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Barcelona Supercomputing Center ~ Red Española de Supercomputación

2009 Annual Report

2009 Annual Report





The 2009 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.





Table of Contents

I About the BSC-CNS

I.1	The BSC-CNS	6
I.2	People of the BSC-CNS	10
I.3	Financial Accounts	20
I.4	Technology Transfer	22
I.5	The New Supercomputing Infrastructure for Europe	24
I.6	Planning a New Home for the BSC-CNS	25

2 Research and Support Activities

2.1	Computer Sciences Department	26
2.2	Earth Sciences Department	30
2.3	Life Sciences Department	34
2.4	Computer Applications in Science & Engineering Department	38
2.5	Operations Department	42
2.6	Management Department	46
2.7	Publications	49

3 Spanish Supercomputing Network (RES)

3.1	Spanish Supercomputing Network (RES)	58
3.2	Universidad Politécnica de Madrid - Magerit Node	62
3.3	Instituto Astrofísico de Canarias - LaPalma Node	64
3.4	Instituto Tecnológico de Canarias - Atlante Node	66
3.5	Universidad de Cantabria - Altamira Node	68
3.6	Universidad de Málaga - Picasso Node	70
3.7	Universidad de Valencia - Tirant Node	72
3.8	Universidad de Zaragoza - Caesaraugusta Node	74
3.9	Astronomy, Space & Earth Sciences (Selected Projects)	76
3.10	Biology and Life Sciences (Selected Projects)	78
3.11	Chemistry and Material Sciences (Selected Projects)	80
3.12	Physics and Engineering (Selected Projects)	82
3.13	RES Project List	84




Mateo Valero,  
Director

Francesc Subirada,  
Associate Director

## 2009 Review

In 2009 the BSC-CNS extended its role as a key infrastructure for Spanish science with further growth of the RES via the addition of a new node, Atlante, the commitment of long-term funding by the Spanish government for the BSC-CNS to host one of the Tier-0 nodes of PRACE, and the ongoing development of training and information sessions for RES users. This latter is particularly important as the true value in the BSC-CNS lies not with its hardware, but in its development and dissemination of knowledge and skills to apply computing power to solve some of the most difficult challenges facing science and society.

### Mission

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

*“Nothing tends so much to the advancement of knowledge as the application of a new instrument.”*  
— Sir Humphry Davy *Elements of Chemical Philosophy* (1812), in J. Davy (ed.), *The Collected Works of Sir Humphry Davy* (1839-40), Vol. 4, 37.

Researchers from across the scientific spectrum, from Biology to Physics to Earth Sciences, and even to the Humanities and Social Sciences, are increasingly leveraging the power of High Performance Computing (HPC) to conduct what is increasingly known as e-Science; modelling situations where experiments are too expensive, highly dangerous, or simply impossible to perform otherwise, and sharing access to unique or distributed scientific facilities, that include data, instruments, computing and communications, regardless of their type and location. e-Science is not just limited to the academic world, with HPC increasingly being used by governments and private industry to solve key challenges and improve competitiveness, as demonstrated by the growth in collaborations between the BSC-CNS and non-academic entities to solve problems as diverse as air pollution modelling to improving yacht designs.

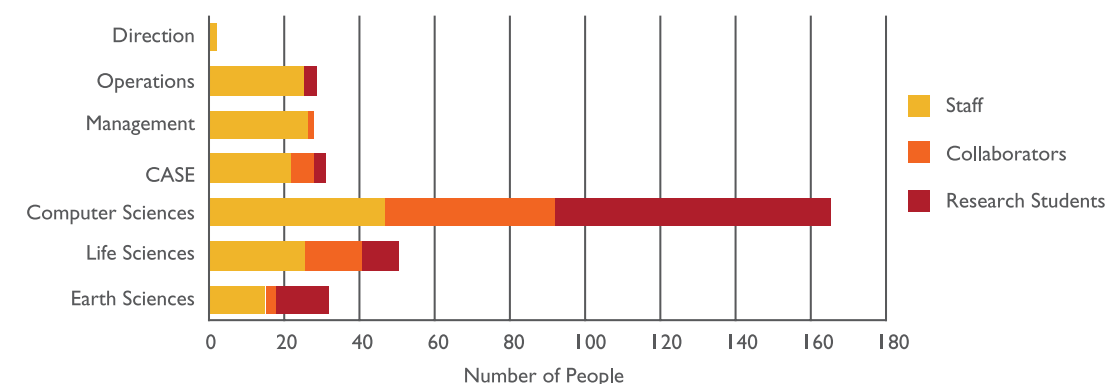
### Powerful Computing

The BSC-CNS is the National Supercomputing Facility in Spain and manages MareNostrum, one of the most powerful supercomputers in Europe, located at the Torre Girona chapel. When last upgraded in 2008, the Top500 list ranked the MareNostrum as the 10th most powerful supercomputer in Europe and 40th in the world.

At the European level, access to HPC computers of leadership class is essential for international competitiveness in all areas of science and engineering. Currently the two main European shortcomings related with Supercomputing are fragmentation and the lack of a strong HPC industry, with a dominance of US, Japanese and Chinese companies. The PRACE initiative was formed to solve these issues. With a budget of more than €400 million already committed for the first five years, PRACE will not only be a major contributor to the European Research Area, but also a stimulator for disruptive science and technologies, providing unique tools to the European scientific community, boosting European competitiveness and positioning itself strategically as a leader rather than follower in the HPC world.

The BSC-CNS has played a leading role in the development of PRACE, and as one of the founding host sites for a Tier-0 node will reap significant advantages, including adding value to other Spanish infrastructures, strengthening the interface between science and industry through interdisciplinary research contacts, attracting young and enquiring minds, creating technology clusters of associated industries and attracting high-tech firms to install R&D facilities nearby, spawning new spin-off products and start-up companies, increasing Spain's international reputation and visibility in scientific and high-tech fields, and improving the trans-European and public-private mobility of researchers and new technologies.

### BSC-CNS People 2009



The BSC-CNS is an attractor of talent. During 2009, some 340 people performed research or provided support at the centre, as compared to a mere 50 back in 2005 when the center was opened. Over one third of staff are of foreign nationality, with over 33 countries represented including: Argentina, Belgium, Brasil, Bulgaria, Canada, China, Chile, Colombia, Cuba, Denmark, Dominican Republic, Ecuador, France, Germany, Greece, Hungary, India, Iran, Ireland, Israel, Italy, Montenegro, Pakistan, Peru, Poland, Portugal, Russia, Serbia, Thailand, Turkey, UK, USA and Spain.



World Map of Countries of Origin

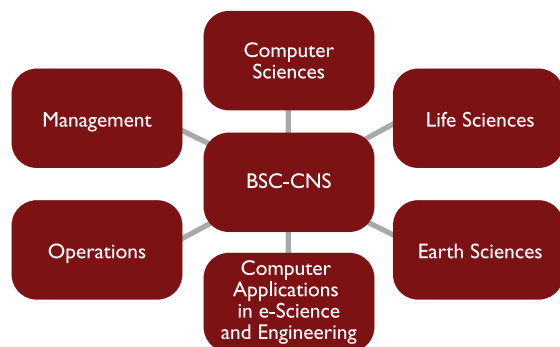
Also attracted to the BSC-CNS are the R&D departments and projects of global high-tech firms. IBM and the BSC-CNS are jointly working on developing the supercomputers of the future, whilst joint projects with Microsoft are applying the concepts of parallelism to the next generation of workstations.

Locally, the BSC-CNS provides sustainable competitive advantage to Spanish firms. The flagship of such projects is with REPSOL in the development of a world-leading technology to process massive amounts of seismic data. This is already being applied in search of remote deposits of oil and gas and in the near future will also be applied to CO2 capture and storage.

Within their respective fields, the research departments of the BSC-CNS continue to build their reputation for excellence at an international level. For example, the Computer Science department is coordinating the European FP7 project VELOX to improve understandings of transactional memory designs by developing an integrated transactional memory stack, from the hardware level, including CPU designs, through to application environments. If successful, such a system could become the tool-of-choice for concurrent programming on multi- and many-core platforms.

## Support and Research

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



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

The Life Sciences department is involved in numerous international projects such as MITIN to model mitochondrial function and insulin signaling in order to better understand complex diseases, and ELIXIR to establish a Europe-wide biological information infrastructure to support the application of life science research to medicine, the environment, bio-industries and society.

Meanwhile, the Earth Sciences department is extending its highly successful CALIOPE project to include Andalusia and the Canary Islands, funded directly by those local governments. CALIOPE is a detailed air quality forecasting system for Spain, with applications in modeling the potential impacts on air quality of proposed developments and industries as well as natural phenomena, thereby providing a useful planning tool as well as a forecasting service.

The Computer Applications in Science and Engineering department further advanced its development of both fundamental numerical modelling issues, such as efficient solving strategies (including preconditioners, parallel strategies and fractional schemes) and applied models, such as simulations of the respiratory system, the brain's arterial system, seismic imaging and sailing boat designs.

The BSC-CNS also continues to develop applied technology systems to provide new tools for solving extremely complex problems. Key amongst these tools is the Alya system, a computational mechanics toolbox specially designed for highly efficient performance in large scale supercomputing facilities. Alya is capable of solving various different physics problems, each with very different modeling characteristics, including airflows, acoustics, thermal flows, solid mechanics, quantum mechanics and more. Another highlight is the Star Superscalar (StarSs) programming model which is being adapted to various platforms to facilitate the parallelisation of applications onto multicore systems.

In addition to the projects undertaken by the BSC-CNS research departments, over 235 external activities utilised some 75 million hours of computation on RES systems. These activities, representing fields of science as diverse as medicine, astrophysics and social sciences, are evaluated for merit and prioritised by an independent Access Committee. Requests for access come from all over Spain, and indeed all over Europe, testifying to both the quality of the RES facilities and the ever increasing demand for supercomputing resources. Requests for access have been steadily increasing above the level of increased computing power and are now more than double the available computing time.

The work carried out by the scientists at BSC-CNS resulted in over 90 journals and book chapter publications, 111 key conference presentations and a number of new patent filings. Additionally, BSC-CNS researchers presented numerous workshops at both national and international levels, and the centre hosted a number of key international events.

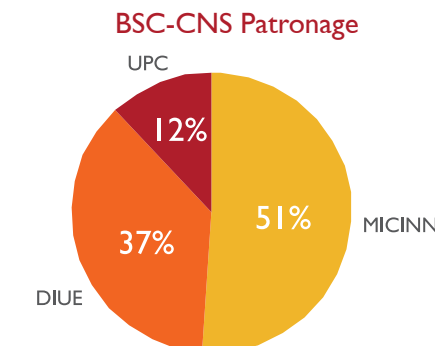
## Broad Access

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

## Patrons of the BSC-CNS

The BSC-CNS is a legally autonomous, public consortium, with three founding partners, the Spanish Ministry of Science & Innovation (MICINN), the Departament d'Innovació, Universitats i Empresa (DIUE) of the Catalan government and the Universitat Politècnica de Catalunya (UPC).

The voting representation is divided between MICINN (51%), DIUE (37%), and UPC (12%).



The income of the BSC-CNS in 2009 was €20.1 M of which €6.6 M corresponded to the ordinary budget coming from the patrons of the BSC-CNS, the Spanish and Catalan Governments; and €8.1 M from competitive projects. Of particular note, €3.9 M of funding was derived from projects with private companies. In 2009, the BSC-CNS participated in 23 competitively funded EU projects, 37 collaborative projects with industry and 14 national projects.

The successes of 2009 would not have been possible without the commitment, hard work, and bright ideas of the staff, students, collaborators and visiting researchers who contributed to the BSC-CNS and continue to build the international reputation of the BSC-CNS as a centre of excellence in High Performance Computing and e-Science.

The Directors wish to express their profound gratitude to all who worked with the BSC-CNS throughout the year, and also give thanks and recognition to the patrons of the BSC-CNS; MICINN, DIUE and UPC for their continued strong support, and to the various funding agencies and private companies who sponsored research and development activities. This continued strong support during a difficult economic period is particularly encouraging and much appreciated.

Mateo Valero, Director

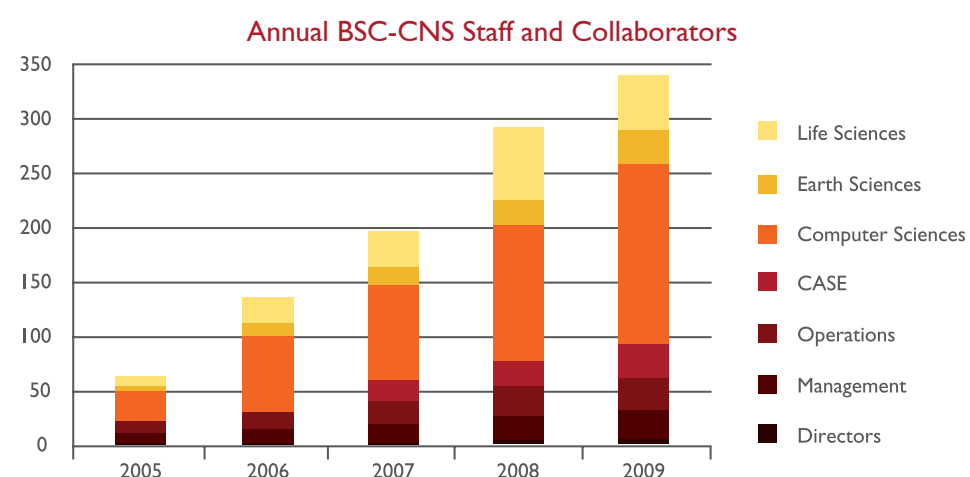
Francesc Subirada, Associate Director



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

As at 31st December 2009, the core staff of the BSC-CNS included 64 permanent positions, 77 dedicated to specific projects and 68 scholarship students. These numbers were significantly augmented by additional staff who participated in the BSC-CNS via a number of programs.

Total personnel who worked at the BSC-CNS throughout the year increased from 302 during 2008 to 340 during 2009, mainly through new temporary and shared staff, resident students, and collaborating and visiting researchers.



**Shared Staff and Human Resource Programs** In addition to its own staff, the BSC-CNS hosts shared staff from other public institutions such as the Technical University of Catalonia (UPC), the Institut de Recerca de Barcelona - Parc Científic de Barcelona - Universitat de Barcelona (IRB-PCB-UB) and the Consejo Superior de Investigaciones Científicas (CSIC).

In 2009 the 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 2009, the BSC-CNS had 91 student researchers associated to several research projects.

**Mobility Programs** The 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. The BSC-CNS is involved in two major mobility programs:



At the Spanish level, the BSC-CNS participates in a national access program called ICTS, whose objective is to leverage the knowledge in supercomputing and eScience from the BSC-CNS. This program, which holds selection meetings every 4 months, allowed 21 researchers to access the BSC-CNS facilities in 2009; their expenses were covered by the Spanish Ministry of Science and Innovation (MICINN).



At the international level, HPC-Europa2 is a consortium of seven leading High Performance Computing (HPC) infrastructures, including the 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 2009 the BSC-CNS hosted 36 of these visitors.





## BSC-CNS Governing Bodies



### Members of the BSC-CNS Board of Trustees as at 31st December 2009

#### President

**Carlos Martínez**, Secretary of State for Research, MICINN

#### Vice President

**Joan Majó**, Commissioner for Universities and Research, DIUE

#### Representatives MICINN

**Montserrat Torné**, Director General for International Cooperation and Institutional Relations, MICINN

**Carmen Peláez**, Vice President of Organization and Institutional Relations, CSIC

**José Ignacio Doncel**, Deputy Director General of Promotion, Technological Infrastructure and Large Facilities, MICINN

#### Invited MICINN

**Luis Eduardo Ruiz López de la Torre Ayllón**, Deputy Director General of International Installations and Organisations

**Francisco Herrada**, Head of e-Science Infrastructures

#### Representatives DIUE

**Josep Ribas**, Director General of Universities

**Joan Roca**, Director General of Research

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

#### Representatives UPC

**Antoni Giró**, Rector

**Josep Casanovas**, Vice Rector of University Policy

**Sebastià Sallent**, Director Foundation i2CAT

#### Representatives BSC-CNS

**Mateo Valero**, Director, BSC

**Francesc Subirada**, Associate Director, BSC

**Ernest Quingles**, Manager, BSC

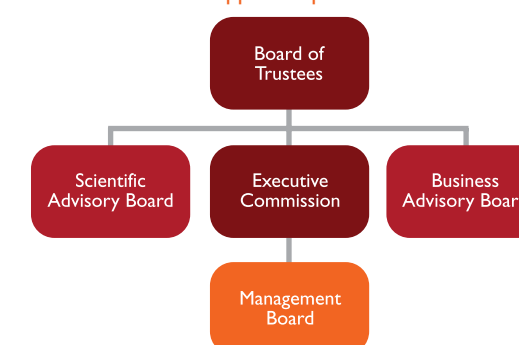
#### Commission Secretaries:

**Mario Maza**, State lawyer

**Javier Zuloaga**, State lawyer

### Strong Governance

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



### Members of the BSC-CNS Executive Committee as at 31st December 2009

#### President

**Montserrat Torné**, Director General for International Cooperation and Institutional Relations, MICINN

#### Vice President

**Joan Roca**, Director General of Research, DIUE

#### Representative MICINN

**José Ignacio Doncel**, Deputy Director General of Promotion, Technological Infrastructure and Large Facilities, MICINN

#### Representative DIUE

**Iolanda Font de Rubinat**, Deputy Director General of Research, DIUE

#### Representatives UPC

**Xavier Gil**, Vice Rector for Research and Innovation

**Josep Casanovas**, Vice Rector for University Policy

#### Representatives BSC-CNS

**Mateo Valero**, Director, BSC

**Francesc Subirada**, Associate Director, BSC

**Ernest Quingles**, Manager, BSC

#### Commission Secretaries

**Mario Maza**, State lawyer

**Javier Zuloaga**, State lawyer

### Management Board

#### Management Board Chairman

**Mateo Valero**, Director

### Management Board Vice-Chairman

**Francesc Subirada**, Associate Director

#### Members

**Jesús Labarta**,  
Computer Sciences Director

**Eduard Ayguadé**,  
Computer Sciences Associate Director

**José María Baldasano**,  
Earth Sciences Director

**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

#### Core Team

**Victoria Ley Vega de Seoane**, Agencia Nacional de Evaluación y Prospectiva

**Ramón Bevide**, Universidad de Cantabria

**Ramón López de Arenosa**, Ministerio de Educación y Ciencia

**José María Cela**, Barcelona Supercomputing Center-Centro Nacional de Supercomputación

#### Biomedicine and Health Sciences Expert Panel

Coordinator: Alfonso Valencia, Centro Nacional de Investigaciones Oncológicas

Assistant: Manuel Palacín, Universidad de Barcelona

#### Chemistry and Material Sciences Expert Panel

Coordinator: Enrique Lomba, CSIC - Instituto de Química Física Rocasolano

Assistant: Mariona Sodupe, Universitat Autònoma de Barcelona

#### Physics and Engineering Expert Panel

Coordinator: Pablo Ordejón, CSIC-ICN Centre d'Investigació en Nanociència i Nanotecnologia

Assistant: Rodolfo Bermejo, Universidad Politécnica de Madrid

#### Astronomy, Space and Earth Sciences Expert Panel

Coordinator: José María Ibáñez, Universidad de Valencia

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



## BSC-CNS Staff and Collaborators during 2009

### Direction

Director: **Mateo Valero**

Associate Director: **Francesc Subirada**

Director Assistant: **Lourdes Cortada**

Associate Director Assistant: **Nuria Sirvent**

PRACE Research Manager: Carlos Mérida

PRACE Research Manager: Eugene Griffiths

Academic Programs Coordinator: Ulises Cortés

### Computer Sciences Department

Computer Sciences Director: **Jesús Labarta**

Computer Sciences Associate Director: **Eduard Ayguadé**

### Autonomic Systems and e-business Platforms

Autonomic Systems and e-business Platforms Group Manager: **Jordi Torres**

Associate Researcher: Mario Macias

Researcher: Vicenç Beltran

Research Support Engineer: Alex Vaque

Associate Researcher: David Carrera

Associate Researcher: Javier Alonso

Associate Researcher: Jordi Guitart

Associate Researcher: Yolanda Becerra

Resident Student: David de Nadal

Resident Student: Ferran Julià

Resident Student: Gemma Reig

Resident Student: Iñigo Goiri

Resident Student: Jorda Polo

Resident Student: Josep Oriol Fito

Resident Student: Uday Kiran

Visitor: Karel Asael

### Computer Architecture for Parallel Paradigms

Computer Architecture for Parallel Paradigms Manager: **Adrián Cristal**

Computer Architecture for Parallel Paradigms Manager: **Osman Unsal**

Senior Researcher: Ibrahim Hur

Junior Researcher: Óscar Palomar

Research Support Engineer: Javier Arias

Research Support Engineer: Oriol Arcas

Resident Student: Adria Armejach

Resident Student: Azam Seyedi

Resident Student: Chinmay Kulkarny

Resident Student: Cristian Perfumo

Resident Student: Ferad Zyulkyarov

Resident Student: Gokcen Kestor

Resident Student: Gulay Yalcin

Resident Student: Ivan Ratkovic

Resident Student: Milan Stanic

Resident Student: Milovan Djuric

Resident Student: Nebjosa Miletic

Resident Student: Nehir Sonmez

Resident Student: Nikola Bezanic

Resident Student: Nikola Markovic

Resident Student: Otto Pflücker

Resident Student: Roberto D'Aprile

Resident Student: Sasa Tomic

Resident Student: Srdjan Stipic

Resident Student: Surthitha Sanyal

Resident Student: Timothy Hayes

Resident Student: Vasilis Karakostas

Resident Student: Vesna Smiljkovic

Resident Student: Vladimir Gajinov

Resident Student: Vladimir Marjanovic

Associate Resident Student: Isidro González

### Grid Computing and Clusters

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

Researcher: Iván Roderó

Researcher: Jorge Ejarque

Researcher: José María Pérez

Researcher: Marta Garcia

Researcher: Raül Sirvent

Associate Researcher: Daniele Lezzi

Associate Researcher: Gladys Utrera

Associate Researcher: Julita Corbalán

Resident Student: Enric Tejedor

Resident Student: Isaac Jurado

Resident Student: Judit Planas

Resident Student: Luis Martinell

Resident Student: Maja Etinski

Resident Student: Pieter Bellens

Resident Student: Rahul Gayatri

Resident Student: Sunny Ranjan

Visitor: Aislan Foina

Visitor: Gabriel Marcel

Visitor: Henrik Akesson

Visitor: Lawrence Eric

Visitor: Lester Abel

Visitor: Masoud Sadjadi

Visitor: Xavier Arroyo

Visitor: Vinoth Elangovan

### Heterogeneous Architectures

Heterogeneous Architectures Group Manager: **Álex Ramírez**

Researcher: Miquel Pericás

Researcher: Yoav Etsion

Associate Researcher: Carlos Álvarez

Associate Researcher: Carlos Villavieja

Associate Researcher: Daniel Jiménez

Associate Researcher: Esther Salami

Associate Researcher: Friman Sánchez

Associate Researcher: Mauricio Álvarez

Resident Student: Antonio Quesada

Resident Student: Aparna Sasidharan

Resident Student: Augusto Vega

Resident Student: Branimir Dickov

Resident Student: Felipe Cabarcas

Resident Student: Milan Pavlovic

Resident Student: Muhammad Shafiq

Resident Student: Paul Carpenter

Resident Student: Tassadaq Hussain

Resident Student: Vladimir Subotic

Visitor: Gurindar Singh Sohi

Visitor: José Miguel Gil

Visitor: Marina García

Visitor: Ozcan Ozturk

Visitor: Ramón Beivide

Visitor: Roberto Hexel

### Network Processors

Network Processors Group Manager: **Mario Nemirovsky**

Associate Researcher: Alejandro Pajuelo

Associate Researcher: Javier Verdú

Resident Student: Ruken Zilan

### Operating System / Computer Architecture Interface

Operating System / Computer Architecture Interface group Manager: **Francisco Javier Cazorla Almeida**

Researcher: Eduardo Quiñones

Researcher: Jaume Abella

Researcher: Roberto Giogiosa

Resident Student: Alessandro Morari

Resident Student: Carlos Boneti

Resident Student: José Carlos Ruiz

Resident Student: Kamil Kedzierski

Resident Student: Leonidas Kosmidis

Resident Student: Marco Paolieri

Resident Student: Petar Radojkovic

Resident Student: Roberta Piscitelli

Resident Student: Víctor Javier Jiménez

Resident Student: Vladimir Cakarevic

Associate Resident Student: Miquel Moretó

Visitor: Emery David Berger

Visitor: Rizos Sakellariou

### Programming Models

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

Researcher: Alex Duran

Researcher: Javier Teruel

Researcher: Roger Ferrer

Associate Researcher: Enric Moracho

Associate Researcher: Juan José Costa

Associate Researcher: Marc González

Associate Researcher: Maria Lluisa Gil

Associate Researcher: Montse Farreras

Associate Researcher: Nacho Navarro

PRACE Research Manager: Ramnath Sai Sagar

Resident Student: Cecilia González

Resident Student: Daniel Cabrera

Resident Student: Javier Bueno

Resident Student: Javier Cabezas

Resident Student: Lluç Álvarez

Resident Student: Lluís Vilanova

Resident Student: Nikola Vujic

Resident Student: Ramon Bertran

Visitor: Carlo Bertolli

Visitor: Dimitry Komatish

Visitor: Nikos Pitsianis

Visitor: Ronald Martin

### Performance Tools

Performance Tools Group Manager: **Judit Giménez**  
 Researcher: Eloy Martínez  
 Researcher: Germán Llorc  
 Researcher: Germán Rodríguez  
 Researcher: Harald Servat  
 Researcher: Juan González  
 Researcher: Kevin Huck  
 Researcher: Marc Casas  
 Researcher: Pedro Antonio González  
 Researcher: Xavier Aguilar  
 Researcher: Xavier Pegenaut  
 Resident Student: Ana Jokanovic  
 Resident Student: Pau Freixes  
 Resident Student: Wahedd Iqbal  
 Visitor: Julio Ramon Beivide Palacio  
 Visitor: Pedro González

### Storage Systems

Storage Systems Group Manager: **Toni Cortés**  
 Researcher: Ernest Artiaga  
 Researcher: Jacobo Giralt  
 Researcher: Jonathan Martí  
 Researcher: Juan González de Benito  
 Researcher: Ramon Nou  
 Resident Student: Albert Miranda  
 Resident Student: Kousik Dheena  
 Visitor: Martin Rehr

### Earth Sciences Department

Earth Sciences Director: **José María Baldasano**  
 Air Quality Group Manager: **Santiago Gassó**  
 Metereological Modelling Group Manager: **Oriol Jorba**  
 Mineral Dust Group Manager: **Carlos Pérez**  
 Senior Researcher: Arnau Folch  
 Senior Reseacher: Pedro Jiménez  
 Researcher: Elies Campmany  
 Researcher: Matthias Piot  
 Resident Student: Alba Badia  
 Resident Student: Ángel Rincón  
 Resident Student: Karsten Haustein  
 Resident Student: Mar Martínez  
 Resident Student: Maria Teresa Pay

Resident Student: Michele Spada  
 Resident Student: Natalia Climent  
 Resident Student: Quinta Ana Pérez  
 Resident Student: Regina Isern  
 Resident Student: Sara Basart  
 Resident Student: Simone Marras  
 Resident Student: Stefany Raquel Hernández  
 Resident Student: Yenny González  
 PhD Student UPC-BSC: Maria Goncalves  
 Research Support Engineer: Albert Soret  
 Research Support Engineer: Eugenio Lopez  
 Technical Project Support: Laura González  
 Technical Support: Cristina Niubo  
 Technical Support: David Carrió  
 Technical Support: Kim Serradell  
 Technical Support: Luca Telloli  
 Visitor: Alexey Cheptsov  
 Visitor: Caubel Aranaud  
 Visitor: Donald Dabdub

### Life Sciences Department

Life Sciences Director: **Modesto Orozco**

#### Computational Genomics

Computational Genomics Group Manager:  
**David Torrents**  
 Researcher: Bárbara Montserrat  
 Researcher: Josep Maria Mercader  
 Resident Student: Carme Vilamala  
 Resident Student: Elisa Durán  
 Resident Student: Leyden Fernández  
 Resident Student: Santiago González  
 Research Support Engineer: Montserrat Puiggrós  
 Research Support Engineer: Valentí Moncunill  
 Research Support Engineer: Xavier Pastor  
 Visitor: Jorge Gulín  
 Visitor: Lucas Damián  
 Visitor: Pierre Pericard  
 Visitor: Santiago Algilaga

#### Electronic and Atomic Protein Modelling

Electronic and Atomic Protein Modelling Group Manager:  
**Victor Guallar**  
 Researcher: Ben Cossins

Researcher: Diego Masone  
 Researcher: Frank Wallrapp  
 Researcher: Ken Borrelli  
 Researcher: Suwipa Saen Oon  
 Associate Researcher: Fátima Lucas  
 Resident Student: Ali Hosseini  
 Associate Resident Student: Israel Cabeza de Vaca  
 Visitor: Evangelos Daskalakis  
 Visitor: Marcela Ayala  
 Visitor: Matthew Jacobson

#### INB-Computational Node

INB-Computational Node Group Manager: **Josep Lluís Gelpí**  
 Researcher: Aida Santaolalla  
 Researcher: Laia Codó  
 Resident Student: Alexis Torrano  
 Software engineer: Dmitry Repchevski  
 Software engineer: Romina Royo

#### Molecular Modelling and Bioinformatics

Molecular Modelling and Bioinformatics Group Manager:  
**Modesto Orozco**  
 Senior Researcher: Ramon Goñi  
 Software engineer: Jordi Camps  
 Visitor: Francesco Raimondi  
 Visitor: Charles Laughton

#### Protein Interactions and Docking

Protein Interactions and Docking Group Manager:  
**Juan Fernández- Recio**  
 Researcher: Albert Solernou  
 Researcher: Athi Narayanan  
 Software engineer: Carles Pons  
 Resident Student: Laura Pérez  
 Resident Student: Solene Grosdidier  
 Resident Student: Xavier Lucas  
 Associate Resident Student: Matthias Pfeifer  
 Visitor: Haydee Valdés  
 Visitor: Fabian Glaser

#### Experimental Bioinformatics Laboratory Platform

Experimental Bioinformatics Laboratory Associate Manager: **Montserrat Soler**  
 Associate Laboratory Support: Maica López

### Computer Applications in Science & Engineering Department

Computer Applications in e-Science and Engineering Director: **José María Cela**  
 High Performance Computational Mechanics Group Manager: **Mariano Vázquez**  
 Physical and Numerical Modelling Group Manager: **Guillaume Houzeaux**  
 Researcher: Albert Farrés  
 Researcher: Alejandro Soba  
 Researcher: Anne Cecile Lesage  
 Researcher: Edgar Alejandro Bea  
 Researcher: Félix Rubio  
 Researcher: Hadrien Calmet  
 Researcher: Herbert Coppola  
 Researcher: Mauricio Araya  
 Researcher: Mauricio Hanzich  
 Researcher: Miquel Català  
 Researcher: Mohammad Jowkar  
 Researcher: Pierre Lafortune  
 Researcher: Raúl de la Cruz  
 Researcher: Rogeli Grima Torres  
 Researcher: Romain Aubry  
 Researcher: Xavier Rubio  
 Researcher: Xavier Sáez  
 Associate Researcher: Carles Serrat  
 Resident Student: Beatriz Eguzkitza  
 Resident Student: Cristina Montañola  
 Resident Student: Cristobal Augusto Samaniego  
 Resident Student: Jelena Koldan  
 Resident Student: Margarida Moragues  
 Resident Student: Ruth Aris  
 Visitor: Karel Asael Barberena  
 Visitor: M<sup>a</sup> Ángeles Moreno  
 Visitor: Paula Villar  
 Visitor: Pedro González  
 Visitor: Petar Mimica



## Operations Department

Operations Director: **Sergi Girona**

### System Administration

Systems Group Manager: **Javier Bartolomé**

Helpdesk: Antonio Espinar

Helpdesk: Ferrán Sellés

Performance Technical: Alejandro Lucero

Performance Technical: Àlex Font

Security and Network: Albert Benet

Security and Network: Juan Carlos Sánchez

System Administration: Gabriele Carteni

System Administration: Guillermo Aguirre

System Administration: Jonathan Evans

System Administration: Jordi Valls

System Administration: Peter Tornyi

System Administration: Sergi Moré

Resident Student: Carles Fenoy

Resident Student: Josep Anguera

### User Support

User Support Group Manager: **David Vicente**

User Support: Joan Josep Iglesias

User Support: Jorge A. Naranjo

Technical Support: Diego Gandia

Technical Support: Jorge Rodríguez

Technical Support: Xavi Abellán

Resident Student: Christian Simarro

Webmaster: Silvina Rusinek

Web Graphic Designer: Jasmina Tomic

SAP Technician: Rubén Ortíz

### Facility Management

Facility Management Group Manager: **Ahmet Senata**

Maintenance Assistant: Albert Riera

### Res Coordination

Technical Coordinator: Montserrat González

## Management Department

Management Director: **Ernest Quingles**

### Finance and Business Administration

Administration, Finance and Human Resources Group

Manager: **Mercè Calvet**

Administration and Finance Account Officer:

Cristina Calonge

Finance Assistant: Judit Soldevila

Accounting Assistant: Ester Bafalluy

Accounting Technical Support: Marina Utges

General Assistant: Eva Vidal

General Assistant: Laura Gutiérrez

General Assistant: Neus Jiménez

Human Resources Officer: Anna Martín

Human Resources Officer: Lara Cejudo

Purchasing Officer: Cristina Vargas

Purchasing Officer: Elena Miró

### Marketing and Communication

Marketing Executive: Renata Giménez

Marketing Communications Officer: Sara Ibáñez

Marketing Assistant: Sonia Castel

ECRI Organization Officer: Eva Comino

MareNostrum Visitors Manager: Oriol Riu

### Project Management

Research Project Manager: Gina Alioto

Research Project Manager: Marta Rosselló

Research Project Manager: Nuria Nadal

Projects Project Officer: Maria Carreras

Associate Researcher: Fermín Sánchez



The financial accounts for 2009 presented here were drawn up following the accounting principles laid out in the General Plan of Public Accounting.

The operating budget of the BSC-CNS Consortium for the fiscal year 2009 was composed of ordinary income derived from contributions by the administrations and organisations that compose it, as well as projects income derived from competitive funding sources and agreements reached with private organisations. This income was then employed to cover expenses, including costs of operations and fulfilment of all financial obligations.



## Income

The Consortium income of €20.126.170 recognised for fiscal year 2009 derived from public administration contributions from the Ministry of Science and Innovation (MICINN), Generalitat de Catalunya (GdC) and European Commission (EC), as well as from agreements, contracts or other collaborative agreements with private organisations. Furthermore, the consolidated budget of the BSC-CNS included the assignment of internal resources carried over from the previous year's provisions.

INCOME	AMOUNT €
Ordinary Income	6,633,087
Ministerio de Ciencia e Innovación	4,288,790
Generalitat de Catalunya	2,344,297
Competitive Income	8,077,795
Ministerio de Ciencia e Innovación	1,310,129
Generalitat de Catalunya	107,973
European Commission	2,784,680
Private Companies	3,875,013
Other Income	5,415,288
Strategic Investment	4,189,938
Overheads / Capital Transfers	1,225,351
<b>TOTAL INCOME</b>	<b>20,126,170</b>

**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.

**Other Income** includes strategic investments, overheads and capital transfers.

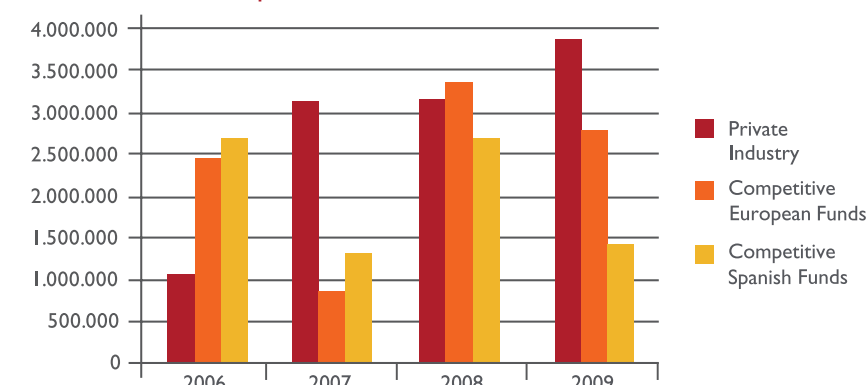
**Strategic Investments** are funds assigned by the Consortium Partners to finance key investments such as the construction of the new building to house the BSC-CNS, increases in supercomputing hardware and the repayment of loans taken out by the Consortium to finance the upgrade of the MareNostrum and the establishment of the RES.

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

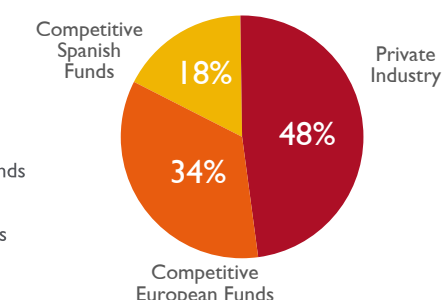
**Capital Transfers** are incomes derived from the yield on the capital accumulated from multiannual reserves for the execution of competitive projects and strategic investments, deposited in different bank accounts.

## Breakdown of Competitive Income

Competitive Income Evolution



Competitive Funding 2009



## Significant Gains in Private Sector Funding

In 2009 the BSC-CNS increased the level of funding from private company sponsored R&D by 23%, highlighting the success of increasing efforts in developing relations with the private sector and technology transfer. Funding from the private sector accounted for 48% of all competitively sourced funds in 2009.

## Expenses

The expenses of the BSC-CNS Consortium in the fiscal year 2009 include all costs associated with personnel, running expenses and investments financed either by the ordinary budget or from project funding derived from competitive grants.

EXPENSES	AMOUNT €		
	Ordinary Budget	Projects Budget	Total
Personnel	4,075,770	2,582,305	6,658,075
Investments	4,786,896	742,504	5,529,400
Current Expenses	3,185,710	1,786,596	4,972,307
Applied Reserves	-	2,966,389	2,966,389
<b>TOTAL EXPENSES</b>	<b>12,048,376</b>	<b>8,077,795</b>	<b>20,126,171</b>

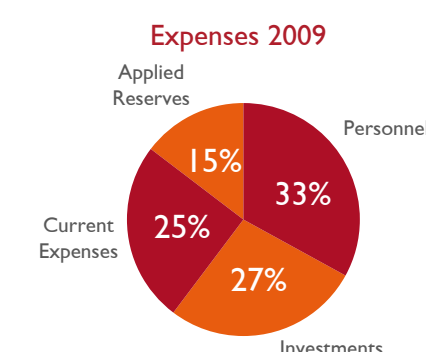
**Personnel** refer to salaries and associated charges directly related to the employment of staff contracted by the BSC-CNS. It does not include salaries and associated charges of visitors or other collaborators who continued to be paid via their originating institution.

**Investments** include all expenditures on computing and scientific equipment and infrastructure.

**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.

**Applied Reserves** are funds not expended in the current year but carried over to future years, and are comprised primarily of two main components; those funds received for strategic investments that have not yet been completed (such as the new BSC-CNS building), and advance competitive project funds secured under various multi-year programs that are progressively applied over the lifetime of each project.

In 2009, the BSC-CNS invited 10 public calls in order to accept 7 supply tenders and 3 services tenders. 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.





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.

Technology Transfer can occur in many ways, including the publication of research results in academic as well as industry journals, licensing of proprietary technology (which is usually protected via patents or copyright) to private industry, spin-off of technology and know-how into a start-up company, joint collaborations with industry in applied research and development of new techniques and products, training of scientists and technicians who then go on to work for private industry, and direct training of workers via short courses, workshops, etc.

It is generally very difficult to patent advances in computer coding and chip design and this limits the opportunities to directly license or spin-off new supercomputing technologies. Although the BSC-CNS does do this when possible, the main focus in technology transfer is in the training of people and joint R&D.

In 2009 the Operations Department expanded its training courses for both RES users and operators of RES nodes, and continued its work to offer improved levels of user support to assist users in overcoming technical issues.

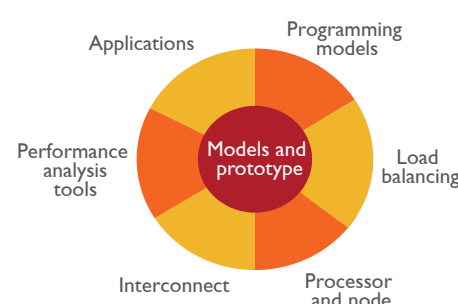
Joint collaboration with private industry continued to grow with a 23% increase in private R&D funding over 2008. Such R&D projects are undertaken at both the system level, via direct collaborations with industry leaders such as IBM and Microsoft, and at the application level, where a significant research effort is dedicated to providing supercomputing based models for solving engineering problems in industrial sectors such as aerospace, transport, energy, medicine, geology, etc.

## IBM MareIncognito

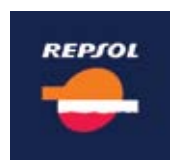


An IBM-BSC joint research project towards a 10+ PF supercomputer, MareIncognito is a bilateral project with IBM under the umbrella of a memorandum of understanding, led by Mateo Valero and Jesús Labarta. It encompasses research in several fields related to supercomputing with the aim to define the technical characteristics and the design of components of interest for a new generation of Petascale supercomputers for the year 2011/12, involving all aspects related to that machine: applications, programming models, performance tools, interconnection and processor architecture, etc.

The MareIncognito Project



## Kaleidoscope (Repsol)



The Kaleidoscope Project led by José María Cela is a “dream team” partnership of top geophysicists, computer scientists and organisations from around the world. It has been initiated by Repsol YPF, a Spanish integrated oil company with large assets in the US Gulf of Mexico, 3DGeo, a leading Houston-based imaging company formed by Stanford University professor and seismic imaging pioneer Biondo Biondi, and the BSC-CNS. The Kaleidoscope Project has privileged access through the BSC-CNS to Cell/BE based systems and technology because the BSC-CNS is one of the few research centres in the world developing libraries and codes for such processors.

The Kaleidoscope Project aims to produce more reliable and faster (by several orders of magnitude) software tools to analyse geo-seismic data and visualise below the thick layers of salt present in the Gulf of Mexico. This will significantly reduce exploration risks and make accessible oil reserves that otherwise would be invisible to the industry.

## BSC-Microsoft Research Centre



The BSC-Microsoft Research Centre, led by Osman Unsal, was established in April 2008 to focus on the way in which microprocessors and software for the mobile and desktop market segments will be designed and interact over the next 10 years and beyond. The advent of many- and multi-core processor computing architectures will make it possible to deliver enormous computa-

tional power on a single chip, with profound implications for the way software is developed. Optimising the design and interaction of hardware and software architectures to take advantage of the new computing power will require tight integration across the industry.

Computer architecture experts at BSC-CNS have teamed up with computer scientists at Microsoft Research Cambridge (MSRC) in the United Kingdom to look for innovative solutions to the challenges and opportunities that massively parallel processing entails. The vision of the centre is of a top-down computer architecture in which software requirements drive the hardware innovation forward rather than letting the hardware design condition software development. In addition to fundamental and applied research in transactional memory, a promising technology that facilitates writing of parallel programs for multi-core processors, hardware support for managed runtimes is being conducted in the initial research projects.

## Other Industry and Institutional Collaborations



### Gas Natural

**Goal:** to study the impact of natural gas-powered vehicles on the air quality in Barcelona and Madrid.



### Sun Microsystems

**Goal:** to propose techniques that allow better exploiting the capabilities of the massive multithreading processors in network servers.



### CISCO Systems Inc.

**Goal:** to model multicore multithreaded architectures in typical network applications and estimate the performance of different architectures.



### SGS TECNOS S.L.

**Goal:** the goal of this collaboration was to perform an impact assessment on the air quality from combined cycle power stations.



### PB Power

**Goal:** to perform air quality modelling.



### BCNEcologia

**Goal:** to perform a simulation for the Air Quality Plan in Catalonia.



### AEMET (The State Meteorological Agency)

**Goal:** 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 characterization studies of atmospheric material.



### CALIOPE

**Goal:** 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

**Goal:** to develop an information system about the air quality forecast and surveillance of the Canary Islands.



### EGMASA Project

**Goal:** 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.

## PRACE - Partnership for Advanced Computing in Europe

### Background

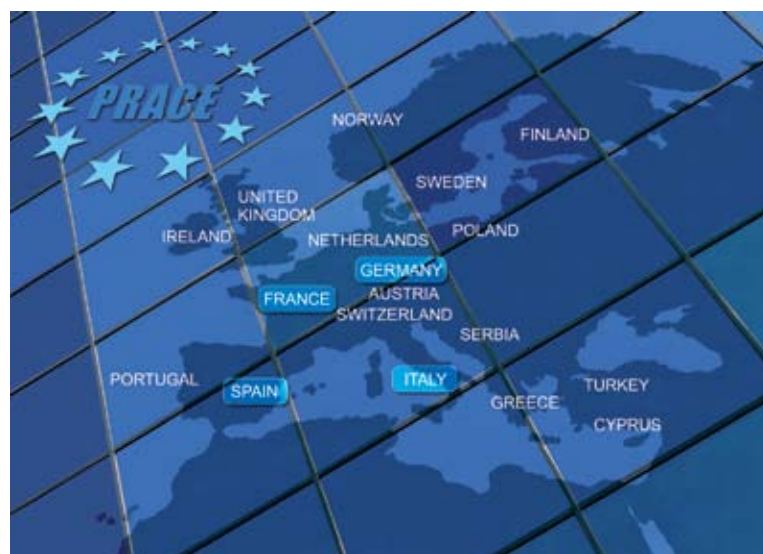


The Partnership for Advanced Computing in Europe, funded in part by the EU's 7th Framework Programme, lays the groundwork for the creation of a persistent pan-European High Performance Computing (HPC) Service, consisting of several tier-0 supercomputing centres. Supercomputers are indispensable tools for solving the most challenging and complex scientific and technological problems through simulations. PRACE will create a top class HPC infrastructure which will be managed as a single European entity. Through PRACE, European scientists and technologists will be provided with world-class leadership supercomputers with capabilities equal to or better than those available in the USA and Japan.

Building a world-class pan-European HPC Service is a highly ambitious undertaking that involves governments, funding agencies, centres capable to host and manage the supercomputers, and the scientific and industrial user communities with leading edge applications. In contrast to Research Infrastructures that focus on a single scientific instrument, an HPC Infrastructure has two unique characteristics: supercomputers serve all scientific disciplines and tier-0 supercomputers have a three year depreciation cycle, as tier-0 implies leading edge services.

PRACE contemplates the collaboration of Hosting Partners (4 to 6), who will host the Tier 0 supercomputing nodes, the European Union, and a number of Non Hosting Partners (between 14 and 16) who will contribute financially to the operating costs of the centres and an aggressive upgrade program that will see each centre upgraded on a 3-4 year cycle.

### BSC-CNS and PRACE



During 2009, PRACE decided on its governance structure, the funding and usage model, and the peer review process. Extensive dissemination and training activities were continued. The six prototypes for Tier-0 systems to be procured in 2010 were installed and assessed in terms of their technical characteristics, performance and total cost of ownership. STRATOS, the PRACE Advisory group for strategic technologies, now involves more than 80 HPC stakeholders, including vendors and academia.

The BSC-CNS will host one of the main Tier-0 nodes and is playing a leading role responsible for preparing the organisational aspects of the future infrastructure, including the legal

and administrative framework. The decision of a legal seat for PRACE was taken with the board finally appointing Brussels (Belgium) as a temporary legal seat for PRACE. Signature-ready documents (statutes and agreement for the initial period) were prepared along with the risk assessment relative to organizational aspects.

A major international workshop on code-porting and scaling was hosted in Barcelona on October 21-23, 2009 to provide participants with the necessary training, education and expertise in programming models and optimization techniques for Cell and GPGPU-based systems that comprise some of PRACE's prototype architectures.

In 2009, the BSC-CNS finalised the planning for its new home, which will begin construction in 2010 and be completed in 2012.



The MareNostrum supercomputer is housed in the Capella Torre Girona in Barcelona. However, currently the majority of the management and research staff of the BSC are housed in several separate facilities belonging to the UPC and Consorci de la Zona Franca. A new building has been approved that will enable all the departments of the BSC-CNS to be housed under one roof.



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



The Chapel Girona

The new building, which will commence construction in 2010 and will be located adjacent to the Capella Girona, has a dedicated section to host a future supercomputer even more powerful than the MareNostrum. The Operations Department has been heavily involved in the design of this new facility and will be responsible for its operation once the building is completed in 2012.

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.





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 architectures, programming and execution environments, resource management layers, etc., bridging what technology offers and application requirements, usually in collaboration with manufacturers.

## Overview

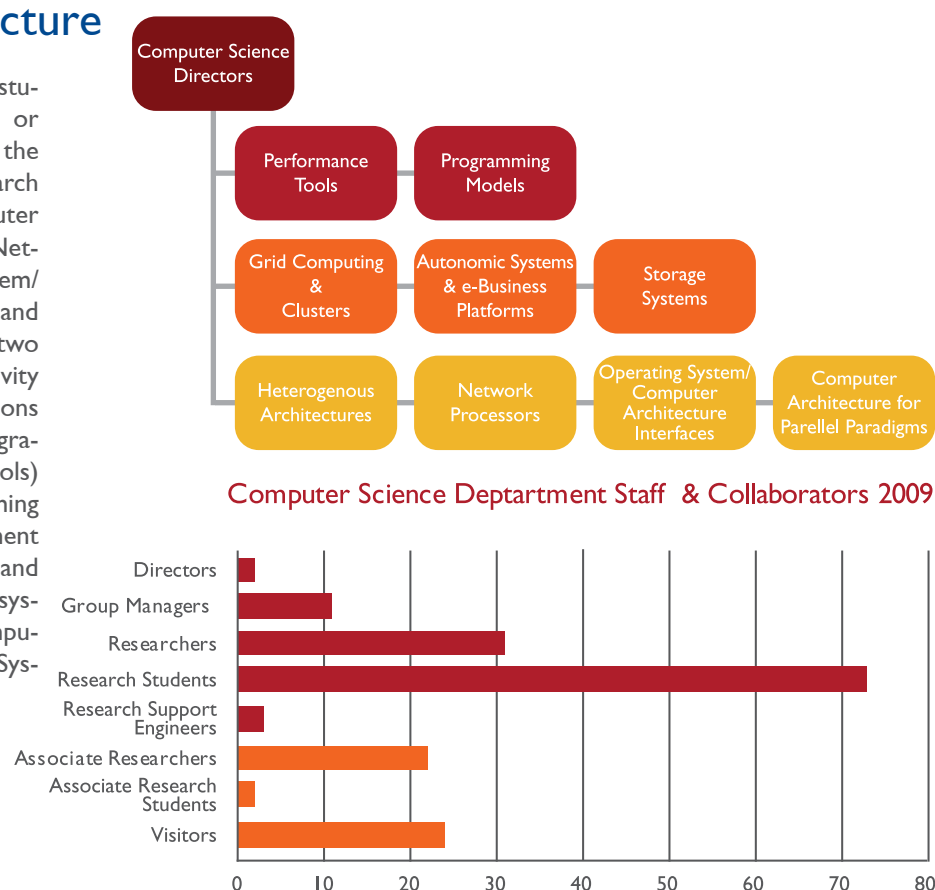
The Computer Sciences department, led by Jesús Labarta and Eduard Ayguadé, is structured in 9 research Groups. Although each Group has its own specialised lines of research and unique projects, the teams often come together to collaborate on larger projects that require vertical integration, such as the MareIncognito project with IBM, whose objective is to develop a prototype Petaflop supercomputer. 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 BSC-CNS has attracted leading computing companies such as IBM and Microsoft to invest heavily in collaborative systems design R&D projects despite the relative youth of the Centre.

## Organisational Structure

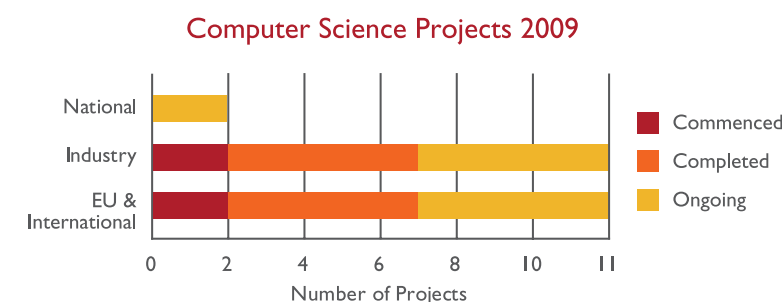
During 2009, some 120 staff and students, and further 46 associated or visiting researchers worked within the Department, organised in 9 research Groups; four focused on Computer Architecture (Parallel Paradigms, Network Processors, Operating System/Computer Architecture Interfaces and Heterogeneous Architectures), two focussed on improving productivity when developing parallel applications on large scale parallel systems (Programming Models and Performance Tools) and three focused on programming models and resource management middleware for distributed cluster and GRID architectures, including file systems (Storage Systems, Grid Computing and Clusters, and Autonomic Systems and e-Business Platforms).



## Key Projects & Networks

During 2009, the Computer Sciences Department participated in:

- ▶ 6 ongoing IST FP6 projects (ACOTES, BE-inGRID, BREIN, SARC, SORMA and XtremOS) and FP7 projects (MERASA and Velox);
- ▶ 2 networks of excellence (HiPEAC and HPC-Europa);
- ▶ The IESP (International Exascale Software Project);
- ▶ The DEISA2 (Distributed European Infrastructure for Supercomputing Applications) consortium;
- ▶ EU COST IC804 action “Energy efficiency in large scale distributed systems”;
- ▶ Several research contracts with companies (IBM, Microsoft and Sun Microsystems);
- ▶ The Spanish Consolider program “Supercomputing and eScience”, coordinating the Basic Research in Supercomputing workpackage.



## Scientific Output

### Impacting the Future of Computing

In collaboration with market leaders such as IBM, Microsoft, Sun and Cisco Systems, as well as other international computing centers and standardization 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. transactional memory), 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 constantly being integrated into new specifications, systems and products.

The research results of the Department have been published in the proceedings of high quality conferences in the area, including International Symposium on Computer Architecture (ISCA), International Conference on Parallel Architectures and Compilation Techniques (PACT), MICRO conference, Symposium on Principles and Practice of Parallel Programming, International Conference on Supercomputing (ICS), International Conference on Parallel Processing (ICPP), International Parallel & Distributed Processing Symposium (IPDPS), and International Conference on Cluster Computing (Cluster). All these are conferences ranked within the A+ and A tiers in the CORE (COmputing REsearch Education) conference classification and with high EIC (Estimated Impact of Conference) in the Computer Sciences Conference Ranking. In addition, other more consolidated research results have been published in prestigious journals in the area.

### Communication & Dissemination 2009

Publishing	
Journal Articles	17
Book Chapters	6
Conference Presentations	
International	36
National	6
Workshops	
Workshops	18
Education	
Theses Read	6



**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. Current trends in service computing are moving towards the creation of virtualized execution environments to run all kind of business applications. The goal is to create large pools of resources where users can run their computing tasks, independently of their nature. These kind of generic computing clusters are known as computing clouds. During 2009 the Group continued efforts to build a self-adaptive execution environment for cloud environments, participating in a number of EU projects (SORMA, Brein, CoreGRID and XtremOS) and several areas of collaboration with IBM Watson. Also during

2009 the group started to address the Cloud energy awareness and joined the network EU COST IC804 action "Energy efficiency in large scale distributed systems".

**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 multicore architectures as well as in highly scalable cluster systems. During 2009 the activities of the Group have focused in developing new features in the Paraver trace analysis tool (automatic analysis and sampling of traces) and tools integration (including multiscale simulation that mixes coarse-grain system simulation with instruction-level simulation). The Group has also been involved in the DEISA2 and HPC-Europa2 projects.

**Programming Models** Led by Xavier Martorell, the Group explores new programming models and their efficient implementation for current and future architectures, ranging from multicore (homogeneous and heterogeneous) architectures with support for accelerators (GPUs, FPGAs, ...) to exascale systems. This exploration is supported with the development of powerful compiler prototypes (Mercurium) and runtime systems (NANOS and StarSs). Based on the ideas behind these proof-of-concept implementations, the team is proposing extensions to the standards to address productivity and performance (partially in the framework of the joint BSC-IBM MareIncognito project). During 2009 the Group also continued the development of programming models for distributed memory architectures, specifically in two directions: supporting distributed shared-memory with NanosDSM, and improving the support for PGAS languages (in collaboration with IBM Watson). The group has continued his involvement in the ACOTES and SARC European projects, and coordinating the programming models cluster and applications task force in the HiPEAC2 Network of Excellence.

**Grid Computing & Clusters** Led by Rosa M. Badia, this Group is researching new programming and execution models, and resource management infrastructures for computational Grids. The team explores solutions in order to simplify application development, enable dynamic exploitation of parallelism at runtime and perform combined scheduling decisions at different levels. The efforts of the Group are focussed mainly in two projects: GRID superscalar and eNANOS. In addition, the Group is participating in a number of EU projects (BEinGRID, Brein, OGFEurope and XtremOS).



**Storage Systems** Led by Toni Cortés, this Group explores appropriate solutions to the scalability of parallel storage systems in large installations (in which very large volumes of data need to be generated and accessed) and file systems for the grid that solve the problems currently found (data location, replication and striping) and that will make these environments more efficient. In 2009 the Group focussed on three areas: file system scalability, Input/Output for Grid systems, and file-system virtualization. Within these, key efforts were the development understanding the data and metadata locality over long periods of time (more than 6 months), the application of COFS for composite file systems, and a number of improvements in the XtremOS project, in particular related to its file system XtremFS.



**Heterogeneous Architectures** Led by Alex Ramírez, this Group, in close interaction with the Programming Models Group, aims to design and evaluate next generation multicore architectures composed of heterogeneous components with a dual purpose: to focus the developments on the actual needs of the applications and the runtime system, and to anticipate the needs of the runtime system for future architectures so that software can be ready when research trends become products. During 2009 the Group has continued its participation in a number of projects (SARC, MareIncognito, ACOTES) with key efforts in integrating the TaskSim environment with the StarSs and NANOS runtime libraries, and exploring the memory architecture of multicore systems with hundreds of accelerators.



**Computer Architecture for Parallel Paradigms** Led by Adrián Cristal and Osman Unsal, this Group does research on architectural support to novel programming models and execution environments for future multicore architectures. The Group constitutes the core of the BSC-Microsoft Research Centre which has mainly focused on lowering the programmability wall raised by new multicore architectures; research areas include Transactional Memory and hardware support for programming language runtimes. During 2009, the Group finalized the development of transactional memory benchmarks and applications, which were released through the group website at [www.bscmsrc.eu](http://www.bscmsrc.eu). In addition the Group has participated in and coordinated the European VELOX project.



**Operating System / Computer Architecture Interface** Led by Francisco J. Cazorla, this Group focuses on three main areas; Kernel/architecture interaction with special emphasis on load balancing in high-performance computing applications, scheduling of network applications in massive multithreading processor architectures, and multicore architectures for hard-real time systems. In 2009 the Group continued its work in the European MERASA project and HiPEAC network of excellence, and in the collaborations in topics related with massively multithreaded architectures with Sun (scheduling of tasks in network applications) and IBM (hardware thread priorities and power consumption).



**Network Processors** Led by Mario Nemirovsky, this Group is conducting research on the massive multithreaded architectures focused on L4-L7 network applications. The Group also analyses the exploitation of parallelism within network processing by improving current parallel programming models and workload management. During 2009 the Group has been involved in a research collaboration with Cisco Systems investigating analytical models to overcome the problems of simulating different realistic network processing scenarios.







José María Baldasano,  
Director of the  
Earth Sciences  
Department

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

## Overview

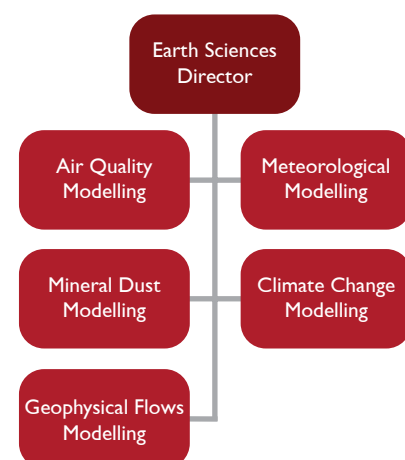
The high performance capabilities of MareNostrum enable the Earth Sciences Department to increase the spatial and temporal resolution of earth systems, in order to improve knowledge of dynamic patterns of air pollutants in complex terrains and interactions and feedbacks of

physico-chemical processes occurring in the atmosphere. Also possible are analyses with high-resolution global circulation models ( $2^\circ \times 2.5^\circ$  to  $1^\circ \times 1^\circ$ ) and downscaling to regional models. This coupling of global and regional climate models will contribute to a detailed description of the impacts of climate change.

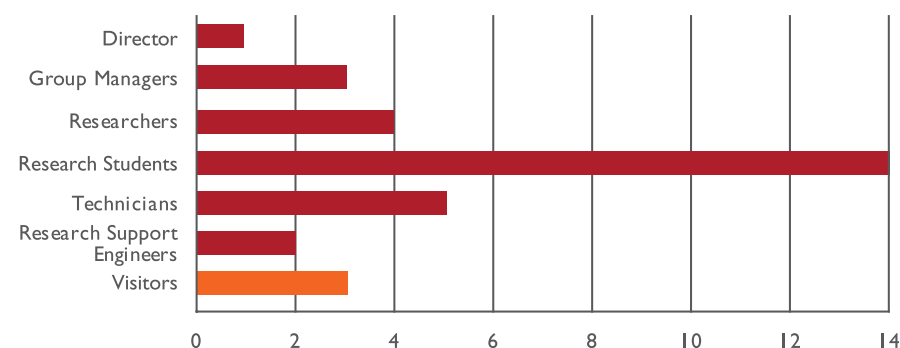
The main topics of research are: high-resolution air quality and meteorological modelling; global and regional mineral dust modelling; and global and regional climate modelling. Currently, the Group maintains daily high-resolution operational air quality forecasts for Europe and Spain ([www.bsc.es/caliope](http://www.bsc.es/caliope)) 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 ([www.bsc.es/projects/earthscience/DREAM](http://www.bsc.es/projects/earthscience/DREAM)).

The Department also collaborates with the World Meteorological Organization (WMO) and the Spanish Meteorological Agency (AEMet) in the creation of the Regional Center for Sand and Dust Storm Warning System (SDS-WAS) covering Europe, northern Africa and the Middle-East. Other research activities involve the diagnosis of the behaviour of Earth System Modelling (ESFM) codes in a supercomputer framework and the improvement of parallel versions of atmospheric models to increase their horizontal and temporal resolution.

## Organisational Structure



Earth Sciences Department Staff & Collaborators 2009

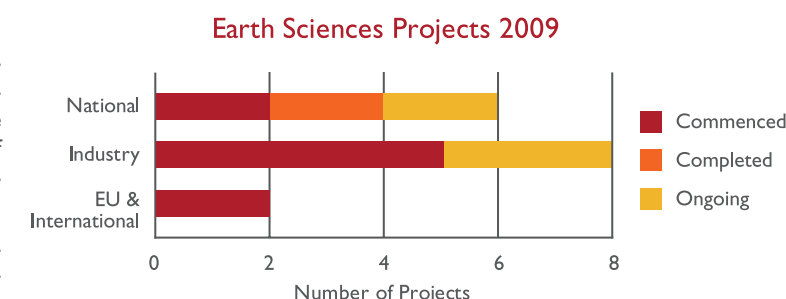


The Department is structured in five Groups that represent the main topics of Earth Sciences research: air quality modelling, mineral dust modelling, meteorological modelling, global and regional climate modelling and geophysical flows. These Groups are interrelated and work in a cooperative form. They 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 2009 some 32 staff and collaborators worked with the Department.



## Key Projects

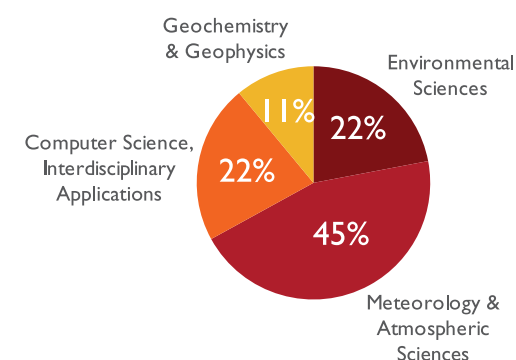
- Continued the new forecast phase of the CALIOPE project, supported by the Spanish Ministry of the Environment, Rural and Marine within the framework of the National Plan of Scientific Research, Development and Technological Innovation 2008-2010;
- Continued the extension of the CALIOPE project to the Canary Islands, funded by Government of the Canary Islands;
- Initiated the extension of the CALIOPE project to the Autonomous Community of Andalusia, funded by the Junta de Andalucía.
- Participated in the European Network for Earth System Modelling (ENES);
- Initiated 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;
- Led the Earth Science work package in the Consolider Program coordinated by the BSC;
- Supported by the Environmental Department of Catalonia Government (Spain), analysed the effects on air quality of introducing a variable speed system in the road network of Barcelona Metropolitan area;
- Continued work on the CICYT project: Coupling of a Fully Online Chemical Mechanism within the Atmospheric Global-Regional UMO Model funded by MICINN; in cooperation with NCEP, NOAA (USA);
- Initiated the Complementary Action: A modelling strategy for the Buenos Aires Volcanic Ash Advisory Center (VAAC). This Project aims at furnishing the Buenos Aires VAAC with the emergent modelling scientific outcomes. It is funded by MICINN;
- Finalised the CICYT Project: Improvement of the DREAM Regional Atmospheric Model of Mineral Dust for the prediction of Saharan Dust events in the Mediterranean and the Canary Islands, funded by MICINN;
- Finalised the CICYT project: High-resolution modelling of atmospheric pollution by anthropogenic and natural particulate matter in the Iberian Peninsula funded by MICINN;
- Initiated the MACC (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;
- 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;
- Actively contributed as a member of the Spanish network RETEMCA (Red Temática de Modelización de la Contaminación Atmosférica);
- Implicated in several projects of technology transfer, such as the participation in two EIAs for Modelling Air Quality of power plants.



## Scientific Output

The diffusion of research results obtained by the Earth Sciences Department has been noteworthy. These results have been presented in a numerous ISI-JCR journals, European and international congresses and symposia organised during 2009, such as the International Technical Meeting on Air Pollution and its Application supported by NATO, Harmonisation within Atmospheric Dispersion Modelling

Journal Publications by Subject Category 2009



for Regulatory Purposes; American Union Geophysical, European Geosciences Union General Assembly Meeting and other congresses organized by the European Meteorology Society (EMS). The number of papers published increased from 51 in 2007 to 59 in 2009, and considerable augmentation of the number of ISI-JCR publications (from 3 in 2007 to 14 in 2009). The JCR publications have an average quality of 2,9 (average ISI Impact Factor) and were distributed over a number of subject categories, as can be seen in the chart.

## Communication & Dissemination 2009

Publishing	
Journal Articles	14
Book Chapters	1
Conference Presentations	
International	35
National	10
Workshops	
Workshops	5
Education	
Theses Read	1

## Air Quality

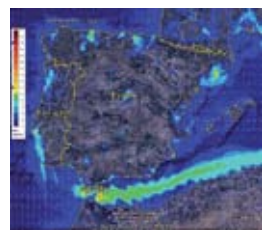


Figure 1 - Air quality modelling system (WRF-ARW/HERMES-EMEP/CMAQ/BSC-DREAM8b) forecast result for NO<sub>2</sub>, visualized in Google Earth

The Air Quality Group focuses its research in 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 2009 the activities were mainly related to the CALIOPE project, funded by the Spanish Ministry of the Environment and Rural and Marine Affairs, whose main objective is to establish an air quality forecasting system for Spain. In this framework, a high-resolution air quality forecasting system, namely WRF-ARW/HERMES-EMEP/CMAQ/BSC-DREAM8b, is being developed and applied to Spain

(4 km x 4 km, 1hr) as well as to Europe (12 km x 12 km, 1hr). The system will provide end-users with an air quality forecasting and assessment service for Spain and Europe with higher detail for some hot spot areas (<http://www.bsc.es/caliope>). During this year enhancements of operational forecast system implementation were introduced, on-line forecast operational evaluation was implemented and Google Earth visualization capabilities were also incorporated (Figure 1).

Air quality models (WRF-ARW/HERMES-EMEP/CMAQ/BSC-DREAM8b) were improved and were also used to assess the effects of hypothetical mitigation measures planned by the regional administration to ameliorate air quality conditions in urban areas, including the effects of introducing a variable speed system in the Barcelona Metropolitan area and comparing emission scenarios based on vehicle fleet composition of Barcelona, differentiating by category (weight, age, fuel) and activity (taxi, public transport vehicles, etc).

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

## Climate Modelling

The Climate Modelling Group investigates the causes and effects of climate change making use of the high spatial and temporal resolution Earth System Models (ESM), in combination with regional disaggregation and downscaling methods to provide regional climate information.

In 2009 the activities of the Climate Modelling Group were mainly related to the EC-Earth project which forges weather forecasting and climate change studies into a single framework under the seamless prediction paradigm. The group worked in dynamical downscaling from EC-Earth version 2. Fully coupled ocean/ice and atmosphere/land models were run for 10 years, starting from 1990 after a spin-up of 250 years, with 20th century boundary conditions (greenhouse gases, aerosols, land use and solar activity) and simulations for the same period were run with MM5 and WRF-Regional Climate Model versions driven by ERA-Interim (EI) reanalysis and EC-Earth. Both models show a systematic cold bias for maximum temperature; however, a warm bias is depicted for the minimum temperature in more northern Europe. The precipitation biases show more varied patterns than temperature and a predominant tendency to underestimate precipitation over Europe (Fig 2). Other key activities, related to EC-Earth project, were porting EC-Earth version 2.1 and 2.2 to MareNostrum and diagnosing the performance of these ESM versions in MareNostrum. EC-Earth version 2.2 is currently being used to perform the simulation runs for the Coupled Model Intercomparison Project Phase 5 (CMIP-5), which will provide future climate change information to be considered in the future IPCC-AR5 report.

The Group also participated in the IS-ENES FP7 project, devoted to fostering the integration of the European climate and Earth system modelling community and the development of Earth System Models (ESM) for the understanding of climate change. The Group evaluated ESMs on the MareNostrum supercomputing architecture and developed a data management tool based on GRID Superscalar.

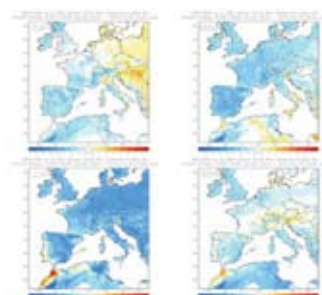


Figure 2 - Seasonal bias of maximum 2-m temperature using MM5 driven by EC-Earthv2.0 simulations for the 1990-2000 period

## Meteorological Modelling

The Meteorological Modelling Group takes advantage of the computing performance of MareNostrum to study mesoscale phenomena, focusing on the improvement of the skills scores of numerical meteorological codes.

In 2009 the Group continued the development of a new on-line global/regional chemical weather prediction system (NMMB/BSC-CHEM) in strong collaboration with the Mineral Dust Modelling group. The system is based on a new multi-scale atmos-

pheric model (NMMB) developed at National Centers for Environmental Prediction (NCEP). The new modeling 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.

In the context of the CALIOPE project, the WRF-ARW model was used to provide meteorological inputs for air quality modelling in the Barcelona area (1km resolution), Andalucía region (2km), Canary Islands (2km), Iberian Peninsula (4km) and Europe (12km). A near-real time evaluation system of surface meteorological fields was implemented to automatically process and evaluate the 2009 forecasts.

In collaboration with the CASE Department, the Group continued the analysis and testing of new atmospheric codes capable of exploiting massively parallel architectures. Ideally tests of dry-adiabatic atmospheres cases are properly solved. Next steps will include the coupling of a transport scheme with the dynamical core and the implementation of a microphysics package to take into account moisture processes.

Research in clean energy resources is also carried on. A solar irradiance forecasting system for Spain by means of numerical weather prediction is under development. The new system aims to provide useful short-term forecasts of solar irradiance for energy production from photovoltaic solar plants, and for improving the management of electrical grid networks. An annual evaluation of the system was performed and post-processing methods to improve the skills of the system are under study.

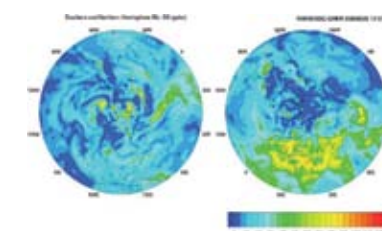


Figure 3 - First simulations with the NMM/BSC-CHEM modeling system on MareNostrum

## Mineral Dust Modelling

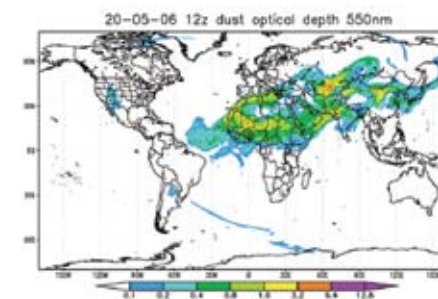


Figure 4 - First Simulations With the NMM/BSC-Dust Dust Modeling System on MareNostrum

The Mineral Dust Group provides daily operational forecasts of mineral dust for North Africa, Middle East, Europe and East Asia based on the Dust Regional Atmospheric Model (DREAM). In 2008 the Group developed a new generation atmospheric mineral dust model (BSC-Dust) coupled on-line to the new generation unified atmospheric model NMMb of the National Centers for Environmental Prediction (NCEP). The new modelling system is intended to be a powerful tool for research and to provide efficient global and regional chemical weather forecasts at sub-synoptic and mesoscale resolutions on MareNostrum supercomputer (Figure 4) including a physically-based dust emission scheme taking into account the effects of saltation and sandblasting, soil moisture and viscous diffusion close to the ground. The World Meteorological Organization (WMO) has launched the Sand and Dust Storm Warning and Assessment System (SDS WAS) that bridges the technological gap between

research and operational services. Regional activities related to modelling, observations and applications are coordinated through the Asia/Central Pacific Regional Centre for SDS WAS at the China Meteorological Agency in Beijing, China. The Regional Centre for Northern Africa, Middle East and Europe is based at the BSC and the AEMet (Spanish Weather Service) in partnership with other operational and research organisations (e.g. ECMWF, MeteoFrance, LISA, LSCE, IFT, EUMETSAT, CNR, AERONET/PHOTONS).

## Geophysical Flows

The main research line of the Geophysical Flows / Physical Volcanology Group during 2009 was modelling atmospheric transport of volcanic ash and aerosols. The main tasks and achievements of the year were:

- ▶ Development, testing and implementation of a new version of the FALL3D code including coupling with global and regional meteorological models, development of a physical model for aggregation of volcanic ash, optimisation for the MareNostrum architecture, parallelisation of the I/O strategy and automatic postprocess.
- ▶ Implementation of the model at several International Institutions including the Buenos Aires Volcanic Ash Advisory Center (project CGL2008-04484-E/CLI entitled "A MODELLING STRATEGY FOR THE BUENOS AIRES VOLCANIC ASH ADVISORY CENTER"), the INGV in Italy, and CORPAIRE in Quito, Ecuador.
- ▶ Parallelisation of the SLAG code aimed at solving the shallow waters equations applied to lava and water flows.
- ▶ Inclusion in the VHub Cyberinfrastructure of the Buffalo University for Volcano Eruption and Hazards Modelling and Simulation.

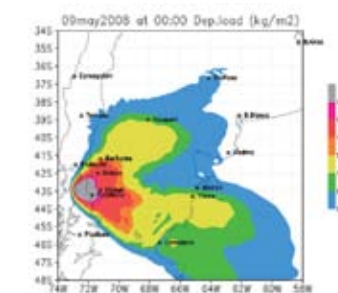


Figure 5 - Ash ground load (in kg/m<sup>2</sup>) from May 2008 Chaitén volcano eruption, Chile. Simulation was done during 2009 at the Buenos Aires VAAC during the installation of the FALL3D program





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 program is tightly integrated in a collaborative effort with the Institute for Research in Biomedicine (IRB).

search 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.

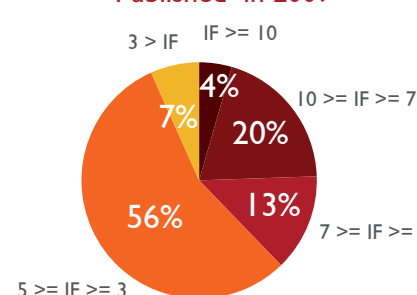
## Joint IRB-BSC Program on Computational Biology



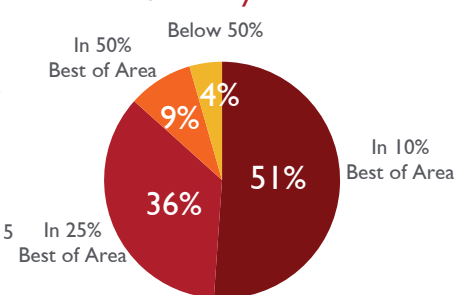
The Computational Biology program was created as a joint venture between the BSC and the Institute for Research in Biomedicine (IRB Barcelona) with the mission to face the computational challenges in molecular biology. The program coordinated by Modesto Orozco includes researchers from the Structural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

The group leaders involved in the program are Victor Guallar (Electronic and Atomic Protein Modeling, BSC-Life Science department), Patrick Aloy (Structural Bioinformatics and Network Biology, IRB Barcelona) and Modesto Orozco (Molecular Modeling and Bioinformatics, IRB Barcelona). Montse Soler is the platform leader of the Experimental Bioinformatics Laboratory (BSC-IRB). The BSC Life Science Program and the Joint IRB-BSC Program on Computational Biology employ researchers from both institutions supported by more than 35 research grants totalling €6M.

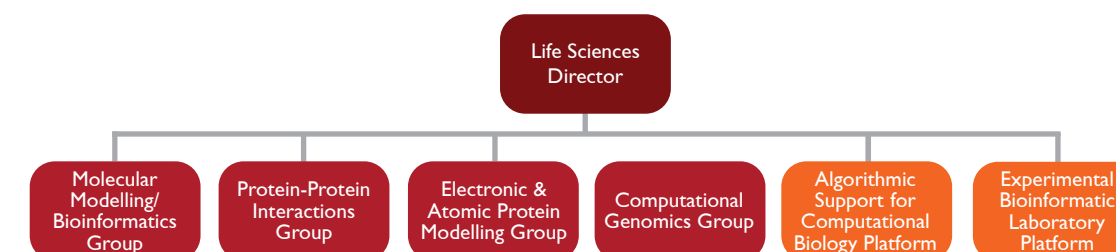
ISI Impact Factor of Articles Published in 2009



Distribution of 2009 Scientific Production by ISI IF Rank

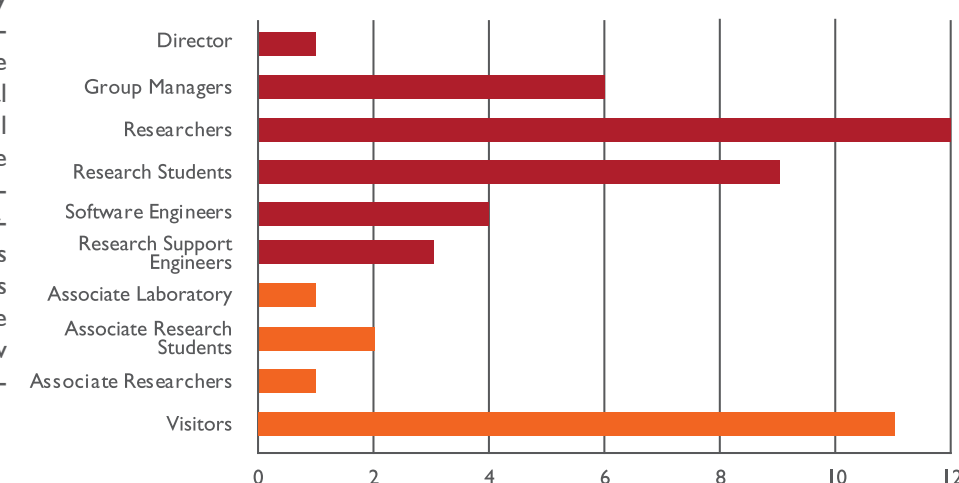


## Organisational Structure



The structure of the Department and the technology platforms in its research program 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 continues to grow strongly, from 37 staff and collaborators in 2006 to 75 in 2009.

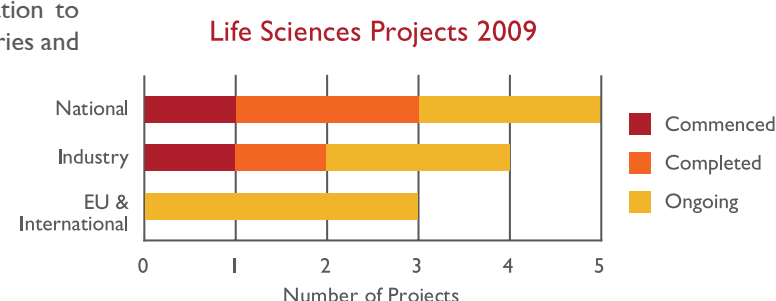
Life Sciences Department Staff & Collaborators 2009



## EU & National Projects

Key activities during 2009 included participation in the following key BSC-CNS projects:

- ▶ MITIN - Integration of the systems models of mitochondrial function and insulin signalling, and its application in the study of complex diseases. Funded by FP7.
- ▶ METAHIT - Metagenomics of the human intestinal tract. Funded by FP7.
- ▶ ELIXIR - To construct and operate a sustainable infrastructure for biological information in Europe to support life science research and its translation to medicine and the environment, the bio-industries and society. Funded by FP7.
- ▶ IMID-Kit - Development of a diagnostic kit for inflammatory diseases mediated by immune mechanisms. Funded by MICINN as a Singular Strategic Project.
- ▶ Genetic Evolution in Vertebrates. Funded by CICYT, Spanish Government.
- ▶ Biochemical Modelling. Funded by CICYT, Spanish Government.
- ▶ Protein Docking Challenges. Funded by CICYT, Spanish Government.



## Scientific Output

The Life Science 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: Discover the mechanisms of biological systems at the molecular scale.

Organised Events:

- ▶ Expanding the Frontiers of Molecular Dynamics, Barcelona 23-25 November 2009
- ▶ Conference on Next Generation Sequencing: Challenges and Opportunities, Barcelona, 1-3 October, 2009
- ▶ CAPRI Barcelona, 9-11 September 2009

Communication & Dissemination 2009	
Publishing	
Journal Articles	46
Book Chapters	0
Conference Presentations	
International	5
National	10
Workshops	
Workshops	0
Education	
Theses Read	3

## Molecular Modelling and Bioinformatics Group

Led by Modesto Orozco, the long term objective of this Group 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. The research effort is focused in three major areas: i) study of small model systems, ii) analysis of stressed or unusual nucleic acids and iii) dynamics of proteins.

## Protein Interaction and Docking Group

Led by Juan Fernández-Recio, this Group aims to study the mechanism and function of proteins in living organisms, with a special focus on the biomolecular interactions at atomic and residue level. Proteins interact to form highly specific complexes that are fundamental for the majority of cellular processes. The prediction and characterization of such complexes has enormous interest,



both at academic level and from a practical point of view. The ultimate scientific goals are: to understand the mechanism of protein-protein association, and to design molecules capable of targeting protein interactions of biomedical interest. The major research areas are: i) development and optimization of protein docking tools, ii) development of new tools for protein structure and function predictions and iii) modelling protein interactions of biological and therapeutical interest.

## Electronic and Protein Modelling Group

Led by Victor Guallar, the overall objective of this lab is to explore the chemical and physical responses to local and global configuration changes in proteins, with emphasis on substrate biochemistry and ligand docking and diffusion. During 2009 the Group continued its research in two key areas: i) Classical simulations using approximate analytical potentials to describe the nuclear energy landscape and ii) Quantum chemistry simulations of electron transfer processes in proteins.



## Computational Genomics Group



Led by David Torrents, the ultimate goal of the research in this Group is the identification and understanding of the molecular and evolutionary processes that determine the biology of genomes, and also the biomedical implications that derive from its malfunction. Increasingly, together with the generation of new genomic sequences, there is a massive and automatic production of functional data associated with these sequences. Based on these datasets and also on detailed experimental data, the Group applies computational approaches to identify, classify and analyse functional genomic regions and regulatory associations between the components of defined biological systems. The key

research lines of the Group are: i) function prediction of regulatory regions in vertebrates, ii) identification of regulatory modules of transcription binding sites conserved in cancer genes, and iii) computational modelling of human complex diseases: diabetes and obesity.

## Algorithmic Support for Computational Biology Platform (ASU-INB Computational Node)

Led by Josep Lluís Gelpi, the platform's main purpose is to facilitate access to biological databases and programs by the bioinformatics community and to support the research Groups in the program. One of the main activities of the node is to coordinate the computational node of the Instituto Nacional de Bioinformática (INB-GN6). The internal structure of the node consists in two subteams: i) external projects support engineers which are assigned to the INB supported projects and help in the implementation and optimization of users applications in the supercomputing environment, and ii) the Web Services and Database development subteam, which is in charge of building web services and web interfaces and create and manage biological databases. During 2009 the ASU has provided external support to the Bioinformatics community in areas such as molecular dynamics simulations, protein-protein interactions and computational genomics. Especially relevant in this area is the collaboration into the IMIDKIT project, where the unit is in charge of creating and managing the epidemiology database.



## Experimental Bioinformatics Laboratory Platform

Led by Montse Soler, this platform was established in January 2008 as part of the IRB-BSC collaboration. The platform is dedicated to implementing advanced experimental approaches that provide computational biologists in the program the opportunity to integrate experimental measurements into their predictions. In 2009 the laboratory was consolidated and extended its work in the areas of systems biology (protein-protein interaction networks) and genome regulation.





José María  
Cela,  
Director of  
the CASE  
Department

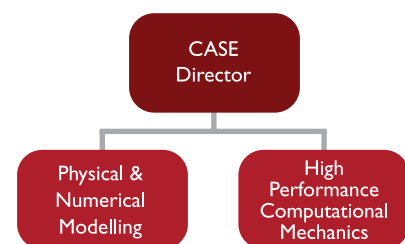
The aim of the Computer Applications in Science & Engineering (CASE) Department is to identify, engage and support user communities in science and engineering that are potential users of High Performance Computing, boosted by its own research lines in High Performance Computational Mechanics.

## Overview

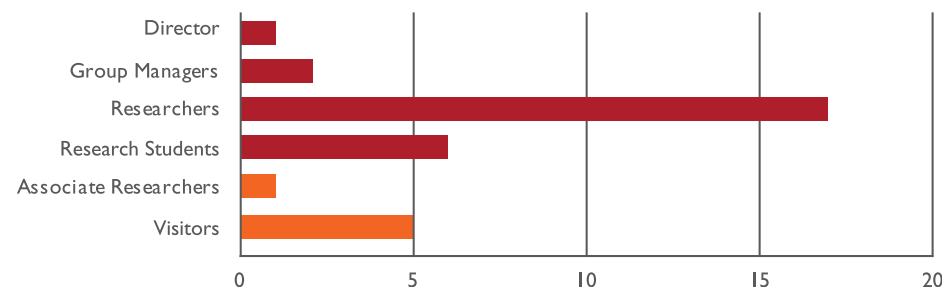
The applications developed by the CASE department are truly multidisciplinary, requiring depth of expertise in many fields. In order to successfully develop these applications, the skills of the CASE team in numerical methods and parallel programming must be complemented by experts in appropriate areas. The Department therefore develops collaborations with other scientific groups, especially those with expertise in areas which the BSC-CNS Groups do not have extensive experience. Examples of institutions with strong research links with CASE include CIEMAT, CSIC, IAC, ICFO, IMDEA and different universities.

The 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.

## Organisational Structure



CASE Department Staff & Collaborators 2009



The CASE Department is led by José María Cela, and although there is high interactivity amongst all the scientists in the Department, the research lines fall naturally in two main Groups; Physical & Numerical Modelling (PNM) and High Performance Computational Mechanics (HPCM).

Each Group consists of 8-10 people at any given time, 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.

## Key Projects

In 2009, the CASE Department carried out work under the scope of the following projects:

### EU funded projects

- ▶ EUFORIA: Generating a software infrastructure for support of the ITER design community.
- ▶ ETSF: Generating a software infrastructure for support of the spectroscopy community; in particular, work was undertaken on the scalability of OCTOPUS.
- ▶ W2PLASTIC: Magnetic Sorting and Ultrasound Sensor Technologies for Production of High Purity Secondary Polyolefins from Waste. The physical problem to be simulated was modeled and validated.
- ▶ DEISA: Continued collaboration, leading work packages 5 and 9, on “Enabling of Applications”.
- ▶ PRACE: Several codes (ALYA, BSIT, CPMD, EUTERPE) were analysed and tuned for PRACE prototypes.

### Enterprise funded projects:

- ▶ Kaleidoscope (REPSOL): With the goal of developing the most powerful seismic imaging tools, an RTM application 10 times faster than any other implementation was developed, specifically developed for running in both IBM's Cell/B.E. processor and GPUs.
- ▶ MareIncognito (IBM): Leading work package 1 for applications porting, some codes (such as SIESTA) were scaled for the MareIncognito architecture.

### 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.
- ▶ ATMOST (Plan Nacional): This project started in 2009 and aims to model ashes and contaminant dispersion in the atmosphere.

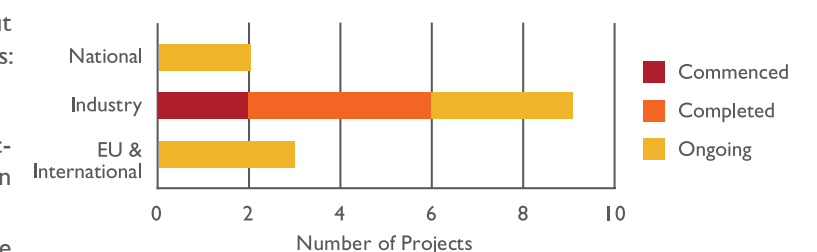
### The CASE department also develops two international collaboration projects in the area of biomechanics:

- ▶ Airflow in the Human Respiratory System: In collaboration with both the Aeronautics and Bioengineering Departments at Imperial College London. A simulation of the complete human respiratory system, including the air surrounding the face, has been carried out. This project is being partially supported by HPC-Europa European project.
- ▶ Cerebral Hemodynamics Model: In collaboration with the CFDLab George Mason University, USA, the Krasnow Institute for Advanced Studies, George Mason University, USA, the Inova Fairfax Hospital, Virginia, USA, the National Center for Computational Biology, UCLA, USA and the Brain Research Institute, Melbourne, Australia. A model of the arterial system of the brain is being developed. A deflated preconditioner with conjugate gradient solver was used to accelerate the pressure solver in this simulation. A speed-up of 10 with respect to the original solver was obtained.

## Scientific Output

Although a large part of the Department's work is private and in-confidence and therefore cannot be published, some important research results of the Department have been presented in congresses and conference lectures as well as a number of scientific publications, including: FEF09 and ParCFD-09, SEG and EAGE conferences in Geophysics, International Conference on Mathematics and Continuum mechanics, as well as the 1st International Conference on Computational & Mathematical Biomedical Engineering.

CASE Projects 2009



Communication & Dissemination 2009

Publishing	
Journal Articles	6
Book Chapters	0
Conference Presentations	
International	9
National	0
Workshops	
Workshops	0
Education	
Theses Read	0

## Physical and Numerical Modelling (PNM)

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.
- ▶ Numerical algorithms to solve the discrete equations efficiently, or to couple a set of algorithms to solve complex physical problems: explicit and implicit schemes, monolithic and fractional algorithms, preconditioners and multigrid.
- ▶ Efficient implementation in a computational mechanics code: distributed/shared memory parallelisation with MPI/OpenMP, code optimisation; architecture dependent implementation (VMX, Cell).
- ▶ Code performance analysis and optimisation.

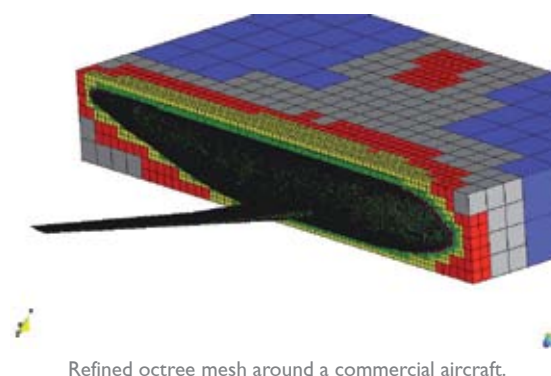
The PNM has recently started a new research line focused on the design of applications specially designed for their use in Social Sciences and policy analysis areas. The group is developing a new simulator capable of executing Agent-Based Models of human societies in a HPC environment, in order to explore:

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

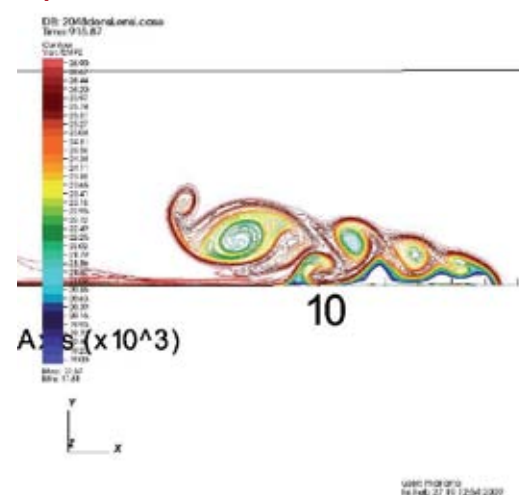
These topics are analyzed from a multidisciplinary approach, as CASE joins efforts with research groups belonging to different disciplines, with diverse perspectives of social interaction (i.e. Archaeology, Demography, Economy, Heritage, History and Sociology).

Within these areas, in 2009 the PNM Group have mainly followed these lines:

- ▶ Efficient solving strategies: preconditioners, parallel strategies, fractional schemes.
- ▶ Octree-like structured mesh generator, now undergoing testing.
- ▶ Stabilisation algorithms for compressible flows for a wide range of Mach numbers.
- ▶ A domain decomposition Chimera scheme for different fluid problems
- ▶ A numerical implementation of Electrophysiology problems in unstructured meshes.
- ▶ A module of Alya for solving large-strain solid mechanics in the total Lagrangian formulation.
- ▶ A free surface module using level sets and a bi-fluid formulation.



Refined octree mesh around a commercial aircraft.



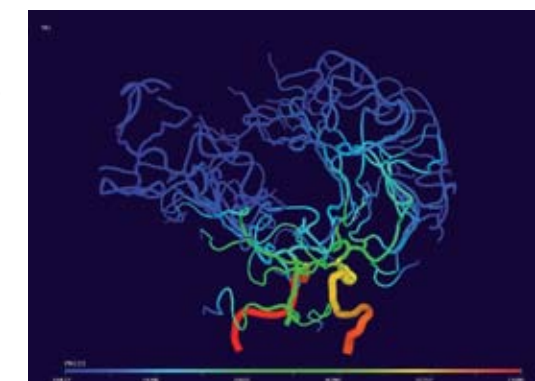
Atmospheric density wave.

## 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 are:

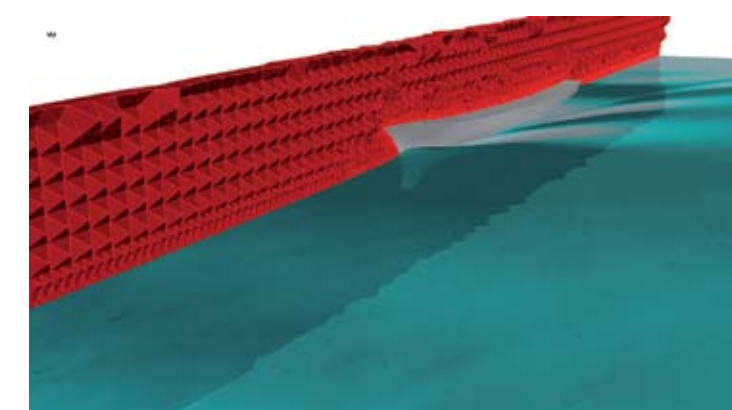
- ▶ Bio-mechanics: Hemodynamics, respiratory system air flow, cardiac simulation.
- ▶ Geophysics: seismic imaging and oil reservoir simulations.
- ▶ Plasma Physics.
- ▶ Atmospheric flows: mesoscale and urban environments.
- ▶ Energetically Efficient Building Design.
- ▶ Ab-initio DFT and TDDFT molecular dynamic simulations.
- ▶ CFD: subsonic and supersonic flows, free surface problems, coupled problems.



Brain arterial system, pressure distribution

Within these fields, in 2009, the HPCM Group developed:

- ▶ A large-strain solid mechanics model for anisotropic cardiac tissue. This model will be coupled with the electrophysiology model to create a cardiac simulator.
- ▶ Hemodynamics simulations of the arterial brain system.
- ▶ Airflow simulations of the whole respiratory system during normal breathing cycles.
- ▶ An RTM seismic imaging facility on GPUs.
- ▶ A dynamic atmospheric mesoscale parallel code.
- ▶ A parallel version of SIESTA code with better load balancing and sparse iterative eigen-solvers.
- ▶ Free surface parallel solver for sailing boats.



Wave system formed by a ship.





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 deve-

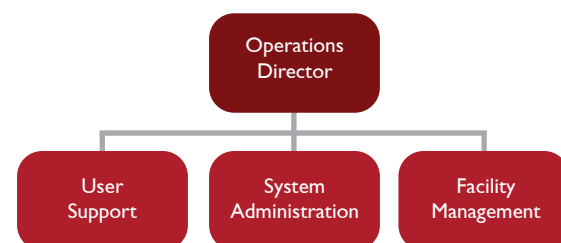
lopment in order to be able to professionally carry out their duties in an environment of constant technological change and advancement.

## Overview

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

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.

## Organisational Structure



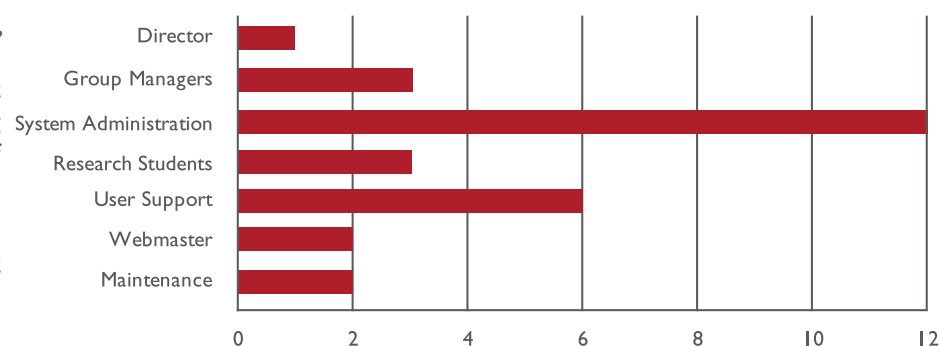
User Support is responsible for direct user support providing detailed knowledge of programming models, libraries, tools and applications, and also is responsible for management of the BSC website, including the electronic management of access applications.

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.

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

Systems Management 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.

Operations Department Staff & Collaborators 2009



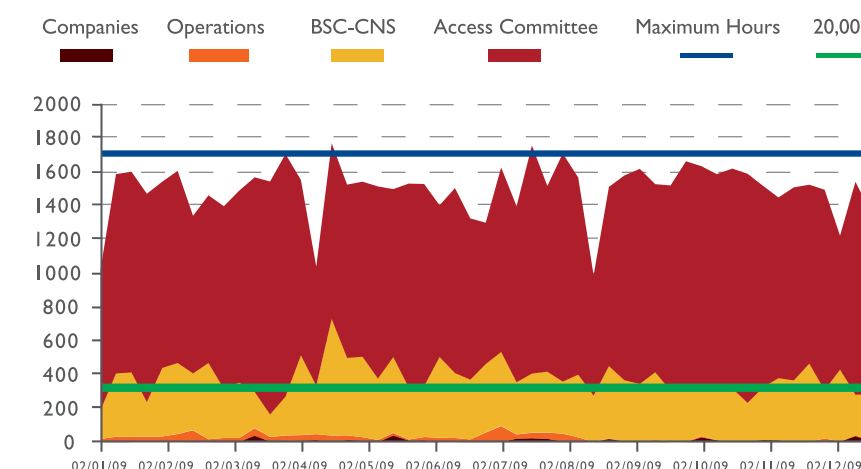
## System Administration

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 Performance 2009

Weekly Use of the MareNostrum in 2009



MareNostrum has been in production the whole year, except for maintenance periods. Using the remaining part of the year as the basis for calculations, the observed system utilization is approximately 82%. In addition to BSC-CNS internal groups, more than 212 external groups accessed to the MareNostrum system.

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

## Training and Seminars

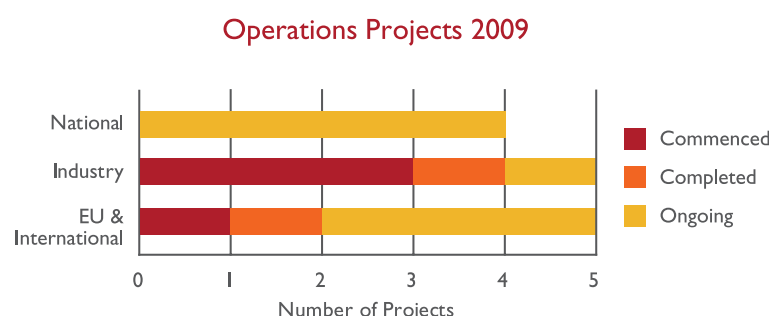
The Operations Department organises technical seminars where engineers share knowledge and experience, for example with manufacturing companies in order to inform attendees about their products and technical processes. During 2009, RES organized a technical seminar related to the upgrade to SLES10 & GPFS 3.2 of the clusters. This seminar took place the 28th and 29th April in Valencia.

## Key Projects and Upgrades 2009

### Software upgrade of MareNostrum

During 2009, MareNostrum was upgraded from Suse Enterprise Linux version 9 Service Pack 3 to Suse Enterprise Linux version 10 Service Pack 2. The upgrade of the operating system has provided the opportunity to upgrade the Global Parallel Filesystem of MareNostrum from version 2.3 to 3.2. Both upgrades have provided new features, better performance and stability of the whole cluster.

Apart from the upgrade on MareNostrum, a plan was performed so all other nodes of the RES were upgraded in the same way that MareNostrum. A workshop made in Valencia was done to coordinate this action.



CNAG Cluster

**CNAG tender preparation** Centro Nacional de Análisis Genómico (CNAG) is a center created in October of 2009 with the mission of promoting the use of modern genomics in Spain, and covers the increasing demand of genome sequencing in research projects.

CNAG plans to acquire 10 sequencing machines, but also requires computer equipment to cover the needs of compute and storage that all post-processing of data generated from the sequencers requires.

BSC helped during 2009 in the computer requirements' collection and design; during 2010 will deploy and administer the CNAG computer infrastructure. As a result, a public tender was prepared and the study of the solutions presented was also carried out, to select which was the best one for the requirements collected.

**Internal database storage expansion** A new controller and disk expansions were acquired and installed to give a total of 28 TB extra to the Life Science and Earth Science databases storage.

**Panasas Filesystem installation** A new filesystem with a capacity of 20 TB has been installed in the Altix machine. This filesystem is also accessible from MareNostrum and is intended to store and share data between both supercomputers.

**Personal equipment Backup system** During 2009 the backup system that was used exclusively for servers and the supercomputers were opened to personal equipment of BSC, so any researcher inside BSC could make backup of their data to the BSC tape storage system.

At the end of 2009, 80 personal computers were introduced and has been using this backup system, with a total tape storage used of 26 TB.

**HSM storage expansion and High-Availability** An expansion of 9 TB of SATA technology was acquired during 2009 to add to the first level of storage of the Hierarchical Storage Management (HSM). Also a second server was acquired so the HSM service can work in a high-availability modality (SAMFS-QFS solution) and also will provide the possibility to access to HSM data from Internet through this new server.

## User Support

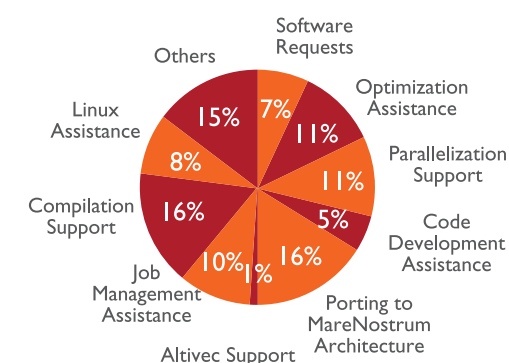
The User Support Group provides assistance with all aspects of scientific computing. This assistance includes general user support, code optimization and parallel model building support, and porting serial and parallel codes for supercomputers such as MareNostrum. The group is also involved in the creation of scripts for ease of use as well as assistance with software packages and tutorials on specialized topics or programs.



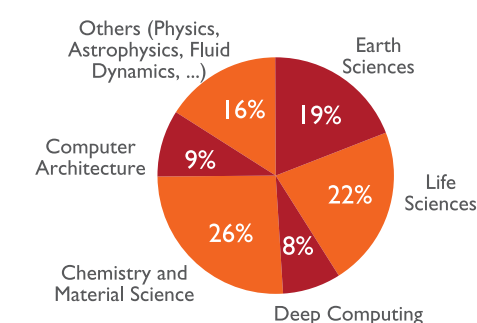
## Support Requests in 2009

The number of support requests received in 2009 was 5836 and these are presented in the figures below, split by support request area and the distribution of requests per month.

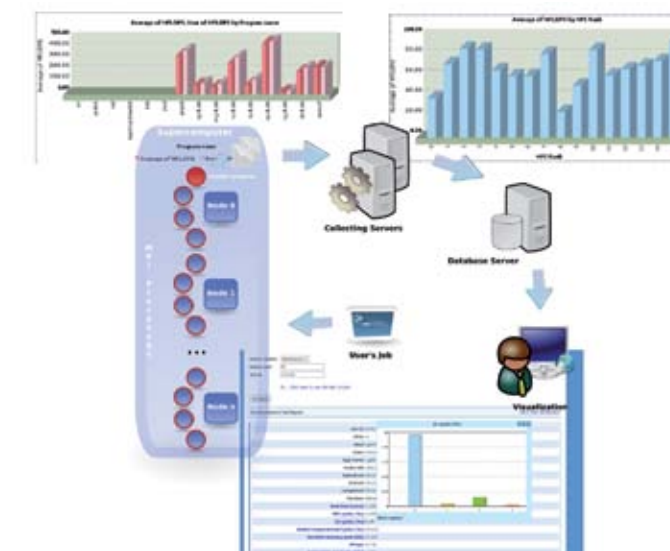
### User Support Requested by Topic 2009



### User Support Requested by Scientific Area 2009



## PerfMiner Project



In 2009 PerfMiner was deployed in MareNostrum, a system for the automated collection, storage and presentation of hardware performance metrics gathered per thread via PAPI across the entire cluster. It enables collection of performance data of the execution of any application running in MareNostrum without user intervention, including serial and parallel programs. Thanks to integration with Slurm, the resource manager, the changes were transparent to the user.

The system, which has negligible performance impact, is able to collect all the data generated by different executions and store it in a database to be analysed and visualised through a web application. A simple query can highlight which programs make better use of resources, if there are differences in performance from the same program across several users, or just produce a general performance report of a certain job.

## Facility Management

The Facility Management Group is responsible for keeping the core BSC-CNS facilities under its purview in a safe and efficient working condition. Key activities include advance data gathering, improving cost tracking and scheduling capabilities, identifying upgrades to major building systems in order to increase comfort, control and to minimize utility costs, and developing close relations with service and material suppliers in order to achieve better discounts and delivery times.

During 2009, several reviews were undertaken to identify priority needs, and to refine planning for the new building which will begin construction in 2010. The Group also contributed significantly to the planning and implementation of a new data centre that will serve the Parc Científic de Barcelona (PCB).







Ernest Quingles,  
Management  
Department  
Director

The key mission of the Management Department is to optimise coordination of the activities of the BSC-CNS and provide consolidated planning and management of support services to better meet the future challenges facing the centre.

Other core objectives include reliable and timely financial reporting, human resources management, and building awareness of the BSC-CNS, its mission, activities and its services. The department also assists other departments in identifying, applying and managing competitive projects, initiating and developing systems and

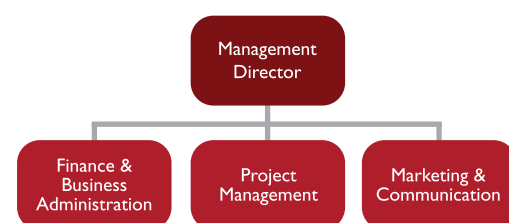
processes to increase the efficiency and effectiveness of staff and the quality of work, and developing electronic management tools.

## Overview

The Management Department, led by Ernest Quingles and supported by Mercè Calvet, was formed in 2007 as part of the internal reorganisation of the management structure of the BSC-CNS.

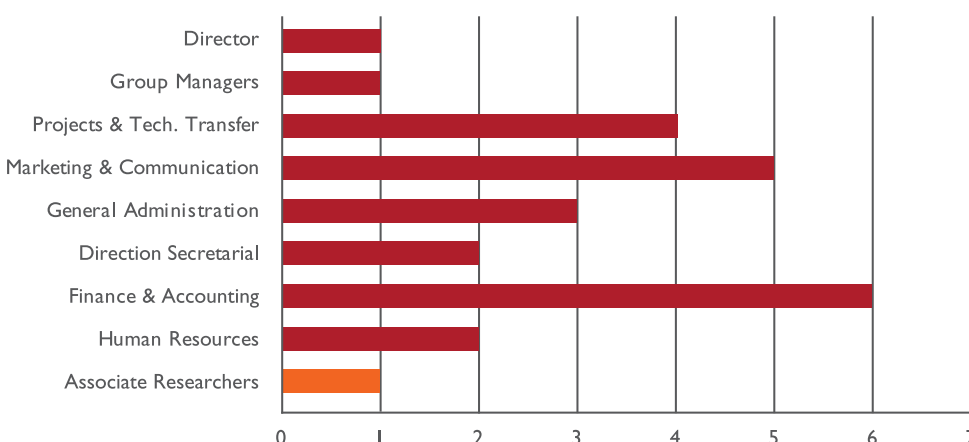
The constant changes at the BSC-CNS arising from its rapid growth, ever-expanding project portfolio, the temporary nature of working facilities pending the dedicated BSC building and the changes in technology and systems that accompany each upgrade cycle, make for a very dynamic environment with often intense and urgent requirements. The Department therefore aims to maintain a certain degree of flexibility and multi-skilling amongst its staff and encourages them to work closely with each other and their key points of contact in other departments.

## Organisational Structure



Management Department Staff & Collaborators 2009

The Management Department is structured in three 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.



## Finance and Business Administration

In 2009 the Finance & Business Administration unit continued improving internal management and reporting systems to support research projects and the increasing daily activity of the centre, as well as to facilitate the integration of new staff and visitors from local universities, and national and international mobility programs.

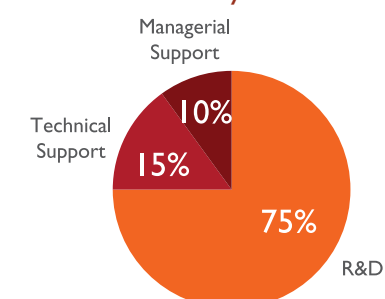
### Finance & Accounting

The Finance & Accounting service is responsible for the financial resources management of the BSC-CNS (expenses, budgets, audits, bank relations, suppliers, receiving payments and budget deviations). The Group also prepares the financial reporting for project audits, working closely with the Project Management Group, and the Marketing & Communication team in preparing budgets. In 2009 the team implemented the SAP BI tool to provide higher levels of fiscal control and better reporting capabilities.

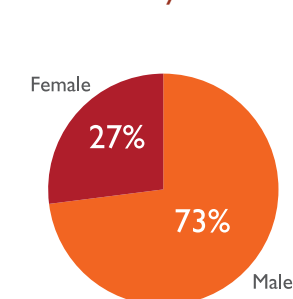
### Human Resources

The Human Resources service is responsible for managing selection processes, hiring and training, job descriptions, labour relations and collective bargaining, planning careers and internal promotion, and preventing work-related accidents. In 2009 various improvements were made in the areas of recruitment, mobility programs and induction processes, and work continued on a career plan for future individualised professional development programs for all BSC-CNS staff.

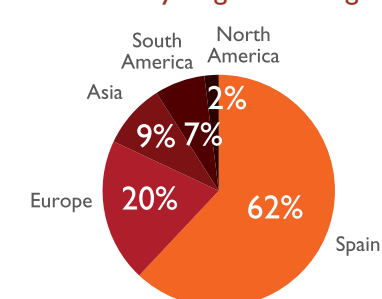
#### 2009 Personnel by Function



#### 2009 Personnel by Gender



#### 2009 Personnel by Region of Origin



## General Administration Support

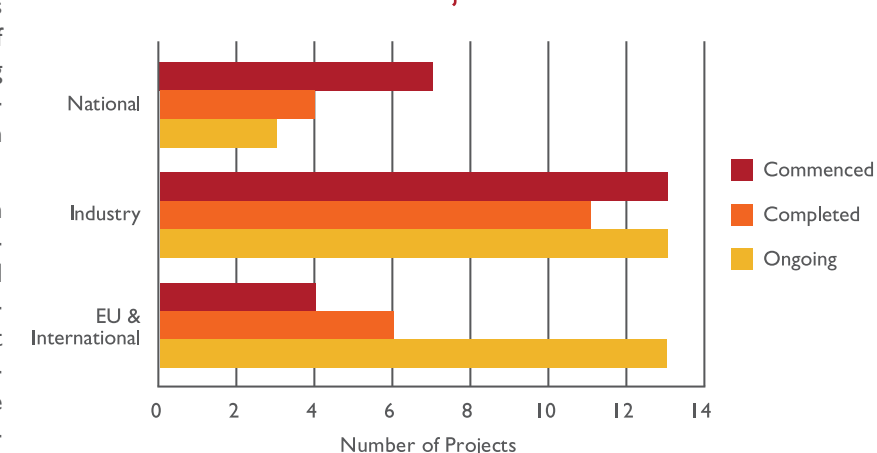
The General Administration service is responsible for activities such as organisation of official meetings, including those of the Access Committee, the Executive Commission, the Board of Trustees and other events. The Group manages travel services, space allocation, supply orders and execution of public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

## Project Management

The Project Management Group is responsible for the management of proposal submissions and ongoing management of publicly funded projects, as well as collaborations with private industry.

In 2009, the BSC-CNS participated in 74 projects, funded by national agencies, the European Commission and private industry. In addition to administering active projects, the Project Management Group assisted BSC-CNS researchers to submit a large number of new project proposals during 2009 to ensure continuity in the project funding pipeline.

#### BSC-CNS Projects 2009



## Marketing & Communication

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

### Visitors

In the course of 2009, the BSC-CNS received a total of 4531 visitors from national and international centres, including universities, research centres, industry and non-profit organisations.

Visitors to the MareNostrum are given a tour of the supercomputer and view a specially prepared video describing the technology used in the centre and the applications resulting from the supercomputing capacity such as all resources included at the RES. The visits can be accommodated depending on the target audience, too.

During this year, the BSC has received different official visits:

- ▶ April: Joan Puigcercós i Oriol Jurqueres
- ▶ July: Cristina Garmendia, Minister of Science and Innovation of the Spanish Government and Diputats del Parlament de Catalunya
- ▶ September: Carme Cubero, Director of Technology and Communications of the Environment Department of the Catalan Government

### BSC-CNS in the Media

During 2009 BSC was mentioned 158 times in national and international newspapers and magazines. Print media have been the ones where BSC has received most coverage, TV and online press are in second place, the third one is radio and the last one wires.

In total, BSC launched 14 press releases in Spanish, Catalan and English that were included on the Press section of the BSC website. All press impacts have also been included in this section. Furthermore, the press team has updated regularly the press dossier of BSC and RES in English, Catalan and Spanish, as well as the BSC-Microsoft Research Center press dossier. This team has also been involved in the launch of various press releases of European Projects (VELOX, MERASA, Hipeac, SARC, HPC-EUROPA, etc.) to the BSC press contacts.

A press conference was organised on the 20th April under the title “Pacte Nacional per a la Recerca i la Innovació (PNRI)” at BSC facilities, where Josep Huguet, Minister of Science and Innovation of the Catalan Government, Jordi Hereu, Major of Barcelona City Council and Mateo Valero, BSC Director addressed the Spanish and Catalan media. During this event the City Council of Barcelona joined the so-called PNRI at Torre Girona.

### Participation in Key Events, Seminars and Workshops

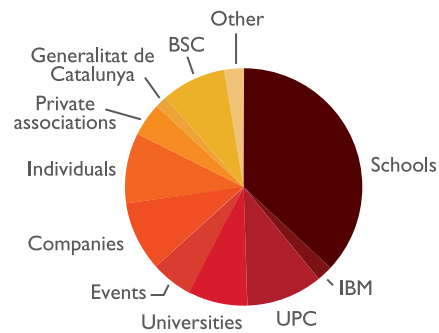
In 2009, BSC-CNS organised the following:

- ▶ ScicomP 15 & SP-XXL, May 18-22, 2009
- ▶ ESA/WMO Expert Consultation Meeting For Development of Satellite Products Relevant to the WMO Sand and Dust Storm Warning Advisory and Assessment system (SDS-WAS), 8-9 September 2009
- ▶ RES Seminar
- ▶ BSC-PRACE code porting and optimization workshop, 21 – 23 October 2009
- ▶ Expanding the frontiers of molecular dynamics simulations in biology, 23-25 November 2009
- ▶ ABC Meeting, 25th November 2009
- ▶ Critical Assessment of Predicted Interaction (CAPRI), 9-11 December 2009

The BSC-CNS also had a significant presence at:

- ▶ Opening of the Instituto Tecnológico de Canarias RES node, 16th February 2009
- ▶ International Supercomputing Conference (ISC2009), Dresden, June 2009
- ▶ Supercomputing (SC'09), November 2009

Visits to the MareNostrum 2009



## Computer Sciences 2009 Publications

### Journals

- » Alejandro Duran, Roger Ferrer, Eduard Ayguadé, Rosa M. Badia and Jesús Labarta, A Proposal to Extend the OpenMP Tasking Model with Dependent Tasks, *International Journal of Parallel Programming*, Volume 37, Issue 3 (2009), pages 292-305, 1/6/2009
- » Alejandro Rico, Alex Ramirez and Mateo Valero, Available task-level parallelism on the Cell BE, *Scientific Programming*, pp. 59-76, vol. 17, no. 1-2, 39845
- » Arnaldo Azevedo, Cor Meenderinck, Ben Juurlink, Andrei Tereckho, Jan Hoogerbrugge, Mauricio Álvarez, Alex Ramirez and Mateo Valero, A Highly Scalable Parallel Implementation of H.264, *Transactions on High-Performance Embedded Architectures and Compilers*, vol. 4, no. 2, 1/9/2009
- » Carlos Luque, Miquel Moreto, Francisco J. Cazorla, Roberto Gioiosa, Alper Buyuktosunoglu, and Mateo Valero, CPU accounting in CMP Processors, *IEEE Computer Architecture Letters*, Volume 9, 1/2/2009
- » Cor Meenderinck, Arnaldo Azevedo, Ben Juurlink, Mauricio Álvarez and Alex Ramirez, Parallel Scalability of Video Decoders, *Journal of Signal Processing Systems*, pp. 173-194, vol. 57, no. 2, 1/11/2009
- » Eduard Ayguadé, Nawal Copti, Alejandro Duran, Jay Hoeflinger, Yuan Lin, Federico Massaioli, Xavier Teruel, Priya Unnikrishnan, Guansong Zhang, The Design of OpenMP Tasks, *IEEE Transactions on Parallel and Distributed Systems*, volumen 20 (number 3), 16/3/2009
- » J. Dongarra, P. Beckman, P. Aerts, F. Capello, T. Lippert, S. Matsuoka, P. Messina, T. Moore, R. Stevens, A. Trefethen and M. Valero. “The International Exascale Software Project: A Call to Cooperative Action by the Global High-Performance Community”. *The International Journal of High Performance Computing Applications*, Vol. 23, No. 4, pp. 309-322, Winter 2009.
- » J. Labarta, E. Ayguadé and M. Valero. BSC Vision Towards Exascale. *International Journal of High Performance Computing Applications*, Vol. 23, no. 4, pp. 340-343. October 2009.
- » Judit Planas, Rosa M. Badia, Eduard Ayguadé and Jesus Labarta, Hierarchical task based programming with StarSs, *International Journal of High Performance Computing Applications*, vol. 23, no. 3, 284 - 299, 1/8/2009
- » Luis Moura Silva, Javier Alonso, Jordi Torres, Using Virtualization to Improve Software Rejuvenation., *IEEE Transactions on Computers*, November 2009 (Vol. 58, No. 11) pp. 1441-1443., 3/11/2009
- » Mauricio Álvarez, Alex Ramirez, Mateo Valero, Arnaldo Azevedo, Cor Meenderinck and Ben Juurlink, Performance Evaluation of Macroblocklevel Parallelization of H.264 Decoding on a cc-NUMA Multiprocessor Architecture, *Avances en Sistemas e Informática*, pp. 219-228, vol. 6, no. 1, 1/6/2009
- » Miquel Moreto, Francisco J. Cazorla, Alex Ramirez, Rizos Sakellariou and Mateo Valero, FlexDCP: a QoS framework for CMP architectures, *ACM SIGOPS Operating System Review, Special Issue on the Interaction among the OS, Compilers, and Multicore Processors*, 1/4/2009
- » Nicolas Poggi, Toni Moreno, Josep Lluís Berral, Ricard Gavalda, Jordi Torres, Self-Adaptive Utility-Based Web Session Management, *Computer Networks Journal*, vol 53, no. 10. 2009. pp.1712-1721. ISSN: 1389-1286, 3/1/2009
- » Oliverio J. Santana, Ayose Falcón, Alex Ramirez and Mateo Valero, DIA: A Complexity-Effective Decoding Architecture, *IEEE Transactions on Computers*, pp. 448-462, vol. 58, no. 4., 1/4/2009
- » Pieter Bellens, Josep M. Perez, Felipe Cabarcas, Alex Ramirez, Rosa M. Badia and Jesus Labarta, CellSs: Scheduling Techniques to Better Exploit Memory Hierarchy, *Scientific Programming*, vol 17, pp. 77-95, 1/1/2009
- » Rosa M. Badia, José R. Herrero, Jesús Labarta, Josep M. Pérez, Enrique S. Quintana-Ortí, Gregorio Quintana-Ortí, Parallelizing Dense and Banded Linear Algebra Libraries Using SMPs, *Concurrency and Computation: Practice and Experience*, volume 21, issue 18, 1/12/2009
- » Rudolf Eigenmann and Eduard Ayguadé. Guest Editor's Introduction (Special issue on IWOMP 2008). *International Journal of Parallel Programming*, vol. 37, no. 3, pp. 247-249. June 2009.

### Book Chapters

- » J. Guitart, M. Macías, O. Rana, P. Wieder, R. Yahyapour, W. Ziegler, SLA-based Resource Management and Allocation, *Market Oriented Grid and Utility Computing, Part III: Policies and Agreements*, Chapter 12, pp. 261-284, 1/11/2009
- » Jakub Kurzak, Hatem Ltaief, Jack Dongarra and Rosa M. Badia, Scheduling for Numerical Linear Algebra Library at Scale, *High Speed and Large Scale Scientific Computing*, pp. 3-26, IOS Press, 1/11/2009
- » M. Duranton, S. Yehia, B. de Sutter, K. de Brosschere, A. Cohen, B. Falsafi, G. Gaydadjiev, M. Katevenis, J. Maebe, H. Munk, N. Navarro, A. Ramirez, O. Teman and M. Valero. “The HiPEAC Vision”. Roadmap of the HiPEAC, network of excellence. *High Performance and Embedded Architectures and Compilers*. European Union. September 2009.
- » M. Macías, G. Smith, O. Rana, J. Guitart, and J. Torres, Enforcing Service Level Agreements using an Economically Enhanced Resource Manager, *Economic Models and Algorithms for Distributed Systems, Autonomic Systems Series, Part II: Service Level Agreements*, Chapter 6, pp. 109-127, 40148
- » M. Valero y J. Mompín. “La Informática en España”. *Ciencia y Tecnología. España Siglo XXI*. Fundación Sistema. Instituto de España. Año 2009, pp. 317-373.
- » T. Püschel, N. Borissow, D. Neumann, M. Macías, J. Guitart, and J. Torres, Extended Resource Management Using Client Classification and Economic Enhancements, *Economic Models and Algorithms for Distributed Systems, Autonomic Systems Series, Part II: Service Level Agreements*, Chapter 7, pp. 129-141, 1/12/2009

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- » Alejandro Duran, Xavier Teruel, Roger Ferrer, Xavier Martorell, Eduard Ayguadé, Barcelona OpenMP Tasks Suite: A Set of Benchmarks Targeting the Exploitation of Task Parallelism in OpenMP, *Proc. of the 2009 International Conference on Parallel Processing (ICPP 2009)*, 22/9/2009
- » Arnaldo Azevedo, Cor Meenderinck, Ben Juurlink, Andrei Tereckho, Jan Hoogerbrugge, Mauricio Alvarez, Alex Ramirez, Mateo Valero, Parallel H.264 Decoding on an Embedded Multicore Processor, *4th International Conference on High-Performance Embedded Architectures and Compilers (HiPEAC'09)*, 12/1/2009



- » Carlos Boneti, Francisco J. Cazorla, Roberto Gioiosa, Chen-Yong Cher, Alper Buyuktosunoglu, Pradip Bose and Mateo Valero, A Dynamic Scheduler for Balancing HPC Applications, In International Conference for High Performance Computing, Networking, Storage and Analysis (SC). Austin, USA, 15/11/2009
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- » Folch, A., Ash cloud modelling using FALL3D, Volcanic Ash Awareness Workshop, Catania, 23-24, 2009
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- » S. Marras, M.Vázquez, O. Jorba, R. Aubry and J. M. Baldasano, A Parallel, Variational Multiscale (VMS) Finite Element Approach to Atmospheric Modeling, ICCSME Conf, Greece, 2009





During 2009 the RES continued its consolidation and increased its computing power with the addition of the new site located at the Instituto Tecnológico de Canarias (ITC). The demand for access to the RES services continued increasing and exceeded more than 200% the time available. Since its creation, the RES has supported more than 1500 scientific projects and has organized seminars for users and technicians.

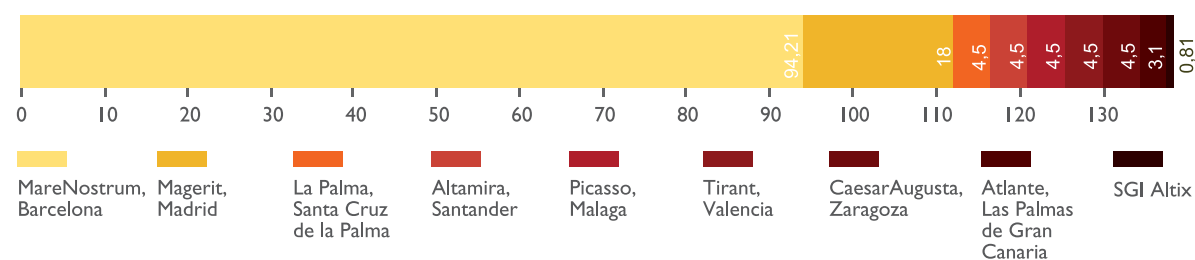


Nodes of the Spanish Supercomputing Network (RES)

## What is the RES?

In July 2006, the Spanish Ministry of Science & Innovation (MICINN) created the Spanish Supercomputing Network (Red Española de Supercomputación - RES) as a response to the need of the Spanish scientific community for increased capacity and accessibility of calculation.

RES Processing Power in TFLOP/s



The RES consists of a virtual distributed infrastructure of supercomputers located in different sites, each of which contributes to the total processing power available to users of different R&D groups in Spain. Generally, each node reserves 20% of capacity for use by researchers at the host institute, and the other 80% is made available to the general scientific community via the Access Committee. The node located at the ITC, which owns its infrastructure, makes available a 20% to the general researchers via the Access Committee.

The total processing capacity of the RES is 138,5 TFLOP/s (138,5 trillion floating point operations per second). The RES is coordinated by the Operations Department of the BSC-CNS, which includes support for global maintenance and upgrades, training of users and technicians, facilitation of access and all aspects of user support.

## RES Usage 2009

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

Allocation of access to RES supercomputer facilities is based on criteria of efficacy, efficiency and transparency, mediated by a double filter system, with potential projects first being evaluated by the ANEP, followed by an evaluation by the Access Committee, composed of a Core Team and four Expert Panels of prestigious scientists external to the BSC-CNS.

The four Expert Panels are defined according to the classification established by the Spanish Foundation of Science and Technology (FECYT).

### The Expert Panels:

- ▶ Astronomy, Space and Earth Sciences
- ▶ Biomedicine and Health Sciences
- ▶ Chemistry and Materials Science and Technology
- ▶ Physics and Engineering

Each of the above areas is chaired by a group leader, who acts as a coordinator, an assistant, and eight experts in the area.

### Access Committee Core Team 2009

- ▶ Ramón López de Arenosa, Ministerio de Educación y Ciencia
- ▶ Victoria Ley Vega de Seoane, Agencia Nacional de Evaluación y Prospectiva;
- ▶ Ramón Beivide, Universidad de Cantabria
- ▶ José María Cela, BSC-CNS

The Access Committee allocates to both Spanish and international researchers more than 25 million computational work hours every four months. In addition to internal research groups, over 235 external activities made use of the RES system in 2009. It is important to note that many scientific projects often request numerous periods of access to the RES in order to perform different work activities (new activities or continuation activities). Each request is treated separately and must pass the evaluation procedure of the Access Committee. Thus the number of activities reported for the RES is greater than the number of projects registered for the year.

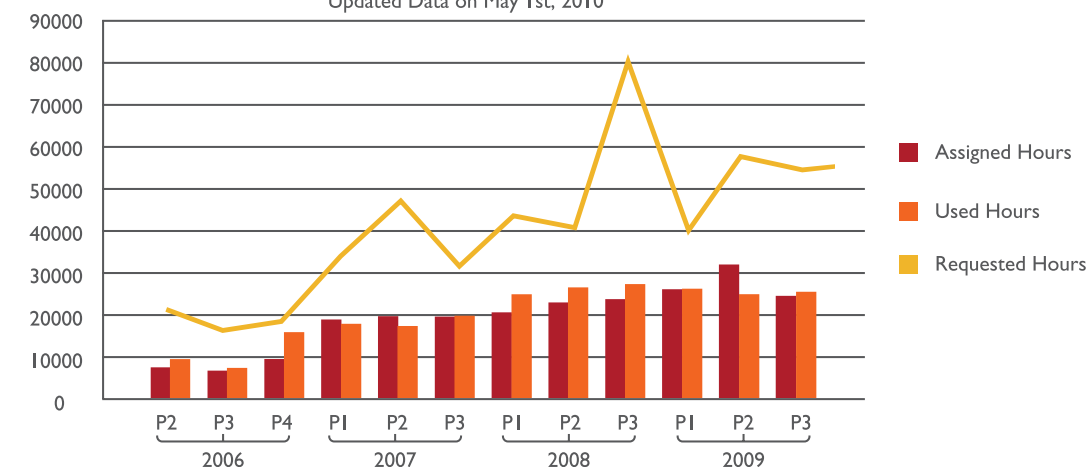
## Access Requests 2009

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

The graph shows the evolution of requested hours (yellow), assigned hours (red) and used hours (orange) over the last four years.

Number of RES Hours

Updated Data on May 1st, 2010



In the four years since the MareNostrum commenced operation, the MareNostrum and other RES nodes have collectively provided 266 million hours of computation. Over the same period 564 million hours were requested, indication that demand is more than double the hours that the RES can supply.

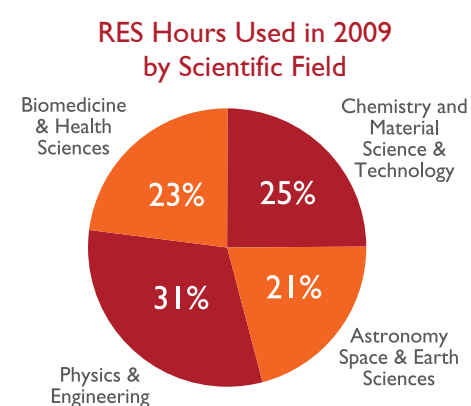


**Broad Impact on Scientific Research** Despite the RES being only a few years old, awareness of the RES and the services it offers has spread quickly. More than 235 R&D activities took advantage of the RES infrastructure in 2009, led by researchers from institutions in over 40 cities in Spain, Europe and overseas.



Cities of Origin of RES Users, 2009

These activities were broadly distributed over many different scientific fields, ranging from climate simulations, to models of biological processes and the simulation of satellite missions. Results of these studies have been presented in conferences worldwide and published in leading scientific journals. Importantly, many of these research activities could not have taken place if it were not for the extremely powerful computing capability offered by the RES, which enables calculations and simulations that would take years on ordinary PCs to be run in very short periods of time. During 2009 the BSC-CNS held seminars to educate potential users about the services available via the RES with the intention of further broadening access to the RES by sectors of the scientific community who have not been traditional users of supercomputers.

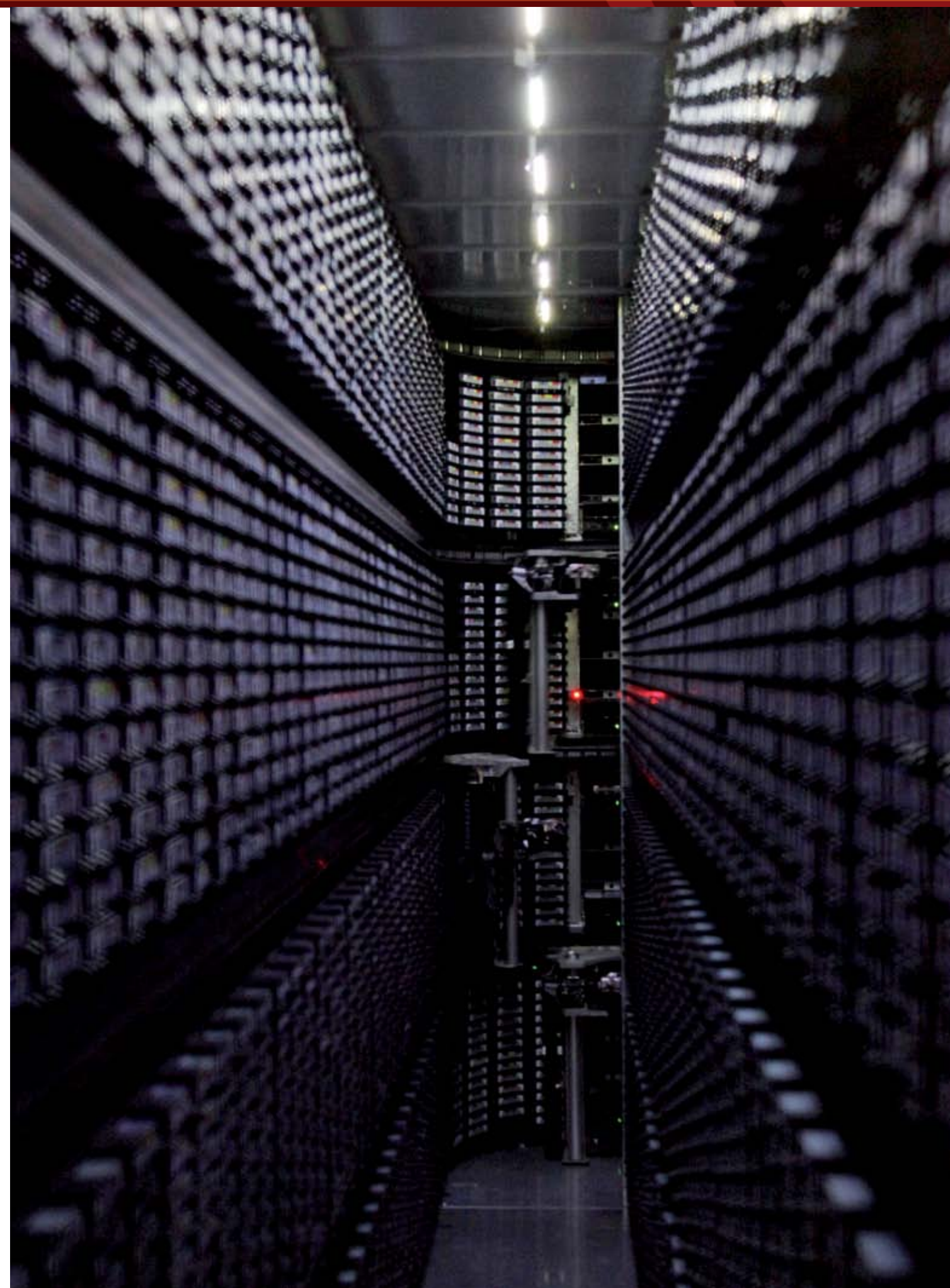


**RES Users Meeting 2009** In September 2009, the RES held its second User Conference in Santander. The meeting was organised jointly by the BSC-CNS (as technical management coordinator), the Physics Institute of Cantabria (IFCA), the mixed center of CSIC and the Cantabria University (as RES node and local organiser.)



The main objective of the meeting was to disseminate and to share the results obtained by different research teams of each area that has access to the RES resources: Astronomy, Space and Earth Sciences; Biomedicine and Health Sciences; Chemistry and Material Sciences; and Physics and Engineering.

There activities included an interactive information session where prestigious researchers that utilise the RES presented many of their activities and the results obtained during the year; and a roundtable debate was held with members of the Access Committee that grants access to RES resources.





## Overview



The MAGERIT Supercomputer

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

Magerit (an ancient name of Madrid) is the name of CeSViMa's supercomputer. Magerit is a cluster of 1204 nodes (1036 eServer BladeCenter JS20 and 168 eServer BladeCenter JS21), that totals 2744 CPUs with 192 TB of storage. All components are interconnected with low latency myrinet network and high bandwidth ethernet network.

When installed, Magerit held 2nd place for Spanish supercomputers in the TOP500 list (November 2006, 2nd in Spain, 9th in Europe and 34th of the world). It held 275th place in the first GREEN500 list of most environmentally friendly supercomputers (November 2007).

## Organisational Structure



The Politechnic University of Madrid (UPM) is devolving the management of CeSViMa to the Faculty of Information Science so the centre is currently undergoing structural re-organisation. However, the organisational structure which predominated in 2009 is shown in the diagram.



The team from left to right: José María Peña, Fernando Limón, Oscar Cubo, Rubén Galeano, Andrés Marín, Oscar Lozano, Borja Chocarro and Victor Maestre.

## Technical and Scientific Highlights 2009

In 2009 the Magerit supercomputer achieved an average load of near 80% with 24x7 availability. This represents a provision of 19 million CPU hours. Projects allocated via the RES access committee used 10,6 million of CPU hours while the rest were assigned by local access committee.

### Key Publications 2009

Oscar Custance and Ruben Perez and Seizo Morita, Atomic force microscopy as a tool for atom manipulation, *Nature Nanotechnology*, 2009.

Nikos Ch. Karayiannis and Martin Kroger, Combined Molecular Algorithms for the Generation, Equilibration and Topological Analysis of Entangled Polymers: Methodology and, *International Journal of Molecular Sciences*, 2009.

Garrido, J.E., Arias, E., Cazorla, D., Cuartero, F., Fernández, I. y Gallardo C. A Distributed Memory Implementation of the Regional Atmospheric Model PROMES, *Int. Journal of Computer Science*, 2009

Ralf Bechstein and Cesar Gonzalez and Jens Schutte and Pavel Jelinek and Ruben Perez and Angelika Kuhnle, "All-inclusive" imaging of the rutile TiO<sub>2</sub>(110) surface using NC-AFM, *Nanotechnology*, 2009

M. P. de Lara Castells and P. Villarreal and G. Delgado-Barrio and A.O. Mitrushchenkov, An Optimized Full-Configuration-Interaction Nuclear Orbital Approach to a "Hard-Core" Interaction Problem, *Journal of Chemical Physics*, 2009

M. Fontelos and U. Kindelan, A variational approach to contact angle saturation and contact line instability in static electrowetting, *The Quarterly Journal of Mechanics and Applied Mathematics*, 2009

Daniel Rodríguez and Vassilis Theofilis, Massively Parallel Solution of the BiGlobal Eigenvalue Problem Using Dense Linear Algebra, *AIAA Journal*, 2009

J.J. Honrubia, J.C. Fernandez, M. Temporal, M. Hegelich and J. Meyer-ter-Vehn, Fast ignition of inertial fusion targets by laser-driven carbon beams, *Physics of Plasmas*, 2009

Robert S. Hoy, Katerina Foteinopoulou, and Martin Kroger, Topological Analysis of Polymeric Melts: Chain-Length Effects and Fast-Converging Estimators for Entanglement Length, *Physical Review E*, 2009

Garrido, J.E., Arias, E., Cazorla, D., Cuartero, F., Fernández, I. y Gallardo C., PROMESPAR: a parallel implementation of the regional atmospheric model PROMES, *Proc. of World Congress of Engineering*, 2009

Helmut G. Katzgraber, H. Bombin, M. A. Martin-Delgado, *Virtual Journal of Nanoscale Science & Technology Virtual Journal of Nanoscale Science and Technology*, 2009

Helmut G. Katzgraber, H. Bombin, M. A. Martin-Delgado "Error Threshold for Color Codes and Random 3-Body Ising Models", *Physical Review Letters*, 2009

Nikos Ch. Karayiannis, Katerina Foteinopoulou, and Manuel Laso Entropy-Driven Crystallization in Dense Systems of Athermal Chain Molecules, *Physical Review Letters*, 2009

Nikos Ch. Karayiannis, Katerina Foteinopoulou, and Manuel Laso, Contact Network in Nearly Jammed Disordered Packings of Hard-Sphere Chains, *Physical Review E*, 2009

J.E. Garrido, E. Arias, D. Cazorla, F. Cuartero, I. Fernández, C. Gallardo., PROMESPAR: A Parallel implementation of the regional Atmospheric Model PROMES, *Proc. of World Congress of Engineering*, 2009

Vassili Kitsios, Daniel Rodríguez, Vassilis Theofilis, Andrew Ooi, Julio Soria, BiGlobal stability analysis in curvilinear coordinates of massively separated lifting bodies, *Journal of Computational Physics*, 2009

M.P. Simens, J. Jimenez, S. Hoyas and Y. Mizuno, A high-resolution code for turbulent boundary layers, *Journal of computational physics*, 2009

Sánchez, K. and Aguilera, I. and Palacios, P. and Wahnón, P., Assessment through first-principles calculations of an intermediate-band photovoltaic material based on Ti-implanted silicon: In, *Phys. Rev. B*, 2009

P. Palacios and K. Sánchez and P. Wahnón, Ab-initio valence band spectra of Al, In doped ZnO, *Thin Solid Films*, 2009

## Key Projects 2009

Magerit provided support to numerous research projects via both RES and local access. The projects that used computing facilities during 2009 are:

**CRP on Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems (ADS)**, Alberto Abánades Velasco (UPM)

**Advanced multiscale nucleo-cellular methods in three dimensional and multigroup geometries for the calculation of reactors of light water**, Carolina Ahnert Iglesias (UPM)

**Statistical modelling of properties and activities of molecules with pharmacological application.**, Gonzalo Fernando Colmenarejo Sánchez (UCM)

**Shock loading and wave propagation in advanced nano-structured materials**, Santiago Cuesta López (UPM)

**Development of a regional climate model with atmospheric-oceanic coupling and the optimisation of code for its execution in massively parallel clusters.**, Rodolfo Bermejo Bermejo (UPM), Fernando Cuartero Gómez (UCLM), Clemente Gallardo andrés (UCLM), Antonio García Dopico (UPM)

**Rapid ignition of blanks of inertial fusion.**, José Javier Honrubia Checa (UPM)

**Simulation of transitional bubbles of separation in low pressure turbines.**, Javier Jiménez Sendín (UPM)

**Mechanical-quantitative study of the Photochemistry and Control of molecules in metal oxide surfaces.**, Maria Pilar Lara Castells de (CSIC)

**Multiscale Modeling of Nanostructured Interfaces for Biological Sensors (MNIBS)**, Manuel Laso Carbajo (UPM)

**Mechano-quantitative in mesoscopic systems.**, Vicente Martín Ayuso (UPM)

**Dynamics, molecular compatability and nanostructures of new generation poleofins.**, Javier Martínez de Salazar Bascuñana (CSIC)

**Massively parallel genetic algorithms: Applications in engineering problems.**, José María Peña Sánchez (UPM)

**Transport in Nanostructures and Proximity Microscopes.**, Rubén Pérez Pérez (UAM)

**Optimisation processes for obtaining bioinformatic knowledge.**, Víctor Robles Forcada (UPM)

**Integrated air quality modeling system in the Iberian Peninsula (SIMCA)**, M<sup>a</sup> Encarnación Rodríguez Hurtado (UPM)

**Operational system for air quality prediction for continental Europe (MM5-CMAQ-EMIMO)**: Regional information services, Roberto San José (UPM)

**Radiation protection and security in high intensity accelerators of the type EVEDA/IFMIF**, Javier Sanz Gozalo (UNED)

**Aero-Acoustic computation and experiment for the prediction and control of noise (ACE-PCOR)**, Vassilis Theofilis (UPM), Eusebio Valero Sánchez (UPM)

**Hiper**, Pedro Velarde Mayol (UPM)

**New photovoltaic materials of intermediate band.**, Perla Wahnón Benarroch (UPM)

**Numerical simulation of the formation of structures in the Universe**, Gustavo Yepes Alonso (UAM)

## Overview



The LaPalma Supercomputer

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

## Organisational Structure

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

The LaPalma Supercomputer Support Team:

Carlos Martín Galán (Senior Engineer), Responsible Technician and the Manager of the Group. Antonio Díaz Chinaa (Senior Engineer), System Administrator. Justo Luna López (Engineer), System Administrator. Ubay Dorta Guerra (Engineer), System Administrator and UserSupport. Ángel de Vicente (Engineer), User Support.



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

## Technical and Scientific Highlights 2009

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

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

### Key Publications 2009

Tortosa Andreu, A., Moreno-Inseris, F. Magnetic flux emergence into the solar photosphere and chromosphere, *Astronomy & Astrophysics*, 2009

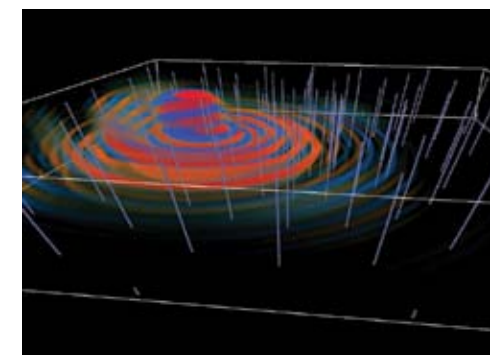
## Key Projects 2009

Aside from the projects assigned by the RES, which utilise approximately 80% of LaPalma's capacity, during 2009 the IAC executed its own scientific projects, among which highlights are:

**Barred galaxies interacting** In recent years, the barred galaxies have become very important in understanding the evolution of disk galaxies and their connection with dark matter theories. The results have been mainly based on numerical simulations of isolated barred galaxies. In this computational project, N-body and N-body+SPH simulations of interacting barred galaxies are performed. The goal of this project is to identify the differences between those bars created or modified by interactions and those self-generated in isolated galaxies. The project also checks if bars evolve in the same way before and after the interaction.

### Propagation of Magnetoacoustic Waves in Magnetic Structures

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



Magnetoacoustic Waves in a Sunspot

### Galaxy Transformations Through Interactions, Mergers and Accretion

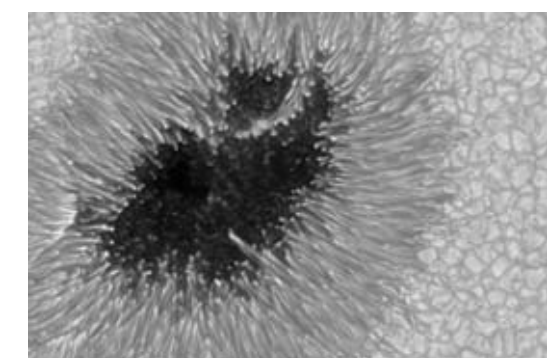
About 8 billion years ago, rapid and violent growth of galaxies was largely complete, but galaxies still must have gone through important transformations to acquire their present-day morphologies, bulge-disk structure, and low star formation rates. This project addresses what types of transformations occur on a disk galaxy when it merges with a smaller galaxy, to determine the role of such minor mergers in galaxy evolution during the last half of the age of the Universe.

### Genetic Algorithm Analyses of Massive Stars

Massive stars are key ingredients in the evolution of the Universe. Their short lifetimes, intense radiation fields and strong stellar winds modify their surroundings on short time-scales. To understand the variety of processes taking place in these stars, a large number of analyses under different conditions are needed using state-of-the-art, realistic model atmospheres. To facilitate this task and concentrate resources on the interpretation of results, the team developed an automatic tool for the model calculation and analysis. This tool was implemented in 2008 and the first applications were run in 2009.

### Image Reconstruction of Photometric and Spectropolarimetric Data by Means of the Multi-Object and Multi-Frame Blind Deconvolution Algorithm (MOMFBD)

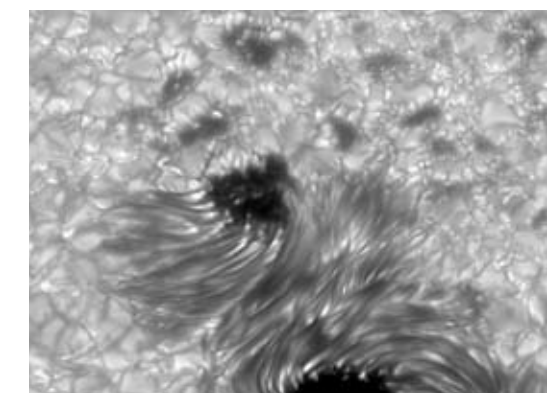
The investigation of the dynamics of the solar fine structure and its magnetic field. This project requires 2D photometric and spectropolarimetric data of the highest angular resolution (better than 0.1 arcsec) which can be only achieved by combining online and post-facto techniques, such as Adaptive Optics and image reconstruction techniques, in order to reduce substantially the image distortions induced by the earth's atmosphere and to further improve the spatial resolution of the observed data sets.



45 min Time Series of Reconstructed Broadband Images Harboring a Large Sunspot

### High Resolution in Solar Physics (Alta Resolución en Física Solar)

Understanding the physics of the Sun increasingly demands the resolution of small features in the solar surface, as those shown in the figure. To achieve this purpose complex and very time consuming computational techniques are required to compensate for the errors induced in the images by the telescope and atmospheric turbulence.



Sunspot Surrounded by Pores, Solar Granulation and "Bright Points"



## Overview



The Atlante Supercomputer

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

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

## Organisational Structure

The technical staff of Atlante is composed by two engineers from ITC (Yeray Gutiérrez Cedrés and María Belén Esteban Sánchez), that are responsible for system management and user support, and a group manager (Juan Francisco Rodríguez Alvarado). There is also a Local Access Committee that shares out the 80% of CPU time amongst users from University of Las Palmas de Gran Canaria, University of La Laguna and ITC.



The Atlante Supercomputer Team:  
M<sup>a</sup> Belén Esteban Sánchez (left, User Support)  
Yeray Gutiérrez Cedrés (right, System Administrator)

## Technical and Scientific Highlights 2009

Atlante was officially inaugurated on 16 February 2009 by Canary Islands Government's President, in the presence of the Rectors of the University of Las Palmas de Gran Canaria and University of La Laguna and the BSC-CNS Associate Director.

Aside from the projects assigned by the RES, which utilise approximately 20% of Atlante's capacity, a total of 17 local projects were accepted by the Local Access Committee throughout 2009.

### Key Publications 2009

L. Cana, D. Grisolia-Santos Numerical simulation of a sea-breeze front at the island of Fuerteventura Geophysical Research Abstracts, Vol. 11 2009

D. Grisolia-Santos, L. Cana Numerical simulations coupling atmospheric and ocean mesoscale models over the Canary Archipelago Geophysical Research Abstracts, Vol. 11 2009

C. Troupin, E. Mason, J.-M. Beckers and P. Sangrà A new mechanism of upwelling generated filaments based on potential vorticity balance EGU Annual Meeting (Vienna) 2009

C. Troupin, J. Aristegui, E. D. Barton, P. Sangrà and J.-M. Beckers Modeling and observation of an upwelling filament off Cape Ghir (NWAfrica) during the CAIBEX campaign VLIZ Young Scientists' day (Oostende) 2009

C. Troupin, J. Aristegui, E. D. Barton, P. Sangrà and J.-M. Beckers Upwelling filaments: a view through 3 different eyes VLIZ Young Scientists' day 2009

R. Lacombe-Perales, D. Errandonea, D. Martinez-Garcia, P. Rodríguez-Hernández, S. Radescu, A. Mujica, A. Muñoz, J. C. Chervin, and A. Polian Raman spectroscopic and ab initio studies of the phase transitions in wolframite-type CdWO<sub>4</sub> at high pressure Physical Review B 2009

Sinhue López, A. H. Romero, P. Rodríguez-Hernández, A. Muñoz First-principles study of the high-pressure phase transitions on ZnAl<sub>2</sub>O<sub>4</sub> and ZnGa<sub>2</sub>O<sub>4</sub>: from cubic spinel to orthorhombic post-spinel structures Physical Review B 2009

F. J. Manjon, D. Errandonea, J. López-Solano, P. Rodríguez-Hernández and A. Muñoz Negative pressure in CaWO<sub>4</sub> nanocrystals Journal of Applied Physics 2009

M. Cardona, R. K. Kremer, R. Lauck, G. Siegle, A. Muñoz, and A. H. Romero Electronic, vibrational, and thermodynamic properties of metacinnabar Bi-HgS, HgSe, and HgTe Physical Review B 2009

S. Radescu, A. Mujica and R. J. Needs Soft-phonon instability in zincblende HgSe and HgTe under moderate pressure: Ab initio pseudopotential calculations Physical Review B 2009

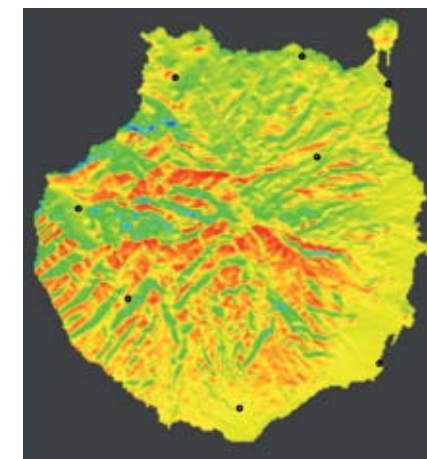
Sinhue López-Moreno, A. H. Romero, P. Rodríguez-Hernández, A. Muñoz Ab initio calculations of the wolframite MnWO<sub>4</sub> under high pressure High Pressure Research 2009

Sinhue López-Moreno, A. H. Romero, P. Rodríguez-Hernández, A. Muñoz Ab initio study of the high pressure phases and dynamical properties of ZnAl<sub>2</sub>O<sub>4</sub> and ZnGa<sub>2</sub>O<sub>4</sub> High Pressure Research 2009

J. López-Solano, P. Rodríguez-Hernández, A. Muñoz Ab initio study of high-pressure structural properties of the LuVO<sub>4</sub> and ScVO<sub>4</sub> zircon-type High Pressure Research 2009

## Key Projects

**Photovoltaic Systems Simulator** The project deals with meteorological data processing to estimate the amount of energy that Photovoltaic Systems allocated in Canary Islands would be able to generate according to the expected weather conditions, which are estimated using Numerical Weather Prediction models (MM5) executed in Atlante supercomputer.



Simulation of Photovoltaic Energy in Gran Canaria

**Atmospheric Numerical Forecast** Modeling using WRF 3.1.1 of relevant weather events in the Canary Islands: formation of sea breezes, local storm phenomena in the Western Isles, effects of topography on the wake of islands or coupling of high resolution models of wind regional ocean models.

**CAIBEX** The main goal of the CAIBEX project is the interdisciplinary study of two upwelling filaments systems; the Cabo Sillero and Cape Ghir upwelling filaments. The project was funded by the Spanish Ministry of Science and Innovation, involving the Universidad de Las Palmas de Gran Canaria, the Universidad de Vigo and the Instituto de Ciencias Marinas de Vigo (CSIC). Among the objectives an important modeling effort was made in order to understand the dynamics responsible for the generation of these structures. Some model runs were performed using Atlante facilities. The main finding is that the Beta effect is the main mechanism involved in the generation of these structures.

**Simulation Studies and Design of Materials and Nanomaterials under Extreme Conditions** From ab initio calculations based on density functional theory studies were performed of electronic and dynamical properties of materials and nano-materials under extreme conditions of high pressure and high temperature. The main focus was on compounds ABX<sub>4</sub>, AB<sub>2</sub>X<sub>4</sub>, etc, some of which are very interesting for geology and have technological applications.

## Overview



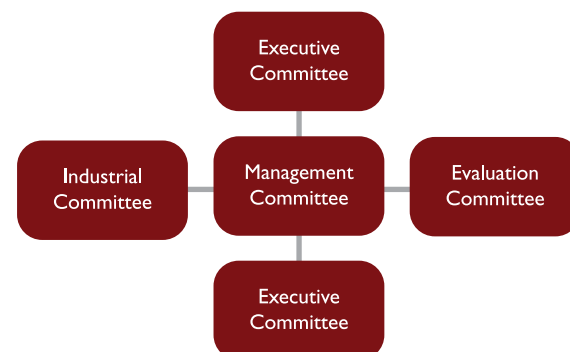
The ALTAMIRA Supercomputer

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

IFCA (Instituto de Física de Cantabria) is a joint center of the University of Cantabria and CSIC with research lines in astrophysics, high energy physics and distributed computing, and participates in several national and European computing projects (including the Spanish e-Science Network, and FP7 projects such as EUFORIA or DORII).

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

## Organisational Structure



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



Luis Cabellos is the system administrator of Altamira

## Technical and Scientific Highlights 2009

In 2009 the Altamira node executed applications corresponding to local users at the University of Cantabria with more than 800.000 hours of CPU time. Key publications and projects resulting from this work are detailed below:

### Key Publications 2009

A. Curto, E. Martínez-González, P. Mukherjee, R. B. Barreiro, F. K. Hansen, M. Liguori, S. Matarrese WMAP 5-year constraints on  $f_{nl}$  with wavelets *Mon. Not. Roy. Astron. Soc.* 393, 615-622 2009

A. Curto, E. Martínez-González, R. B. Barreiro improved constraints on primordial non-Gaussianity for the Wilkinson Microwave Anisotropy Probe 5-yr data *Astrophys. J.* 706:399-403 2009

Raul Guanche, Inigo J. Losada, Javier L. Lara Numerical Analysis of Coastal Structures Stability. *Coastal Engineering ELSEVIER* .56 (5-6). Pp. 543-558 2009

Isabel Campos, Enol Fernandex, Luis Cabellos, Marcin Plociennik, Michal Owsiak, Bernard Guilletminet, Alejandro Soba Modelling mixed work-flows between Grid and HPC in EUFORIA 3rd Iberian Grid Infrastructure Conference, Valencia IBERGRID Proceedings 2009

P. Albella, J. M. Saiz, J. M. Sanz, F. González and F. Moreno Nanoscopic Surface Inspection by analyzing the linear polarization degree of the scattered light *Optics Letters*, Vol. 34, Issue 12, pp. 1906-1908 2009

J. M. Sanz, P. Albella, F. Moreno, J. M. Saiz and F. González Application of the Polar Decomposition Method to Particle Scattering Systems Volume 110, Issues 14-16, September-November 2009, Pages 1369-1374 2009

M. Vallejo, M. Rada, L. Buelta, I. Cabria, F. Rodríguez, and A. Mañanes Aggregate model for the vibrational properties of hydroxyapatites TNT2009, *Trends in Nanotechnology* 2009, Barcelona (Spain) 2009

C. Martínez, R. Bevide, E. M. Gabidulin Perfect Codes from Cayley Graphs over Lipschitz Integers *IEEE Transactions on Information Theory* Vol. 55, No 8, pp. 3552-3562 2009

Lee S, Molina LM, Lopez MJ, et al. Selective Propene Epoxidation on Immobilized Au6-10 Clusters: The Effect of Hydrogen and Water on Activity and Selectivity *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*, 48, 1467 2009

C. Pedraza, J. Castillo, P. Huerta, J. Cano, J. L. Bosque, J. I. Martínez Speeding up combinational synthesis in an FPGA cluster *Proceedings of the International Conference on Parallel Computing* 2009

C. Pedraza, J. Castillo, P. Huerta, J. Cano, J. L. Bosque, J. I. Martínez FPGA Cluster Accelerated Boolean Synthesis *Proceedings of the 9th International Conference Computational and Mathematical Methods in Science and Engineering*, (CMMSE2009), pp. 806 - 816 2009

G. Rodríguez, R. Bevide, C. Minkenberg, J. Labarta and M. Valero, Exploring Pattern-aware Routing in Generalized Fat Tree Networks *Proc of the IEEE International Conference on Supercomputing, ICS* 2009. Pp. 276-285 2009

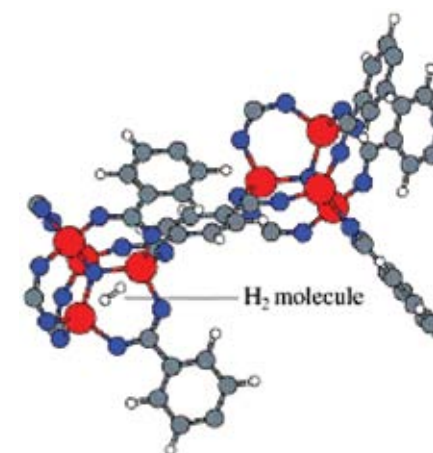
D. Suárez, T. Monreal, F. Vallejo, R. Bevide and V. Viñals Light NUCA: A proposal for bridging the inter-cache latency gap *Proc. of Design, Automation & Test in Europe Conference & Exhibition* 2009

J. Castillo, Jose L. Bosque, E. Castillo, P. Huerta, J. I. Martínez. Hardware accelerated Montecarlo financial simulation over low cost FPGA cluster *Proceedings of the International Symposium on Parallel and Distributed Processing* 2009, pp. 1 -8 2009

## Key Projects 2009

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

**Storage of hydrogen in MOF-5** Led by Angel Mañanes Pérez, a study on the storage of hydrogen in MOF-5. MOF-5 is highly porous and one of the most highly hydrogen absorptive substances. The DACAPO program was used in the Altamira to resolve DFT equations for solid materials.



Molecular Scheme of the MOF-5 Material

### Cornell Multi-grid Coupled Tsunami Model

Led by Ernesto Mauricio González Rodríguez, this activity is part of the European TRANSFER project (Tsunami Risk AND Strategies For the European Region) which aims to improve understanding of tsunamis, in particular on European coastlines. Studies on floods of Cádiz and the Balearic Islands were run on Altamira.

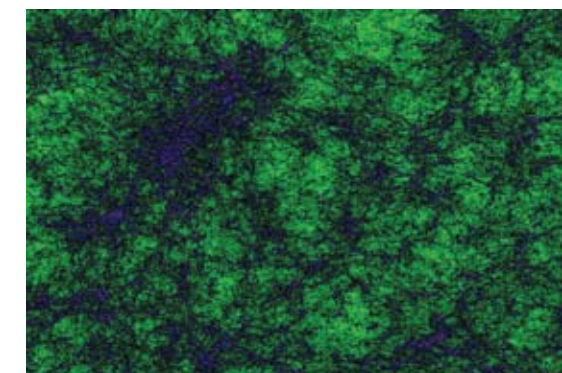
**Testing Gaussianity of CMB Maps** Led by Enrique Martínez, the Group of Cosmic Microwave Background (CMB) of the Physics Institute of Cantabria undertook a number of different analysis projects. The Altamira was used in the analysis and detection of compact sources utilising data from the CMB Group. The project is financed by the National Research Plan.

### Modelling of the structural mechanical response in high-rise buildings under real fire

Led by Jorge A. Capote Abreu, a study and simulation of the propagation of fire in tall buildings, in order to predict the behaviour of fire in real situations. The Altamira supercomputer was used to resolve the fluid dynamic equations with which the fire was simulated. The project is financed by a Plan Nacional.

### Simulation at a Grand Scale of the N-body Universe

Led by Jose María Diego, simulations of the universe utilising the Gadget-2 program. Gadget-2 is a highly parallelisable program and by using the Altamira it has been possible to run small simulations in reasonably short times, utilising up to 64 processor per execution. Larger simulations are planned for future execution periods.



Simulated Maps of Structures in the Universe

### Wave-structure interaction by the use of TRUCHAS

Led by Iñigo Losada, a study in the 3-dimensional behaviour of wave structures using the TRUCHAS numerical method. The study also aims to validate the numerical results obtained by the Laboratory of the Oceanographic and Coastal Engineering Group (IH Cantabria).

### Light scattering by micro-nano particles located on substrates

Led by Pablo Alvella Echave, a study in the detection of defects in the microstructures of substrates used in the diffusion of light. The Altamira supercomputer was needed to advance from 2D calculations to 3D calculations and thereby enable the study of further situations. The project is financed by a Plan Nacional.



## Overview

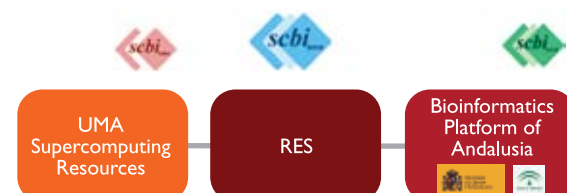


The Picasso Supercomputer

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

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

## Organisational Structure



The SCBI draws on 12 years of experience of the Computational Laboratory of the UM in running production supercomputers to support scientific research in several fields. It also incorporates a recently created research infrastructure, the Bioinformatics Platform of Andalusia, whose mission is to provide computational resources and commercial software licenses, and to transfer knowledge and experience on bioinformatics research to the scientific community in Andalusia.

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

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



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

## Technical and Scientific Highlights 2009

In 2009, Picasso offered 3.7 million CPU hours, of which 80% was made available to the RES and the rest was made available to the local scientific community.

### Key Publications 2009

Julio F. Fernández and Juan J. Alonso, Equilibrium spin-glass transition of magnetic dipoles with random anisotropy axes on a site-diluted lattice, *Physical Review B* 79, 214424, 2009

A. Navarro, R. Asenjo, S. Tabik and C. Cascaval, Load balancing using work-stealing for pipeline parallelism in emerging applications, *ACM 23rd International Conference on Supercomputing*, 2009

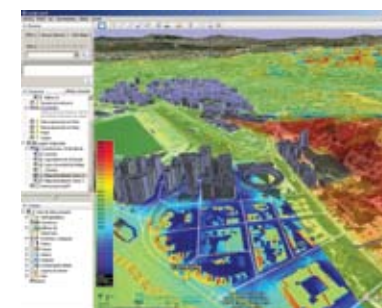
A. Navarro, R. Asenjo, S. Tabik and C. Cascaval, Analytical Modeling of Pipeline Parallelism, *ACM-IEEE International Conference on Parallel Architectures and Compilation Techniques (PACT)*, 2009

R. Castillo, F. Corbera, A. Navarro, R. Asenjo, E.L. Zapata, Conflict Analysis for heap-based Data Dependence Detection, *International Conference on Parallel Computing. ParCo* 2009, 2009

A. Tineo, F. Corbera, A. Navarro, R. Asenjo, E.L. Zapata, On the automatic detection of heap-induced data dependences with interprocedural shape analysis, *International Workshop on Advanced Distributed and Parallel Network Applications (ADPNA)*, 2009

## Key Projects 2009

**Parallel Programming Models and Compilers** Group on Parallel Programming Models and Compilers from the Computer Architecture Department of the University of Málaga.



Projection of an Insolation Model on the Earth Surface, Using Google Earth.

In collaboration with George Almasi and Calin Cascaval and related with the project Parallel Programming and PGAS languages at IBM T.J. Watson Research Center, this Group has built on its experience in 2008 to improve its n-body algorithm (Barnes-Hut) using the IBM UPC compiler (xlupc). The Unified Parallel C (UPC) language is a parallel extension of the C language that provides a shared memory view of the physically distributed memory implemented in the Group's IBM machine (pablo). This abstraction leads to a productive approach to the problem of exploiting an MPP architecture.

Also the Group enhanced its library-based (STL-like) approach to provide a higher level of abstraction in order to more productively develop parallel codes based on recursive data structures for MPP architectures. This library enhances the performance of the UPC run-time when dealing with pointer-based algorithms. Two important considerations will be to exploit the overlapping of communications and computations when possible and to also take advantage of that usually, in particular regions of the code, the traversed data structure is simpler than the real stored data structure.

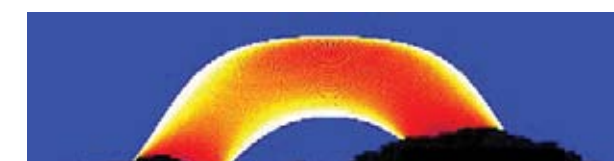
### High Precision Model of Solar Radiation

Luis F. Romero, researcher from the Parallel Applications Group of the Computer Architecture Group of the University of Málaga.

In 2008 a high precision model of the incoming solar radiation was developed. This model has enabled the elaboration of an high resolution Insolation Atlas for more regions of the world. Merely analysing the shadows projected by tall buildings involves a large amount of CPU time (about 9700 hours for one map); however, the high degree of parallelism obtained enabled the utilisation of up to 128 CPUs with efficiency close to 100%.

The city of Málaga was awarded the "Eurocities Innovation Award 2009" for this project.

**Andalusian Platform for Genomics, Proteomics, and Bioinformatics Research** Bioinformatics Platform of Andalusia



Integration of Energy Received from Sun for an Specific Location on Earth Taking Into Account Horizon Elevation.

In collaboration with researchers of the Department of Molecular Biology and Biochemistry of the University of Málaga, three-dimensional folding models of enzymes and other proteins are being computed to study their structural and functional characteristics. The predicted characteristics represent a valuable resource to understand the function of this enzyme in amino acid metabolism.

The Group is also developing high performance computing workflows using its own tools to process data from genomics and proteomics projects which involve a large amount of input data which has to be analysed. These locally produced tools include SEQTRIM, FULL-LENGTHER and ALIGNMINER.

**Molecular Modelling in rare diseases** Group on Molecular Modelling, specialised in rare diseases, from the Department of Molecular Biology and Biochemistry of the University of Málaga.

Homology model of the human MTHFR in two views (lower structure is rotated about 90° with respect to the upper one). The cofactor and the residues A222 and V218 are depicted in green sticks, whereas the α5 helix is coloured in yellow. Graphical representation of the residue positional fluctuations as Z-scores of the p.A222V (b) and the double mutant (c) systems.

The Group belong to the CIBERER (Biomedical Network Research Centre on Rare Diseases) which was created to consolidate stable cooperative research structures, and is intended to foster basic and clinical excellence research, with marked stress on transferring this to the patients' bedsides. The Group's work inside the CIBERER is centered on basic research.

Also the Group does protein structure network analysis and molecular dynamics simulations to increase the knowledge of protein interaction in live organisms.

**Statistical physics** Group on Statistics Physics and Scattered Fields, from the Department of Applied Physics of the University of Málaga.

The Group develops models and numerical simulations to research the collective behaviour of many particles systems.

The arrangement of magnetic nanoparticles and molecular magnets is researched, exploring the physical limits of information storage in magnetic devices.

Also the behaviour of nanoparticles suspensions in watery environments is researched, for biotechnical and biomedicine applications.

### Bioinformatics and information technologies

This groups belongs to the INB (Instituto Nacional de Bioinformática) (National Bioinformatics Institute) and has as its main focus the application of information technologies to bioinformatics. It has developed a new parallel algorithm to do large microarray quantile normalization.

## Overview



The TIRANT Supercomputer

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

## Organisational Structure

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

## Technical and Scientific Highlights 2009

In 2009, Tirant offered 3.7 million CPU hours of which some 80% was made available to the RES and the rest was made available to all the scientific community of the Valencia region, including researchers at the University of Valencia.



From the left: Alejandro Soriano - System Analyst, Josep Vicent Sala - System Analyst, Salvador Roca - IT Group Director, Gabriel Aparicio - System Analyst, Jose María González - Operator

### Key Publications 2009

Bordas, P., Bosch-Ramon, V., Paredes, J. M., and Perucho, M., Non-thermal emission from microquasar/ISM interaction, *Astronomy and Astrophysics*, Volume 497, Issue 2, pp.325-334, 2009

E. Ramos, J.E. Roman, S. Cardona-Serra, J.M. Clemente-Juan., Parallel implementation of MAGPACK package for analysis of high-nuclearity spin clusters, *Computers & Chemical Engineering*, 2009

E. Ramos, J.E. Román, S. Cardona, J.M. Clemente, E. Coronado, Paralelización de Magpack: Propiedades Magnéticas de Sistemas Anisótropos de Alta Nuclearidad, *XX Jornadas de Paralelismo*, A Coruña, 2009

E. Ramos, J.E. Román, S. Cardona, J.M. Clemente, E. Coronado, Simulación de propiedades magnéticas de moléculas usando la librería de cálculo de valores propios SLEPc, *XIX Jornadas de Paralelismo - Castellón*, e-Treballs d'Informàtica i Tecnologia, 8 ISBN: 978-84-8021-676-0, 2009

Erik Strandberg, Santi Esteban-Martín, Jesús Salgado, and Anne S. Ulrich, Orientation and Dynamics of Peptides in Membranes Calculated from 2H-NMR Data, *Biophysical Journal* Volume 96 3223-3232, 2009

Santi Esteban-Martín, Erik Strandberg, Gustavo Fuertes, Anne S. Ulrich, and Jesús Salgado, Influence of Whole-Body Dynamics on 15N PISEMA NMR Spectra of Membrane Proteins: A Theoretical Analysis, *Biophysical Journal* Volume 96 3233-3241, 2009

S. Esteban-Martín, H.J. Risselada, J. Salgado, S.J. Marrink., Stability of asymmetric lipid bilayers assessed by molecular dynamics simulations., *JACS*, 131:15194-15202, 2009

Esteban-Martín Santi, Giménez Diana, Fuertes Gustavo, Salgado Jesús, Orientational Landscapes of Peptides in Membranes: Prediction of 2H NMR Couplings in a Dynamic Context., *Biochemistry*, vol.48 n.48 pp:11441-11448, 2009

Blanquer, I.; Carrión, A.; Hernández, V.; Pignatelli, M.; Tamames, J., A Comparison Between mpiBLAST on Supercomputers and High-Throughput BLAST on Grid Infrastructures., *First EELA-2 Conference*, Bogota, Colombia. Proceedings of the First EELA-2 Conference. Madrid: Editorial CIEMAT. ISBN: 9788478346004, 2009

Violeta López-Canut, Maite Roca, Juan Bertrán, Vicent Moliner and Iñaki Tuñón, Theoretical Study of Phosphodiester Hydrolysis in Nucleotide Pyrophosphatase/Phosphodiesterase. Environmental Effects on the Reaction Mechanism, *JACS Articles*, 2009

V. Gimenez, D. Palao et al., Kaon oscillations in the Standard Model and Beyond using Nf=2 dynamical quarks, *27th International Symposium on Lattice Field Theory*, Beijing, China, pp.258, 2009

F. Bernardoni, P. Hernández, N. Garron, S. Necco and C. Pena, Mixed action computations on fine dynamical lattices, *27th International Symposium on Lattice Field Theory*, Beijing, China, 2009

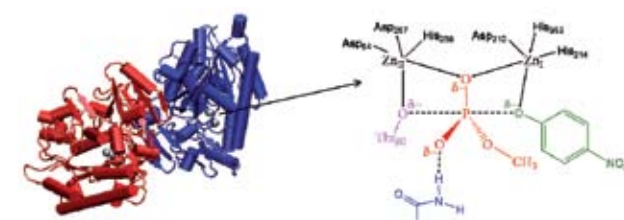
Aznar, E.; Coll, C.; Marcos, M. D.; Martínez-Mañez, R.; Sancenón, F.; Soto, J.; Amorós, P.; Cano, J.; Ruiz, E., Borate-Driven Gatelike Scaffolding Using Mesoporous Materials Functionalised with Saccharides, *Chem. Eur. J.*, 2009, 15, 6877., 2009

## Key Projects 2009

**Coupling of gold catalyzed hydrogenation of nitroaromatics with selective alcohol oxidation** Led by Mercedes Boronat Zaragoza, the general objective is to prepare hybrid organic-inorganic nanoporous and mesoporous materials and use them as sensors, catalysts and for H2 storage.

**Analysis of CRISPR Sequences present in Metagenomes** Led by Francisco Rodríguez-Valera, the research line in exploratory metagenomics concentrates mostly on the microbiota of the Mediterranean Sea, producing archives, in the form of metagenomic libraries and gene sequences in databases. It represents an invaluable genetic heritage useful for specialized studies.

**Enzymatic hydrolysis of phosphoesters. A free energy surface exploration** Understanding the mechanism of the enzymatic catalysis enables the creation of artificial catalysts with industry oriented purposes. Led by Ignacio Tuñón, this project tries to elucidate the mechanism of one of them: the hydrolysis of phosphoesters done by an alkaline Phosphatase.



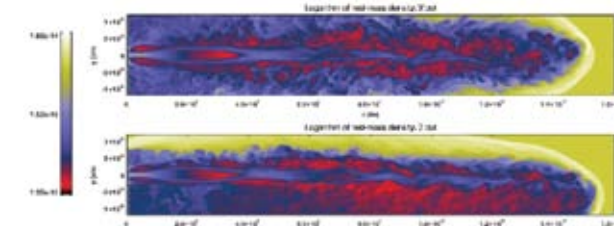
Schematic representation of the putative TS of the phosphodiester hydrolysis in the NPP active site

**Explaining blazars and gamma-ray bursts with numerical relativistic magneto-hydrodynamics** Led by Miguel Ángel Aloy Torás, this project is related to coupling relativistic plasma (magneto-)hydrodynamics to non-thermal emission in order to provide synthetic models that explain the observed electromagnetic patterns of some astrophysical sources (blazars, gamma-ray bursts and relativistic jets).

**Flavour Physics from Mixed-action Lattice QCD** The goal of the project led by Pilar Hernández is to determine the low-energy couplings of the Chiral Lagrangian that are relevant in flavour physics, beyond the quenched approximation.

**Numerical simulations of hadron properties** Led by Vicent Giménez Gómez the main goal is to quantitatively describe and predict, using numerical simulations of the Quantum Chromodynamics (QCD), the properties of hadrons, mesons and baryons, like the proton and the neutron which form the nucleus of all the atoms.

**3D simulations of relativistic jets** The aim of the project led by Manuel Perucho Pla is to simulate two aspects of relativistic jets in the Universe: to apply a theoretical model for the development of instabilities in the extragalactic jet of M87 and to study the interaction between jets in microquasars and their environments, particularly, in simulating the influence from strong winds in massive companion stars on the evolving jets rising from the compact object in the X-ray binary.



Microquasar Jets With RATPENAT (3D Simulations)

**Study of the cavitation phenomena in Diesel injector nozzles** In Diesel engines, it is well known that the characteristics of the internal nozzle flow have a strong impact on the spray and its atomization, and therefore in the efficiency of the combustion process. This is particularly true when cavitation occurs in the fuel injector nozzles under the high pressures at which operate modern Diesel engines. As demonstrated by the numerical results obtained from the CNS node Tirant by the group led by Fco. Javier Salvador Rubio, cavitation can be modeled to explain in depth important phenomena such as the mass flow collapse or the increment of effective velocity induced by cavitation.

**Magnetic properties of high-nuclearity spin clusters and mixed-valence clusters** The project led by Juan Modesto Clemente is focused on developing a parallel version of the integrated applications of MAGPACK library by using SLEPc library. The main aim is to be able to measure different magnetic properties, both thermo-dynamics and optics, of high-nuclearity spin clusters.

**Refolding of an amphitropic protein at the lipid membrane interface** The group led by Jesús Salgado is exploring the mechanisms of refolding and activation in lipid membranes of proteins from the Bcl-2 family. These proteins regulate physiological cell death by controlling the release of apoptotic inducers from mitochondria. Bcl-2 proteins activate by binding and inserting into the outer mitochondrial membrane, where they change their constitutive water-soluble state to a membrane bound state, able to distort the lipid bilayer and form proteolipidic pores. They investigate the structural changes accompanying the formation of protein/membrane complexes, both in the protein and the lipid bilayer, using atomistic and coarse grained molecular dynamics simulations.



## Overview



The CAESARAUGUSTA Supercomputer

Located at the Faculty of Science of the University of Zaragoza, the CAESARAUGUSTA supercomputer was one of the initial seven founding nodes of the RES. It is managed by the Supercomputing Area of the Institute for Bio-computation and Physics of Complex Systems (BIFI).

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

## Organisational Structure

CAESARAUGUSTA is maintained by technical staff of the Supercomputing Area at BIFI. This includes hardware and software administration as well as first level user support, all of which is 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 2009, the members of the local Access Committee were:

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



CAESARAUGUSTA Operations Team (from left to right): Javier Alcázar Luque (BIFI's sysadmin), Arturo Giner (BIFI's sysadmin), Guillermo Losilla (BIFI's computing manager), Alfonso Tarancón (BIFI's secretary professor & Head of the Computing Area)

## Technical and Scientific Highlights 2009

2009 was a year of consolidation for CAESARAUGUSTA with a total of 9 local projects accepted by the local Access Committee, utilising 800.000 hours of CPU time. These activities have produced numerous scientific results and publications.

### Key Publications 2009

L.A. Fernandez, V. Martín-Mayor, S. Perez-Gaviro, A. Tarancon and A.P. Young, Phase transition in the three dimensional Heisenberg spin glass: Finite-size scaling analysis, *Physical Review B* 80, 024422 (2009), 2009

P. Echenique, The many-body expansion of potential energy functions as a cost-saving approximation in ab-initio molecular dynamics simulations, IV National Conference BIFI2009, February 2009, Zaragoza, Spain, 2009

Angarica, V.E., Cuesta-Lopez, S., Estrada, J. and Sancho, J., A computational study of the mutational space of the LDL-r LA5 module: in silico prediction of disease-like phenotypes in a conformational disease, International Workshop Angel Ramirez Ortiz in memoriam, Madrid, Spain (Poster Presentation), 2009

Angarica, V.E., Cuesta-Lopez, S., Estrada, J. and Sancho, J., Using Molecular Dynamics to study the conformational changes of the LDL-r LA5 module upon mutation, Congress BIFI 2009, Zaragoza, Spain (Oral Presentation), 2009

Angarica, V.E., Cuesta-Lopez, S., and Sancho, J., Exploring the mutational space of the LDL-r module using molecular dynamics: connecting SNPs to abnormal phenotypes in a conformational disease, XXXII Congress of the Spanish Society for Biochemistry and Molecular Biology, Oviedo, Spain, 2009

Velez, E.; Alberola, A.; Polo, V. J., Broken Symmetry Density Functional Theory Studies on Spin-Crossover Materials, *Physical Chemistry A*, 2009, 113, 14008-14013, 2009

model system from which to derive a unified theory of the glassy state (glass is one of the most common, yet mysterious states of condensed matter). Interest in spin glasses also extends outside of condensed matter physics because there has been a fruitful exchange of ideas between the spin glass community and researchers in other

branches of science such as computer scientists working on combinatorial optimization. Simple analytical approximations predict that spin glasses have a finite temperature transition, but whether this actually occurs (or is an artifact of the approximations used) has remained unclear, at least for a variety known as "Heisenberg spin glasses". The advent of a new generation of simulation algorithms, finite-size scaling analysis and parallel computers have meant that at last a serious attempt can be made to fully understand the phase transition in Heisenberg spin glasses. This investigation was carried out at Caesaraugusta (Zaragoza), Mare Nostrum (Barcelona Supercomputing Center) and in the CINECA (Bologna, Italy, thanks to the European DEISA initiative).

**Many-body expansion of the quantum chemical energy surface of biological molecules. Towards a new type of force fields.** Led by Pablo Echenique (BIFI, Theoretical Physics Department UZ), The calculation of potential energy surfaces (PESs) of flexible molecules using quantum chemical methods is a computationally expensive task. In this project, Caesaraugusta was used to investigate whether or not such a surface can be expanded in its different many-body terms and this expansion be truncated at orders that make the calculation feasible at the same time that the approximated PES is accurate enough for practical purposes.

**QM / MM Simulations of Proteins with Special Optical Properties** Led by José Luis Alonso (BIFI, Theoretical Physics Department UZ), the group modified Octopus, a computer code for simulation of systems based on Time Dependent Density Functional Theory, so that simulations of biomolecules are more reliable. Also calculated were the absorption spectra of the fluorescent protein GFP in several conformations and using different theoretical approaches. This biomolecule was chosen due to its huge practical interest (the Nobel Prize in Chemistry 2008 rewarded its discovery and further works on it because of its important medical usefulness).

**Prediction of conformational diseases from simulation** Led by Javier Sancho Sanz (BIFI, Department of Biochemistry and Molecular and Cellular Biology UZ), Familial hypercholesterolemia is a conformational disease linked to mutations in the gene encoding the low-density lipoprotein receptor. A high percentage of these mutations have been found in the seven small modular binding repeats of the receptor. Taking advantage of its small size, the group planned an in depth MD study of module LA5, that represents a possible tool to improve genetic diagnosis as well as to gain insights into the molecular basis of diseases related to protein miss-folding. 20 ns simulations were run in explicit solvent of all the mutants arising from non-silent, non-miss-sense single nucleotide mutations aiming at developing an anticipated computational diagnosis strategy and to assess the structural implications of every possible SNP and its probability to give rise to disease. It was found that the dynamical evolution of mutants is quite different depending on the residues changed. In this regard, mutants involving residues of the ion binding cage and the disulfide bridges can be clustered together in a RMSD vs SASA profile. In this profile it was also found that the dynamical behavior of these "sensible" mutations is different from the one observed for mutations involving tail residues and Single Nucleotide Polymorphisms (SNPs) that have not been reported previously as related to the disease. A more detailed analysis of the trajectories using Principal Component Analysis proved that mutations in some specific positions cause distortions in the 3D struc-

ture which might result in a miss-folding of the mutants. A group of SNPs were identified which have not been previously described that could be related to the disease, given the fact that mutations cause important structural changes that could lead to species unable to fold properly. This kind of approach would be of great guidance to experimentalists mapping the mutational space of this gene to identify new pathologic mutations related to Familial Hypercholesterolemia.

**Broken Symmetry Density Functional Theory Studies on Spin-Crossover Materials** Led by Victor Polo (BIFI, Department of Physical and Organic Chemistry, UZ), this project studies the phenomena of spin crossover using density functional theory based methodologies. Compounds presenting spin crossover are characterised by equilibrium between two electronic states with different spin multiplicities which can be switched by variation of temperature or external conditions. In a first step, these processes have been simulated computationally for isolated molecules and future research will be done in order to understand cooperative effects in spin transitions leading to hysteresis effects.

**Molecular Simulations on the Critical Properties and High-Pressure Volumetric Behavior of Hydrocarbons in Supercritical Carbon Dioxide** Led by Victor Polo (BIFI, Department of Physical and Organic Chemistry, UZ), using Monte Carlo simulations, this project attempts to understand the solvent behavior of carbon dioxide in supercritical conditions. When the critical point located at 72.9 atm and 31.1°C is reached, CO<sub>2</sub> forms a fluid state with excellent solvent properties which are used for extraction processes. By means of pair density analysis on extensive simulations using molecular mechanics, the clustering of CO<sub>2</sub> molecules around small hydrocarbons and their volumetric implications were determined.

**A step by step algorithm for combining diagnostic tests** Led by Luis Mariano Esteban, a step by step algorithm for estimating the parameters of a linear classifier which combines several measures was analysed. Diagnosis in medicine is not an easy task, and it is usual to carry out a large number of tests in order to predict various aspects of diseases. In this context, how to combine the results of these multiple tests becomes a key point in obtaining a good discrimination rule for diseased and non-diseased states. A step by step approach was considered in order to build linear models which combine multiple markers. This is a distribution-free approach which had not previously been sufficiently explored. The optimisation criterion is to maximise the area under the Receiver Operating Characteristic (ROC) curve.

The algorithm is applied to different simulated data sets and its performance is evaluated. Diagnostic tests produce many measurements ranging from continuous to discrete variables. Thus, in order to include all these possible situations, different scenarios have been considered in this work. We have performed several simulation studies, each based on 1000 or 10000 simulation runs. Each scenario requires a computation that can reach several days.

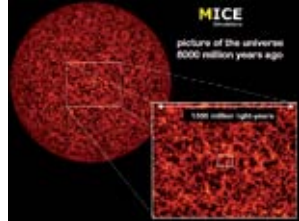
Simulations results show the good performance of the step by step method. This work has been accepted to be published in the *Journal of Applied Statistics*: "A step by step algorithm for combining diagnostic tests", *JApplStats* (accepted 1-Feb-2010)

## Key Projects 2009

**Heisenberg Spin Glasses: Large Lattices at Low Temperatures** Led by Víctor Martín Mayor (BIFI, Theoretical Physics Department UCM), Spin-glasses are disordered magnetic alloys with very unusual behaviour. Interest in spin glasses goes far beyond just this class of materials, however, because they provide a convenient



### Large numerical simulations for dark-energy surveys, Pablo Fosalba, Instituto de Ciencias del Espacio (IEEC-CSIC)



Simulated image of the galaxy distribution over the entire celestial sphere

**Abstract** How did the large-scale structure of the universe, such as galaxies, clusters of galaxies, superclusters, etc. form? Is gravity responsible for it? How is the structure formation process affected by the presence of the mysterious dark-energy density that drives the observed accelerated expansion of the universe?

Using the most powerful supercomputers in Europe, MareNostrum, the project is developing the largest cosmological dark matter simulations to date, involving thousands of millions of particles in volumes of several thousands of million light-years a side.

The aim is to reproduce with unprecedented detail the history of the universe, from much before the first stars formed up to nowadays, and determine how well future astronomical surveys can answer these fundamental open questions.

**Results** The project has produced the largest cosmological simulations to date involving up to 100 thousand million dark-matter particles in a volume comparable to all the observable universe. Using these simulations it is possible to reproduce what current and planned astronomical surveys will see with unprecedented detail. In particular, the simulations have been used to interpret the clustering statistics of current galaxy catalogues, how quasars formed and evolved, and the first all-sky map of the weak-lensing distortion produced by the dark-matter distribution on the light emitted by distant galaxies was produced. Ultimately these simulations will be used to predict how well future astronomical surveys will determine the nature of the dark-energy that is responsible for the observed accelerated expansion of the universe. Usage of the Marenostrum supercomputer is essential to the project as the simulations require thousands of billions of computations to complete them. This is only possible using thousands of computers working in parallel over about one month, as opposed to hundreds of years using a single processor.

**Publications** Measuring Baryon Acoustic Oscillations along the line of sight with photometric redshifts: the PAU survey, N.Benitez, et al. *ApJ*, 691, 241, 2009; Simulating the universe with MICE: I. The abundance of massive halos, M.Crocce, P.Fosalba, E.Gaztanaga, F.Castander. Submitted to *MNRAS*, 2009

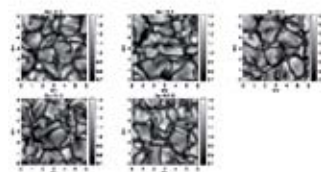
### Magneto-convection And Wave Simulations Of Solar And Stellar Atmospheres, Elena Khomenko, Instituto de Astrofísica de Canarias

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

**Results** Six long time series of solar 3D magneto-convection simulations were completed with different amounts of magnetic flux from 0 to 125 G. These simulations are found to reflect well the observed properties of the quiet solar regions and to reproduce correctly the shapes of solar spectral lines profiles. Current work is focused on the main task of the project: influence of the magnetic field effects and 3D effects on the abundance determination of chemical elements. The first results show that this effect can be important. Future work will include solar models with larger field and models of other stars.

Also analysed was the three-dimensional wave propagation and mode transformation in a sunspot model with the help of several successful simulation runs. These simulations showed a number of new interesting features regarding the possibility of the wave energy propagation into the high atmospheric layers in sunspots. The most energetic 5-minute solar waves were found to propagate hardly any energy upwards due to the cut-off and mode transformation effects. These simulations enabled for the first time the study of the transformation of the Alfvén mode in realistic conditions.

**Publications** Magneto-acoustic waves in sunspots: first results from new 3D nonlinear magnetohydrodynamic code. Felipe, T., Khomenko, E., Collados, M. *The Astrophysical Journal*, 2010, submitted; Mode transformation and frequency change with height in 3D numerical simulations of magneto-acoustic wave propagation in sunspots. Felipe, T., Khomenko, E., Collados, M. *Astronomical Notes*, 2010, in press; Solar abundance determination from three-dimensional magneto-convection simulations. Fabbian, D., Khomenko, E., Moreno-Inseris, F., Nordlund, A. *The Astrophysical Journal Letter*, 2010, in preparation



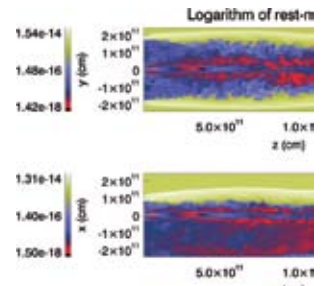
Emerging continuum intensity in solar magneto-convection simulations with different amount of magnetic flux. The images show an increasing number of bright points in intergranular lanes with increasing flux, in agreement with observations.

### Relativistic Outflows In Astrophysics, Manel Perucho Pla, Universitat de Valencia

**Abstract** Relativistic jets are a common feature of radio-loud Active Galactic Nuclei and X-ray Binary Star Systems. The Group investigates the physics of extragalactic relativistic jets in several different contexts: 1) The evolution of jets from X-ray binaries, in the frame of the interaction between the jets and the stellar wind from the companion -massive- star; 2) the generation of observable structures and the deceleration of jets due to the growth of fluid instabilities and/or stellar mass loss; 3) the evolution and properties of kiloparsec-scale FRI jets, and 4) the long-term evolution and feedback of kiloparsec-scale FRII jets in the intergalactic environment, especially concerning the cosmological implications that this process may have. By using own developed code, RATPENAT, in supercomputers, the Group obtained interesting information in this field.

**Results** The 3D simulations of the interaction between microquasar jets and winds from massive stars demonstrated that this interaction could be responsible for the absence of radio-jets in some massive X-ray binary stars, and also produced sites suitable for the production of high-energy emission observed. Simulations of the jet in M87 showed that the observed jet deceleration is not easily reproduced within the frame of the growth of instabilities, as some models predict. Thus, other mechanisms have to be tested, e.g., mass-load from stars. In the field of long-term evolution of extragalactic jets, this work, which is still being analysed, already shows interesting results with respect to the FRI-FRII dichotomy (dynamics and disruption of jet flows due to different nonlinear processes) and the role of these jets in the “cooling” problem and galaxy evolution at cosmological scales. The use of supercomputational resources is crucial due to the extreme size and duration of the simulations. Further work should deepen understandings in the physics of relativistic outflows in astrophysics from different perspectives and scenarios.

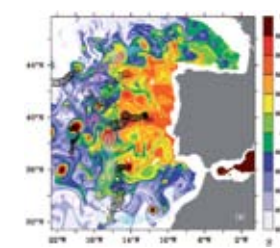
**Publications** Stability of three-dimensional relativistic jets: implications for jet collimation. Perucho, M., Martí, J.M., Cela, J.M., Hanasz, M., de la Cruz, R., Rubio, F. *Astronomy & Astrophysics*, submitted; 3D simulations of wind-jet interaction in massive X-ray binaries. Perucho, M., Bosch-Ramon, V., Khangulyan, D. *Astronomy & Astrophysics Letters*, 512, 4, March-April, 2010.; High-energy emission from the jet-wind interaction in massive X-ray binaries. Bosch-Ramon, V., Khangulyan, D., Perucho, M. *Astronomy & Astrophysics*, in preparation.; When jets die. Perucho, M., Quilis, V., Martí, J.M. In preparation; Jet deceleration in M87: instabilities vs mass load. Perucho, M., Hardee, P.E., Martí, J.M. In preparation.; Numerical simulations of FRI jets: the first kiloparsecs. Perucho, M., Laing, R., Martí, J.M. In preparation.



Map of the rest-mass density cut along the axis of a microquasar jet interacting with a wind from a massive star. The wind from the star impacts the jet in the X-Z plane (bottom panel), disturbing the whole structure of the jet and causing its disruption and deceleration.

### Seismic Oceanography: High-resolution Numerical Simulations Of The Ocean Circulation Off Iberia, Nuno Serra, University of Hamburg

**Abstract** The boundaries between the Mediterranean Water (MW) and the surrounding Atlantic water present conditions to form thermohaline fine-structures due to double diffusion and intrusions. These small-scale processes play a yet not fully understood role in the mixing of MW and in the decay of MW eddies forming at depth off Iberia. Conventional in situ measurements can only resolve these phenomena vertically. Seismic reflection measurements were recently shown to horizontally image small scales in the ocean (order of 10m), however, the lack of direct observations or detailed simulations renders the seismic interpretation difficult. An ocean model forced by atmospheric reanalysis data was applied at high-resolution to the ocean off Iberia. The simulations have enabled the understanding of some mixing processes that can be mapped by the seismic method.



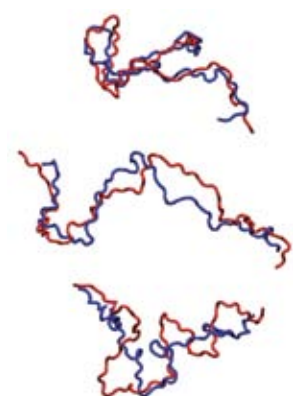
Instantaneous distribution of model salinity at 1100m depth, showing the presence of sub-mesoscale anticyclonic vortices of MW origin. Selected trajectories of model floats are superimposed.

**Results** The generation of subsurface dipolar eddies within the MW layers off the Iberian coast was numerically simulated using the computational resources provided by the BSC-CNS. The mechanisms leading to the generation of these oceanic structures are small in scale and therefore, to face the needed horizontal high-resolution, supercomputing resources were of utmost importance. The surface expression of the mid-depth dipoles, previously identified in satellite remote sensing data (sea surface temperature, chlorophyll concentration and sea surface height), was further investigated with the simulations. The presence of MW dipoles (Fig. 1) was shown to influence the development of coastal upwelling filaments, which are upper ocean phenomena. The surface circulation induced by the dipoles causes the upwelling filaments to extend offshorewards (Fig. 2) and thus to enhance the transport of physical, chemical and biological properties into the open ocean, with potential impact on the coastal zone ocean productivity. The analysis of the simulations will continue focusing on the mixing and decay of the MW vortices, of importance to the maintenance of the ocean stratification in the Atlantic thermocline.

**Publications** Surface expression of Mediterranean Water dipoles and their contribution to the shelf/slope - open ocean exchange. Serra, N., I. Ambar & D. Boutov. *Ocean Science*, 6, 191-209, 2010.



### Determination Of Native Ensembles For Proteins Using Ensemble Restrained Simulations, Xavier Salvatella, Institute for Research in Biomedicine (Previously at the Department of Chemistry, University of Cambridge)



Examples of the range of structural corrections induced by refinement, where the SCM ensemble members are shown in red and the refined ensemble members are shown in blue.

**Abstract** A description of the relationship between the structure and the function of proteins is not complete without a thorough understanding of protein dynamics. Methods are available for the characterisation of the average structure of proteins but, by contrast, the development of approaches to generate native ensembles, that simultaneously describe the structure and the dynamics of the protein, is still at its infancy. The goal of this research project is the development of procedures for the generation of such ensembles using ensemble molecular simulations restrained by the results of NMR experiments.

**Results** Residual dipolar couplings are probes of the dynamical properties of biomolecules that are used to study the relationship between macromolecular motion and biological function. To date this powerful strategy is only applicable to molecules that do not undergo shape changes, preventing the study of multidomain and unstructured proteins. This limitation is circumvented by computing the alignment tensors of the ensemble members at each step and, in a first application, determining an ensemble of conformations that describes denatured ubiquitin. In analogy to dynamic refinement of folded proteins, Statistical Coil Models are used as a starting configuration because they are the best available descriptions of unstructured proteins. It was found that refinement causes structural corrections and yields an ensemble that is in agreement with the measured

RDCs and presents inter-residue interactions between strands beta1 and beta2, also observed in other studies, and can be cross-validated against RDCs. This method increases the range of systems that can be studied using RDCs and is likely to yield new insights in how the large scale motions of macromolecules relate to function.

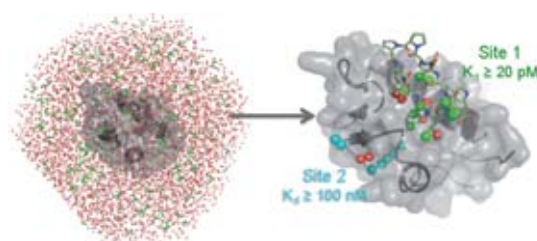
**Publications** Refinement of ensembles describing unstructured proteins. Esteban-Martin S, Fenwick R. B. and Salvatella X. (2010). J. Am. Chem. Soc. 132, 4626-4632.

### Optimization And Applications Of MDmix, A Druggability Index Based On First Principles, Xavier Barril, ICREA & Universitat de Barcelona

**Abstract** Advances in molecular biology, genomics, proteomics and systems biology offer the possibility to expand the number and quality of potential therapeutic targets. Unfortunately, many targets with a sound biological rationale are pharmacologically inaccessible because they do not bind drug-like molecules. Failing to recognise this can lead to a waste of resources, but concentrating on 'classical' target classes leads to a waste of opportunities. The quantitative prediction of a target's druggability (i.e. its potential to be modulated by drugs) is, therefore, crucial in drug discovery. The Group recently developed a new druggability index based on first principles. The aim is to refine the methodology, apply it to drug discovery and extend its applicability to other biological problems.

**Results** A new method was developed to detect binding sites and to quantify the maximal binding affinity that a ligand may achieve for them. In contrast with other published methods, it is based on first-principles molecular simulations and is not trained on a dataset. As such, it is particularly suited to study binding sites that do not fall into the main target classes (e.g., protein-protein interfaces). Furthermore, the strategy provides very detailed information about the interaction preferences of the binding sites and can be extremely effective in providing a new perspective on the target of interest.

The method is useful for selection of new pharmacological targets and was successfully applied to identify previously unknown drug binding sites. The main drawback of the method is that, reliant on state-of-the-art molecular dynamics simulations, it is computationally very demanding. Having access to a supercomputing facility enables predictions to be obtained in a matter of days, and to apply the method to a large set of potential pharmacological targets.

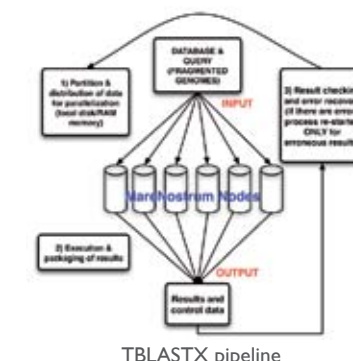


Molecular dynamics simulations with explicit solvent can be used to predict the drug binding sites on the surface of proteins. This is exemplified here with MDM2, an anticancer target.

### Use Of TBLASTX To Find Regions Of Homology Among Multiple Large-size Full Genomes, Roderic Guigó, Centro de Regulación Genómica

**Abstract** The predictive power of many bioinformatic tools makes use of similarities between genomes, which can be detected by the computationally intensive algorithm TblastX. The Genome Bioinformatics group led by R. Guigó uses MareNostrum to run TblastX to find regions of homology (in the form of High-Scoring pairs -HSPs-) between 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.

**Results** In 2009 the Group contributed to the annotation of the Cow Genome with the help of the computation power of MareNostrum to TBLASTX the cow genome against both the mouse and human genome assemblies. The homology-based gene prediction program SGP was one of the prediction tools used in the annotating the Cow genome. SGP predictions for several mammalian genome can be found at: <http://genome.ucsc.edu/cgi-bin/hgGateway>. All SGP-based predictions can be downloaded from: <http://genome.crg.es/genepredictions/index.html>



### Targeting The Plasticity Of Abl And C-Src Tyrosine Kinases Through Mutagenesis And Atomically Detailed Large-scale Molecular Dynamics Simulations, Francesco L. Gervasio, Centro Nacional de Investigaciones Oncológicas

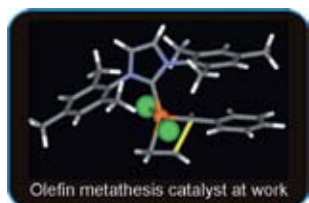
**Abstract** In most protein kinases, conformational changes connect catalytically active and inactive conformations. Many kinase inhibitors, including the approved cancer drugs imatinib and sorafenib, selectively target a specific Abl tyrosine kinase conformation, but the function and mechanism of the conformational change remain unclear. Using single point mutations and large scale accelerated molecular dynamics simulations of the c-Src and Abl kinase, the conformational changes involved in activation and drug binding in these tyrosine kinase were studied, resulting in a deeper understanding of the role played by specific active-site residues.

**Results** Molecular Dynamics complemented by metadynamics was used to understand how this single point mutation can affect the DFG flip. First, 1 μs long simulations have shown that the mutation destabilizes a cluster of hydrophobic residues. This cluster is in the DFG region and in the wild-type c-Src stabilizes the DFG-in conformation. This evidence has now been corroborated by thermal unfolding experiments (collaboration with the CNIO NMR unit). A guess reactive coordinate was built from the available crystallographic structures of c-Src and Abl. It was optimised in free energy space with the PCV and biased simulations were run of the DFG flip in the wt and mutant c-Src. The free energy profiles of the flip confirmed that the specific LEU to ILE mutation in the hydrophobic cluster close to the DFG motif considerably lowers the free energy barrier of the flip. An important role of the protonation state of the Asp in the DFG motif was also discovered.



The active conformation of c-Src kinase is shown in the figure. From left to right: open, intermediate and close conformations. The DFG is in CPK representation and the activation loop in color.

### Ab initio Molecular Dynamics Simulations Of Ru-Catalyzed Olefin Metathesis Reaction, Luigi Cavallo, University of Salerno



Olefin metathesis catalyst at work

**Abstract** The dynamic behavior of Ru-complexes relevant to olefin metathesis, the Nobel 2005 reaction, was investigated. This reaction is very important to the petrol chemistry as well as the pharma industry. Ab initio molecular dynamics simulations performed with BSC-CNS facilities facilitated the study of the evolution of the catalysts during a deactivation reaction that simply inactivates an otherwise active and expensive catalyst, and the investigation of the dynamic flexibility of these catalysts to relate activity with catalyst structure. Better understanding of the chemistry of these catalysts can be used by experimental chemists to design better catalysts. These kinds of extremely expensive simulations are only possible at state-of-the-art computational centres.

**Results** Dynamics simulations were performed to investigate the deactivation reaction promoted by addition of CO to Grubbs 2nd generation catalysts. The simulations showed the complete decourse of the reaction from the starting and active catalyst to the experimentally characterised deactivation products, offering mechanistic insights simply impossible to obtain with static methods. Also studied was the dynamic characterisation of 11 Ru-NHC complexes relevant to olefin metathesis. The simulations indicated that the flexibility of the N-substituents of the NHC ligand is strictly dependent on the ortho-groups on the N-substituents, and that even a single methyl group restricts remarkably rotation around the N-substituent bond. The results also rationalised the catalytic stability and reactivity of different complexes.

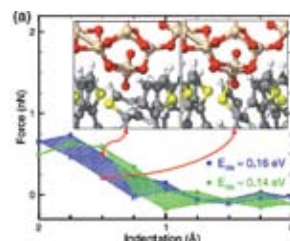
**Publications** Exploring the Reactivity of Ru-Based Metathesis Catalysts with a PI-Acid Ligand Trans to the Ru-ylidene Bond. Poater A., Correa A., Ragone F., Cavallo L. J. Am. Chem. Soc. 2009, 131, 9000.; Flexibility of N-Heterocyclic Carbene Ligands in Ru-Complexes Relevant to Olefin Metathesis and Their Impact in the First Coordination Sphere of the Metal. Ragone F., Poater A., Cavallo L. J. Am. Chem. Soc. 2010, 132, in press.; The Mechanics of Olefins Metathesis from a Theoretical Perspective 18 International Symposium on Olefin Metathesis. Cavallo L. Leipzig 2-7 August 2009.

### Interaction Of Atoms And Molecules With Metals And Metallic Oxides Characterized By First-principles Calculations And Simulations Of Surface Imaging Techniques, Rubén Pérez, Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid

**Abstract** The aim of this activity is to gain insight into the interaction of atoms and molecules with metals and metallic oxides combining first-principles simulations with state-of-the-art experimental techniques. Within this broad field, two topics were focused on: (1) Understanding energy dissipation in dynamic AFM experiments; and (2) the calculation of stress-strain characteristics in different compounds, including alkaline-earth tungstates. These subjects are relevant from both a basic perspective and in prospective technological applications: phase-imaging enhances significantly the resolution on polymers and biological samples, while tungstates are key compounds to design instrumentation for low-background particle physics experiments and the implementation of Raman lasers.

**Results** Variation of the phase shift of a vibrating tip across a heterogeneous surface gives rise to a powerful source of spatial contrast. Simple analytical models show that the phase lag is related to the local energy dissipation on the surface. A combined experimental and theoretical approach was taken to establish the atomistic origin of energy dissipation. It was shown that the energy transferred by a single nano-asperity to a sexithiophene monolayer is about 0.15 eV/cycle. The configuration space sampled by the tip depends on whether it approaches or withdraws from the surface. The asymmetry arises because of the presence of energy barriers among different deformations of the molecular geometry. This is the source of the material contrast provided by the phase-shift images. Regarding the stress-strain calculations, the dynamics of different materials were studied, including wolframite MnWO<sub>4</sub>, ZnAl<sub>2</sub>O<sub>4</sub> and ZnGa<sub>2</sub>O<sub>4</sub>, and LuVO<sub>4</sub> and ScVO<sub>4</sub> zircon-type under high pressure. These results were compared with Raman scattering results in order to gain knowledge both on the material behavior, and on the accuracy of the formalism to describe stress and strain in the DFT codes.

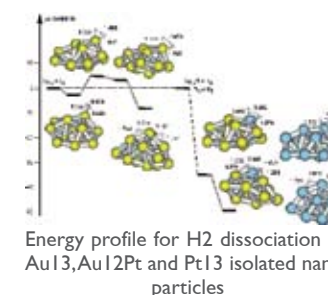
**Publications** Molecular energy-dissipating processes in oligothiophene monolayers determined by phase-imaging force microscopy. N.F. Martínez, V.V. Kaminski, C.J. Gómez, C. Albonetti, F. Biscarini, R. Pérez and R. García. Nanotechnology 20,434021 (2009). (invited article in the special issue to mark the 20th volume of Nanotechnology); Ab initio calculations of the wolframite MnWO<sub>4</sub> under high pressure. Sinhue López-Moreno, A. H. Romero, P. Rodríguez-Hernández and A. Muñoz. High Pressure Research, 29, 578-581 (2009); Ab initio study of the high pressure phases and dynamical properties of ZnAl<sub>2</sub>O<sub>4</sub> and ZnGa<sub>2</sub>O<sub>4</sub>. Sinhue López-Moreno, A. H. Romero, P. Rodríguez-Hernández and A. Muñoz. High Pressure Research, 29, 573-577 (2009); Ab initio study of high-pressure structural properties of the LuVO<sub>4</sub> and ScVO<sub>4</sub> zircon-type. J. López-Solano, P. Rodríguez-Hernández and A. Muñoz. High Pressure Research, 29, 582-586 (2009).



Force-distance curves at a hollow position between molecules (green, circles) and over a sulfur atom (blue, squares) for a Si oxide nanoasperity indenting on a sexithiophene monolayer.

### Supported Metal Nanoparticles As Chemoselective Hydrogenation Catalysts, Avelino Corma Canós, Instituto de Tecnología Química UPV-CSIC

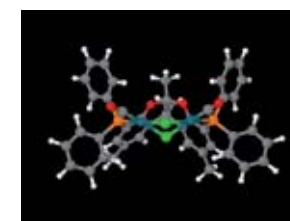
**Abstract** Selective hydrogenation of multifunctional molecules is an important target for the research in catalysis and the industrial production of fine chemicals. While gold nanoparticles supported on TiO<sub>2</sub> are highly chemoselective for the hydrogenation of the nitro group in substituted nitroaromatics, platinum nanoparticles supported on TiO<sub>2</sub> are highly active but not chemoselective. High selectivity is only achieved when the surface of the Pt nanoparticles is decorated with partly reduced oxide particles (TiO<sub>x</sub>) that are formed as a result of high-temperature reduction pretreatment. The nature of these TiO<sub>x</sub> particles and the mechanism of selective hydrogenation of the nitro group of nitrostyrene on these decorated Pt catalysts is being investigated from a theoretical point of view.



**Results** To improve the activity of Au/TiO<sub>2</sub> catalysts toward hydrogenation without decreasing chemoselectivity, a number of isolated and supported Au, Pt and Au-Pt nanoparticles were investigated by means of DFT calculations. H<sub>2</sub> dissociation on Pt and Au-Pt nanoparticles is considerably faster than on Au, because H<sub>2</sub> adsorption on Pt atoms is dissociative and no activation barriers are involved. The high chemoselectivity of Au/TiO<sub>2</sub> catalysts does not exist in Pt/TiO<sub>2</sub> catalysts no matter how small the Pt particles are, but can be preserved in Au-Pt/TiO<sub>2</sub> catalysts if the Au/Pt ratio is high enough as to keep Pt atoms isolated and not at the active metal-support interface. The knowledge provided by the computational study has enabled the improvement of the performance of currently used hydrogenation catalysts.

**Publications** Origin of the Different Activity and Selectivity toward Hydrogenation of Single Metal Au and Pt on TiO<sub>2</sub> and Bimetallic Au-Pt/TiO<sub>2</sub> Catalysts. Mercedes Boronat and Avelino Corma, Langmuir, DOI: 10.1021/la101752a

### Wide Bite-angle Ligands: New Catalysts For Old And New Reactions, Carles Bo Jane, ICIQ



Cl-Bridged Dinuclear Rhodium Catalyst bearing JOLE Ligand

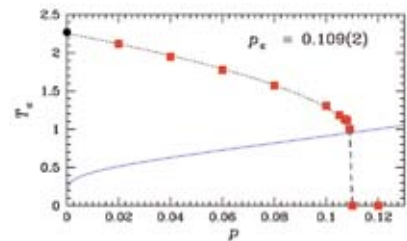
**Abstract** Homogeneous catalysis using transition metal complexes is a key area of research in modern chemistry. Many catalytic reactions are now widely used and the development and design of new ligands in order to improve such reactions is a very active field. Among these ligands, phosphine based ligands are very popular in organometallic chemistry, especially in homogeneous catalysis. Newly developed dinuclear rhodium complexes bearing wide bite-angle phosphine ligands exhibit unprecedented activity in the carbonylation of methanol, one of the most important industrial applications to produce acetic acid. A complete understanding of the reaction mechanisms throughout the catalytic cycle, and especially during the rate-limiting step, is still missing and will greatly help the understanding of such reactions and the design of new catalysts.

**Results** The Group successfully managed to compute energies and vibrational frequencies of very large molecules up to 115 atoms with heavy metallic atoms using relativistic density functional theory (DFT) methods. This would have been quite challenging using the Group's own computing cluster, but thanks to MareNostrum the research is able to be performed. However, there are still some discrepancies between experimental and theoretical results that induce more work from both sides, especially from the computational point of view. The processing of the data requires some time as both experimental and theoretical groups have to collaborate to get the results published. Results from previous research on a similar application (Computational modeling of nanocages: giant polyoxometalates, organic capsules and molecular vessels) have recently been published (see below).

**Publications** Water Oxidation at a Tetra Ruthenate Core Stabilized by Polyoxometalate Ligands: Experimental and Computational Evidence To Trace the Competent Intermediates. A. Sartorel, P. Miró, M. Carraro, E. Salvadori, S. Romain, G. Scorrano, M. Di Valentin, A. Llobet, C. Bo, M. Bonchio. J. Am. Chem. Soc., 131, 16051, 2009; Towards a Computational Treatment of Polyoxometalates in Solution using QM Methods and Explicit Solvent Molecules. P. Miró, J. Bonet Ávalos, J. M. Poblet. C. Bo. Can. J. Chem., 87, 1296, 2009



## Decoherence Effects In Topological Quantum-Computing Models, Miguel A. Martin-Delgado, Universidad Complutense de Madrid



“ $p_c$ – $T_c$ ” phase diagram for the random 3-body Ising model. For “ $p > p_c$  approx 0.109” the ferromagnetic order is lost. The dotted line is a guide to the eye, the black circle represents the analytically-known transition temperature of the 2D Ising model. The blue (solid) line represents the Nishimori line, where quantum computation is reliable below the error threshold “ $p_c$ ”.

**Abstract** Quantum technologies, including topological quantum computation (TQC), are emerging technologies which have the potential to revolutionise computing and science. However, sensitivity to quantum noise or decoherence makes most of the current quantum computing schemes prone to error and nonscalable. Error correction software can, in principle, solve this problem, but this requires a much higher fidelity of the basic components of the computer than currently can be achieved and introduces an undesirable overhead. Here the decoherence effects due to external noise on a topologically protected system are studied. In this proposal Monte Carlo simulations are performed of statistical mechanics counterparts of the topological quantum models for TQC in order to determine the error tolerance.

**Results** Enhanced quantum information stability does not imply a lower noise tolerance. Improving the computational capabilities of a quantum information system generally comes at the price of decreased robustness against

environmental noise. This trade-off has been one of the hardest nuts to crack for scientists. However, in a recent letter, Katzgraber, Bombin and Martin-Delgado have shown that this is not necessarily the case, provided the data are encoded using topological color codes—a new form of topological quantum computer—that allows for the implementation of complex quantum operations, such as quantum distillation, teleportation, and dense coding, to name a few. Topological color codes preserve a high error tolerance for quantum operations without performance trade-offs. To estimate the error tolerance, Katzgraber et al. mapped the problem onto a novel statistical model with random interactions that correspond to the faulty bits. The exhaustive analysis has been carried with the help of supercomputers around the world, including the MareNostrum at the BSC-CNS, using highly-optimised large-scale Monte Carlo simulations.

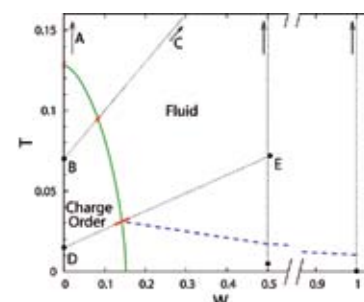
**Publications** Error Threshold for Color Codes and Random 3-Body Ising Models. Helmut G. Katzgraber, H. Bombin, M. A. Martin-Delgado. Phys. Rev. Lett. 103, 090501 (2009). arXiv:0902.4845

## Monte Carlo Simulation Of Disordered Electronic Systems, Matteo Palassini, Universitat de Barcelona

**Abstract** Correlated electron systems provide a concrete laboratory example of a “complex system” in which simple interactions give rise to a nontrivial, intricate structure. The research focuses on the Coulomb glass, a state occurring in disordered localized electron systems. The goal is to elucidate both the equilibrium thermodynamic properties of these systems and their glassy dynamics. These issues were investigated using large-scale Monte Carlo simulations with the parallel tempering algorithm, as well as with kinetic Monte Carlo and optimisation algorithms.

**Results** Investigations of the fundamental properties of the “Coulomb glass”, a state occurring in disordered insulators at low temperature, resulted in the determination with great accuracy of the correlation gap in the single-particle density of states. For large disorder, for the first time the validity of a prediction by Efros and Shklovskii was validated, which has important consequences for understanding the hopping electrical conductivity in disordered insulator. A crossover was also discovered at small disorder due to the presence of the charge-ordered phase; The influence on the density of states of the boundary conditions in the Ewald method was clarified analytically and numerically; Equilibrium correlations in two dimensions were studied and a behaviour similar to the three dimensional case was found, strengthening the demonstration of the absence of an equilibrium glass phase. The short-range Random Field Ising Model was also studied, identifying a clear difference from the Coulomb glass. This sheds light on the peculiar correlations induced by the long-range interactions; The nature of avalanches induced by the addition of a charge were characterised.

**Publications** Phase diagram, correlation gap, and critical properties of the Coulomb glass. Martin Goethe and Matteo Palassini. Physical Review Letters 103, 045702, July 2009.; Numerical study of the equilibrium thermodynamics of the Coulomb glass. Martin Goethe and Matteo Palassini. Annalen der Physik 18, 868, December 2009.



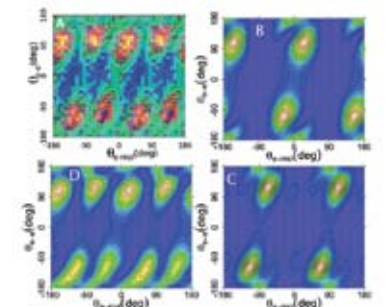
Phase diagram of the Coulomb glass. The lines represent the paths of the simulations used to determine the diagram.

## Nuclear And Electronic Dynamics In One- And Multi-photon Ionization Of Atoms And Molecules By Ultrashort Pulses And Synchrotron Radiation, Fernando Martin Garcia, UAM

**Abstract** Theoretical progress to accurately describe non dissociative and dissociative ionisation of molecules exposed to synchrotron radiation and ultrashort uv/xuv laser pulses was achieved by including both the electronic and nuclear degrees of freedom. This is essential to describe the delicate interplay between the electronic motion and the molecule's vibration, especially in those cases where ionisation occurs in a time scale comparable to that of the vibrational motion. In this project these methods were extended to study two-photon double ionisation of He and H2 as well as molecular autoionisation by using pump-probe strategies.

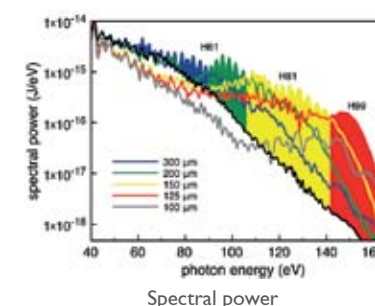
**Results** Thanks to the advanced parallel paradigms and the computational power of MareNostrum, converged results were obtained for the following problems: - One-photon double ionisation of the Hydrogen molecule at high photon energies. This proved the appearance of classical interference effects in the double ionisation of H2, and explained recent experimental results. - Two-photon double ionisation of H2. Fully differential and integrated cross sections in the photon energy range 26-30 eV are being obtained, to deliver what are believed to be the first converged results in this field. - Pump/probe theoretical calculations in H2 were carried out, using an attosecond pump and a femtosecond probe, including doubly excited states. As far as is known, these are the first pump probe calculations ever done for a molecular system including all electronic and vibrational degrees of freedom.

**Publications** Double-slit, confinement, and non-Franck-Condon effects in photo ionization of H2 at high photon energy. J. Fernández, O. Fojón, and F. Martín. Phys. Rev. A 79, 023420 2009



TDCS at photon energy of 160 eV plotted as function of angle of faster electron with molecular axis and angle between electrons. (a) Experiments with circular polarization of Ref. (Science 318, 949 (2007)) with ECS calculations superimposed as white contours. Data include all energy sharings between 78% and 96%. (b) ECS calculations for parallel polarization for ejection energy of 108 eV (99% energy sharing). (c) Corresponding calculations for perpendicular polarization. (d) Calculations for circular polarization.

## Scaled Attosecond Physics, Carles Serrat, ICFO - UVIC



**Abstract** The Scaled Attosecond Physics research project aims at studying the coherent motion of electron wavepackets inside atoms and molecules on attosecond timescales, considering the generation and propagation of high order harmonics (HHG) driven by high-energy phase-stable few-cycle long-wavelength laser pulses. The interaction of mid-IR laser light with noble gas atoms and coherently prepared systems such as alkalis for HHG were investigated. The low conversion efficiency of HHG is one of the biggest obstacles for practical applications and this project investigates new techniques for enhanced harmonic photon yield.

**Results** The generation of coherent light was extensively studied in the short wavelength region of the electromagnetic spectrum by high harmonic generation (HHG), and important advances were made. The low yield of HHG especially for high photon energies, combined with a lack in tunability, often prevents many exciting applications from HHG, such as the visualisation of atoms, molecules and nano-materials, or recording dynamic behavior of chemical reactions at the electronic level. A feasibility study was performed to enhance and control the photon yield, especially near the high harmonics cutoff, tunable to high soft-X-ray energies, by adding a DC electric field periodically in space along the HHG interaction region and also by using carrier envelope phase dynamics with Bessels beams.

The Maxwell-Schrödinger equations solver that was used for the numerical simulations is extremely time-consuming for the conditions of interest, which can only be resolved through parallel intensive computations. The code is fully parallelised with typical runs of 48-72 hours using 128-256 nodes in MareNostrum. The interprocess communication is tightly coupled and therefore the simulations benefit significantly from the high velocity interprocess communication system of a supercomputer such as MareNostrum.

**Publications** Modulated phase matching and high-order harmonic enhancement mediated by the carrier-envelope phase. D. Faccio, C. Serrat, J. M. Cela, A. Farrés, P. Di Trapani, J. Biegert. Physical Review A 81, 011803(R) (2010); All-Regions Tunable High Harmonic Enhancement by a Periodic Static Electric Field. C. Serrat, J. Biegert. Physical Review Letters 104, 073901 (2010). To be Highlighted in Nature Photonics, May 2010

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