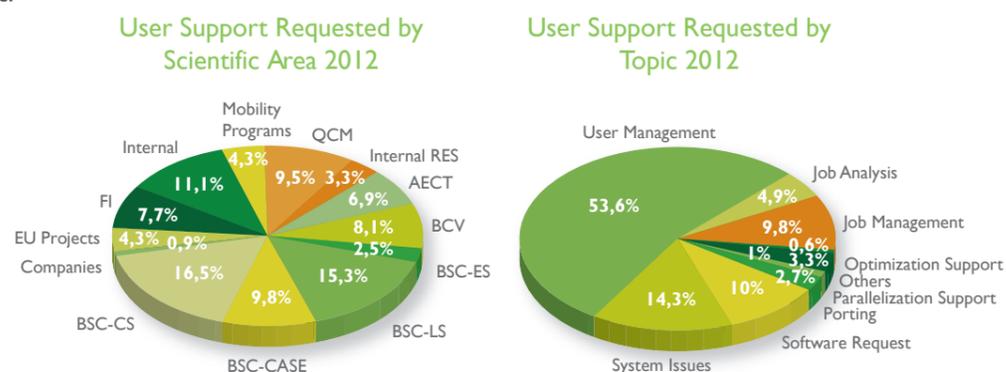
### » User Support

The User Support Group provides assistance with all aspects of scientific computing. This assistance includes general user support, code optimisation and parallel model building support and porting serial and parallel codes for supercomputers such as 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 specialised topics or programs. The Group is also in charge of the SC virtual reality and 3D visualisation system, the BSC-CNS official website, the Intranet and the graphical design activities.

Some 5422 support requests were received in 2012 as presented in the figures below, split by support request area and by topic.



### Highlighted Projects

#### ► iCORDI

The User Support group is coordinating the participation of BSC-CNS in iCORDI. It is the premier global forum charting, demonstrating and driving convergence between emerging global data infrastructures. iCORDI focuses on coordinating a series of cross-infrastructure experiments on global interoperability with a selected group of projects and communities. Each prototype addresses a specific community-driven use case identifying best-of-breed solutions and the remaining challenges.



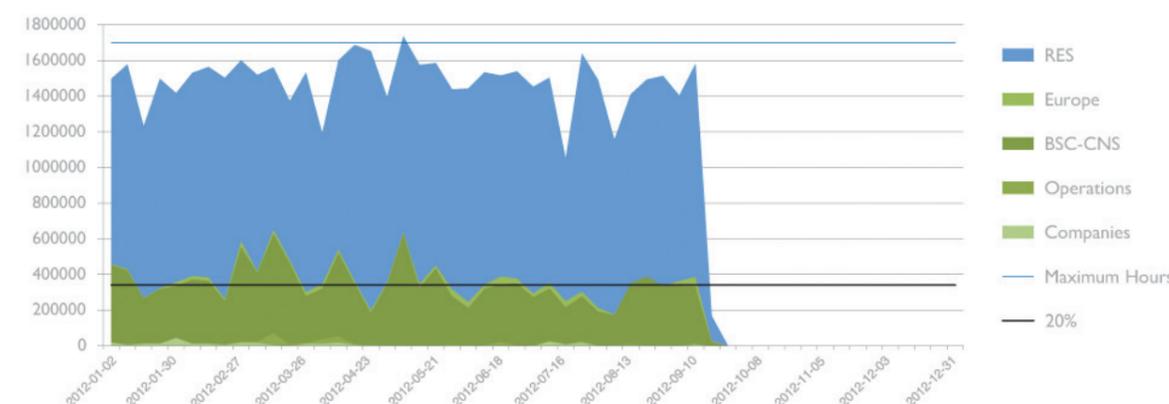
The iCORDI Prototype Programme is developed in synergy with the iCORDI Analysis Programme, which is devoted to analysing data organizations and solutions as they emerge from the various scientific communities, and the iCORDI Workshop Programme, which covers the investigation data infrastructure convergence and reaching out to new research communities. All these activities are part of the RDA (Research Data Alliance) organisation. BSC-CNS is a key contributor, acting as Work Package leader and heavily involved in the core tasks of the project.

#### MareNostrum Performance 2012

MareNostrum was in full production until 17<sup>th</sup> of September for 2012. Using the operative part of the year as the basis for calculations, the observed system utilisation was approximately 82%. In addition to BSC-CNS internal groups, more than 288 external groups accessed the MareNostrum system.

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

#### Weekly Use of the MareNostrum in 2012



### » Facility Management

The mission of Facility Management (FM) is to keep 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:

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



#### Finished MareNostrum III facility upgrade

All facility installations were upgraded to support the new MareNostrum III supercomputer. Electricity consumption will be around 1 MW, which is some 30% higher than for the old MareNostrum, while computing power has been multiplied by 10.

- ▶ 2 new electrical transformers with 2KVA each were installed,
- ▶ 2 new air conditioning chillers providing a total of 2202, 6 kW were installed in a noise-cancellation building,
- ▶ Racks are water cooled with Rear Door Heat Exchangers (RDHx) improving energy efficiency.

#### ► BMS (Building Management System)

In the scope of the facility upgrade, a control system (BMS) was deployed that allows monitoring and automation of all electrical and mechanical infrastructure.

#### Highlight features include:

- ▶ Collection and real-time monitoring of all facility parameters,
- ▶ Alarm notification,
- ▶ Automatic rotation between different redundant components,
- ▶ Automatic temperature control in all water circuits and room temperature,
- ▶ Remote control of the infrastructure.



Chill Water Exchanger



Ernest Quingles, Management Department Director

The key mission of the Management Department is to optimise coordination of the activities of BSC-CNS and provide consolidated planning and management of support services in order to better meet future challenges. Other core objectives include reliable and timely financial reporting, human resources management, and building awareness of 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.

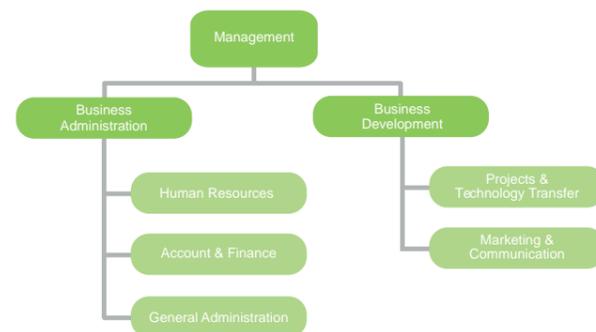
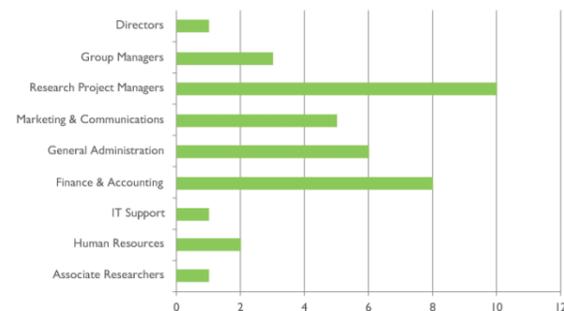
» Overview

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 BSC-CNS and constantly changing needs resulting from 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 2012



» Finance and Business Administration

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

Finance & Accounting

The Finance & Accounting Group is responsible for the financial resources management of all BSC-CNS activities (expenses, budgets, audits, bank relations, suppliers, receiving payments and controlling budget deviations). Adhering to current financial legislation and accountancy norms, they manage and safeguard financial resources, supported by the Administration group. The Group also prepares financial reports for project audits in coordination with the project management office and principal researchers. Due to the difficult economic environment and public funding delays, the role of controller has expanded significantly to manage relations with banks and negotiate conditions with suppliers and clients. To provide better support a new procurement unit is being developed which will work closely with purchasing staff.

In 2012 the Group continued working on a SAP BI Tool with a system upgrade for better reporting capabilities, and developed new finance queries. Work also progressed on the automation of certain data analysis and exploitation processes.

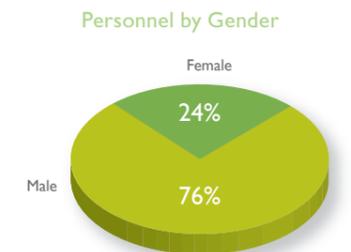
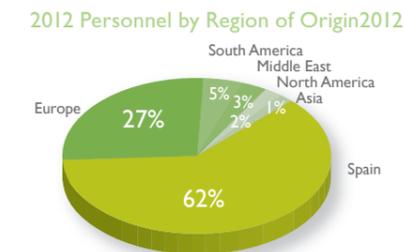
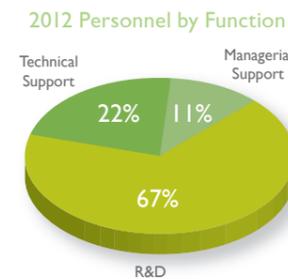
**Human Resources** The Human Resources Group is responsible for managing selection processes, hiring and training,



ning, job descriptions, labour relations and collective bargaining, planning careers and internal promotion, and preventing work-related accidents. In 2012 the Group continued work on a professional development system for all BSC-CNS staff. In order to facilitate improved motivation and retention of talent, a new web tool was designed to manage the BSC-CNS Staff Professional Development Plan. The tool will facilitate annual reporting and evaluation, monitoring of staff development and training, and facilitates the creation of evaluation and progress reports by groups and also at individual level.

Training needs of different departments and groups were identified, and a plan was established for providing internal training to BSC-CNS personnel. The training actions developed for this period included two types: professional development of personal skills needed for work (leadership, teamwork, and communication) and development of knowledge and skills to facilitate mobility and help the integration and internationalization of BSC-CNS staff.

BSC-CNS continues to attract researchers from all over the world and currently 38% of its researchers are from abroad (39 countries). In 2012 the Group produced the "Welcome Guide BSC-CNS", which will be available in 3 languages, to facilitate recruitment processes and the adaptation of BSC-CNS staff new to Barcelona life. The Group also actively disseminated the new positions available under the Severo Ochoa program via 16 different media of European scope, filling 95% of the vacancies with excellent candidates. All selection procedures were performed in compliance with disclosure, merit, competition and gender equality requirements.



**General Administration** 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 institutional events. The Group manages travel services, space allocation and new offices requirements, purchasing services and execution of public tender processes as well as providing general administrative support, logistic and reception services, such as receiving visiting researchers, official representatives and invited speakers.

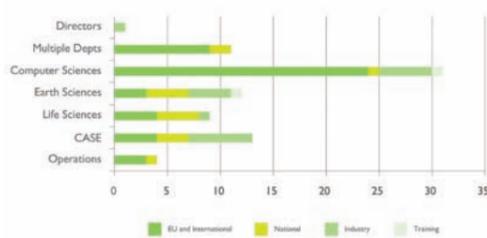
In 2012, BSC-CNS published 11 public calls in order to accept 6 supply tenders, 3 services tenders and 2 works tenders. A total of 51 administration contracts were signed during the year. The purchasing unit's activities increased significantly, especially with the works tenders that were held to start the 2nd phase construction of the new BSC-CNS building and adapt the technical services at the new site for the new supercomputer. Both actions will be funded with grants from the European Regional Development Fund (FEDER).



» Project Management

**Project Management Office** The BSC-CNS Project Management Office (PMO) consists of seven experienced project managers who work closely with the centre's Principal Investigators. PMO is responsible for: detecting and communicating research funding opportunities; coordinating and contributing to project proposals; managing contract negotiations, and managing all legal, financial and administrative aspects of contracts and projects. This includes both publicly funded projects and collaborations with private industry. PMO also maintains a comprehensive database of project information and extracts reports used to analyse the centre's performance in various areas. PMO is also responsible for following and anticipating developments in relevant funding programmes and helping the centre to adapt to changing requirements. The aim is to increase BSC-CNS's capacity to leverage competitive funding and professionally manage results-oriented research. In 2012, BSC-CNS participated in 81 projects (excluding personnel grants), 43 were funded by the extremely competitive Framework Seven Programme of the European Commission (FP7). Eight of these FP7 projects were led by BSC-CNS in which the centre coordinated a total of 55 partners based throughout Europe and

BSC-CNS Projects 2012



Latin America. Two of the 81 were COST-funded projects for the international coordination of nationally funded research. 14 were funded using Spanish National or Catalan funds and 22 were research activities funded by companies. In addition to managing active projects, the Project Management Office assisted BSC-CNS researchers in submitting 142 new project proposals to help ensure continued funding for BSC-CNS research activities, including proposals for 61 personnel grants.

**Strategic Projects Area** The Strategic Projects Area of BSC-CNS works on coordinating activities linked to prioritising and road mapping future research (European Technology platform for High Performance Computing ETP4HPC), definition of organisation and management of international research infrastructures (PRACE, EUDAT) and technology transfer (participation in the proposed Spanish node of the EIT ICT Labs) among others.



» **Marketing & Communication** The BSC-CNS Communications team 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 2012, BSC-CNS received a total of 5221 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 a talk about the centre, our technology and our research lines. The visits are tailored depending on the target audience.



**BSC-CNS in the Media** BSC-CNS was mentioned 545 times in national and international newspapers and magazines in 2012. 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 17 press releases in Spanish, Catalan and English, all posted on the Press section of the BSC-CNS website. All identified press impacts were also included on the web.

**Web and Social Media** In 2012 the Communications team made a major effort to strengthen BSC-CNS's web presence and social media networks. More than 50 articles were published on the corporate website and 800 posts were made, mainly on Facebook and Twitter. During this period, the number of Facebook fans increased by 120% and the number of Twitter followers, by 278%. A Youtube Channel was also created.

**Internal Communication** In the area of internal communication, the Communications team launched the BSC-CNS Newsletter, now published every four months, and coordinated the development of the social plan.

**Events, Seminars and Workshops** In 2012, BSC-CNS hosted and organized the following events: EUDAT User Forum, May 7-8 / BIO-NMR Meeting, March 12-14 / En los orígenes de la mente humana, May 21 / Mateo'12: Multicore Architectures and Their Effective Operation 2012, June 28-29 / PUMPS Summer School, July 2-6 / Jornada Usuarios de la RES / HPC Advisory Council (Málaga), September 12-13 / Computational biology: From genomes to cells and systems, October 14-20 / 24th ACCENT/ GLOREAM Workshop, October 17-19 / SLURM User Group Meeting, October 9-10 / First EUDAT conference, October 22-24 / II Lectures on Atmospheric Mineral Dust, November 5-9 / BSC-CNS Annual Meeting, December.

**Participation in international supercomputing conferences** The Communications team prepared the BSC-CNS presence in International SuperComputing12 and SuperComputing12 exhibitions and coordinated logistics resulting in the presence of BSC-CNS researchers in these prestigious conferences.

**Dissemination of European and National Projects** The Communications team also carried out BSC-CNS dissemination actions for 20 European and national projects. PRACE, Mont-Blanc and EUDAT were the projects with the most dissemination assigned to BSC-CNS in 2012.

## » Computer Sciences 2012 Publications

### Journals

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- » Baldasano, J. M., "**El transporte de contaminantes en el área de Barcelona**", Observatori Fabra, 11 July, 2012. Barcelona. Spain, 2012
- » Baldasano, J. M., "**La ingeniería ambiental como disciplina básica hacia la sostenibilidad**", CMU Ramon Llull, 26 November, 2012. Barcelona, Spain, 2012
- » Baldasano, J. M., "**La situación actual de la gestión de residuos en España**", Congreso Nacional del Medio Ambiente (CONAMA 12). Valorización energética como parte de la solución integral de la gestión de residuos (ST-9), 26-30 November, 2012. Madrid, Spain, 2012
- » Baldasano, J. M., "**Projecte ESCAT: Objectius, Metodologia i necessitats computacionals**", Generalitat de Catalunya, 23 October, 2012. Barcelona. Spain, 2012
- » Maria Gonçalves, A. Barrera-Escoda, J. M. Baldasano, J. Cunillera, "**Estudi de regionalització climàtica dinàmica a alta resolució sobre Catalunya**", Reunió Grup d'Experts en Canvi Climàtic a Catalunya (GECCC), 28-29 June, 2012. Monestir de les Avellanés, Spain, 2012

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- » A. Badia, Oriol Jorba, "**Evaluation of the gas-phase results of the online NMMB/BSC-CTM model at regional and global scales**", 24<sup>th</sup> ACCENT/GLO-REAM Workshop, 17-19 October, 2012. Barcelona, Spain, [http://www.bsc.es/gloream/sites/default/files/pdf\\_web/session2\\_pdf/GLOREAM2102-Badia\\_Oriol\\_Evaluation\\_NMMB\\_BSC-CTM-abstract.pdf](http://www.bsc.es/gloream/sites/default/files/pdf_web/session2_pdf/GLOREAM2102-Badia_Oriol_Evaluation_NMMB_BSC-CTM-abstract.pdf), 2012
- » Baldasano, J. M., "**WCES panel: Weather and Air Quality**", PRACE Scientific Case Update Workshop, 15 March, 2012. Dublin, Ireland, 2012
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- » K. Haustein, "**Development of an atmospheric modeling system for regional and global mineral dust prediction: Application to Northern Africa, Middle East and Europe**", 2012
- » Sara Basart, "**Desert dust characterization in Northern Africa, Middle East and Europe through regional dust modelling, and satellite-borne and ground-based observations**", 2012
- » Simone Marras, "**Variational Multiscale Stabilization of Finite and Spectral Elements for Dry and Moist Atmospheric Problems**", 2012

## » Life Sciences 2012 Publications

### Journals

- » Adams, David, Altucci, Lucia, Antonarakis, Stylianos E, Ballesteros, Juan, Beck, Stephan, Bird, Adrian, Bock, Christoph, Boehm, Bernhard, Campo, Elías, Caricasole, Andrea, Dahl, Fredrik, Dermitzakis, Emmanouil T, Enver, Tariq, Esteller, Manel, Estivill, Xavier, Ferguson-Smith, Anne, Fitzgibbon, Jude, Flicek, Paul, Giehl, Claudia, Graf, Thomas, Grosveld, Frank, Guigó, Roderic, Gut, Ivo, Helin, Kristian, Jarvius, Jonas, Küppers, Ralf, Lehrach, Hans, Lengauer, Thomas, Lernmark, Ake, Leslie, David, Loeffler, Markus, Macintyre, Elizabeth, Mai, Antonello, Martens, Joost Ha, Minucci, Saverio, Ouwehand, Willem H, Pelicci, Pier Giuseppe, Pendeville, Hélène, Porse, Bo, Rakyán, Vardhman, Reik, Wolf, Schrappe, Martin, Schübeler, Dirk, Seifert, Martin, Siebert, Reiner, Simmons, David, Soranzo, Nicole, Spicuglia, Salvatore, Stratton, Michael, Stunnenberg, Hendrik G, Tanay, Amos, David Torrents, Valencia, Alfonso, Vellenga, Edo, Vingron, Martin, Walter, Jörn, Willcocks, Spike, "**BLUEPRINT to decode the epigenetic signature written in blood**", Nature biotechnology, 30, 3, 224-6, 2012
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- » Barbany, Montserrat, Morata, Jordi, Tim Meyer, Lois, Sergi, Modesto Orozco, de la Cruz, Xavier, "**Characterization of the impact of alternative splicing on protein dynamics: the cases of glutathione S-transferase and ectodysplasin-A isoforms**", Proteins, 80, 9, 2235-49, 2012
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- » Carrillo, Oliver, Charles A. Laughton, Modesto Orozco, "**Fast Atomistic Molecular Dynamics Simulations from Essential Dynamics Samplings**", J. Chem. Theory Comput., 2012
- » Cossins, Benjamin P, Hosseini, Ali, Guallar, Victor, "**Exploration of Protein Conformational Change with PELE and Meta-Dynamics**", Journal of Chemical Theory and Computation, 8, 959-965, <http://pubs.acs.org/doi/abs/10.1021/ct200675g>, 2012
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- » Djebali, Sarah, Lagarde, Julien, Kapranov, Philipp, Lacroix, Vincent, Borel, Christelle, Mudge, Jonathan M, Howald, Cédric, Foissac, Sylvain, Ucla, Catherine, Chrast, Jacqueline, Ribeca, Paolo, Martin, David, Murray, Ryan R, Yang, Xiping, Ghamsari, Lila, Lin, Chenwei, Bell, Ian, Dumais, Erica, Drenkow, Jorg, Tress, Michael L, Josep L Gelpi, Modesto Orozco, Valencia, Alfonso, van Berkum, Nynke L, Lajoie, Bryan R, Vidal, Marc, Stamatoyannopoulos, John, Batut, Philippe, Dobin, Alex, Harrow, Jennifer, Hubbard, Tim, Dekker, Job, Frankish, Adam, Salehi-Ashtiani, Kourosh, Reymond, Alexandre, Antonarakis, Stylianos E, Guigó, Roderic, Gingeras, Thomas R, "**Evidence for transcript networks composed of chimeric RNAs in human cells**", PLoS one, 7, 1, e28213, 2012
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- » Eva Maria Novoa, Lluís Ribas de Pouplana, Modesto Orozco, "**Small Molecule Docking from Theoretical Structural Models**", Computational Modeling of Biological Systems Biological and Medical Physics, Biomedical Engineering, 75-95, 2012
- » Fernandez-Recio, Juan, Verma, Chandra, "**Theory and simulation: complexity and emergence**", Current opinion in structural biology, 22, 2, 127-9, 2012
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- » Tomato Genome Consortium, "**The tomato genome sequence provides insights into fleshy fruit evolution**", Nature, 485, 7400, 635-41, 2012
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- » David Torrents, "**Application of modern genomics to biomedicine**", International Workshop: ParBioHet. Brasilia, Brazil, 2012
- » David Torrents, "**Genomics, from DNA sequence to chromatin**", EMBO course: Bioinformatics for Microbial Genomics and Metagenomics. Rabat, Morocco, 2012
- » David Torrents, "**Modern Genomics**", Computational Biology Meeting, RISC, 2012
- » Josep Ll. Gelpi, "**DISCRETE – a novel package for the simulation of protein dynamics using the Discrete Molecular Dynamics method**", High Performance Computing in Computational Chemistry and Molecular Biology: Challenges and Solutions provided by ScalaLife project, 2012
- » Juan Fernández Recio, "**Conformational flexibility in protein-protein association: application to docking predictions**", Bio-NMR 2012. Barcelona, Spain, 2012
- » Juan Fernández Recio, "**Docking and hot-spot prediction for drug discovery targeting protein-protein interactions**", IV International Conference BIFI on Protein Targets: Discovery of Bioactive Compounds, Zaragoza, Spain, 2012
- » Juan Fernández Recio, "**Integration of low-resolution data into all-atom protein docking**", 243<sup>rd</sup> American Chemical Society meeting, San Diego, US, 2012
- » Juan Fernández Recio, "**New challenges for protein docking in the interactomics era**", ICM User Group Meeting 2012, San Diego, US 2012
- » Modesto Orozco, "**Challenges in the dynamic representation of protein dynamics**", CECAM meeting High performance computing in computational chemistry and molecular biology. Lausanne. Switzerland, 2012
- » Modesto Orozco, "**Expanding the frontiers of dynamics calculations of macromolecules**", WE-Hareus Seminar, Bad Honnef, Germany, 2012
- » Modesto Orozco, "**Exploring protein dynamics in the postgenomic era**", CECAM meeting Exploring protein interactions through theory and experiments, Lausanne, Switzerland, 2012

- » Modesto Orozco, "**Exploring protein dynamics in the Post-Genomic era**", Plenary Lecture 1<sup>st</sup> meeting of the Chemical Biology Group RSEQ, Santiago, 2012
- » Modesto Orozco, "**Multi-level simulation of DNA**", UK-Distinguish Scientist Tour, Bristol University, 2012
- » Modesto Orozco, "**Multi-level simulation of DNA**", UK-Distinguish Scientist Tour, Nottingham University, 2012
- » Modesto Orozco, "**Multi-scale view of DNA and chromatin**", Telluride meeting on coarse-grained representation of structure and dynamics of macromolecules, Telluride, CO, USA, 2012
- » Modesto Orozco, "**New approaches for the study of protein dynamics in the post-genome scenario**", Max Planck workshop on Emerging dynamics view of proteins, Dresden, Germany, 2012
- » Modesto Orozco, "**Protein dynamics simulation in the PostGenome Era**", UK-Distinguish Scientist Tour, Belfast University, 2012
- » Modesto Orozco, "**Simulating unusual nucleic acids in unusual environments**", Conformational diversity and application of G-Quadruplexes, Sitges, 2012
- » Modesto Orozco, "**The dry part of the genomic projects**", IMPCC Workshop on Biobanking in Predictive Medicine, Barcelona, 2012
- » Modesto Orozco, "**The dry side of biology: when computers meet microscopes**", Intel Leadership Conferences on HPC for Life Sciences, Brussels, 2012
- » Víctor Guallar, "**Mapping ligand migration in Hemoglobins with PELE**", XVII Oxygen Binding and Sensing Proteins, Parma (Italy), 2012
- » Víctor Guallar, "**PELE: low cost protein-ligand dynamics and induced fit**", Discovery Chemistry Congress, Munich (Germany), 2012
- » Víctor Guallar, "**PELE: low cost protein-ligand dynamics and induced fit**", International BIC symposium, University of Canterbury, Christchurch (New Zealand), 2012
- » Víctor Guallar, "**Protein-Protein and Protein-Ligand refinement**", Schrodinger European Meeting, Brussels (Belgium), 2012
- » Víctor Guallar, "**QM/MM Methods: Following Electrons in Complex Systems**", Cecam meeting on: Spin states in Biochemistry and inorganic chemistry, Zaragoza, 2012

## National Conferences

- » Josep Ll. Gelpi, "**FlexPortal: An integrated platform for the study of macromolecular flexibility**", 6<sup>th</sup> Annual SME Support Forum Barcelona, October, 2012
- » Modesto Orozco, "**DNA from the electron to the chromosome**", XXVIII Reunión anual de la Xarxa de Referència en Química Teòrica i Computacional, Barcelona, 2012
- » Modesto Orozco, "**In Silico Biology**", 50 years of the Catalan Society of Biology, Barcelona, 2012

## Workshops

- » "**BioNMR**, (<http://mmb.irbbarcelona.org/BioNMR2012>)", 2012
- » "**DESMOND European hands-on workshop**", 2012
- » "**EMBO Workshop in Computational biology**, (<http://events.embo.org/12-comp-bio/>)", 2012

## Theses

- » Diego Masone, "**Dynamical mapping of protein-protein interactions**", 2012

## » Computer Applications in Science & Engineering (CASE) 2012 Publications

### Journals

- » A Costa, Arnau Folch, G Macedonio, Giaccio, B, Isaia, R, Smith, V.C, "**Quantifying volcanic ash dispersal and impact of the Campanian Ignimbrite super-eruption**", Geophysical Research Letters, 39, <http://dx.doi.org/10.1029/2012GL051605>, 2012
- » Arnau Folch, "**A review of tephra transport and dispersal models: Evolution, current status, and future perspectives**", Journal of Volcanology and Geothermal Research, 235 - 236, 96 - 115, <http://www.sciencedirect.com/science/article/pii/S0377027312001588>, 2012
- » B. Eguzkitza, G. Houzeaux, R. Aubry, Mariano Vázquez, "**A Parallel coupling strategy for the Chimera and Domain Decomposition methods in Computational Mechanics**", Computers & Fluids, In Press, 2012
- » C. Scaini, Arnau Folch, M. Navarro, "**Tephra hazard assessment at Concepción Volcano, Nicaragua**", Journal of Volcanology and Geothermal Research, 219-220, 41-51, 2012
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- » M.S. Osoro, Arnau Folch, E. Collini, G. Villarosa, A. Durant, G. Pujol, J.G. Viramonte, "**Validation of the FALL3D model for the 2008 Chaitén eruption using field, laboratory and satellite data**", Andean Geology, 40, 2012
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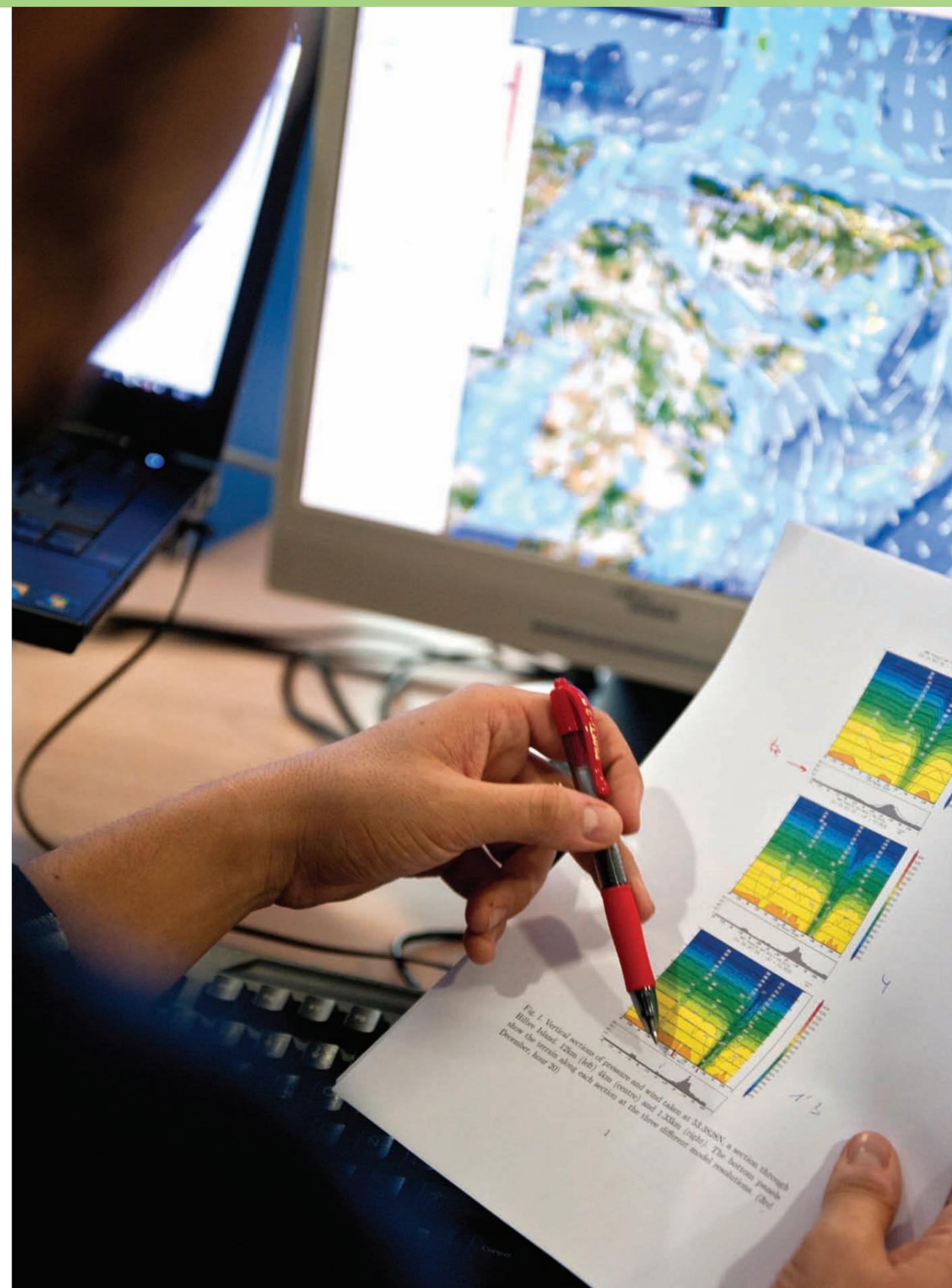
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### Book Chapters

- » Cristina Montaña-Sales, Xavier Rubio-Campillo, José Ma. Cela, J. Casanovas-García, A. Kaplan-Marcusán, P. Fonseca, "Formal Languages for Computer Simulation: Transdisciplinary Models and Applications", Formal Languages for Computer Simulation: Transdisciplinary Models and Applications, Submitted 2012
- » Óscar Peredo, Ortiz, Julian M., Abrahamsen, Petter, Hauge, Ragnar, Kolbjørnsen, Odd, "Multiple-Point Geostatistical Simulation Based on Genetic Algorithms Implemented in a Shared-Memory Supercomputer", Geostatistics Oslo 2012, 17, 103-114, [http://dx.doi.org/10.1007/978-94-007-4153-9\\_9](http://dx.doi.org/10.1007/978-94-007-4153-9_9), 2012

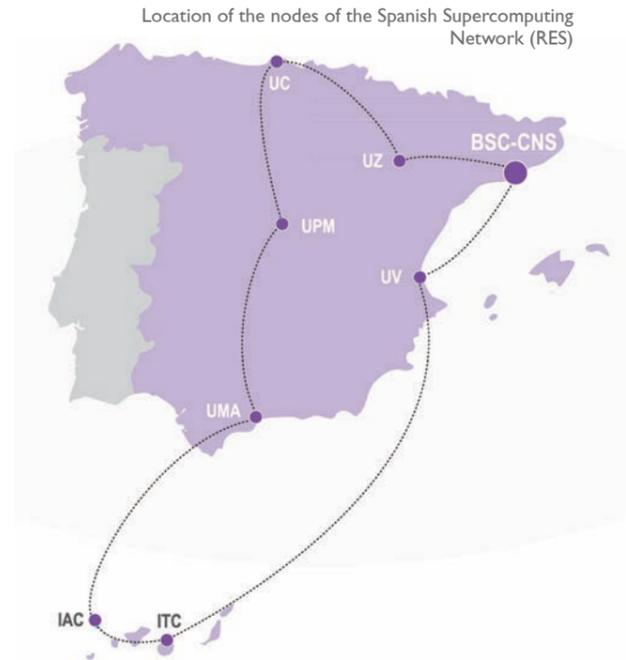
### International Conferences

- » Aguado-Sierra J, Aris R, Houzeaux, Guillaume, Mariano Vázquez, "A framework for anti-arrhythmic drugs testing using a multi-scale computational heart employing Alya Red", UT Austin - Portugal Workshop on Modeling and Simulation of physiological systems, 2012
- » Aguado-Sierra J, Vázquez M, "Multiple Ion Channel Block Simulations on a computational, transmurally heterogeneous, fully coupled, electro-mechanic model of the human heart in a geometrically accurate anatomical model to assess torsadogenic risk", Bioengineering UK 2012, 2012
- » Bernardo Rondelli, Xavier Rubio-Campillo, Alexis Torrano, Miquel Ramírez, Carla Lancelotti, Matthieu Salpeteur, Victoria Reyes-García, Marco Madella, "Applying the ODD protocol in agent-based modeling of past socio-ecological dynamics", Computer Applications in Archaeology, Southampton, 2012
- » Ekinhe García, Roger Sala, Xavier Rubio-Campillo, Robert Tamba, "Multi-Scale Exploration of the Archaeological Site of Puig Ciutat (Oristà, Catalunya)", European Association of Archaeologists Conference, Helsinki, 2012
- » F. DiMaio, P. Rem, S. Lofti, S. Serranti, G. Bonifazi, M. Hu, V. Burganos, E. Skouras, F. Cucchietti, Mariano Vázquez, "Cement and Clean Aggregates from CDW: The C2CA Project", International Conference on Solid Waste Technology and Management, Philadelphia (US), 2012
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- » M. Avila, Arnau Folch, G. Houzeaux, B. Eguzkitza, L. Prieto, D. Cabezón, "Onshore Wind Farm Modelling", Congreso Latinoamericano de Ingeniería del Viento, 2012
- » M.C. Rojo Ariza, Xavier Rubio-Campillo, Francesc Xavier Hernández, "Mapping Spanish Republican Airfields: Using GIS for interpreting Air Warfare", Computer Applications in Archaeology, Southampton, 2012
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- » Vladimir Puzyrev, Jelena Koldan, Josep de la Puente, Houzeaux, Guillaume, José Ma. Cela, "A Massively Parallel Nodal 3D Finite-Element Approach to CSEM Problems", AGU Fall Meeting, 2012
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- » Xavier Rubio-Campillo, Alexis Torrano, Jose Maria Cela, Bernardo Rondelli, Andrea Balbo, Miquel Ramírez, Carla Lancelotti, Matthieu Salpeteur, Victoria Reyes-García, Marco Madella, "Pandora's box: the challenge of exploring social simulation models with supercomputers", Computer Applications in Archaeology, Southampton, 2012
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During 2012, the RES continued to provide world-class High Performance Computing resources and services to meet the ever-increasing demand of the Spanish and international scientific communities. Despite the augmentation of available resources, the amount of requests exceeded available capacity by 30%. A total of some 200 projects were developed during the year. The RES also organised training sessions for both technicians managing the infrastructure, and scientists, as well as seminars to enhance the dissemination of scientific results. Since the creation of the RES in 2006, more than 2050 projects have been awarded access to the network, illustrating the relevance and need of access to supercomputing facilities in Spain.



Despite the difficult economic situation, long term planning bore fruit in 2012, with upgrades of several RES supercomputers and a resultant increase in HPC resources available to users. The supercomputers upgraded (or in the process of upgrading) include MareNostrum (BSC-CNS), LaPalma (IAC), Altamira (UC), Pablo Picasso (UM), Tirant (UV), the new Memento supercomputer at BIFI (UZ), and Atlante (ITC).

### » Vision ESFRI of the European HPC service and how fit RES and PRACE in it

European HPC-facilities are organised in a pyramid according to the volume of computing resources offered and the number of systems which provide them. The shared European vision is to encourage and support the creation of an overall European HPC ecosystem involving all stakeholders: HPC service providers, grid infrastructures, scientific and industrial user communities, and the European HPC hardware and software industry.



The RES, as a national and local-level HPC service provider is intended to provide tier-1 and tier-2 level infrastructure. The upgraded MareNostrum III, as a PRACE infrastructure, will provide tier-0 service to Europe, and service at tier-1 level to Spain via the RES network. The other RES nodes will provide tier-1 or 2 service according to their capabilities.

### » RES history, main goals, resources and members

The Spanish government created the Spanish Supercomputing Network (Red Española de Supercomputación) in July 2006 as an answer to the need of the Spanish scientific community for intensive calculation resources, considering supercomputing infrastructure and services to be a decisive asset for the scientific and technological development of the country.

RES Processing Power in TFLOP/s in December 2012



The RES consists of a distributed virtual infrastructure of supercomputers located in different sites and each contributes to the total processing power available to users of different R&D groups in Spain. Its operation is coordinated by the Operations Department of BSC-CNS, which includes support for global maintenance and upgrades, training of users and technicians, facilitation of access and other aspects related to user support.

### » Access protocol and allocations in the RES

All the computing capacity offered is made available to the general scientific community via public calls, with applications submitted via a web interface, and are evaluated by a single Access Committee.

The allocation of access to the supercomputing facilities is based on criteria of efficacy, efficiency and transparency.

The evaluation process is mediated by a double filter system, with potential projects first being evaluated by the ANEP (National Agency of Evaluation and Prospective) if they have not been previously evaluated by other relevant national or international institutions, followed by a review by the RES Access Committee. This is composed of a Core Team and four Scientific Expert Panels formed by prestigious scientists external to BSC-CNS and 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 panel is composed of a coordinator, an assistant, and eight reviewers.

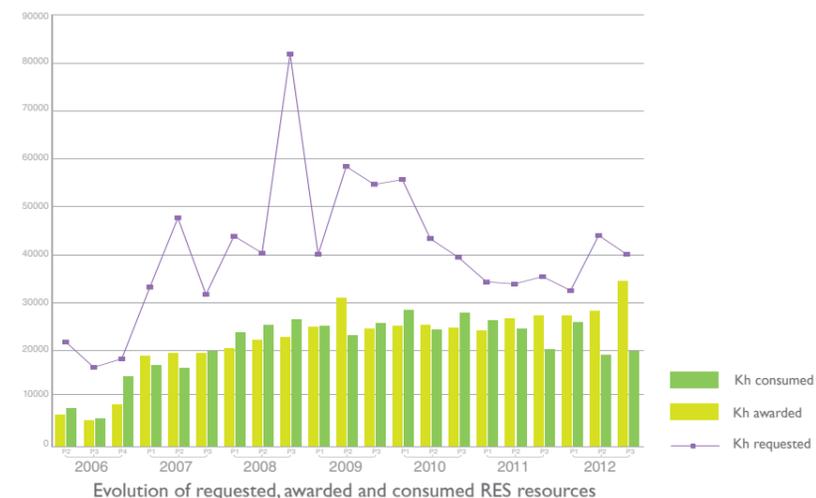
#### The Access Committee Core Team in 2012

- ▶ Joaquin Serrano, MINECO
- ▶ Julio Bravo, ANEP
- ▶ Alfonso Tarancón, BIFI-Universidad de Zaragoza
- ▶ Eduard Ayguadé, BSC-CNS

During 2012 more than 89 million hours were awarded by the Access Committee in 3 calls for applications. In addition to internal research groups, more than 200 research projects made use of the RES system in 2012. It is important to note that many scientific projects often request several periods of access during the year (each access lasts 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 and usage of RES resources 2012

Following the publication of the list of awarded activities by the Access Committee, the technicians at the RES nodes take over the logistical processes, including scheduling the users, preparing their software for loading and running, and ensuring access to results data and also statistics on the performance of the code, so as to facilitate future code improvements.



The graph left shows the evolution of requested, assigned and used hours since the founding of the RES. It clearly shows how demand is always higher than the resources offered, and how any upgrades in capacity are quickly absorbed.

### » CURES, the RES Users Committee

CURES was established in 2010 to provide advice and feedback to the RES management on the current state and future delivery of the resources and services provided. Therefore, CURES aims to promote the effective use of the facilities by sharing information on experiences in using the different systems, suggesting new research and technology directions in scientific computing and, above all, voicing user concerns.

To this end CURES undertakes various communication activities, such as holding regular meetings, establishing shared databases, and posting information. Furthermore, with the CURES cooperation, in 2012 was deployed the first Survey on RES User Satisfaction and the gathered data supplied an important input to be analysed.

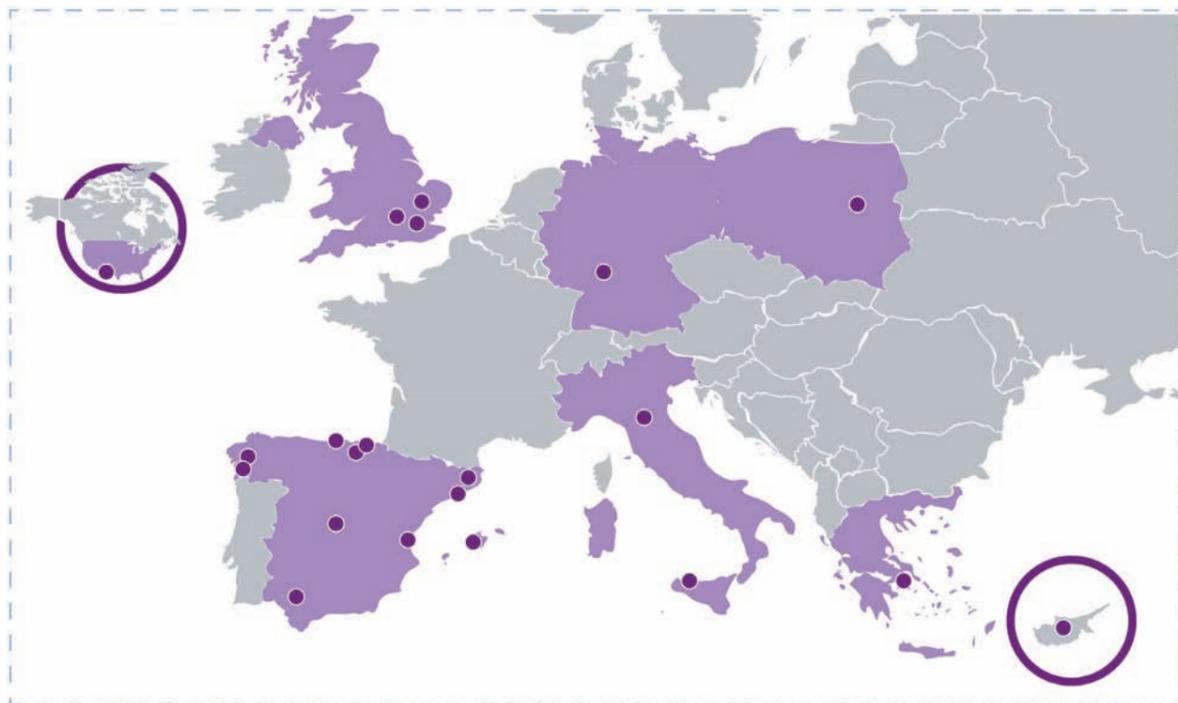
#### The CURES members in 2012

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

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.

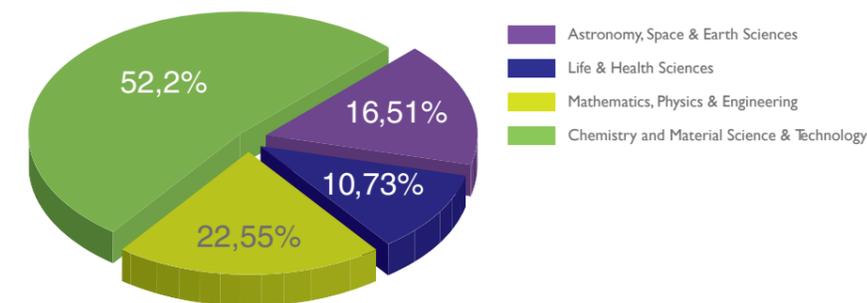
### Broad Impact on Scientific Research

The importance of the RES lies in that it not only supports research in computing, but also research in many other fields, facilitating simulations and calculations to produce scientific results that would otherwise have been impossible to obtain, or at least in such short timeframes, using traditional computers.



Geographical precedence of the RES users

The different research activities carried out on RES supercomputers during 2012 were led by some of the most prominent researchers from institutions all over Spain, Europe and overseas, and covered a huge range of scientific fields, whose results were disseminated in seminars and conferences all over the world, in prestigious peer-reviewed journals, and also to broader audiences via the BSC-CNS website and social networks.



Percentage of RES resources used by Scientific Area

### » 6th 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. The 2012 meeting took place on 12<sup>th</sup> September in Málaga and was organised in co-operation with the HPC Advisory Council, a network of experts from some of the leading global HPC companies, which held its first meeting in Spain the following day.

At the RES User Meeting, in addition to general RES issues, users were updated on the scheduled upgrades for the various RES nodes, progress on the PRACE initiative, and the objectives of the Mont-Blanc project. More information is available at [www.bsc.es/res-and-hpcac-spain-conference-2012](http://www.bsc.es/res-and-hpcac-spain-conference-2012).



Poster of the 6<sup>th</sup> RES User Conference

### » RES User Trainings

A total of seven RES User meetings were organised in 2012, almost one in each city hosting a RES node. The aim of these meetings was to inform local scientific communities of the resources and support services provided by BSC-CNS and the RES, and how to request the use of the PRACE European infrastructure for supercomputing.

Some 126 attendees participated in the meetings that took place in Madrid, Málaga, Tenerife, Valencia, Zaragoza and Barcelona.

The programme, presentation documents and other data is published on the website <http://www.bsc.es/bsc-res-and-prace-2012>.



Poster of the Dissemination Meetings

### » Scientific seminars

In 2012, due to the shortage of funding, the RES did not financially support or directly organise any scientific seminars.

However, the RES did provide logistic support to the Bio-NMR workshop in March, cooperating in the dissemination, invitation of speakers and provision of information on supercomputing resources. Bio-NMR is an event co-organised by the IRB (Institute for Research in Biomedicine), Barcelona University, BSC-CNS, ISMAR, Elixir, GERMN RSEQ, and the RES.

The Bio-NMR project is financed by the European Commission's Framework Programme 7 and the workshop brought together more than 80 leaders in the synergistic use of computation and NMR to discuss present approaches and future avenues in this multidisciplinary and rapidly evolving field. Additionally were explained that computational tools have been crucial for the full exploitation of the wide variety of parameters that can be measured by NMR. The programme and another details can be found in the website <http://mmb.irbbarcelona.org/BioNMR2012/sciprogram.htm>.

### » Technical seminars

Two very specific sessions were held during 2012 in order to promote the cooperation between the RES sites and share experiences in the deployment of tasks.

**Migration of Cluster Slurm+Moab to Slurm v2.3.** Further to a half-day workshop on SLURM & MOAB which took place in 2011, a follow-on video conference was scheduled to continue the discussion in 2012, and then a training session was scheduled 27-28<sup>th</sup> March, for technicians to learn how to migrate to the new version of SLURM. The training was conducted by the performance engineers at BSC-CNS during the two days in which the cluster in Zaragoza was migrated so the attendees benefited from first-hand practical experience on the migration deployment.



Work developed to upgrade Tirant

**Upgrade of the Tirant node.** In November 2012, a three-day workshop was held whose main purpose was to observe the upgrade of the Tirant supercomputer by means of replacing the JS20 blades with JS21 blades and developing the necessary modifications of the system. The meeting was conducted by the system engineers at BSC-CNS and provided the attendees experience to be able to deploy the same tasks in their own supercomputers.



## » Overview



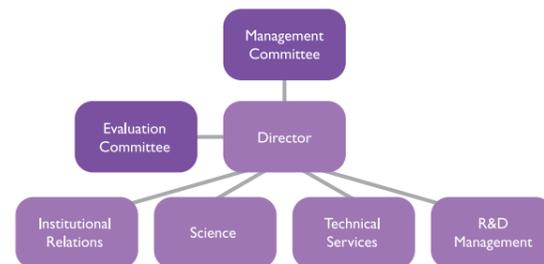
Magerit Supercomputer

CeSViMa (Supercomputing and Visualization Centre 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 a 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. CeSViMa's supercomputer is called Magerit (the ancient recorded name of Madrid). The second version of this supercomputer is a cluster of 245 nodes PS702, that provides almost 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.

## » Organisational Structure



CeSViMa Team as of January 2013



## » Technical and Scientific Highlights 2012

## Key Publications 2012 • Journals

- ▶ Nikos Ch. Karayiannis, Rohit Malshe, Martin Kroeger, Juan J. de Pablo and Manuel Laso, Evolution of fivefold local symmetry during crystal nucleation and growth in dense hard-sphere packings.
- ▶ Nikos Ch. Karayiannis, Rohit Malshe, Martin Kroeger, Juan J. de Pablo and Manuel Laso, Evolution of fivefold local symmetry during crystal nucleation and growth in dense hard-sphere packings.
- ▶ Perla Wahnón, José C. Conesa, Pablo Palacios, Raquel Lucena, Irene Aguilera, Yohanna Seminovski and Fernando Fresno, V-doped SnS<sub>2</sub>: a new intermediate band material for a better use of the solar spectrum.
- ▶ R. Strandberg and I. Aguilera, Evaluation of vanadium substituted In<sub>2</sub>S<sub>3</sub> as a material for intermediate band solar cells.
- ▶ R. San Jose, J.L. Pérez and R.M. Gonzalez, Sensitivity analysis of two different shadow models implemented into EULAG CFD model: Madrid experiment.
- ▶ Y. Seminovski, P. Palacios, P. Wahnón and R. Grau-Crespo, Band gap control via tuning of inversion degree in CdIn<sub>2</sub>S<sub>4</sub> spinel.
- ▶ J.A. García, J.M. Peña, S. McHugh and A. Jérusalem, A model of the spatially dependent mechanical properties of the axon during its growth.
- ▶ Santiago Muelas, Antonio LaTorre and José María Peña, A new methodology for the automatic creation of adaptive hybrid algorithms.

ology for the automatic creation of adaptive hybrid algorithms.

- ▶ Antonio LaTorre, Santiago Muelas and José María Peña, A MOS-based dynamic memetic differential evolution algorithm for continuous optimization: a scalability test.
- ▶ Martínez-Mateo, D. Elkouss and V. Martín, Blind Reconciliation. J. Bobadilla, F. Ortega, A. Hernando and A. Arroyo, A balanced memory-based collaborative filtering similarity measure.
- ▶ A. Hernando, J. Bobadilla, F. Ortega and J. Tejedor, Incorporating reliability measurements into the predictions of a recommender system.
- ▶ Y. Seminovski, P. Palacios and P. Wahnón, Effect of van der Waals interaction on the properties of SnS<sub>2</sub> layered semiconductors.

## Proceedings

- ▶ Roberto Santana, Santiago Muelas, Antonio LaTorre and Jose M. Peña, A direct optimisation approach to the P300 speller
- ▶ Antonio LaTorre, Santiago Muelas and José María Peña, Benchmarking a hybrid DE-RHC algorithm on real world problems

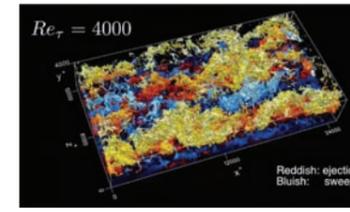
## Conference

- ▶ Foyzur Rahman, Daryl Posnett, Israel Herraiz and Premkumar Devanbu, Size Matters. Does Bias?

## » Key Projects 2012



**Blue Brain Project, José María Peña Sánchez (CeSViMa)** The Universidad Politécnica de Madrid (UPM) and Instituto Cajal (IC) from Consejo Superior de Investigaciones Científicas (CSIC) are involved in the Blue Brain Project (BBP) with an initiative named Cajal Blue Brain. Different research groups and laboratories from Spanish institutions take part in this initiative, grouping together a large number of scientist, engineers and practitioners. Spanish participation falls into two main themes: 1) Functional and anatomical microorganisation of the cortical column, and 2) Biomedical technology development (potentially transferable to other applications). UPM, as a core participant, is deeply involved in setting the objectives and visions of the BBP. Data analysis, optimisation and visualisation software of the BBP are researched in collaboration with UPM. IC intensively collaborates in micro anatomical studies of neuronal cells, their morphology and function. The Cajal Blue Brain Project attracted major industrial partners, which are closely engaged in setting the objectives of the project. The Cajal Blue Brain Project is hosted by the Universidad Politécnica de Madrid (UPM) in the Montegancedo Campus, supported by two of its research centres, the Centro de Tecnología Biomédica (CTB) and the Centro de Supercomputación y Visualización de Madrid (CeSViMa).

The 3D structure of turbulent channels up to  $Re_{\tau} = 4000$ 

flows with high enough Reynolds numbers to be truly multiscale, as well as the possibility of performing conceptual experiments on them. These new capabilities should enable elucidation, once and for all, of the physics underlying the multiscale transfer processes in turbulence in the next five years, especially in shear flows near walls. That will allow the formulation of more realistic engineering models, but the immediate goal of the proposal is to answer the fundamental questions that have resisted two centuries of attack by physicists and engineers. An important part of the work will involve adapting simulation codes to the new computer architectures expected in the next few years. Neither large-scale computing nor data mining are trivial activities, but the group has specialised in both during the past 20 years, particularly for the study of turbulence.

## Multiscale dynamics of turbulent flows, Adrián Lozano Durán (UPM)

Turbulence is a fundamental unsolved problem, at whose core are the multiscale processes that transfer, for example, energy across the inertial range of scales, or momentum across wall-bounded shear flows. Moreover, turbulence is also key to applications from industrial design and energy generation to climate dynamics, where the worst uncertainties lie, due to modelling limitations. Its practical computation and control have been hindered by empirical models and boundary conditions, in large part because of insufficient understanding of these multiscale transfer processes. Direct simulations, without approximation, are expensive, but the past few years have seen the appearance of larger computers and reasonably-priced disks that allow, for the first time, the compilation of time-resolved data sets of canonical turbulent

## Other Projects

- ▶ QUITEMAD: Cryptography, Computation and Simulation, Miguel Ángel Martín-Delgado Alcántara (CeSViMa)
- ▶ QUITEMAD: QUINFOG, Juan José García Ripoll (CeSViMa)
- ▶ QUITEMAD: GICC-UPM, Vicente Martín Ayuso (CeSViMa)
- ▶ QUITEMAD: MIC, David Pérez García (CeSViMa)
- ▶ INTI, Juan Luis Sampedro (CeSViMa)
- ▶ Third generation prediction system of air quality, Roberto San José García (UPM)
- ▶ Parameter Control of Genetic Algorithms, Juan Antonio Fernández del Pozo de Salamanca (UPM)
- ▶ Design, Synthesis and Characterization of High Efficiency Advanced Photovoltaic Materials, Perla Wahnón Benarroch (UPM)
- ▶ White rapid ignition of Inertial Fusion, José Javier Honrubia (UPM)
- ▶ Modelling of Synthetic and Biological Micromolecules Through a Hierarchical Multiscale Approach, Nikos Karayiannis (UPM)
- ▶ Determination of the Stress-optical coefficient and plateau modulus from atomistic simulations of polyethylene melts, Vicente Lorenzo (UPM)
- ▶ Mining Software Repositories, Israel Herraiz Tabernero (UPM)
- ▶ Collaboration Institute of Nuclear Fusion, José Manuel Perlado Martín (UPM)
- ▶ Evaluation of similarity metrics applied to recommendation systems, Jesús Bobadilla Sancho (UPM)
- ▶ Behavioural Simulation in proteins involved in the assembly of the hydrogenase solution, Juan Imperial Ródenas (UPM)
- ▶ Algorithm Parallelisation of optimisation applied to the segmentation of multispectral images, Consuelo Gonzalo Martín (UPM)
- ▶ Application of statistical physics to the mechanics of granular media, Rafael Jimenez (UPM)
- ▶ Heterogeneous domain decomposition methods for aerodynamical simulations, Carlos Castro Barbero (UPM)
- ▶ Primer Extractor Browser Plugin, David Perez del Rey (UPM)
- ▶ Heart visualisation and supervised classification, María Montoya (CNIC)
- ▶ Distributed supercomputing application to genomic sequence analysis and enzymatic modelling, Juan Imperial Ródenas (UPM)
- ▶ Monte Carlo Method in competitive problem solving, Alfonso Rodríguez-Paton (UPM)
- ▶ Towards a novel oxide electronics ab initio many body calculation of the electronic properties of interfaces between transition metal oxides, Ángel Rubio Secades (País Vasco)
- ▶ Mesoscale atmospheric reanalysis IPRA using 3DVAR over the Iberian Peninsula, Jon Saenz (País Vasco)
- ▶ Constraints on inflationary models of the universe based on CMB data, Enrique Martínez González (Cantabria)
- ▶ Interactions between Peptides and Membranes Studied by all-atom free Energy Calculations, Carmen Domene (Reino Unido)
- ▶ Carbon nanostructures and hydrogen production and storage by first-principles calculations and scanning probe techniques, Rubén Pérez Pérez (Madrid)
- ▶ Properties of epitaxial graphene on Ru(0001), Manuel Alcami Pertejo (Madrid)
- ▶ Numerical study of disordered localised electronic systems using energy minimisation, Matteo Palassini (Cataluña)
- ▶ Insensitivity to symmetry breaking in the very excited spectrum, Felipe J. Llanes Estrada (Madrid)
- ▶ Light scattering properties of nonspherical atmospheric aerosols for radiative transfer applications: the ALFA database (extension), Francisco José Olmos Reyes (Andalucía)
- ▶ Identification of genes involved in Parkinson's disease and essential tremor phenotypic spectrum, Pau Pastor (Navarra)
- ▶ Coupling WRF to a wave model through a joint sea surface roughness description, Agustín Sánchez-Arcilla (Cataluña)
- ▶ Numerical simulations of massive separated flows: flow over a stalled NACA airfoil, Assensi Oliva (Cataluña)
- ▶ Extending parallel capabilities of the general purpose Kratos Solver, Riccardo Rossi (Cataluña)
- ▶ Design and Characterisation of Advanced Photovoltaic Materials with High Efficiency, Perla Wahnón Benarroch (Madrid)
- ▶ Tuning of inversion degree and band gap control in MgIn<sub>2</sub>S<sub>4</sub> and CdIn<sub>2</sub>S<sub>4</sub> thio-spinels, Pablo Palacios Clemente (Madrid)
- ▶ Theoretical Characterisation of the optimized geometry and energy levels in a hybrid nanostructure, Pablo Palacios Clemente (Madrid)
- ▶ Ketonic decarboxylation over metal oxides: MgO and ZrO<sub>2</sub>, Mercedes Boronat (Valencia)
- ▶ Binding of glycosylated surfactants to concanavalin A, Antoni Planas (Italia)
- ▶ Evidence of Conformational Selection in a Glycosyltransferase Structure, Antoni Planas (Italia)
- ▶ Catalysis modelling: gold nanoparticles supported on yttrium modified anatase as efficient WGS and CO oxidation catalysts, Javier Fernández Sanz (Andalucía)
- ▶ Study of the transport properties of nanotubes in solution and lipid bilayers, Rebeca García Fandiño (Galicia)

» Overview



The LaPalma Supercomputer

Financed by the Ministry of Economy and Competitiveness (MINECO), LaPalma super-computer is one of the eight nodes belonging to the RES. It is located in the "Centro de Astrofísica de La Palma (CALP)", in Breña Baja. The upgrade of MareNostrum in December 2012 allowed LaPalma to double its capacity.

The installation of La Palma was a strategic step with the objective 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 therefore reinforce the telecommunication development on the island.

» Organisational Structure

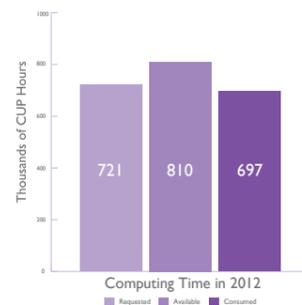
The Time Assignment Commission manages the percentage of the CPU time of LaPalma. Its members come from different divisions of the Instituto de Astrofísica de Canarias (IAC). For administration and management of the supercomputer node, the Instituto de Astrofísica de Canarias (IAC) makes available its IT support team and additionally has employed one engineer dedicated full-time to fulfil these functions.



The LaPalma Supercomputer Systems & Support Team: **Carlos Martín Galán** (Senior Engineer), Responsible Technician and the Manager of the Group. **Antonio Díaz Chinae** (Senior Engineer), System Administrator. **Justo Luna López** (Engineer), System Administrator. **Ubay Dorta Guerra** (Engineer), System Administrator and User Support. **Antonio Dorta Lorenzo** (PhD), User Support. **Victor Plasencia Darías** (Operator), User Support.

» Technical and Scientific Highlights 2012

At the end of 2012 LaPalma doubled the number of cores but kept the number of nodes. Now, with 1024 PowerPC cores, the maximum processing capacity has been increased from 4.5 TFLOP/s to almost 9 TFLOP/s. The power consumption has however increased only by 20%. LaPalma, installed in a controlled environment room of 32 square metres, has now two terabytes of principal memory in addition to its 38.5 TB of hard-disc data storage. The headquarters of IAC and its observatories are connected to LaPalma via a 10Gbps link, of which the supercomputer can use up to 4Gbps. In 2012 LaPalma provided roughly 810k hours of CPU time for IAC researchers. Their projects consumed 86% of available time.



» Key Publications 2012

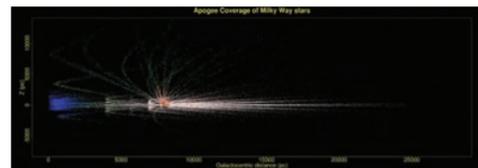
**Journals** • Fabbian, D.; Moreno-Inertis, F.; Khomenko, E.; Nordlund, Å, "Solar Fe abundance and magnetic fields. Towards a consistent reference metallicity". *Astronomy & Astrophysics*, Volume 548, A35 (2012) • Maercker, M.; Mohamed, S. et al, "Unexpectedly large mass loss during the thermal pulse cycle of the red giant star R Sculptoris", *Nature*, 490, 232 (2012).

**Posters** • Parviainen, H "Systematic Search for Secondary Eclipses from the CoRoT Light Curves", *Observing Planetary Systems II ESO Workshop*, Santiago de Chile, March 5-8, 2012.

**Thesis** • M.T. Tapia "Minor Merger Effects On Galaxy Evolution", 2012 (thesis advisor M. Balcells).

» Key Projects 2012

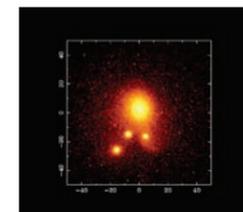
**DAPAPOGEE: Automated Data Processing for APOGEE (PI.: Carlos Allende Prieto)** APOGEE, the Apache Point Observatory (APO) Galactic Evolution Experiment, is one of the surveys included in the current activity of the Sloan Digital Sky Survey (SDSS-III), in which the IAC is heavily involved. The instrument, a 300-fiber high-resolution IR spectrograph, was installed at APO in 2011. The project has generated a flood of data, over 100,000 spectra of about 30,000 stars, and recently improved the data analysis pipeline. In addition to computers at Virginia and New Mexico in the USA, the team processed its data using LaPalma to derive atmospheric parameters and chemical abundances with optimisation algorithms. The results are being used to create a 3D map of the chemical compositions of stars in the



Simulated distribution of the stars observed by APOGEE

disk and bulge of the Milky Way in detail (see Figure), with the ultimate goal of shedding light on the formation and chemical evolution of our Galaxy. The infrared observations made by APOGEE can pierce through the interstellar dust, reaching regions inaccessible to optical instrumentation. One of the latest full runs for the APOGEE Stellar Parameters and Chemical Abundance Pipeline (ASPCAP) was performed on LaPalma supercomputer.

**Galaxy transformations through interactions, mergers and accretion (PI.: 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



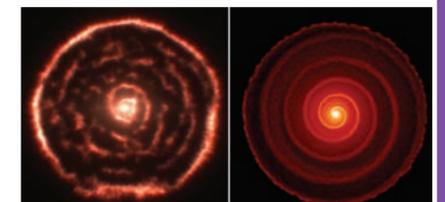
Typically massive galaxies accrete 5 to 10 smaller galaxies in the last 10 billion years

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 analyse 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.

**Smoothed Particle Hydrodynamic Simulations of the symbiotic binary, R Aquarii (PI.: Romano Corradi)**

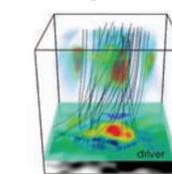
Jets are a common phenomenon in astrophysics, playing an important role in the evolution of stellar systems by carrying mass, energy, and momentum, and probably serve a role similar to a relief valve where energy densities are uncontrollable. Launching jets from magnetised accretion disks is the

most popular explanation. Unfortunately, most jets are so distant that it is not possible to resolve the immediate environment of the outflow sources, and many contain large amounts of dust that veils the outflows within opaque cocoons. However the subject of study, the highly evolved symbiotic star R Aquarii (R Aqr) is one of the closest stellar jets (200 pc) and is bright, active and with relatively low extinction. The project entails a comprehensive study of R Aqr, in particular a programme of multi-epoch imaging over several years to reveal the evolution of the R Aqr outflows in real-time. This accurate observational study is contrasted 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.



On the left is the ALMA observation of circumstellar environment of R Sculptoris and on the right is a cross-section through the 3D hydrodynamics simulation of the interacting binary star system

**Propagation of magnetoacoustic waves in magnetic structures (PI.: Elena Khomenko)**

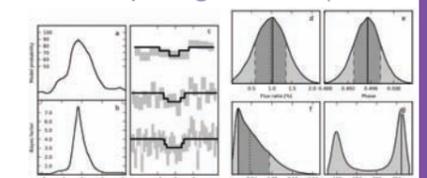


Simulation of wave propagation in the Sun's atmosphere driven by spectropolarimetric observations by IBIS

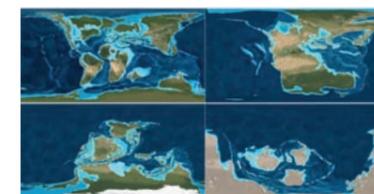
Local helioseismology of solar active regions will be able to provide information about sub-surface magnetic fields to be used by magnetic dynamo models, in order for which the physics of waves in magnetised regions has to be well understood. Forward numerical simulations have become a preferred approach in recent years to attack the complex non-linear physics of waves in non-trivial magnetic field configurations. The project aims to understand: (a) Mechanisms of excitation of waves in sunspots. (b) Physics of umbral flashes and running penumbral waves. (c) Identify wave types dominating helioseismological velocity signals detected in active regions. (d) Analyse consequences of the strong magnetic field of sunspots onto helioseismology measurements and determination of sub-photospheric structure of solar active regions.

**Bayesian analysis of secondary transits from the CoRoT and Kepler light curves (PI.: Hannu Parviainen)**

This project uses methods based on Bayesian model comparison to assess whether the light curves for stars with known transiting planets observed with the CoRoT and Kepler space telescopes feature a secondary transit signal.



**The Earth in time as a template for the characterisation of inhabitable exoplanets (PI.: María Esther Sanromá Ramos)**

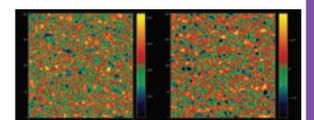


Global views of the Earth's continental distribution

To date, more than 850 exoplanets have been detected outside the Solar System. Even though most of these are gas giants, evolving observational capabilities are enabling the discovery of planets in the super-Earth mass range. To facilitate characterisation of future exoearth detections, observation and characterisation of the Solar System rocky planets, including Earth, will be essential to aid in interpreting observational data. This project aims to characterise earth-like planets throughout studying the photometric and spectroscopy variability of our own planet. That is, to study the Earth as if it were an exoplanet observed from an astronomical distance. Because extrasolar planets are expected to exhibit a wide range of ages and evolutionary stages, the team aims to study the Earth as it is today, and also at different epochs of its history, such as 90, 340 or 500 Ma ago.

**NLTE inversion of CaII lines in a sunspot/Photospheric O abundance (PI.: Hector Socas Navarro)**

The time requested is actually for two different projects that require running the same code on different data sets. The first project is an improved analysis of a high-quality dataset that was inverted back in 2004 (Socas-Navarro 2005), this time with a new version of the code that incorporates new physical ingredients. The results will then be used by Khomenko et al as an initial model for a MHD wave simulation. The second project seeks to determine the solar O abundance for a 3D photospheric model obtained by inverting data from the Hinode satellite (Socas-Navarro 2011).



Horizontal cut of the 3D model near the base of the photosphere

» Overview

Atlante supercomputer joined the RES on February 16<sup>th</sup> 2009, becoming its 8<sup>th</sup> 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 Supercomputer

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 was upgraded due to the installation of MareNostrum3, by virtue of the agreement between RES nodes. Atlante offers now 96TB of storage disk.

» Organisational Structure

The technical staff of Atlante comprises a computing engineer from ITC (María Belén Esteban Sánchez), who is 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.



M<sup>a</sup> Belén Esteban Sánchez (System Administrator and User Support)

» Technical and Scientific Highlights 2012

In 2012 Atlante's local access granted 12 local projects corresponding to Canary islands's Companies and Researchers. They ran 997K hours of CPU time, related to the following projects:

» Key Publications 2012

Journals

- Inmaculada Menéndez, Emma Pérez-Chacón, José Mangas, Esperança Tauler, Johann P. Engelbrecht, Edward Derbyshire, Luis Cana, Ignacio Alonso. Dust deposits on La Graciosa Island (Canary Islands, Spain): texture, mineralogy and a case study of a recent plume dust transport. Journal Catena. Ed.: Elsevier.

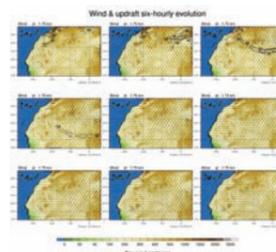
PhD Thesis

- Pedro Gonzalez-Morales. Multi-Source Modelling of Helioseismic Waves in the Sunspots and Quiet Sun.

» Key Projects 2012

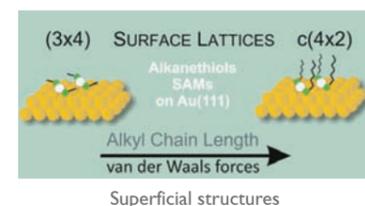
Atmospheric numerical prediction

In the framework of a multidisciplinary research project (characterisation and modelling of the Saharan dust deposition in La Graciosa), the group contributed to modelling a high resolution wind field of an event in March 2004, showing that Saharan air flows are able to lift and carry particles of coarse sand, which appear in La Graciosa.



Panel dust episode 2004

DFT calculation of the surface structures of different adsorbates on transition metals

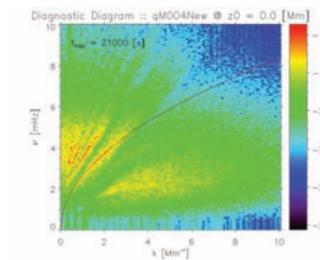


Thiol self-assembled monolayers (SAMs) on Au(111) were established as a model system in modern surface science, in addition to their numerous applications in Nanotechnology. These molecules adsorb on the gold surface as thiolates yielding ordered, commensurate lattices, the most usual being the (3 3)-R30 and its related c(4 2) superlattice. In this work the team ran vdW-DFT calculations to investigate the role of hydrocarbon chain length for the purpose of selecting the surface structure (that contains thiolate-Auad species) for MT, BT, and HT on the Au(111) surface.

Propagation of magnetoacoustic waves in magnetic structures

The cluster Atlante is being used to perform multi-source modelling of wave propagation into realistic magnetic and non-magnetic solar atmospheres for helioseismic purposes. The magnetic atmosphere represents an average sunspot model.

Both atmospheric models were perturbed using two different models of random sources, one of them was masked in height following an isothermal profile and in amplitude following a isomagnetic profile, the other one not. The team found that the unmasked source model gave a realistic wave-field for the quiet sun model and unrealistic results for the sunspot model. The opposite behaviour was found for the masked source model. These numerical results were confirmed recently using SDO/HMI sunspot data by Zhao & Chou (2012). Currently this work continues to its natural 3D extension.

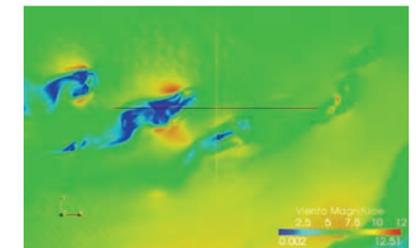


Wave dispersion diagram

Figure shows wave dispersion diagram corresponding to the unmasked multi-source model into the quiet sun atmosphere at photospheric level ( $z_0 = 0$  Mm). The time series interval is 21000 s. The red line is the g-mode dispersion relation.

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, make it essential to use forecasting techniques to try to predict solar radiation. This makes possible to organise 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.



Coastline wind

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 discretisation of the Navier-Stokes equations. To this end, the Code Saturne flow solver was extensively used on Atlante, leading to the assessment of power levels, lift/drag/moment coefficients and stability derivatives needed to design a working prototype in the short term future.

### » Overview

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 centre of the University of Cantabria and CSIC with research lines in astrophysics, high energy physics and distributed computing. It participates in several national and European computing projects.

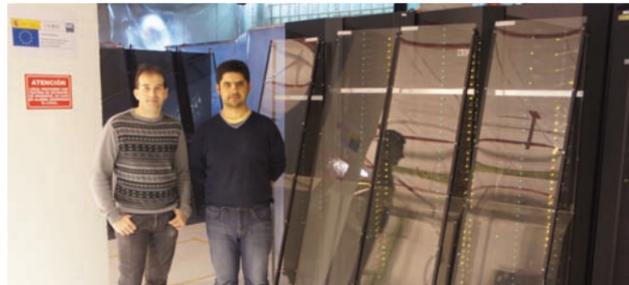
The main research areas of the Computer Architecture Group (ATC) of the University of Cantabria are the analysis, design, and evaluation of parallel computers, covering their principal aspects from programming to the lower hardware levels.

The ALTAMIRA node was upgraded in June 2012 with the installation of a new system at IFCA datacenter room. The system was presented on 3<sup>rd</sup> October 2012.

The current systems in the ALTAMIRA node is composed of 158 IBM-iDataPlex servers interconnected with Mellanox InfiniBand fabric. Also, ALTAMIRA has a small GPU based cluster, with 5 IBM servers, each one with 2 GPU cards, and a cluster with IBM POWER7 blades, with capacity for up to 700 processes to execute intensive CPU applications.

### » Organisational Structure

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



Miguel Angel Nuñez and Luis Cabellos



### » Technical and Scientific Highlights 2012

In 2012 the Altamira node executed applications corresponding to local users at the University of Cantabria with more than 2 millions hours of CPU.

### » Key Publications 2012

- ▶ Falocco, S.; Carrera, F.J.; Corral, A.; Laird, E.; Nandra, K.; Barcons, X.; Page, M.J.; Digby-North, J.; Averaging the AGN X-ray spectra from deep Chandra fields. *Astronomy & Astrophysics*, Volume 538, id.A83, 14 pp.

### » Key Projects 2012

#### Differential expression in Schizophrenia

Led by Jesús Sainz this project aims to find abnormalities in the transcriptome expression of individuals affected by schizophrenia and to characterise the genes modulated by anti-psychotics currently used in the clinic. The goal is to facilitate the design of diagnostic tests and the development of improved treatments of the disease.

#### Genomic characterization of human tumours

Ignacio Varela leads a new research line in IBBTEC (Instituto de Biomedicina y Biotecnología de Cantabria) that uses the newly developed ultrasequencing technologies (NGS) to characterise at the genomic level human and mouse tumours

in order to identify new molecular mechanisms involved on tumour progression and metastasis that could be used as therapeutic targets. This line is at the moment funded by the National Research Plan and a proposal for ERC funding is under evaluation.

Altamira is used for the analysis of the NGS genomic data. This group also provides analysis support for NGS data to several collaborators in different institutions like IFIMAV (Spain), WTSI (UK), LRI (UK) or NCI (US).

#### Constraints on inflationary models of the universe based on CMB

Enrique Martinez leads a Cosmic Microwave Background Radiation (CMB) research group. The CMB represents an essential tool for the research in Modern Cosmology.

There are a large number of ground-based, balloon-borne and satellite experiments both current and planned. The existence of the CMB is a proof of the primordial explosion widely-known as Big-Bang. The anisotropies of the black body radiation temperature measured in different directions of the sky provide valuable information about the primordial epochs of the universe and its evolution.

The standard inflation theory, developed in the 1980's and nowadays widely accepted, predicts that these anisotropies follow very closely a Gaussian distribution. The detection of non-Gaussian deviations in the CMB would have far-reaching consequences for our understanding of the universe.



The ALTAMIRA Supercomputer

### » Overview



The Picasso Supercomputer

Pablo Picasso is a RES node 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. It 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. These include 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 include a virtual 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

The SCBI draws on 15 years of experience of the Computational Laboratory of the University of Málaga in running production supercomputers to support scientific research in several fields. It also incorporates a multidisciplinary 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.



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

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 2012

In 2012, PABLO consolidated the services it offers researchers, providing service to several new users that have still not published but with promising research going forward. Also in 2012, all the resources of the SCBI were updated, and in 2013 these new computer resources will be available to users, with more cores, more disk space and a wider selection of systems. Four different systems will be offered, all under the control of the same queue manager, thereby enabling users to select the one which best matches their research needs.

### » Key Publications 2012 • Please, check the online version of this report to see other publications of Pablo Picasso Node.

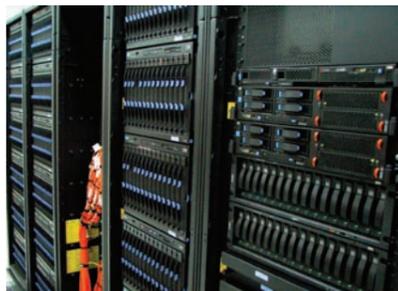
- ▶ Carlos A. Fuentes-Almagro, María-José Prieto-Álamo, Carmen Pueyo, Juan Jurado. Identification Of Proteins Containing Redox-Sensitive Thiols After Prdx1, Prdx3 And Gclc Silencing And/Or Glucose Oxidase Treatment In Hepa 1-6 Cells, *Journal Of Proteomics*, Volume 77, 21 December 2012, Pages 262-279, Issn 1874-3919, 10.1016/j.jprot.2012.08.025. (<http://www.sciencedirect.com/science/article/pii/S187439191200646x>)
- ▶ Aguilar-Melero P, Prieto-Álamo Mj, Jurado J, Holmgren A, Pueyo C. *J Proteomics*. 2013 Feb 21;79:161-71. Doi: 10.1016/j.jprot.2012.12.005. Epub 2012 Dec 28. Proteomics In Hepg2 Hepatocarcinoma Cells With Stably Silenced Expression Of Prdx1.
- ▶ Pablo Ameigeiras, Yuanye Wang, Jorge Navarro-Ortiz, Preben E Mogensen, Juan M Lopez-Soler. Open Access Traffic Models Impact On Ofdma Scheduling Design. *Eurasip Journal On Wireless Communications And Networking*. February 2012, 2012:61.
- ▶ Ameigeiras, P.; Azcona-Rivas, A.; Navarro-Ortiz, J.; Ramos-Munoz, J.J.; Lopez-Soler, J.M., "A Simple Model For Predicting The Number And Duration Of Rebuffering Events For Youtube Flows," *Communications Letters, IEEE*, Vol.16, No.2, Pp.278, 280, February 2012. Doi: 10.1109/Lcomm.2011.121311.111682. Url: <http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&number=6109192&isnumber=6146702>
- ▶ J. Barrios, A. Pietrus, G. Joya, A. Marrero, And H. De Arazoza. A Differential Inclusion Approach For Modelling And Analysis Of Dynamical Systems Under Uncertainty. *Soft Computing - A Fusion Of Foundations, Methodologies And Applications*, Pages 1-15, 2012. Doi: 10.1007/S00500-012-0889-2.
- ▶ Xugang Guo; Jordan Quinn; Zhihua Chen; Hakan Usta; Yan Zheng; Yu Xia; Jonathan Hennek; Rocío Ponce Ortiz; Tobin J. Marks; Antonio Facchetti. Dialkoxibithiazole: A New Building Block For Head-To-Head Polymer Semiconductors. *J. Am. Chem. Soc.* 2013, 135, 1986 – 1996
- ▶ Zhou, Nanjia; Guo, Xugang; Ponce Ortiz, Rocío; Li, Shiqiang; Zhang, Shiming; Chang, Robert P. H.; Facchetti, Antonio; Marks, Tobin. J. Bithiophene Imide And Benzodithiophene Copolymers For Efficient Inverted Solar Cells. *Advanced Materials* 2012, 24, 2242 - 2248.
- ▶ Huang, Hui; Ponce Ortiz, R.; Chen, Zhihua; Newman, Christopher; Usta, Hakan; Lou, Sylvia; Youn, Jangdae; Noh, Yong-Young; Baeg, Kang-Jun; Chen, Lin X.; Facchetti, Antonio; Marks, Tobin. J. Combining Electron-Neutral Building Blocks With Intramolecular "Conformational Locks" Affords Stable, High-Mobility P-And N-Channel Polymer Semiconductors. *J. Am. Chem. Soc.* 2012, 134, 10966-10973.

- ▶ Boudreault, Pierre-Luc; Hennek, Jonathan; Loser, Stephen; Ponce Ortiz, Rocío; Eckstein, Brian; Facchetti, Antonio; Marks, Tobin. J. New Semiconductors Based On 2,2'-Ethyne-1,2-Diylbis[3-(Alk-1-Yn-1-Yl)Thiophene] For Organic Opto-Electronics. *Chem. Mater.* 2012, 24, 2929-2942
- ▶ Ponce Ortiz, R.; Brisset, Hugues; Vidélot-Ackermann, Christine. Perfluoroarene Units In Distyryl-Oligothiophene Analogues: An Efficient Electron Density Confinement Preventing N-Type Transport In Organic Thin Film Transistors. *Synth. Met.* 2012, 162, 857-861.
- ▶ Ponce Ortiz, Rocío; Herrera, Helena; Seoane, Carlos; Segura, José L.; Facchetti, Antonio; Marks, Tobin. J. Rationale Design Of Ambipolar Organic Semiconductors Is Core Planarity Central To Ambipolarity In Thiophene-Naphthalene Semiconductors? *Chem. Eur. J.* 2012, 18, 470-484.
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- ▶ F. Rodríguez-Llansola, D. Hermida-Merino, B. Nieto-Ortega, F.J. Ramírez, J. T. López Navarrete, J. Casado, B. Escuder, W. Hayes, J. F. Miravet. Self-Assembly Studies Of A Chiral Bisurea-Based Superhydrogelator *Chem. Eur. J.* 18, Pág. 14725-14731 (2012)
- ▶ B. Nieto-Ortega, V.J. Nebot, J.F. Miravet, B. Escuder, J.T. López Navarrete, J. Casado, F.J. Ramírez. Vibrational Circular Dichroism Shows Reversible Helical Handedness Switching In Peptidomimetic L-Valine Fibrils *J. Phys. Chem. Lett.* 3, Pág. 2120-2124 (2012)
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- ▶ Xiaozhang Zhu, Hayato Tsuji, Juan T. López Navarrete, Juan Casado, And Eiichi Nakamura. Carbon-Bridged Oligo(Phenylenevinylene)s: Stable -Systems With High Responsiveness To Doping And Excitation *J. Am. Chem. Soc.* 134, Pág. 19254-19259 (2012)
- ▶ R. González-Cano, H. Herrera, J.L. Segura, J. T. Lopez Navarrete, M.C. Ruiz Delgado, J. Casado. Conformational Control Of The Electronic Properties Of An Alpha-Beta Terthiophene: Lessons From A Precursor Towards Dendritic Hyperbranched Oligo- And Polythiophenes. *Chem. Phys. Chem.* 13, Pág. 3893-3900 (2012)
- ▶ T. Pappenfus, K.B. Schliep, A. Dissanayake, T. Ludden, B. Nieto-Ortega, J. T. Lopez Navarrete, M.C. Ruiz Delgado, J. Casado. Organic Materials In The Undergraduate Laboratory: Microscale Synthesis And Investigation Of A Donor-Acceptor Molecule. *J. Chem. Ed.* 89, Pág. 1461-1465 (2012)
- ▶ Julio F. Fernández And Juan J. Alonso. Pair Correlation Function For Spin Glasses. *Phys. Rev. B* 86, 140402(R) – Published 9 October 2012. Url: <http://prb.aps.org/abstract/prb/v86/i14/e140402>. doi: 10.1103/physrevb.86.140402
- ▶ Rafael M. Luque-Baena, Juan M. Ortiz-De-Lazcano-Lobato, Ezequiel López-Rubio, Enrique Domínguez, Esteban J. Palomo. A Competitive Neural Network For Multiple Object Tracking In Video Sequence Analysis. *Neural Process Lett* (2013) 37:47-67 Doi 10.1007/S11063-012-9268-3.
- ▶ Rodrigo Prado Martins, Carmen Aguilar, James E Graham, Ana Carvajal, Rocío Bautista, M. Gonzalo Claros And Juan J Garrido. Pig Infections By Salmonella Enterica Serovar Typhimurium: An Insight Into The Molecular Mechanisms Carried Out In Mesenteric Lymph-Nodes By Host And Pathogen. *Veterinary Research* [http://www.veterinaryresearch.org/Imedia/8372036159073134\\_Article.Pdf](http://www.veterinaryresearch.org/Imedia/8372036159073134_Article.Pdf)

### » Key Projects 2012

2012 was a highly productive year, with numerous publications and very interesting research. One example can be seen in a video made by the physical oceanography research group of the University of Malaga about the Strait of Gibraltar.

## » Overview

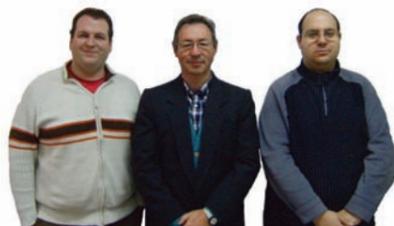


The TIRANT Supercomputer

The RES node located at the University of Valencia was inaugurated in January 2008. The supercomputer's name Tirant refers to the main character in the "Tirant lo Blanc" novel written by a Catalan author Joanot Martorell in 1490. The node is installed in a specially designed data centre and is managed by technicians of the Servei d'Informàtica de la Universitat de València (SIUV). The SIUV has a long experience in managing supercomputers and has been central to the university's efforts in the field of scientific computing since 1978. 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. In December 2012, Tirant was upgraded as a consequence of the installation of MareNostrum III, by virtue of the agreement between RES nodes. Tirant now has 2048 processors and 4 TB of distributed memory.

## » Organisational Structure

Tirant is managed by technicians from SIUV who report to the systems group director and who are responsible for the system management (dealing with hardware problems, installation and configuration of system software) and user support (compiling scientific programs, managing the system queue, solving user problems). The RES access committee is responsible for assigning CPU hours to Tirant users by evaluating new projects. In addition, a local access committee (CARS) receives and evaluates scientific projects from all Valencia and is responsible for the distribution of local hours among them.



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

## » Technical and Scientific Highlights 2012

In 2012, Tirant offered more than 3 million CPU hours, of which 1,25 million (40,5%) hours were used by the scientific community of Valencia, including researchers at the host University. The rest was consumed by RES users.

## » Key Publications 2012

- M. Roca, J.L. Pascual-Ahuir, I. Tuñón. Reversibility and Diffusion in Mandelythiamin Decarboxylation. Searching Dynamical Effects in Decarboxylation Reactions. *Journal of the American Chemical Society*, 134(25), pp 10509–10514, 2012
- J. Aranda, M. Roca, I. Tuñón. Substrate promiscuity in DNA methyltransferase M.Pvull. A mechanistic insight. *Organic & Biomolecular Chemistry*, 10(28), pp 5395–400, 2012
- F. Payri, R. Payri, F.J. Salvador, J. Martínez-López. A contribution to the understanding of cavitation effects in Diesel injector nozzles through a combined experimental and computational investigation. *Computer and Fluids*, vol. 58, 88–101, 2012.

- F. J. Salvador, J. Martínez-López, M. Caballer, C. De Alfonso. Study of the influence of the needle lift on the internal flow and cavitation phenomenon in diesel injector nozzles by CFD using RANS methods. Accepted for publication in *Energy Conversion and Management*, 2012
- A. Pulido, M. Boronat, A. Corma. "Propene epoxidation with H<sub>2</sub>/H<sub>2</sub>O/O<sub>2</sub> mixtures over gold atoms supported on defective graphene: A theoretical study" *Journal of Physical Chemistry C*, 116, 19355–19362, 2012
- M. Boronat, D. Combita, P. Concepción, A. Corma, H. García, R. Juárez, S. Laursen, J. Lopez-Castro. "Making C-C bonds with gold: identification of selective gold sites for homo- and cross-coupling reactions between iodobenzene and alkynes" *Journal of Physical Chemistry C*, 116, 24855–24867, 2012

## Contributed talks and posters 2012

- **Invited talk:** I. Tuñón "Dynamical Effects in Enzymatic Catalysis Advances in Quantum Chemistry: Interfacing Electronic Structure with Dynamics", June 20–22, 2012, University of Minnesota, Minneapolis, USA
- **Poster:** J. Aranda, M. Sanchez-Tarín, M. Roca, I. Tuñón. "Molecular Mechanism and Long Molecular Dynamic Simulation of Taql N6-Adenine-Methyltransferase", ESPA2012, Barcelona, 26–29 Junio 2012
- **Presentation (Oral):** I) Mathematical Modelling in Engineering & Human Behaviour 2011. September 2012. Universitat Politècnica de València, Spain.

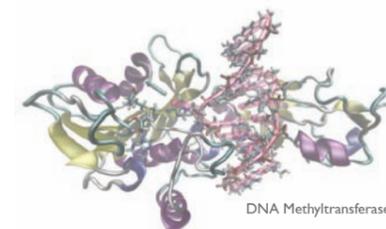
- 2) A. Pulido, M. Boronat, A. Corma. "Propene epoxidation with H<sub>2</sub> and O<sub>2</sub> over gold atoms supported on defective graphene: a theoretical study", GOLD 2012, 6th international conference on gold science technology and its applications. Tokyo.
- **Poster:** S. Laursen, D. Combita, M. Boronat, A. Corma. "Directed design of gold-based heterogeneous catalysts for the Sonogashira coupling reaction from first-principles calculations", ICC 2012, 15<sup>th</sup> International Congress on Catalysis. Munich.

## » Key Projects 2012

**Theoretical study of the DNA methyltransferase family by means of QM/MM simulations** • During 2012, the group led by Ignacio Tuñón undertook a theoretical study of the reaction mechanism that catalyses the enzyme N6 adenine methyltransferase, by means of the exploration of the potential energy surface and the localisation and characterisation of the stationary structures using the hybrid methodology quantum mechanics / molecular mechanics (QM/MM). They performed molecular dynamics simulations (MD) using QM/MM to obtain the potential of mean force and thus calculate the activation barriers. Primary results show that the mechanism of the N6 adenine methyltransferase

consists of the methylation of the adenine N6 and afterwards a hydrogen transfer from this nitrogen to a water molecule.

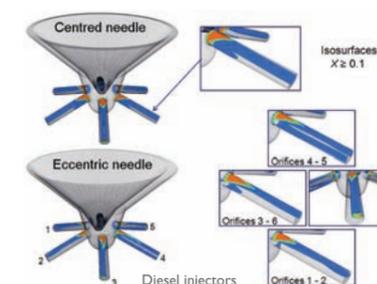
consists of the methylation of the adenine N6 and afterwards a hydrogen transfer from this nitrogen to a water molecule.



DNA Methyltransferase

## » Study of the cavitation phenomena in Diesel injector nozzles

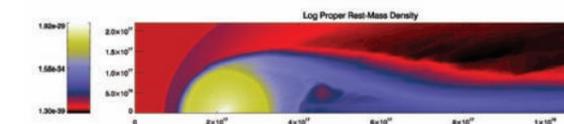
In its third year, the project led by Javier Salvador uses Tirant to simulate the cavitation phenomena in diesel injector nozzles, and continues to obtain new and interesting results. The project studies the influence of the inclination of the diesel injector nozzle holes upon the internal flux on its inner side. The inclination depends on the geometry of the combustion chamber and the results provide practical knowledge as to how this hole inclination modifies the flow injected by the different holes. The project also performed simulations to study the influence of the eccentricity on the flow spread in the holes and in the cavitation pattern.



Diesel injectors

## » Study of detailed physical processes taking place in relativistic jets in Active Galactic Nuclei

The group led by Manel Perucho studied the interaction between a cloud of gas or stellar wind interacting with the jet flow. The objective was to study the mass-load process of the jet, which may lead to deceleration and disruption in the long-term, together with the radiative implications that this interaction may have, mainly in the very-high-energy bands of the spectrum. The results obtained show that the interaction between a supersonic relativistic flow and a gas cloud gives rise to a very strong shock, which propagates through the cloud, increasing its temperature and pressure and thus, its volume. Another set of simulations was used to study the interaction between shock waves in blazars. This work was motivated by the observations of the blazar CTA 102 after a strong radio flare in 2006. The work, included in the PhD thesis of Christian M. Fromm, was defended last January at the University of Bonn, with grade Summa cum Laude.

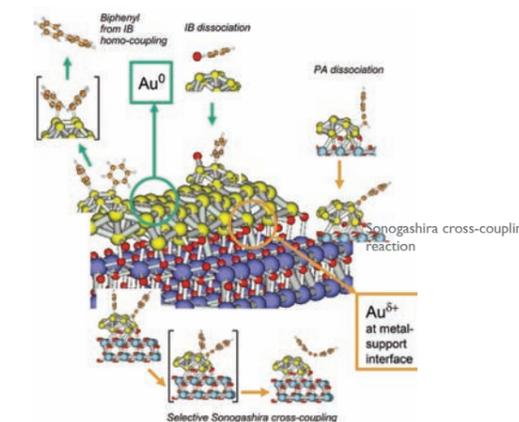


**Study of the Type I myotonic dystrophy** Type I myotonic dystrophy (DMI) is a hereditary multisystem disease. At a molecular level, the DMI is produced by the anomaly expansion of CTG trinucleotides in the 3'-UTR region of DMPK gene. The group led by Ruben Artero studied the macromolecular interaction between RNA and MBNL1 pro-

tein, by means of molecular dynamics simulations. The nanosecond scale simulation allows the observation of common structural patterns that characterize this sequence and give it the ability to interact with MBNL1 protein and also with polyamidic ligands.

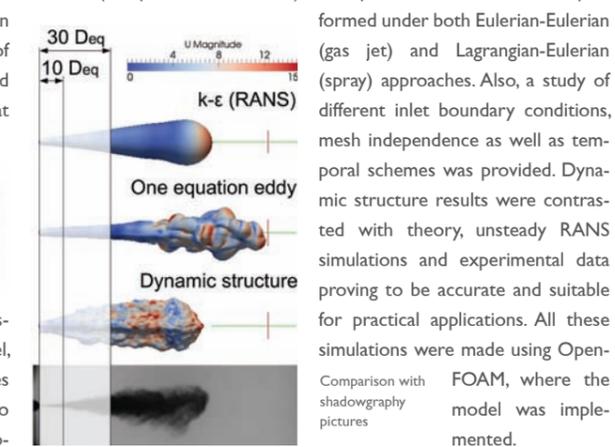
## » Stability and reactivity of gold nanoparticles stabilised by organic ligands

The synthesis of colloidal gold nanoparticles with controlled size and shape is of great interest in several fields such as materials science, biotechnology, and catalysis. The properties of the synthesised gold nanoparticles are influenced by the nature and concentration of the ligands used to stabilise them. In this project, the group led by Mercedes Boronat studied the stability and reactivity of gold nanoparticles passivated by thiolate and citrate ligands, and their performance in several reactions: propene epoxidation, Sonogashira cross-coupling, and oxidation of thiols to disulfide was investigated by means of DFT calculations.



## » Engineering LES of diesel sprays: viscous versus non-viscous models

There is an increasing awareness and concern in society about pollutant emissions. In the case of Diesel engines, there are two problems: soot and NO<sub>x</sub>. It is well known that there exists a direct relation between emissions and instantaneous values of both temperature and fuel concentration fields inside engines. Great efforts both in experimental and theoretical studies of spray atomization and dispersion have been performed in recent years. In this work, the classical LES turbulent models were compared with a non-viscous turbulent model with a specific source term for spray simulations (dynamic structure). The goal is to perform reliable LES of sprays under diesel-like conditions with a low computational cost (comparable with RANS). A comparison of the models was performed under both Eulerian-Eulerian (gas jet) and Lagrangian-Eulerian (spray) approaches. Also, a study of different inlet boundary conditions, mesh independence as well as temporal schemes was provided. Dynamic structure results were contrasted with theory, unsteady RANS simulations and experimental data proving to be accurate and suitable for practical applications. All these simulations were made using Open-



Comparison with shadowgraphy pictures FOAM, where the model was implemented.

### » Overview

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 interdisciplinary 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 2012, the members of the local Access Committee were:

- **Pablo Ibáñez Marín.** Professor at the Computing and Systems Engineering Department and member of the Computer Architecture Group UZ (gaZ)
- **Luis Rández García.** Professor at the Applied Mathematics Department and member of Instituto Universitario de Matemáticas y Aplicaciones UZ (IUMA)
- **Alfonso Tarancón Lafita.** Professor at the Theoretical Physics Department and Director of the Institute of Biocomputation and Physics of Complex Systems UZ (BIFI)

### » Technical and Scientific Highlights 2012

In 2012 CAESARAUGUSTA's local Access Committee granted a total of 13 local projects, running 366.000 hours of CPU time. These activities have produced numerous scientific results and publications.

### » Key Publications 2012

#### Journals

- "Genetic predisposition to early recurrence in clinically localized prostate cancer". Borque A, Del Amo J, Esteban LM, Ars E, Hernández C, Planas J, Arruza A, Llarena R, Palou J, Herranz F, Raventós CX, Tejedor D, Artieda M, Simon L, Martínez A, Carceller E, Suárez M, Allué M, Sanz G, Morote J. *BJU Int.* 2012 Jul 3. doi: 10.1111/j.1464-410X.2012.11333.x
- "Modelos predictivos de recidiva bioquímica en el cáncer de próstata tras tratamiento local". A. Borque Fernando, L. M. Esteban Escaño, G. Sanz Sáiz y L.A. Rioja Sanz. *Validez de los nomogramas. Archivos Españoles de Urología.* 2012; 65 (1)
- "Value of perineural invasion, lymphovascular invasion and multicentricity in radical prostatectomy specimens as a predictors of biochemical relapse in organ-confined prostate cancer" Marta Allué; Angel Borque; Luis Mariano Esteban; Gerardo Sanz; Jokin del Amo; Ricardo Ponz; Juan Morote. *Journal of Urology.* 187 - 4, pp. e595 – e596.2012
- "Postoperative nomogram predicting the probability of biochemical recurrence after radical prostatectomy for prostate cancer", M. Allué; A. Borque; L.M. Esteban; G. Sanz; J. del Amo; R. Ponz; J. Morote. *European Urology Supplements.* 11 - 1, pp. e977 – e977a. 2012
- "Construction of Nomograms for Predicting the Development of Metastases and Biochemical Failure in Cancer of Prostate Treated With Radiation Therapy From Patients of Spanish Cancer Prostate Register (RECAP)", J. Torrecilla; A. Boladeras; M.A. Cabeza; J. Jove; A. Zapatero; L.M. Esteban; I. Henríquez; M. Casaña; C. González; J.L. Mengual. *International Journal of Radiation Oncology Biology Physics.* 84 - 3S, pp. S376 - S377. 2012
- "Ion Movements Responsible of the Dielectric Properties of Na12, K12 and Na4Ca4 A-Zeolites", J. Gracia, M. Escuin, R. Mallada, N. Navascues, J. Santamaría, It's going to be submitted to *Journal of Physical Chemistry C.*
- "Influence of mesh structure on 2D full shallow water equations and SCS cur-

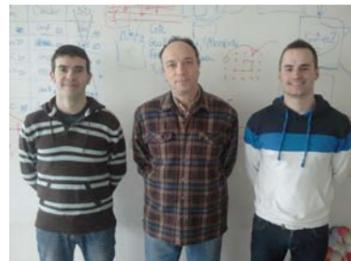
- ve number simulation of rainfall/runoff events", Daniel Caviedes-Voullième, Pilar García-Navarro, Javier Murillo, *Journal of Hydrology, Volumes 448-449, 2 July 2012, Pages 39-59*
- "Preprocess static subdomain decomposition in practical cases of 2D unsteady hydraulic simulation", A. Lacasta, P. García-Navarro, J. Burguete, J. Murillo, *Computers & Fluids, In Press, Available online 29 March 2012*
- "Finite volumes for 2D shallow-water flow with bed-load transport on unstructured grids", Alberto Serrano-Pacheco, Javier Murillo & Pilar García-Navarro, *Journal of Hydraulic Research Volume 50, Issue 2, April 2012, pages 154-163*
- "Wave Riemann description of friction terms in unsteady shallow flows: Application to water and mud/debris floods", J. Murillo, P. García-Navarro, *Journal of Computational Physics, Volume 231, Issue 4, 20, 2012, Pages 1963-2001*
- "A Riemann solver for unsteady computation of 2D shallow flows with variable density", J. Murillo, B. Latorre, P. García-Navarro, *Journal of Computational Physics, Volume 231, Issue 14, 2012, Pages 4775-4807*
- "A large time step 1D upwind explicit scheme (CFL > 1): Application to shallow water equations", M. Morales-Hernandez, P. García-Navarro, J. Murillo, *Journal of Computational Physics, Volume 231, Issue 19, 1 August 2012, Pages 6532-6557*
- "Augmented versions of the HLL and HLLC Riemann solvers including source terms in one and two dimensions for shallow flow applications", J. Murillo, P. García-Navarro, *Journal of Computational Physics, Volume 231, Issue 20, 15 August 2012, Pages 6861-6906*

#### Contributed talks

- "External and internal boundary conditions treatment in a Large Time Step explicit method for river flows", M. Morales-Hernandez; P. García-Navarro, *HIC 2012 - 10th International Conference on Hydroinformatics, Hamburg, Germany, July 2012*



The CAESARAUGUSTA Supercomputer



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

- "Influence of mesh topology and resolution on the rain-runoff simulation with a 2D shallow-water model for a Pyrenean catchment", Caviedes-Voullième, D., García-Navarro, P., Murillo, J., *HIC 2012 - 10th International Conference on Hydroinformatics, Hamburg, Germany, July 2012*
- "A compromise between computational load and refinement criteria in two-dimensional hydraulic simulation: a real case", A. Lacasta, M. González-Sanchis, J. Murillo, P. García-Navarro, *HIC 2012 - 10th International Conference on Hydroinformatics, Hamburg, Germany, July 2012*
- "Flood Lamination Strategy Based on a Three-Flood-Diversion-Area System Management", H. Nouasse; P. Charbonnaud; P. Chiron; J. Murillo; M. Morales; P. García-Navarro; G. Perez, *20th Mediterranean Conference on Control and Automation, Barcelona, June 2012*

### » Key Projects 2012

**Numerical Simulation of Unsteady Free Surface Flows** Pilar García Navarro (UZ). Computational Hydraulics involves the study of free surface flow dynamics using numerical solutions of non-linear equations. 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 consists of replacing equations by numbers so that they provide information on the spatial and temporal evolution of the flow field.

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. The numerical schemes were extended 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.

**Algorithms for combining diagnostic tests that increase the discrimination capacity of predictive models in oncology** Gerardo Sanz (Métodos Estadísticos. UZ). Management of prostate cancer is a complex decision-making issue. Validated and user-friendly predictive tools are extremely convenient in this decision process. In this context, it is important to evaluate the performance of different algorithms to develop better predictive models. The research group analysed the building of models that achieve a greater ability to discriminate between different disease states. In addition, non parametric approaches were implemented in R programming language, and also examined different measures to identify new markers in order to improve models for cancer recurrence.

**Overcoming data suppression in geographical and sectoral information through genetic algorithms** Domingo Pérez Ximénez-de-Embún (UZ). Missing data represents a relevant statistical challenge of research for social scientists. The objective is first, to impute missing numbers for regional data released by the Bureau of Economic analysis, particularly Table 25 (employment by industry), and second, to propose a new method using genetic algorithms and also taking into account a third dimension of information, time trends. In the first stage uncertainty is reduced by a recursive strategy taking into account information of sectoral and spatial dimensions. In the second stage an initial candidate with imputed values is created. In the third stage a genetic algorithm is carried out to obtain an imputed candidate that fulfils all spatial and sectoral constraints besides a minimization of the time deviations. The proposed method leads to consistent missing values imputation.

**Ion Movements Responsible of the Dielectric Properties of Na12, K12 and Na4Ca4 A-Zeolites** J. Gracia, M. Escuin, R. Mallada, N. Navascues, J. Santamaría. (INA, UZ). The project analyses the temperature distribution in Linde Type A Na12, K12 and Na4Ca4 zeolites under MW radiation. Also, Density Functional Theory is used to discern the movements of the most labile cations

- "A Predictive and Transitory Nutrient Uptake Model across Experimental and Numerical Analysis", González-Sanchis, M., Murillo, J., Vermaat, J., Comín, F., García-Navarro, P., *Ecohydraulics 2012, Vienna, Austria, September 2012*
- "Evaluation of the applicability of a coupled model of groundwater and surface flow using field data", Caviedes-Voullième, D., González-Sanchis, M., García-Navarro, P., Murillo, J., González, E., Comín F., *International Conference on Fluvial Hydraulics - River Flow 2012, San Jose, Costa Rica, September 2012*
- "Numerical simulation of groundwater-surface interactions by external coupling of the 3D Richards equation and the full 2D shallow-water equations", Caviedes-Voullième, D., Murillo, J., García-Navarro, P., *XIX Conference on Computational Methods in Water Resources, Urbana-Champaign, Illinois, USA, June 2012*

in model dehydrated Linde Type A Na12, K12 and Na4Ca4 zeolites. For each composition, different relaxation processes were found 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, is described according to transition state theory. The calculated enthalpy barriers,  $\text{Na12} < \text{K12} < \text{Na4Ca4}$ , for the most probable cation jumps are inverse to the heated curves measured under common conditions. Discrepancies between the theoretical and reported experimental activation energies appear due to intermediate compositions or multipart jumps.

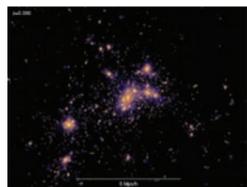
**Large orbital magnetic moment in Pt13 clusters** O. Bunau, J. Bartolomé, F. Bartolomé and L-M. Garcia (ICMA, UZ). Recent experimental data show that small Pt clusters supported in the NaY zeolite are magnetic and show an unexpectedly large orbital moment, the highest ever reported in Pt compounds. An extensive study was performed of Pt13 clusters embedded in a Na-Y zeolite, including structural refinements for various geometries involving the isolated clusters and calculating the corresponding X-ray absorption and magnetic circular dichroism spectra, from the joint perspective of pseudopotential plane waves calculations and real space multiple scattering theory. Taking into account the spin-orbit coupling is shown to improve significantly the previous scalar relativistic results. The ensemble of Pt13 clusters is found to be dominated by a non-magnetic cubeoctahedral geometry. Several isomers were studied which yield a magnetic signature, whose abundance was estimated by direct comparison with the experiment. The orbit and spin contribution to the magnetic moment are disentangled, giving a relative strength of  $0.31 \pm 0.01$ , in excellent agreement with the values extracted on the XMCD spectra. The project therefore provides theoretical proof of the extraordinary orbital magnetization in Pt13 clusters. However, calculations of isolated clusters severely underestimate the total magnetic moment deduced experimentally, which may hint to an electron exchange between the zeolite and the Pt13 particles.

**1 Dimensional Potts Glass** Alfonso Tarancón (BIFI, UZ). This project aims at the simulation of the one dimensional Potts Glass with interactions strength that can be tuned using a parameter, called  $\sigma$ , as function of distance. The key idea is to use the disordered version of the Potts Model (used in diverse fields from Biology to Economics), where interactions between single elements of the model are basically random in nature, and introduces frustration. Single interactions are either drawn from a Bimodal or Gaussian distribution, and are mediated by a quantity that goes proportional to  $r^{-\sigma}$  where  $r$  is the geometrical distance between elements (which are on a line with periodic boundary condition, and hence a ring) and  $\sigma$  is an exponent which can be tuned. Tuning the  $\sigma$  parameter permits access to different versions of the model, from the long range to the nearest neighbours version, and hence by studying the variation of the phase transitions as a function of  $\sigma$ , different behaviours can be observed: mean field, non mean field or anything that happens in between.

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

**Abstract** • The MareNostrum Numerical Cosmology Project (<http://astro.ft.uam.es/marenostrum>) is an international collaboration with the aim of using the exceptional capabilities of the MareNostrum supercomputer 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 for simulations, based on different techniques, SPH (GADGET, GASOLINE) and AMR (ART, RAMSES). All of them are fully MPI+OpenMP parallelised.

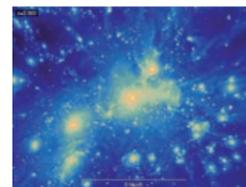
**Results** • During the year 2012 the project extended its study on the structure formation in the Universe at different scales ranging from the very large ones with volumes of billions of light years across (MUSIC project) to our very local neighbourhood in the Universe (CLUES project). More than 15 publications in high impact journals were published during the year 2012. Also, a number of different websites were set up with specific details of the simulations as well as to provide access to the numerical results.



The stellar component of the most massive cluster in the MUSIC database



MUSIC clusters shown in the process of merging

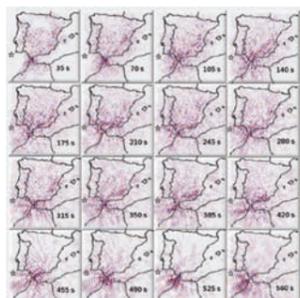


The gas distribution of the most massive cluster in MUSIC database

**Publications** • **How many radio relics await discovery?** Nuza, S. E., Hoefl, M., van Weeren, R. J., Gottlöber, S., and Yepes, G., Monthly Notices of the Royal Astronomical Society, Volume 420, Issue 3, pp. 2006-2019., 420, 2006, 2012 • **CLUES on Fermi-LAT prospects for the extragalactic detection of Mu nu SSM gravitino dark matter**, Gómez-Vargas, G.A., Fornasa, M., Zandanel, F., Cuesta, A.J., Muñoz, C., Prada, F., and Yepes, G., Journal of Cosmology and Astroparticle Physics, Issue 02, article id. 001, pp. (2012)., 2, 1, 2012 • **Modelling the fraction of Lyman break galaxies with strong Lyman emission at  $z \approx 7$** , Forero-Romero, Jaime E., Yepes, Gustavo, Gottlöber, Stefan, and Prada, Francisco, Monthly Notices of the Royal Astronomical Society, Volume 419, Issue 2, pp. 952-958., 419, 952, 2012

• For more related publications, please see the online version of this report

### Time reversal imaging of continuous seismic sources, Daniel Stich, Instituto Andaluz de Geofísica



Snapshots of backpropagating coda waves for the December 17<sup>th</sup> 2009 earthquake in the Atlantic Ocean. Constructive interference in the Gulf of Cadiz and Betic Range can be clearly appreciated for reverse time 140s to 280s. For large reverse times, artefacts dominate the snapshots

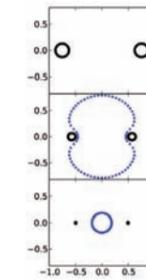
**Abstract** • Most laws in physics, including the elastodynamic wave equation, are time reversal invariant. While the direction of processes in nature is prescribed by the 2nd principle of thermodynamics, in numerical simulations the direction can be inverted. In earthquake seismology, time reversal approaches have been used recently to image characteristics of tectonic earthquakes as well as more exotic seismic sources by numerically back-propagating recorded wavefields. Unlike proper inversion, time reversal needs virtually no a priori assumptions of the processes involved. The project applies time reversal to elucidate the nature of peculiar propagation effects on surface waves in the Gibraltar Arc area, focusing on resonance effects in deep sedimentary basins that act as continuous secondary sources contributing to the complexity in recorded seismograms.

**Results** • Time reversal was applied to different coda wave windows for 5 earthquakes in the Iberia-Maghreb region, with source location in the Atlantic Ocean, Spain and Algeria. Time reversed late surface waves give information on which structural features control regional wave propagation, without any a priori information. The images obtained shows focussing mainly in four regions: The Gulf of Cadiz sedimentary basin, West Alboran sedimentary basin, Gibraltar, and the Betic chain. For Gibraltar and the Betic chain, coherence appears at a late stage of the time reverse simulations, indicating a contribution of delayed direct surface waves from these regions, consistent with lower group velocities identified previously. On the contrary, coherence in deep sedimentary basins appears early in the time reverse simulations, and for earthquakes

for different source region. The project interprets this observation due to prolonged resonance that represents a continuous secondary source of seismic surface waves that become dominant in the wavefield after the direct waves and linear multipathing effects. These secondary surface wavefields appear to be generated at the lateral borders of the sedimentary basins.

for different source region. The project interprets this observation due to prolonged resonance that represents a continuous secondary source of seismic surface waves that become dominant in the wavefield after the direct waves and linear multipathing effects. These secondary surface wavefields appear to be generated at the lateral borders of the sedimentary basins.

### Black hole dynamics in alternative theories of gravity, Helvi Witek, DAMTP, Centre for Mathematical Sciences, University of Cambridge



Snapshots of simulations of a binary black hole system, depicting the BH position (black circles) and the position of the cosmological apparent horizon (blue curves) as seen by an observer at  $r=0$  at different time slices of the numerical evolution

**Abstract** • Formulated by Einstein in 1916, General Relativity passed many stringent tests and is now accepted as the standard theory of gravity. Nevertheless, most experiments can only probe its weak-field regime, while the strong curvature regime remains essentially unexplored. In this regime the dynamics of black holes can sensibly differ from GR, with dramatic and potentially observable effects. A strong motivation to study generic theories of gravity comes from cosmology. Indeed, modified theories of gravity could help to explain cosmological observations. The project seeks to explore the dynamics of BH space-times in modified theories of gravity fully non-linearly, thus investigating these more realistic (cosmological) models, in the highly non-linear, strong-curvature regime.

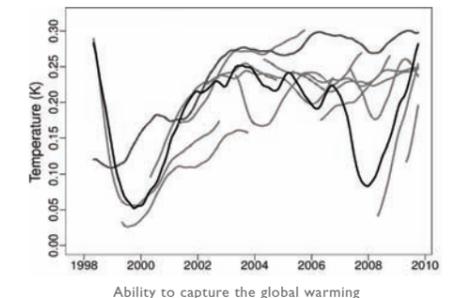
**Results** • Both periods of the present grant were dedicated to extend numerical relativity methods to beyond-gravity theories and cosmological spacetimes in order to study exciting phenomena in these setups in the highly dynamical, strong-field regime. Thanks to BSC-CNS computational resources, the project made significant progress in further developing and testing the numerical code and is the first group to accomplish successful

simulations of single and binary black hole systems in asymptotically deSitter spacetimes. As an example, the attached figure depicts snapshots of a binary BH evolution in asymptotically dS, showing the position of the BHs as well as the cosmological apparent horizon at different time slices of the evolution. Preliminary results were reported in various international conferences and invited seminars and this very fruitful work is expected to continue in the coming year. The help and support of the team at BSC-CNS and the high-performance computing facilities at MareNostrum were invaluable in order to accomplish the presented results.

**Publications** • M.Zilhao, V.Cardoso, L.Gualtieri, C.Herdeiro, U.Sperhake and H.Witek, "Dynamics of black holes in de Sitter spacetimes", Phys. Rev. D85, 104039 (2012)

### Slow down of the global warming in the early XXIst century, Francisco J. Doblas-Reyes, Institut Català de Ciències del Clima

**Abstract** • The observed global mean near-surface temperature underwent a plateau during the early 21<sup>st</sup> century. Most of this global warming slow down has been ascribed to the internally generated climate variability in previous literature. Some authors also suggest a substantial contribution of the minimum in solar activity that occurred in during this period. The project proposes to initialise near-term climate predictions every year from 1995 to 2005 and to compare them to un-initialised counterparts in order to assess the relative contributions of internally generated versus externally forced climate signal to the plateau. The contribution of the solar cycle will then be assessed by performing the same experiments again but applying a constant solar activity in time instead of applying the observed 11-year solar cycle.

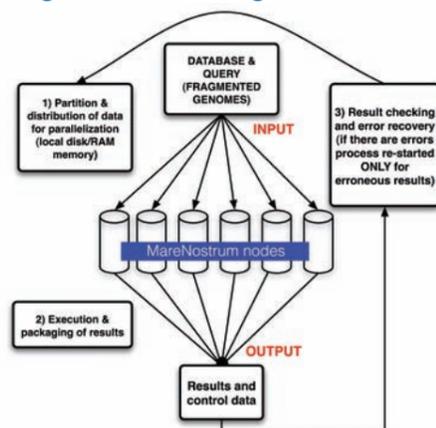


Ability to capture the global warming

**Results** • The Climate Forecasting Unit (CFU) produced retrospective climate predictions initialized every year from 1995 to 2011, in which the global mean near-surface temperature plateau observed in the last decade is reproduced with an error which does not exceed 0.03K in the first three forecast years. This excellent performance of the EC-Earth forecast system was therefore submitted for publication to Nature Climate Change and is currently under revision. Due to the embargo policy on the results published in Nature journals, those results can not be distributed before the online publication. A full report at the end of the next application period will be then provided.

**Publications** • Guemas V., Doblas-Reyes F., Andreu-Burillo I., Asif M., 2013, Retrospective prediction of the global warming slowdown in the last decade, revised for Nature Climate Change, NCLIM-12111103A.

### Use of TBLASTX to find regions of homology among multiple large-size full genomes, Roderic Guigó, Centro de Regulación Genómica



**Abstract** • At the Genome Informatics laboratory (genome.crg.es), part of the "Centro de Regulació Genómica" (CRG) in Barcelona, MareNostrum is used to run the computationally intensive algorithm TBLASTX to find regions of homology (in the form of High-Scoring pairs -HSPs-) between two full genomes (i.e. Mouse vs. Human). Running TBLASTX to find potentially conserved regions between different species is an essential component of the homology-based gene prediction tool SGP which has been developed by the group. Generally, TBLASTX comparison among species with large genomes, such as Human and Mouse, would require 7-10 days on a 20-25 processor grid. However, MareNostrum's processing speed and especially parallelisation potential allows the same work to be performed in approximately 10 hours (on 256 CPUs and excluding queuing time). This is important because it enables execution of

TBLASTX to find homologies among many different genomes at the same time, in a reasonable time frame, which would be impossible to achieve locally or using a smaller computer grid. This, in turn, enables the development and improvement of SGP for large genome species to a level which would be unattainable by using a smaller grid.

**Results** • During the years in which the project utilised MareNostrum, contributions were made to the annotation of several mammalian genomes. Namely, the data generated was used in the pilot phase of the International ENCODE project in order to help identify the functional elements in 1% of the human genome (TBLASTX of Human vs Mouse) and the homology-based gene prediction program SGP was also one of the prediction tools used in the annotating the Cow genome. SGP predictions for several mammalian genome can be found here: <http://genome.ucsc.edu> while locally all SGP-based predictions can be downloaded from: <http://genome.crg.eu/genepredictions>.

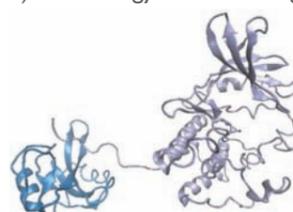
### Modelling Protein-protein interactions in protein kinases with a multiscale molecular dynamics approach, Francesco Luigi Gervasio, Centro Nacional de Investigaciones Oncológicas

**Abstract** • The identification, description and prediction of protein-protein interaction (PPI) is central to both functional and structural biology. A large number of these interactions are transient and lead to continuously forming and dissociating complexes. This complicates the use of structural methods. Moreover, most proteins undergo conformational transitions upon binding, undermining the efforts of developing simple computational methods based on shape complementarity and electrostatics. This is the case of protein-kinases (PK) involved in cell signalling. Here, we propose to study PK protein complexes by using fully solvated all-atom molecular dynamics simulations, free energy methods and a novel coarse-grained approach based on the combination of a structure-based protein potential with a bioinformatics prediction method.

**Results** • "First, we have obtained atomically detailed understanding of the conformational transition and the reference FESs of the two important oncogenic proteins cSRC and CDK2. To that aim we run long (500ns) all-atom explicit solvent molecular dynamics simulations with the Amber 99SB-ILDN\* force field and the code GROMACS 4.0. The free energies were calculated with the Metadynamics/parallel tempering (PT-MetaD) free energy method using the PLUMED plug-in. PT-MetaD is extremely expensive from a computational point of view, as it requires several parallel replicas (28/30 replicas) of the system running at the same time at different temperatures. We tried to use metadynamics without PT, which requires less computational resources, but the resulting free energy surface reconstruction suffered from hysteresis and it was difficult to converge it sufficiently.

The converged free energies were used to fine-tune our coarse-grained potential, which was able to reproduce semi-quantitatively the free energies of the fully atomistic PT-metaD. The results are described in Ref. 1. Using our new coarse-grained force-field we started studying PPI (See figure)."

**Publications** • M. D'Abramo, O. Rabal, J. Oyarzabal, F.L. Gervasio. **Conformational selection vs. induced fit effects in PI3K kinases.** *Angew. Chemie Intl. Ed.*, 51, 642–646, 2012

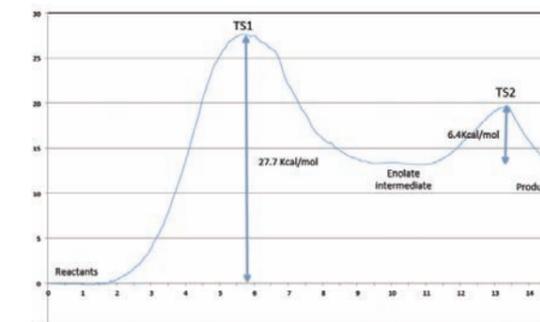


MD simulation performed with our new CG potential showing the SH2 approaching the Src kinase domain. The correct crystallographic position and significant conformational changes are well described by the CG potential

### Simulation of the enzyme reaction mechanism in helicobacter pylori type II 3-dihydroquinase trimer using QM/MD hybrid methods, Federico Gago, Universidad de Alcalá

**Abstract** • By using a combination of classical molecular dynamics simulations in explicit solvent and quantum mechanical calculations in the active site region, the project expects to gain further insight into the catalytic mechanism of Helicobacter pylori type II 3-dihydroquinase. Each of the steps of the reaction will be studied in atomic detail: formation of the Michaelis-Menten complex, formation and stabilization of the transition state (TS), evolution of the TS towards the products of the reaction, and exit of the product. Alternative mechanisms will be explored in order to select the most plausible one.

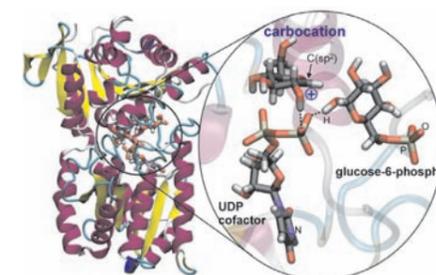
**Results** • Results to date have allowed the project to pinpoint Asp89 as a crucial amino acid for catalysis because the carboxylate on its side chain can act as a Lewis base to withdraw the phenolic proton of Tyr22. At the same time, the guanidinium group of Arg17 that interacts with the ketone acts as a Lewis acid and increases the acidity of the C2-axial proton of shikimic acid. A site-directed mutant has confirmed the prediction and further work (study of isotopic effects) is in progress to support the claims prior to publication.



Energy profile over the reaction coordinate explored during the QM/MM simulations

### The molecular mechanism of trehalose-6-phosphate synthase, 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 glycogen, starch or cellulose (polymers). One of the most puzzling aspects in the field of glycobiology is the catalytic mechanism of glycosyltransferases, the enzymes responsible for the formation of the glycosidic bond. A very unusual mechanism with little chemical precedence ("front-face") has been proposed. Yet the lack of mechanistic insight does not allow to conclude whether this mechanism is feasible in the enzyme environment. In our project we plan to elucidate whether the front-face mechanism is feasible for glycosyltransferases.



Molecular 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

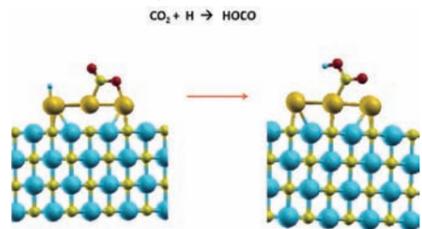
**Results** • By means of ab initio metadynamics dynamics techniques we demonstrated that the "front-face" type mechanism is feasible thanks to the formation of a positively-charged species (a carbocation) with an extremely short half-life that moves quickly from the donor to the acceptor. The modelled enzyme is glycosyltransferase trehalose-6-phosphate synthase (OtsA), which participates in the final synthesis of trehalose, a disaccharide of great importance in nature. Given their absence in mammalian biology, trehalose synthesising and processing enzymes offer attractive inhibition targets. Glycosyltransferases are responsible for the structure of many carbohydrates and, therefore, the knowledge of their mechanism of action will help to modify their function, thereby improving the synthesis of known carbohydrates and new structures. It will also contribute to the design of inhibitors for those GTs that are involved in infectious diseases. The large-scale simulations needed to perform this project were possible only if using high supercomputing facilities such as provided by MareNostrum.

### Publications

- Rojas-Cervellera, V., Ardèvol, A., Boero, M., Planas, A. and Rovira, C. (2013), **Formation of a Covalent Glycosyl-Enzyme Species in a Retaining Glycosyltransferase.** *Chem. Eur. J.* doi: 10.1002/chem. 201302898
- Victor Rojas-Cervellera, Ernest Giralt, and Carme Rovira, Staple Motifs, **Initial Steps in the Formation of Thiolate-Protected Gold Nanoparticles: How Do They Form?** *Inorganic Chemistry* 2012 51 (21), 11422-11429

### Testing Au/TiC as a potential catalyst for CO<sub>2</sub> hydrogenation, Dr. Francesc Illas, Universitat de Barcelona

**Abstract** • Activation of CO<sub>2</sub> is important to reduce the concentration of this greenhouse gas in the earth atmosphere. Heterogeneous catalysis is likely to provide one of the most efficient ways to activate this rather inert molecule and to turn it into a useful chemical. Unfortunately, existing catalysts are not efficient or not active enough to be used on a large scale basis. The project explores the possibility of using a new class of catalysts based on Au nanoparticles supported on TiC as opposed to the common type of metal supported catalysts where supports are made of oxides. By combined use of experiment and theoretical calculations it was shown that Au/TiC systems are active towards hydrodesulfuration reactions as well as to H<sub>2</sub> and O<sub>2</sub> dissociations. The project explores the catalytic activity of Au/TiC systems towards CO<sub>2</sub> hydrogenation to formic acid.



Initial step for CO<sub>2</sub> hydrogenation on a Au/TiC model catalyst

**Results** • The catalytic activity of Au/TiC systems towards CO<sub>2</sub> hydrogenation to formic acid is being explored. COOH and HCOO intermediates found and characterized. Transition state search in progress.

**Publications** • CO<sub>2</sub> Activation and Methanol Synthesis on Au/TiC and Cu/TiC Catalysts: Au-C and Cu-C Interactions and the Effects of Charge Polarization on Chemical Reactivity, A. B. Vidal, L. Feria, J. Evans, Y. Takahashi, P. Liu, K. Nakamura, F. Illas and J. A. Rodriguez, *J. Phys. Chem. Lett.*, 3 (2012) 2275-2280

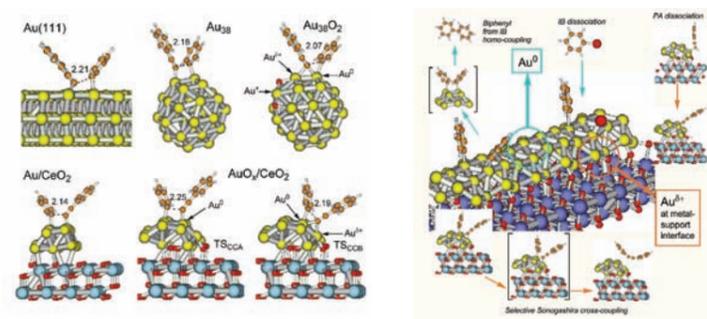
### Gold-catalyzed C-C bond forming reactions: identification of the selective active sites, Avelino Corma Canós, Instituto de Tecnología Química UPV-CSIC

**Abstract** • The Sonogashira coupling between aryl halides and alkynes, typically catalysed by palladium in homogeneous phase, allows to obtain products widely used as intermediates in the synthesis of polymers, natural products and bioactive compounds. It was recently presented that a heterogeneous Au/CeO<sub>2</sub> catalyst is also able to promote this reaction with 89% selectivity towards the desired cross-coupling product, while selectivities obtained with Au/SiO<sub>2</sub> or Au/TiO<sub>2</sub> catalysts are really low, of the order of 20%. A DFT study of the reaction mechanism on different gold catalyst models will allow to establish how the Sonogashira reaction occurs on gold metal nanoparticles, and which are the active and selective sites leading to the desired cross-coupling product.

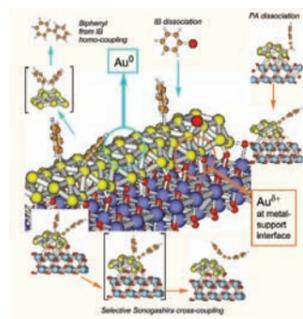
**Results** • The elementary steps involved in the mechanism of the homo- and cross-coupling reactions between IB and PA were investigated with DFT methods on several models containing neutral and cationic gold sites with different coordination number. Calculations show that IB dissociates on metallic Au atoms, the same sites that catalyse undesired IB homo-coupling. PA is activated on both metallic and cationic sites present at the metal-support interface, and the barrier for the desired cross-coupling is lower if both reactants are activated at different sites. This means that the selectivity toward the Sonogashira product is promoted if the catalyst contains both neutral and cationic sites. Several Au/CeO<sub>2</sub> catalysts containing different ratios of metallic/cationic Au sites were synthesized, and the experimental study of their catalytic performance shows that cationic gold plays a key role in the cross-coupling reaction. These conclusions explain the diversity of selectivity results reported in the literature on different gold catalysts, and have driven the synthesis of the most selective heterogeneous gold based catalyst ever reported.

Several Au/CeO<sub>2</sub> catalysts containing different ratios of metallic/cationic Au sites were synthesized, and the experimental study of their catalytic performance shows that cationic gold plays a key role in the cross-coupling reaction. These conclusions explain the diversity of selectivity results reported in the literature on different gold catalysts, and have driven the synthesis of the most selective heterogeneous gold based catalyst ever reported.

**Publications** • Mercedes Boronat, Diego C. Ombita, Patricia Concepción, Avelino Corma, Hermenegildo García, Raquel Juárez, Siris Laursen, Juan de Dios López-Castro. **Making C-C bonds with gold: identification of selective gold sites for homo- and cross-coupling reactions between iodobenzene and alkynes.** *Journal of Physical Chemistry C*, 116, 24855-24867, October 2012

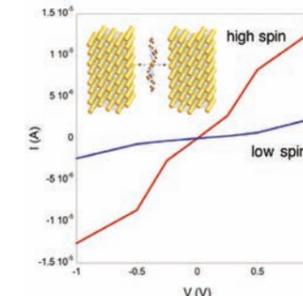


Transition state for the C-C bond forming step over different gold catalysts models



Schematic representation of the different elementary steps in the mechanism of Sonogashira cross-coupling reaction catalyzed by Au nanoparticles supported on CeO<sub>2</sub>

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



Spin Crossover Fe(II) complex sandwiched by two gold electrodes showing the difference of conductivity between the high and low spin states

**Abstract** • Some polynuclear transition metal complexes, known as single molecule magnets (SMM), show a slow relaxation of the magnetization 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. Spin crossover systems show a spin transition usually caused by an external stimuli, such as temperature pressure, light, current and so on. The switch of the magnetic properties causes also different conductivity properties. Theoretical methods using density functional methods allow to understand and rationalize the experimental data and to point out new synthetic targets in these families of magnetic systems.

**Results** • Molecular magnetic systems were considered as an alternative to replace the metal alloys in storage devices such as hard disks. The small size of the molecules in comparison with the domains of the alloys would result in a considerable increase of capacity. Also, the presence of quantum tunnelling in single-molecule magnets has opened the possibility to employ such a system for use as qubits in Quantum Computing.

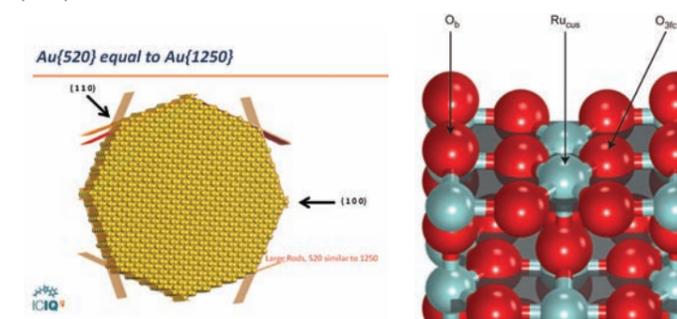
**Publications** • E. Cremades, S. Gomez-Coca, D. Aravena, S. Alvarez, E. Ruiz, "Theoretical Study of Exchange Coupling in 3d-Gd Complexes: Large Magnetocaloric Effect Systems", *J. Am. Chem. Soc.* 2012, 134, 10532-10542 • F. J. Muñoz Lara, A. B. Gaspar, D. Aravena, E. Ruiz, M. C. Muñoz, M. Ohba, R. Ohtani, S. Kitagawa, J. A. Real. "Enhanced bistability by guest inclusion in Fe(II) spin crossover porous coordination polymers", *Chem. Commun.*, 2012, 48, 4686-4688 • G. Magadur, J.-S. Lauret, G. Charron, F. Bouanis, E. Norman, V. Huc, C.-S. Cojocaru, S. Gómez-Coca, E. Ruiz, T. Mallah, "Charge Transfer and Tunable Ambipolar Effect Induced by Assembly of Cu(II) Binuclear Complexes on Carbon Nanotube Field Effect Transistor Devices", *J. Am. Chem. Soc.*, 2012, 134, 7896-7901 • S. Gómez-Coca, E. Ruiz "Exchange coupling and magnetic anisotropy of exchanged-biased quantum tunnelling single-molecule magnet Ni<sub>3</sub>Mn<sub>2</sub> complexes using theoretical methods based on Density Functional Theory" *Dalton Trans.* 2012, 41, 2659-2666 • D. Aravena, E. Ruiz, "Coherent transport through spin-crossover single molecules" *J. Am. Chem. Soc.* 2012, 134, 777-779.

### Growth of Gold Nanoparticles and Nanorods and Wires: DFT Study, Nuria Lopez, ICIQ

**Abstract** • The properties of gold nanoparticles depend on their morphology. The project's goal is to employ DFT to unravel the role of the different compounds employed in the synthetic routes that can provide different morphologies.

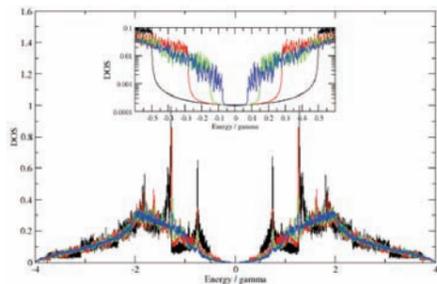
**Results** • The results obtained through DFT were employed to set up a mesosized model by inclusion of the energies as a function of the chemical potential of the surfactant. This was done for the first time and will enable assessment of the differences between different preparations, the role of counter ions and the nature of solvent effects. A publication with these results is being prepared.

**Publications** • G. Novell-Leruth, N. Lopez, in preparation • **In situ surface coverage analysis of RuO<sub>2</sub>-catalysed HCl oxidation reveals the entropic origin of compensation in heterogeneous catalysis.** Detre Teschner, Gerard Novell-Leruth, Ramzi Farra, Axel Knop-Gericke, Robert Schlögl, László Szentmiklósi, Miguel González Hevia, Hary Soerijanto, Reinhard Schomäcker, Javier Pérez-Ramírez, Núria López. *Nature Chemistry* 4, 739-745(2012)



Gold nanoparticles showing the different orientations of potential surface planes

### Charge and Spin Transport in Topological Insulators, Stephan Roche, Catalan Institute of Nanotechnology (ICN) Barcelona



DOS for slabs based upon the Dirac semimetal phase with varying thickness from 6 layers (black), 12 layers (red) to 24 layers (blue)

**Abstract** • This project aims to explore charge and spin mesoscopic transport in disordered topological insulators by using advanced multiscale computational methodologies that will maximally crosslink state-of-the-art ab initio methods and real space order N implementations of Kubo-Greenwood transport methods, accounting for spin-orbit coupling. The elaborated computational strategy will offer unique possibilities for in-depth scrutiny of quantum transport phenomena beyond conventional semi-classical treatments and mean field approaches, allowing quantitative comparison with experiments, and providing guidance for further technological breakthroughs.

**Results** • The influence of surface geometry on the electronic structure of topological insulator films was studied, and it was found that the

low-energy states are localized in the surface layers. The project demonstrated a tunability of the electronic properties by changing the surface termination. This includes both a change of the number and in the position of Dirac cones in the electronic structure which opens new possibilities to study real topological insulators like Bi<sub>2</sub>Se<sub>3</sub> by using simplified models. Localisation phenomena were investigated by examining the extension of the wavefunctions in presence of disorder. This complex problem could only be solved using High-Performance Computing infrastructure. It is found that wavefunctions remain delocalised even for very strong disorder which points towards favourable electronic properties. Finally, the project scrutinised the stability of surface-state spin textures. It was found that the spin polarisation changes with increasing disorder which could be used as a tool to assess the quality of real materials by spin polarized spectroscopy. This leads to fundamental insight into topological insulators a class of materials which holds great promise for diverse future applications.

**Publications** • D. Soriano, F. Ortmann, and S. Roche, “Three-Dimensional Models of Topological Insulator Films: Engineering of Dirac Cone and Robustness of the Spin Texture” *Physical Review Letters* (in press), arXiv: 1210.6534v1 /

### Metal-insulator transition in graphene, Andrey V. Malyshev, Universidad Complutense de Madrid

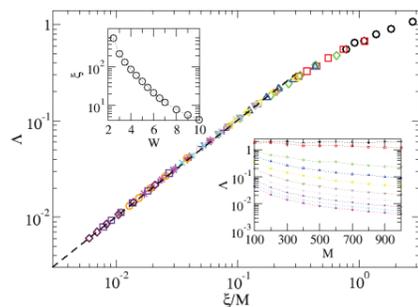
**Abstract** • The main aim of the proposed work is to study theoretically the nature of the electronic states in disordered graphene. This will shed light on the recent debate about the possible existence of the metal-insulator transition

in graphene. It is known that although disorder should lead to localization, in two dimensional systems the sample may appear metallic when too small systems sizes are used. The challenge of this project is to study disordered graphene numerically for large enough system sizes to uncover the true nature of electronic states in graphene.

**Results** • The project modified the standard transfer-matrix method in order to study a truly 2D graphene sample. The TMM determines the localization length LL, but in order to compare systems with different sizes, one investigates the dependence of the reduced localization length  $rLL = LL/M$  on the width M of the system. In the localized regime rLL decreases with M since LL remains finite in the thermodynamic limit. On the other hand, rLL increases for extended states. It is worth noting that one must perform this investigation over the complete energy spectrum of graphene, in order to

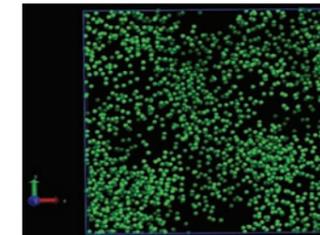
find out whether the MIT takes place at the centre of the band energy or in the tails. This is a large computational task. The results obtained by the use of the RES resources show that sates ographene sheets seem to be localized (for both kind of edges) although certain energy regimes can be identified where the results are clearly inconclusive at present. In order to describe the transmission properties of a system with infinite width, the data was fitted for different sizes in a single curve with the election of a suitable scaling parameter. The presence of one branch is a signature of localised states.

**Publications** • C. González-Santander, F. Domínguez-Adame y R. A. Römer: **Localization of states on graphene-type lattices. Poster awarded by EPL at 8<sup>th</sup> International Workshop on Disordered Systems**, Benasque, Spain 2012 and by Keren Prize at TNT 2012 Trends in Nanotechnology, Madrid, Spain 2012



Scaling function obtained by fitting the results for ZZ at E=0 for disorders W=2 to W=10 and system sizes up to 700x700 atom sites

### Self organization and structure formation in biomimetic active suspensions, Ignacio Pagonabarraga, University of Barcelona



Structures developed by attractive active colloids. The flows induced by their intrinsic activity give rise to evolving and heterogeneous aggregates, with large fluctuations in density

**Abstract** • This project focuses on the study of the basic physical mechanisms which allow active materials to self organise, exploiting a coarse grained approach to face the multiscale nature of these systems with appropriate coupling to the embedding solvent. The project will analyse both the essential features of such spontaneous aggregates as well as their mechanical implications, addressing three different kinds of materials, namely molecular motors, microrobots and wet granulates. The simulations will both analyse the basic properties and performance of ensembles in such systems, and also help to address their impact.

**Results** • The project analysed the interplay between the internal motion of self-propelling particles and their attractions. The emergence of clusters induced by activity was quantified, the relevance of adhesion in favouring the formation of fractal aggregates was identified, and the relevance of internal activity in controlling

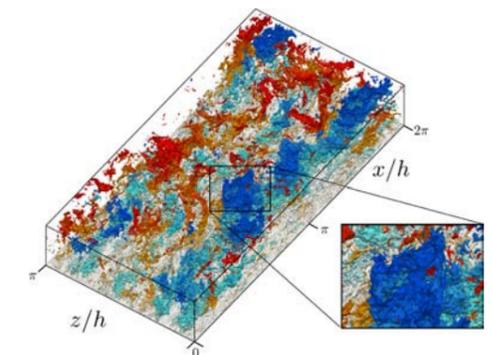
different types of morphologies was clarified, helping to understand experimental results of auto-catalytic colloids and how the hydrodynamic and chemical coupling compete to favour emerging patterns. The cooperative motion of molecular motors and their role in cytoplasmic streaming in plant cells was also analysed, giving insight to tune and control the transport of minute quantities of liquids at the microscale of active matter.

**Publications** • I. Pagonabarraga, **Adsorbed colloids relax slowly**, *Journal: Nature Materials* 11, 99 (2012) • P. Magaretti, I. Pagonabarraga and D. Frenkel, **Running faster together: large hydrodynamic coupling of molecular stepping motors**, *Journal: Phys. Rev. Lett.* 109, 168101 (2012) • F. Alarcon and I. Pagonabarraga, **Spontaneous aggregation and global polar ordering in squirming suspensions**, *Journal: J. Mol. Liq.* (in press) • I. Llopis, I. Pagonabarraga, M. Consentino-Lagomarsino and C.P. Lowe, **Cooperative motion of intrinsic and semiflexible swimmers**, *Phys. Rev. E* 87, 032720 (2013) • I. Pagonabarraga, I. Llopis, **The structure and rheology of sheared model swimmer suspensions**, *Soft Matter* 9, 7174 (2013)

### Time-resolved evolution of vorticity and momentum cascades in turbulent channels, Javier Jiménez Sendin, School of Aeronautics, Universidad Politécnica Madrid, Spain

**Abstract** • In recent years, the dynamics of the buffer layer of wall-bounded turbulent flows have been reasonably well understood. Different models have been proposed to explain the logarithmic region, but some of them are in disagreement from the dynamical point of view. The project's goal is the study of the temporal evolution of coherent structures in a turbulent channel with  $Re_{\tau} = 4000$ , using DNSes sequences with temporal separations among fields short enough for individual structures to be tracked. Special attention will be paid to the dynamics of the structures, and their relation with a physical direct and inverse cascade.

**Results** • The temporal evolution of eddies in a turbulent channel was studied using time-resolved direct numerical simulation data at  $Re_{\tau} = 4000$ . Eddies are born at all distances from the wall, although with higher probability near it, where the shear is strongest. Most of them stay small and do not last long. However, one family of eddies becomes large enough to attach to the wall while they reach into the logarithmic layer. They are geometrically self-similar with sizes and lifetimes proportional to their distance from the wall. Eddies associated with ejections move away from the wall, and their base attaches early in their lives. Conversely, sweeps move towards the wall and attach later. Both remain attached for 2/3 of their lives. In the streamwise direction, eddies are advected and sheared by the local mean velocity. The methodology has proven very promising.



Ejections (cold) and sweeps (hot) in a turbulent channel

**Publications** • “Dynamics of wall-bounded turbulence”, J. Jiménez and G. Kawahara, chapter in Ten chapters in turbulence (P.A. Davidson, Y. Kaneda & K.R. Sreenivasan, eds.), Cambridge U. Press, pp. 221–268, January (2013) • “Direct numerical simulations of wake-perturbed separated boundary layers”, A.G. Gungor, M.P., Simens and J. Jiménez, *ASME J. Turbomach.*, 134, 061024 (2012) • “A code for direct numerical simulation of turbulent boundary layers at high Reynolds numbers in BG/P supercomputers”, G. Borrelli, J.A. Sillero and J. Jiménez, *Computers and Fluids*, 80, 37–43 (2013), DOI: 10.1016/j.compfluid.2012.07.004

## » Astronomy, Space & Earth Sciences

### Highlighted Projects

- » **Black hole dynamics in alternative theories of gravity** -Helvi Witek, DAMTP, Centre for Mathematical Sciences, University of Cambridge
- » **Slow down of the global warming in the early XXIst century** -Francisco J. Doblas-Reyes, Institut Català de Ciències del Clima
- » **The Marenostro Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe** -Gustavo Yepes, Universidad Autonoma de Madrid
- » **Time reversal imaging of continuous seismic sources** -Daniel Stich, Instituto Andaluz de Geofísica

### 2012 Projects

- » **Black-holes in non-asymptotically flat spacetimes** -Ulrich Sperhake, CSIC-IEEC Barcelona
- » Building an improved catalog of gravitational waves from neutron star mergers -Jose Antonio Font Roda, Universidad de Valencia
- » **Calibrating high order finite difference methods for evolving black hole binaries** -Sascha Husa, Universitat de les Illes Balears
- » **Chemical Evolution of the Universe** -Patricia Tissera, Instituto de Astrofísica de Andalucía
- » **Constraints on inflationary models of the universe based on CMB data** -Enrique Martínez Gonzalez, Instituto de Física de Cantabria
- » **Constraints on inflationary models of the universe based on CMB data** -Enrique Martínez Gonzalez, Instituto de Física de Cantabria
- » **Coupling wave-current-sediment transport (ROMS-SWAN) models in a high resolution coastal area.** -Manel Grifoll, LIM/UPC
- » **Coupling WRF to a wave model through a joint sea surface roughness description** -Agustín Sánchez-Arcilla, Laboratori d'Enginyeria Marítima (LIM), Universitat Politècnica de Catalunya (UPC)
- » **Gaia: Simulation of Telemetry Stream** -Jordi Torra i Roca, Universitat de Barcelona (UB), Departament d'Astronomia i Meteorologia
- » **GALACTICA: GALaxies interACTing In a Cosmological hAbitat** -Rosa Domínguez, Univ Autonoma Madrid
- » **Impact of Charge and Spin on Black-Hole Collisions** -Ulrich Sperhake, CSIC-IEEC Barcelona
- » **Impact of Solar Forcing on Future Climate Change Using a Chemistry Climate Model** -Natalia Calvo Fernández, Universidad Complutense de Madrid
- » **Implementation of a High-Res Ensemble Kalman Filter for the Wetern Mediterranean** -Victor Homar Santaner, Universitat de les Illes Balears
- » **Light scattering properties of nonspherical atmospheric aerosols for radiative transfer applications: the ALFA database (extension)** -Francisco José Olmo Reyes, University of Granada
- » **Light scattering properties of nonspherical particles for radiative transfer applications: the ALFA database (extension 2)** -Francisco José Olmo Reyes, University of Granada
- » **Magneto-convection and wave simulations of solar and stellar atmospheres** -Elena Khomenko, Instituto de Astrofísica de Canarias
- » **Mesoscale atmospheric reanalysis IPRA using 3DVAR over the Iberian Peninsula** -Jon Saenz, UPV/EHU
- » **Methods for evolving black hole binaries** -Sascha Husa, Universitat de les Illes Balears
- » **Numerical simulations of black-hole dynamics for use in experiment and observation** -Ulrich Sperhake, CSIC-IEEC Barcelona
- » **Radiative MHD shocks in density structured accretion streams of classical T Tauri stars** -Salvatore Orlando, INAF - Osservatorio Astronomico di Palermo
- » **Relativistic extragalactic jets: Interaction with stellar winds** -Manel Peruchó Pla, Universitat de València
- » **Relativistic Outflows: Dynamics, mass-load and high-energy emission** -Manel Peruchó Pla, Universitat de Valencia
- » **Sea ice initial conditions for seasonal to decadal predictions** -Francisco J. Doblas-Reyes, Institut Català de Ciències del Clima
- » **Simulations of dynamics of partially ionized solar atmosphere** -Elena Khomenko, Instituto de Astrofísica de Canarias
- » **Superradiant instabilities in astrophysical systems** -Helvi Witek, DAMTP, Centre for Mathematical Sciences, University of Cambridge
- » **The Chemical Evolution of the Universe** -Patricia Tissera, Instituto de Astrofísica de Andalucía
- » **The link between multidimensional and spherically symmetric simulations: characterization of convection in 3D and the role of the chemical composition and stellar mass on mixing in classical novae** -Jordi José, UPC
- » **The sizes of massive galaxies from redshift 2.5 to the present** -Marc Balcells, IAC/ING

## » Biology and Life Sciences

### Highlighted Projects

- » **Modelling Protein-protein interactions in protein kinases with a multiscale molecular dynamics approach.** -Francesco Luigi Gervasio, Centro Nacional de Investigaciones Oncológicas
- » **Simulation of the enzyme reaction mechanism in helicobacter pylori type II 3-dihydroquinase trimer using QM/MD hybrid methods** -Federico Gago, Universidad de Alcalá
- » **The molecular mechanism of trehalose-6-phosphate synthase** -Carme Rovira, Parc Científic de Barcelona
- » **Use of TBLASTX to find regions of homology among multiple large-size full genomes** -Roderic Guigó, Centro de Regulación Genómica

### 2012 Projects

- » **Amphipathic helices discovery on Mycoplasma genitalium glycosyltransferase structure by means of explicit membrane molecular dynamics simulations.** -Antoni Planas, Laboratory of Biochemistry, IQS - Universitat Ramon Llull
- » **Catalytic mechanism of the Complex II family enzyme Succinate:quinone oxidoreductase (SQR)** -Marcel Swart, Universidad de Girona

- » **Diversity, distributions and function in aquatic microbes investigated with next-generation sequencing technologies** -Ramiro Logares-Haurie, Instituto de Ciencias del Mar, CMIMA, CSIC
- » **Evidence of Conformational Selection in a Glycosyltransferase Structure?** -Antoni Planas, Laboratory of Biochemistry, IQS - Universitat Ramon Llull
- » **Exploring a 3D model of N- and C-Terminal regions of CPTI proteins** -Carme Rovira, Parc Científic de Barcelona
- » **Exploring a novel non-competitive inhibition mechanism of GSK3: Allosteric regulation by the marine compound palinurin** -Fco. Javier Luque Garriga, Faculty of Pharmacy, University of Barcelona
- » **Generating a design space for somitogenesis** -James Sharpe, Center for Genomic Regulation
- » **Identification of genes involved in Parkinson's disease and essential tremor phenotypical spectrum** -Pau Pastor, CIMA
- » **Mechanistic insight into N-glycan processing by ab initio metadynamics** -Carme Rovira, Parc Científic de Barcelona
- » **Multi-scale Simulations of Derivatized Carbon Nanotubes - Interactions with Membranes, Water and Ions** -Mark S.P. Sansom, Oxford University (Biochemistry Department)
- » **Reverse-engineering embryo segmentation patterning in flies: exploring different scenarios** -Johannes Jaeger, EMBL/CRG Research Unit in Systems Biology
- » **Reverse-engineering mutant gene regulatory networks in Drosophila** -Johannes Jaeger, EMBL/CRG Research Unit in Systems Biology
- » **Structure-based drug design studies against influenza A virus** -Fco. Javier Luque Garriga, Faculty of Pharmacy, University of Barcelona
- » **Study of the transport properties of nanotubes in solution and lipid bilayers** -Rebeca García Fandiño, Universidad de Santiago de Compostela
- » **Targeting the Dimerization Interface of Leishmania Trypanothione Reductase in the Search for New Drugs** -Federico Gago, Universidad de Alcalá
- » **The structure and dynamics of neuropeptides in cell membranes** -Slawomir Filipek, University of Warsaw, Faculty of Chemistry
- » **Transmembrane Ion Transport through alpha, gamma-Peptide Nanotubes** -Rebeca García Fandiño, Universidad de Santiago de Compostela
- » **Virtual Screening towards the Discovery of Pharmacological Chaperons with Therapeutic Potential for Retinitis Pigmentosa** -Francesca Fanelli, University of Modena and Reggio Emilia

## » Chemistry and Material Sciences

### Highlighted Projects

- » **Gold-catalyzed C-C bond forming reactions: identification of the selective active sites** -Avelino Corma Canós, Instituto de Tecnología Química UPV-CSIC
- » **Growth of Gold Nanoparticles and Nanorods and Wires: DFT Study** -Nuria Lopez, ICIQ
- » **Single-Molecule Magnets: Magnetism on Surfaces and Quantum Transport** -Ei-seo RUIZ, Universitat de Barcelona
- » **Testing Au/TiC as a potential catalyst for CO2 hydrogenation** -Francesc Illas, Universitat de Barcelona

### 2012 Projects

- » **1,3-dipolar cycloaddition of azomethine ylide to graphene sheets** -Josep M. Luis, Universitat de Girona
- » **A study of the supramolecular structures of a chiral regioregular poly thiophene, and the role-playing between the solvent and the metal effects on the formation of chiral aggregates** -Joan Torras Costa, UPC
- » **Ab initio metadynamics simulations of the binding of peptides to gold nanoparticles** -Carme Rovira, Parc Científic de Barcelona
- » **Ab Initio Molecular Dynamics Study of** -Luis Rodriguez, UAB
- » **Ab initio molecular dynamics study of aqueous non polar species close to a graphene sheet** -Elvira Guardia, UPC
- » **Ab initio study of organic molecule solvation by ionic liquids** -Thomas Schafer, POLYMAT, UPV/EHU
- » **Accurate methods for the theoretical prediction of polymorphic crystalline materials of technological interest: magnetic materials having bi-stable properties** -Juan Jose Novoa Vide, University of Barcelona
- » **Catalysis modeling: gold nanoparticles supported on yttrium modified anatase as efficient WGS and CO oxidation catalysts** -Javier Fdez Sanz, Universidad de Sevilla
- » **Computer Modeling to Gain an Atomistic Insight into the Energy Storage Processes Mediated by Ceria** -Konstantin NEYMAN, Departament de Química Física, Universitat de Barcelona
- » **CPMD study of the crystal thermal effects on the NCBDTA magnetic crystal: Vibrational thermal effect or phase transition?** -Juan Jose Novoa Vide, University of Barcelona
- » **Characterizing the non-covalent interactions at play in the molecular recognition processes** -Jose Andres Fernandez, Universidad del País Vasco
- » **De novo design of enzymes** -Kendall N. Houk, University of California, Los Angeles (UCLA), Department of Chemistry and Biochemistry
- » **Defects mediated enhancement of TiO2 photocatalysis in the visible range: understanding of the wet electron states by ab initio techniques** -Angel Rubio, University of the Basque Country UPV/EHU
- » **Design and Characterization of Advanced Photovoltaic Materials with High Efficiency** -Perla Wahnón, Universidad Politécnica de Madrid
- » **Design of new catalysts for methanol synthesis: performance of Au/TiC** -Francesc Illas, Universitat de Barcelona
- » **Dynamics and formation processes of defect complexes in magnesium oxide from first-principles order-N simulations** -Oscar Paz, ICMA-B-CSIC
- » **Electronic Properties of CdSe Quantum Dots Used as Light Captors in Sensitized Solar Cells** -Javier Fdez Sanz, Universidad de Sevilla
- » **Equilibrium properties of Silicon Quantum dots for Solar Cells Application: Study of diameters and dopants (EU project FP7-NMP-245977)** -Albert Cirera Hernández, Universitat de Barcelona
- » **First principles investigation of Ni/ceria nanocatalysts for water-gas shift reaction** -Maria Verónica Ganduglia-Pirovano, Instituto de Catalis y Petroleoquímica, CSIC

- » **First principles study of the Supramolecular assembly of conductive 1D Pt-based structures** -Angel Rubio, University of the Basque Country UPV/EHU
- » **First-principles Forces and Currents to characterize carbon nanostructures and oxide surfaces** -Ruben Perez, Universidad Autónoma de Madrid
- » **First-principles scanning probe calculations for the characterization of intermolecular interactions and the charge distribution at the atomic scale** -Rubén Pérez, Universidad Autónoma de Madrid
- » **First-principles studies of two-dimensional electron gases in complex oxides superlattices** -Javier Junquera, Universidad de Cantabria
- » **Formation and stabilization of electropores in cell membranes: a Molecular Dynamics study** -Ramon Reigada, University of Barcelona
- » **FP7-NMP-245977:Equilibrium and Transport Properties of Silicon Quantum Dots for Tandem Solar Cells** -Albert Cirera Hernández, Universitat de Barcelona
- » **Gold-catalyzed C-C bond forming reactions: identification of active sites for phenylacetylene homocoupling in homogeneous and heterogeneous gold catalysts** -Avelino Corma Canós, Instituto de Tecnología Química UPV-CSIC
- » **Graphene heterostructures with 2D nanosheets** -Miguel Pruneda, CIN2 (CSIC-ICN)
- » **Graphene supported gold catalysts for propene epoxidation with molecular O<sub>2</sub>** - Mercedes Boronat, Instituto de Tecnología Química UPV-CSIC
- » **Ice crystallization** -Carlos Vega, Universidad Complutense de Madrid, Fac.Ciencias Químicas, Dep.Química Física I
- » **Interplay between local interface chemistry and longer-range structure** -Emilio Artacho, University of Cambridge
- » **Investigation of the non-Einstein decrease of viscosity in nanocomposite materials** -Florian Müller-Plathe, Technische Universität Darmstadt
- » **Ketonic decarboxylation over metal oxides: MgO and ZrO<sub>2</sub>** -Mercedes Boronat, Instituto de Tecnología Química UPV-CSIC
- » **Low cost new materials for energy storage systems** -Elena Arroyo, Universidad Complutense de Madrid
- » **Magnetism and Transport Properties of Magnetic Molecules on Surfaces and Nanostructured Systems** -Eliseo RUIZ, Universitat de Barcelona
- » **Modeling dynamic materials: the case of a solvent-responsive coordination cage** -Agustí Lledós, UAB
- » **Modelling Ni/ceria systems as potential water-gas shift catalysts for hydrogen production** -Maria Veronica Ganduglia-Pirovano, Instituto de Catalis y Petroleoquímica, CSIC
- » **Molecular design of high-grade nonlinear optical materials: alkides and electrides** -Heribert Reis, National Hellenic Research Foundation
- » **Optical response of silver nanoparticles to femto- and attosecond pulses: the role of the nanoparticle size and geometry** -Angel Rubio, University of the Basque Country UPV/EHU
- » **Optical response, excitons and electronic correlations in TiO<sub>2</sub> nanomaterials: novel insights from a fully ab-initio many-body perturbation theory approach** -Angel Rubio, University of the Basque Country UPV/EHU
- » **Optical, electronic and dynamical properties of confined water in carbon nanotubes** -Alejandro Perez Paz, Universidad del Pais Vasco UPV/EHU
- » **Palladium-catalyzed oxidations in water** -Gregori Ujaque, UAB
- » **Phosphine dissociation from Grubbs' catalysts in toluene: an explicit solvent ab initio molecular dynamics modeling** -Agustí Lledós, UAB
- » **Photofragmentation of amino acids and nucleobases using quantum molecular dynamics** -Yang Wang, UAM
- » **PNOF theory:Towards biological applications** -Jesus Mari Ugalde Uribe-txeberria, UPV/EHU
- » **Properties of epitaxial graphene on Ru(0001)** -Manuel Alcamí, UAM
- » **QM/MM metadynamics Studies on the beta-Galactosidase Catalytic Mechanism** -J. J. Barbero, CIB
- » **Quantitative prediction of Charge Density Wave instabilities in low dimensionality crystals** -Pablo Ordejón, CIN2 (CSIC-ICN)
- » **Quantum nonlocal effects in plasmonic nanostructures: bridging the gap between fully atomistic approaches and the classical descriptions of their electronic response** -Angel Rubio, University of the Basque Country UPV/EHU
- » **Reversal of spin-state preferences** -Marcel Swart, Universidad de Girona
- » **Role of hopanoids in the mechanical properties of model bacterial membranes and function of mechanosensitive channels** -Juan Manuel Vanegas, Universitat Politècnica de Catalunya
- » **Ru-catalyzed hydrogen transfer reactions in water** -Gregori Ujaque, UAB
- » **Search for a silver based selective catalyst for propylene epoxidation with molecular O<sub>2</sub>** -Mercedes Boronat, Instituto de Tecnología Química UPV-CSIC
- » **Selective inactivation of one catalytic site in the the double-strand DNA cleaver homing endonuclease I-Dmol** -Antonio Sánchez Torralba, Centro Nacional de Investigaciones Oncológicas
- » **Self-assembly ofTCNQ and TCNQ derivatives on Graphene and metal surfaces** -Manuel Alcamí, UAM
- » **Simulations of chemical reactions of diverse interest** -F.Javier Aoz, Universidad Complutense de Madrid
- » **Structure and reactivity of silicate nanoparticles** -Stefan Bromley, Universitat de Barcelona
- » **Structures, energetics, and phase transitions of self-assembled monolayers of alkylthiolates on various metal surfaces** -Yang Wang, UAM
- » **Study of reactivity and regioselectivity of La@C<sub>2v</sub>(9)-C<sub>82</sub>** -Marcel Swart, Universidad de Girona
- » **Tailoring molecular reactivity on monolayers of Cu adsorbed on Ru(0001)** -Yang Wang, UAM
- » **Theoretical Characterization of the optimized geometry and energy levels in an hybrid nanostructure** -Pablo Palacios Clemente, Universidad Politécnica de Madrid
- » **Towards a novel "oxide electronics": ab initio many body calculation of the electronic properties of interfaces between transition metal oxides** -Angel Rubio, University of the Basque Country UPV/EHU
- » **Towards catalysts of new generation:Active sites of ionic Pt in nanostructured ceria** -Konstantin NEYMAN, Departament de Química Física, Universitat de Barcelona
- » **Tuning of inversion degree and band gap control in MgIn<sub>2</sub>S<sub>4</sub> and CdIn<sub>2</sub>S<sub>4</sub> thio-spinels** -Pablo Palacios Clemente, Universidad Politécnica de Madrid
- » **Understanding the dynamics of water-silicate interactions at the nanoscale** -Stefan Bromley, Universitat de Barcelona

## » Physics and Engineering

### Highlighted Projects

- » **Charge and Spin Transport in Topological Insulators** - Stephan Roche, Catalan Institute of Nanotechnology (ICN) Barcelona
- » **Metal-insulator transition in graphene** - Andrey V. Malyshev, Universidad Complutense de Madrid
- » **Self organization and structure formation in biomimetic active suspensions** - Ignacio Pagonabarraga, University of Barcelona
- » **Time-resolved evolution of vorticity and momentum cascades in turbulent channels** - Javier Jiménez Sendin, School of Aeronautics, Universidad Politécnica Madrid, 28040-Madrid, Spain

### 2012 Projects

- » **Ab initio calculation of linear responses in graphene nanostructures** - Francisco Javier García de Abajo, Instituto de Optica - CSIC
- » **Ab-initio study of electronic and optical properties of metal-free dyes on ZnO substrate for dye-sensitized solar cells** - Umberto De Giovannini, University of the Basque Country
- » **Analysing the parallel capabilities of HySEA multi-GPU solver.Application to the simulation of tsunamis generated by landslides** - Manuel Jesús Castro Díaz,
- » **Anisotropic Heisenberg spin-glasses on the GPU** -Victor Martin Mayor, Universidad Complutense de Madrid
- » **Calculation of the thermoelectric properties of the SrZrO<sub>3</sub>(5)/SrRuO<sub>3</sub>(1) heterostructure and its variation with temperature** - Javier Junquera, Universidad de Cantabria
- » **Disconnected contributions for the eta' and the nucleon form factors from GPU's** - Alexandrou, University of Cyprus
- » **Dynamic structure factor of Bulk Metallic Glasses determined by Molecular Dynamics simulation** - Daniel Crespo, Universitat Politècnica de Catalunya
- » **Dynamics of turbulent transport in tokamaks and stellarators** - Luis Raul Sánchez Fernández, Universidad Carlos III de Madrid
- » **Electromagnetic and Gravitational Emissions from Compact Objects** - Milton Ruiz, University of the Balearic Islands
- » **Exploring new frontiers in turbulent natural convection flows** - Assensi Oliva, Universitat Politècnica de Catalunya
- » **Extending parallel capabilities of the general purpose Kratos Solver** - Riccardo Rossi, CIMNE
- » **Extending Parallel CFD capabilities of Kratos, a general purpose FE solver.** - Riccardo Rossi, CIMNE
- » **Fast ignition of inertial fusion targets** - Javier Honrubia, Universidad Politécnica de Madrid
- » **First principles calculation of the thermoelectric properties of electron-doped SrTiO<sub>3</sub> and hole-doped LaRhO<sub>3</sub> in thin-film configuration** - Javier Junquera Universidad de Cantabria
- » **Flavour Physics from Mixed-action Lattice QCD** - Pilar Hernández Gamazo, Instituto de Física Corpuscular-Universidad de Valencia
- » **Hybrid substructuring domain decomposition methods for computational fusion** - Santiago Badia, Universitat Politècnica de Catalunya & Centre Internacional de Mètodes Numèrics en Enginyeria
- » **Interface engineering in multifunctional oxides** - Jorge Iniguez, Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC)
- » **Massively parallel Smoothed Particle Hydrodynamics scheme using GPU clusters** - Ramon Gómez Gesteira, Universidade de Vigo
- » **Molecular dynamics simulations of the sintering and coalescence of CuAg core-shell nanoparticles** - Christian Lorenz, Kings College London
- » **New CG-type Eigensolvers in the SLEPc Library** - Jose E. Roman, Universidad Politécnica de Valencia
- » **Nuclear and electron dynamics in diatomic molecules probed with attosecond pulse trains and infrared pulses** - Fernando Martin, UAM
- » **Numerical simulations of massive separated flows: flow over a stalled NACA airfoil** - Assensi Oliva, Universitat Politècnica de Catalunya
- » **Numerical study of disordered localized electronic systems using energy minimization** - Matteo Palassini, Universitat de Barcelona
- » **Phase-field modeling of fracture in ferroelectric ceramics** - Irene Arias, Universitat Politècnica de Catalunya
- » **Physical mechanisms involved in transport and in confinement transitions in plasmas** - Luis García Gonzalo, Universidad Carlos III de Madrid
- » **SAIL: lighth quark mass dependence of two-hadron energies in Lattice QCD** - Assumpta Parreno García, University of Barcelona
- » **Scalable and Dynamic Performance Tuning for Large-Scale Parallel Applications** - Anna Sikora, Departamento de Arquitectura de Computadores y Sistemas Operativos, Universidad Autónoma de Barcelona.
- » **Scaled Attosecond Physics** - Carles Serrat, Universitat de Vic
- » **Self assembly in active suspensions** - Ignacio Pagonabarraga, University of Barcelona
- » **Simulation of the Entrainment Effects in Turbulent Boundary Layers** - Javier Jiménez Sendin, School of Aeronautics, Universidad Politecnica Madrid, 28040-Madrid, Spain
- » **Strain tuning of ferroelectric-antiferrodistortive coupling in PbTiO<sub>3</sub>/SrTiO<sub>3</sub> superlattices** - Javier Junquera, Universidad de Cantabria
- » **Testing new optimization methods for mixed action simulations** - Pilar Hernández Gamazo, Instituto de Física Corpuscular-Universidad de Valencia
- » **Three-body problem in non-relativistic Chromodynamics and with the Cornell model** - Felipe J. Llanes Estrada, Univ. Complutense
- » **Time-resolved electron dynamics in atoms using X-Ray Free Electron Lasers and Ultra-short pulses** - Alicia Palacios, Universidad Autónoma de Madrid
- » **Towards the understanding of shear-layer instability mechanisms for drag reduction by means of advanced turbulence modeling** - Assensi Oliva, Universitat Politècnica de Catalunya
- » **Tuning of the electronic state of a 2-dimensional electron gas in PbTiO<sub>3</sub>/SrRuO<sub>3</sub> interfaces** - Javier Junquera, Universidad de Cantabria
- » **Turbulent natural convection in enclosed cavities. On the role of transitional thermal boundary layers in the flow structure** - Assensi Oliva, Universitat Politècnica de Catalunya
- » **XUV/X-ray laser pulses for ultrafast electronic control in molecules** - Fernando Martin, UAM

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