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Barcelona Supercomputing Center ~ Red Española de Supercomputación

2010 Annual Report



2010 Annual Report





The 2010 Combined Annual Report of the Barcelona Supercomputing Center - Centro Nacional de Supercomputación (BSC-CNS) and the Spanish Supercomputing Network (RES) summarises the various support and research activities for the year and provides a short description of the two organisations.



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2010 Review



Mateo Valero,
Director

Francesc Subirada,
Associate Director

We are pleased to report that in 2010 the BSC-CNS continued to build strongly on the growth and achievement of previous years. A number of research departments were highly successful in attracting new competitive funds, and the services provided to the Spanish scientific community via the Spanish Supercomputing Network (RES) were further augmented with the addition of a new node, Atlante in the Canary Islands, and via increased offerings of training seminars and workshops. Although the economic crisis has somewhat blunted its strong growth expectations, the BSC-CNS is privileged to continue to receive support across the political spectrum, recognition of its strategic importance within the Spanish scientific framework and the excellence of its scientific and technical activities. This was exemplified with the inauguration in Barcelona of the PRACE distributed European supercomputing research infrastructure involving 20 countries, within which the BSC-CNS has a leadership role.

Mission

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

Spain is suffering under a prolonged and profound economic crisis. The growth and success of the BSC-CNS stands in stark contrast to the reduced activities of many key Spanish firms and the closure of many businesses, both small and large. That is not to say that the BSC-CNS has been insulated from the crisis, indeed, many BSC-CNS staff were affected by the general salary reductions of the public sector, and the decrease in funds available for both studentships and research grants has been keenly felt.

However the crisis itself has been a source of great motivation for BSC-CNS staff. Many believe that it is only through strong efforts to fundamentally change the fabric of Spanish science and industry that Spain will be able to arise from the crisis and regain a premier economic and industrial leadership role within both European and global markets. By positioning itself at the forefront of European efforts to compete head-to-head with the United States for leadership in High Performance Computing architectures and software systems, the BSC-CNS is betting that the modern model it has adopted of an independent research centre, coupled with the strong creativity and dedication of local researchers, and the ability of Barcelona as a city and a scientific nexus to attract top international talent, will forge a first class team with sufficient breadth and depth to challenge the world's best supercomputing research centres.

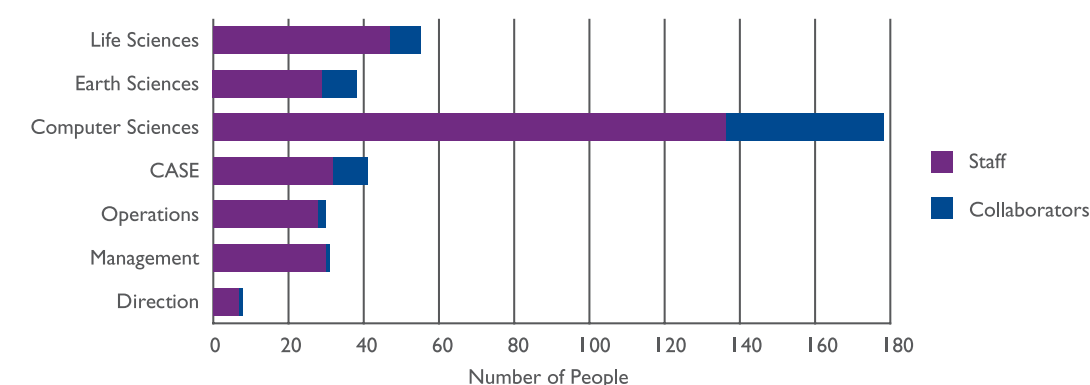
Powerful Computing

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 2006, the Top500 list ranked the MareNostrum as the 10th most powerful supercomputer in Europe and 40th in the world.

The promise that this vision brings is a future in which key computing technologies are developed here in Barcelona, in partnership with the world's leading computing companies, that a new generation of computer architects, programmers and technicians are trained in Barcelona with skills that make them sought after worldwide, and that local businesses are able to gain significant competitive advantage by being the first to adopt HPC advances.

During 2010, significant progress was made in this direction with the reaffirmation of the BSC-CNS as one of only four confirmed European hosting sites for the Tier-0 super computing nodes of the future, under the Europe-wide PRACE program. Work has begun on the new building adjacent to the MareNostrum facility, which will house the new supercomputer and serve as the new headquarters for the BSC-CNS. The Spanish Supercomputing Network (RES) has also continued to expand, with the consolidation of a new node in the Canary Islands, Atlante. The 8th member of the network, Atlante is located at the Science and Technology Park of the University of Las Palmas de Gran Canaria, and tackles a diverse range of projects, from the study of photovoltaics to simulations of ocean currents. Requests by scientists for access to the RES has continued to grow, with demand reaching double the available computing time. Allocation of time is managed by the Access Committee, whose dedication and professionalism in selecting the best scientific projects to run on the MareNostrum and other RES nodes is deeply appreciated.

BSC-CNS People 2010



The BSC-CNS continues to attract talented young researchers from across the globe. During 2010, some 381 people performed research or provided support at the centre, as compared to a mere 50 back in 2005 when the centre was opened. Over 40% of staff are of foreign nationality, with over 40 countries represented including: Argentina, Austria, Belgium, Brasil, Bulgaria, Canada, Colombia, Cuba, Denmark, Ecuador, France, Germany, Greece, Hungary, Chile, China, India, Iran, Ireland, Israel, Italy, Japan, Korea, Mexico, Montenegro, Netherlands, Pakistan, Peru, Poland, Portugal, Romania, Russia, Serbia, Slovakia, Switzerland, Thailand, Turkey, United Kingdom, USA and Spain.



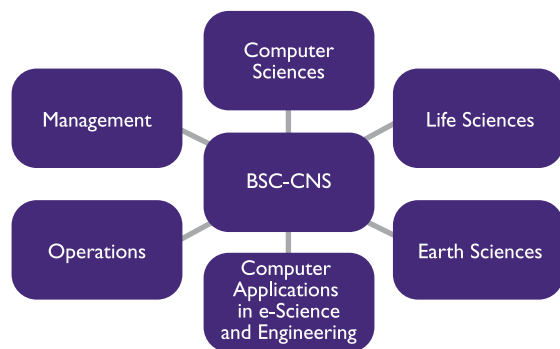
World Map of Countries of Origin

The BSC-CNS has developed strong relationships with the research departments of a number of global high-tech firms, which grow in scope from year to year. 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. In 2010, the BSC-CNS was named by NVIDIA as the first CUDA Research Centre in Spain, recognising broad-based research successes in leveraging the NVIDIA CUDA technology and GPU computing. On the Spanish front, the collaboration with REPSOL has also grown, with significant efforts being invested in the further development and refinement of BSC-CNS technology to process massive amounts of seismic data in order to identify remote sub-sea deposits of oil and gas. Supporting and enhancing the competitiveness of Spanish industry is a key objective of the BSC-CNS and one which is receiving increasing focus, with efforts being made to reach out to local industry and facilitate the adoption of HPC technologies.

In the academic arena, the scientific output of BSC-CNS scientists consistently features in top publications and conferences. Each research department within the BSC-CNS both conducts highly specific, in-depth research as well as collaborating with other departments on broader, multi-disciplinary strategic projects.

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 Science & Engineering (CASE), and Management.



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

The Computer Sciences Department is at the forefront of many areas of HPC research, involved in some 19 international projects during 2010, including coordinating the FP7 Velox project to develop new programming tools and the HiPEAC and HPC-Europa networks of excellence, as well as projects with industry leaders, collaborating with IBM to develop next generation Petaflop supercomputers, with NVIDIA on CUDA architecture for using GPUs in massively parallel applications, and with Microsoft to develop new programming systems for multicore architectures.

The Life Sciences Department is deeply involved in a number of cutting edge international projects such as MITIN, METAHIT and ELIXIR which range from development of disease models through to the establishment of biological information infrastructures. The IMID-Kit project funded by MICINN as a singular strategic project aims to develop a diagnostic kit for inflammatory diseases, while a newly secured, highly prestigious Advanced ERC grant will seek to develop new drug design tools.

The Earth Sciences Department is focussed on developing integrated climate models with ever increasing resolution, such as the CALIOPE project to provide detailed air quality forecasting systems for Spain. CALIOPE is increasingly being adopted by regional governments around Spain to model impacts on air quality of industrial and urban activities as well as natural phenomena.

The Computer Applications in Science and Engineering Department continued to advance development of both modelling tools, such as the ALYA platform, with general applications across numerous physical systems, and highly specific models of important biomechanical systems such as airflow in the human respiratory system, the brain's arterial system, and electromechanical simulations of the heart.

In addition to the projects undertaken by the BSC-CNS research departments, over 400 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.

Broad Access

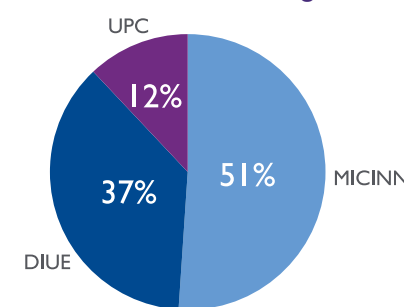
The powerful resources of the MareNostrum Supercomputer and the RES nodes are accessed by a broad spectrum of Spanish and international scientists. Computing time is allocated by the Access Committee, composed of a Core Team and four Expert Panels of prestigious Spanish scientists external to the BSC-CNS.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

The work carried out by the scientists at BSC-CNS resulted in over 88 journals and book chapter publications, 129 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.

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%).

BSC-CNS Patronage



The income of the BSC-CNS in 2010 was €18.5 M of which €11.1 M corresponded to the ordinary budget coming from the patrons of the BSC-CNS, the Spanish and Catalan Governments; and €7.4 M from competitive projects. Of particular note, €1.4 M of funding was derived from projects with private companies. In 2010, the BSC-CNS participated in 30 competitively funded EU projects, 21 collaborative projects with industry and 18 national projects.

The successes of 2010 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

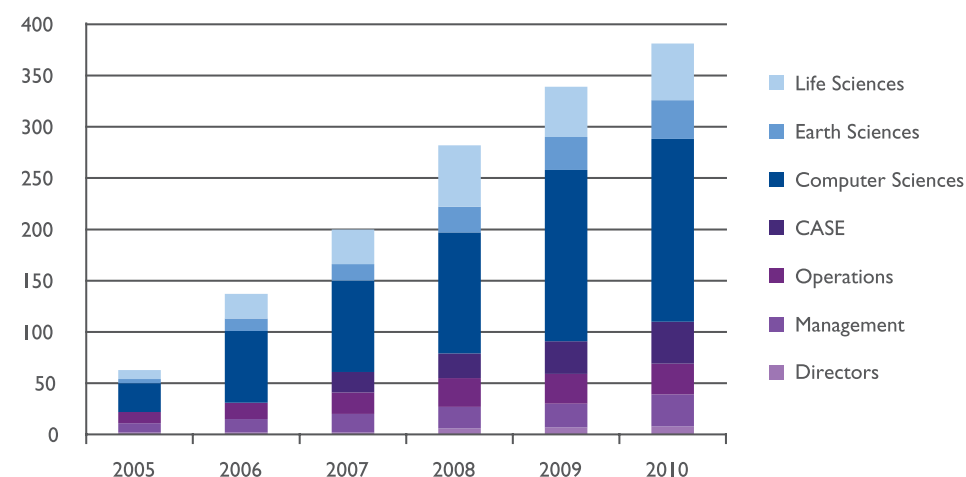
Francesc Subirada, Associate Director

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 2010, the core staff of the BSC-CNS included 92 permanent positions, 95 dedicated to specific projects and 74 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 339 during 2009 to 381 during 2010, mainly through new temporary and shared staff, resident students, and collaborating and visiting researchers.

Annual BSC-CNS Staff and Collaborators



Shared Staff and Human Resource Programs In addition to its own staff, the BSC-CNS hosts shared staff from other public institutions such as the Technical University of Catalonia (UPC), the Institute for Research in Biomedicine (IRB) and the Consejo Superior Investigaciones Científicas (CSIC). In 2010 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 2010, the BSC-CNS had 100 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 6 researchers to access the BSC-CNS facilities in 2010; 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 2010 the BSC-CNS hosted 64 of these visitors.



BSC-CNS Governing Bodies



Members of the BSC-CNS Board of Trustees as at 31st December 2010

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Felipe Pétriz, Secretary of State for Research, MICINN

Vice President

Joan Majó, Commissioner for Universities and Research, DIUE

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Francisco Montero, Vice President of Organization and Institutional Relations, CSIC

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

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Iolanda Font de Rubinat, Deputy Director General of Research

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Antoni Giró, Rector

Josep Casanovas, Vice Rector of University Policy

Sebastià Sallent, Director Fundació i2CAT

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Francesc Subirada, Associate Director, BSC

Ernest Quingles, Manager, BSC

Commission Secretaries:

Mario Maza, State lawyer

Javier Zuloaga, State lawyer

Members of the BSC-CNS Executive Committee as at 31st December 2010

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

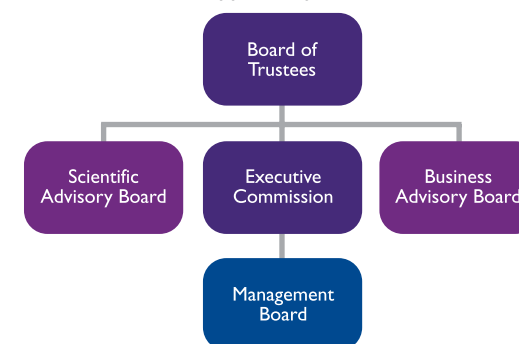
Representatives UPC

Ana Pérez, Vice Rector for Research and Innovation

Josep Casanovas, Vice Rector for University Policy

Strong Governance

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



Representatives BSC-CNS

Mateo Valero, Director, BSC

Francesc Subirada, Associate Director, BSC

Ernest Quingles, Manager, BSC

Commission Secretaries

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

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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 Beivide, 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"

RES Users' Committee (CURES)

Area Physics and Engineering (FI) representative

Javier Jiménez Sendín, **Fernando Martín García**

Area Chemistry and Material Sciences (QCTM) representative

Rubén Pérez, **Núria López**

Area Biomedicine and Health Sciences (BCV) representative

Carme Rovira, **Francisco Javier Luque**

Astronomy, Space and Earth Sciences (AECT) representative

Jordi Torra, **Vacancy available**

RES Management and technicians representative

Sergi Girona

BSC-CNS Staff and Collaborators during 2010

Direction

Director: **Mateo Valero**

Associate Director: **Francesc Subirada**

Director Assistant: **Lourdes Cortada**

Associate Director Assistant: **Judith Camba**

PRACE Research Manager: Carlos Mérida

Academic Programs Coordinator: Ulises Cortés

Facility Management Consultant Operations:

Ramon Pallisa

Travel Administrative Student: Sara Mula

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**

Senior Researcher: Vicenç Beltran

Associate Researcher: David Carrera

Associate Researcher: Javier Alonso

Associate Researcher: Jordi Guitart

Associate Researcher: Mario Macías

Associate Researcher: Yolanda Becerra

Resident Student: Gemma Reig

Resident Student: Iñigo Goiri

Resident Student: Jordà Polo

Resident Student: Josep Oriol Fito

Resident Student: Zeus Gómez

Research Support Engineer: Alexandre Vaqué

Visitor: Anastasios Papagiannis

Visitor: Cristian González

Visitor: Valeria Quadros

HPC Europa Visitor: Alessandro Cilardo

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

Resident Student: Adrià Armejach

Resident Student: Azam Seyed

Resident Student: Cristian Perfumo

Resident Student: Ferad Zyulkyarov

Resident Student: Gokçen Kestor

Resident Student: Gokhan Sayilar

Resident Student: Gulay Yalcin

Resident Student: Isidro González

Resident Student: Ismail Ege Akpinar

Resident Student: Ivan Ratkovic

Resident Student: Milan Stanic

Resident Student: Milovan Duric

Resident Student: Nebojsa Miletic

Resident Student: Nehir Sonmez

Resident Student: Nikola Bezanic

Resident Student: Nikola Markovic

Resident Student: Oriol Arcas Abella

Resident Student: Otto Pflücker

Resident Student: Sasa Tomic

Resident Student: Srdjan Stipic

Resident Student: Sutirtha Sanyal

Resident Student: Timothy Hayes

Resident Student: Vasileios Karakostas

Resident Student: Vesna Smiljkovic

Resident Student: Vladimir Gajinov

Associate Research Support Engineer: Javier Arias

Associate Research Support Engineer: Oscar Palomar

Visitor: Ferran Ollé Pla

Grid Computing and Clusters

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

Senior Researcher: Vassil Nikolov Alexandrov

Researcher: Javier Alvarez

Researcher: Jorge Ejarque

Researcher: José Maria Pérez

Researcher: Marta García

Researcher: Raül Sirvent

Associate Researcher: Daniele Lezzi

Associate Researcher: Julita Corbalán

Associate Researcher: Marc Casas Guix

Resident Student: Aislan Foina

Resident Student: Francesc Lordan

Resident Student: Vinoth Krishnan

Resident Student: Jan Ciesko

Resident Student: Judit Planas

Resident Student: Maja Etinski

Resident Student: Pieter Bellens

Resident Student: Rahul Gayatri

Resident Student: Roger Rafanell Mas

Resident Student: Vladimir Marjanovic

Associate Resident Student: Enric Tejedor

Research Support Engineer: Lluís Martinell

Visitor: Vanessa Ramírez

HPC Europa Visitor: Annika Schiller

Heterogeneous Architectures

Heterogeneous Architectures Group Manager: **Álex Ramírez**

Senior Researcher: Yoav Etsion

Researcher: Miquel Pericas

Associate Researcher: Carlos Alvarez

Associate Researcher: Carlos Villavieja

Associate Researcher: Esther Salami

Associate Researcher: Friman Sánchez

Associate Researcher: Mauricio Alvarez

Associate Researcher: Roberto Hexsel

Resident Student: Antonio Quesada

Resident Student: Fahimed Yazdanpanah

Resident Student: Alejandro Rico

Resident Student: Augusto Vega

Resident Student: Branimir Dickov

Resident Student: Felipe Cabarcas

Resident Student: Karthikeyan Palavedu

Resident Student: Milan Pavlovic

Resident Student: Muhammad Shafiq

Resident Student: Tassadaq Hussain

Associate Research Support Engineer: Paul Carpenter

Visitor: Luis Hernando

HPC Europa Visitor: Ozcan Ozturk

Network Processors

Network Processors Group Manager: **Mario Nemirovsky**

Associate Researcher: Alejandro Pajuelo

Associate Researcher: Javier Verdú

Resident Student: Mauro Pisano

Resident Student: Ruken Zilan

Visitor: Daniele Busin

Operating System / Computer Architecture Interface

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

Senior Researcher: Eduardo Quiñones

Senior Researcher: Jaime Abella

Researcher: Roberto Gioiosa

Resident Student: Qixiao Liu

Resident Student: Alessandro Morari

Resident Student: Bojan Maric

Resident Student: Vivek Sabbineni

Resident Student: José Carlos Ruiz

Resident Student: Kamil Kedzierski

Resident Student: Leonidas Kosmidis

Resident Student: Marco Paolieri

Resident Student: Muhammad Ismail

Resident Student: Petar Radojkovic

Resident Student: Roberta Piscitelli

Resident Student: Víctor Javier Jiménez

Resident Student: Vladimir Cakarevic

Associate Resident Student: Miquel Moreto

Visitor: Emery Berger

Programming Models

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

Senior Researcher: Gabor Janos

Senior Researcher: Alejandro Durán

Researcher: Roger Ferrer

Researcher: Xavier Teruel

Associate Researcher: Daniel Jiménez

Associate Researcher: Isaac Gelado

Associate Researcher: Juan José Costa

Associate Researcher: Marc González

Associate Researcher: Marisa Gil

Associate Researcher: Montserrat Farreras

Associate Researcher: Nacho Navarro

Resident Student: Diego Luis Caballero De Gea

Resident Student: Bastien Frank

Resident Student: Cecilia González

Resident Student: Daniel Cabrera

Resident Student: Javier Bueno

Resident Student: Javier Cabezas

Resident Student: Lluç Alvarez

Resident Student: Lluís Vilanova

Resident Student: Michail Alvanos

Resident Student: Nikola Vujic

Resident Student: Ramon Bertran

Resident Student: Sara Royuela

Resident Student: Víctor García

Visitor: Carlo Bertolli

Visitor: Ioanna Tsalouchidou

HPC Europa Visitor: Matteo Comin

Performance Tools

Performance Tools Group Manager: **Judit Giménez**

Senior Researcher: José Carlos Sancho Pitarch

Senior Researcher: Kevin Huck

Research Manager Prace: Ramnath Sai Sagar Thumbavanam Padmanabh

Researcher: Eloy Martínez

Researcher: Francisco Javier Pegenaute

Researcher: Germán Rodríguez

Researcher: Germán Llorc

Researcher: Harald Servat

Researcher: Pedro Antonio González

Associate Researcher: Xavier Andrade

Resident Student: Ana Jokanovic

Resident Student: Oscar Amorós

Resident Student: Víctor López

Resident Student: Vladimir Subotic

Technical Support Res Project: Juan González

HPC Europa Visitor: Cristian Grozea

Storage Systems

Storage Systems Group Manager: **Toni Cortés**

Researcher: Ernest Artiaga

Researcher: Jacobo Giralt

Researcher: Jan Wiberg

Researcher: Jonathan Martí

Researcher: Juan González De Benito

Researcher: Ramon Nou Castell

Researcher: Thanos Makatos

Junior Researcher: Paul Hermann Lensing

Junior Researcher: Matthias Werner Brugger

Resident Student: Albert Miranda

Resident Student: Kousik Dheena

Earth Sciences Department

Earth Sciences Director: **José María Baldasano**

Senior Researcher: Arnau Folch

Researcher: Matthias Piot

Associate Researcher: Carlos Pérez

Associate Researcher: Enric Terradellas

Associate Researcher: Maria Goncalves

Associate Researcher: Pedro Jiménez

Resident Student: M del Mar Martínez

Resident Student: Simone Marras

Research Support Engineer: Albert Soret

Research Support Engineer: David Carrio

Air Quality

Air Quality Group Manager: **Santiago Gassó**

Researcher: Elies Campmany i Pons

Researcher: Valentina Sicardi

Resident Student: Gina Ferrer

Resident Student: Kasja Witlox

Resident Student: M Teresa Pay

Resident Student: Regina Margarita Isern

Resident Student: Yenny González

Research Support Engineer: Cristina Niubó

Research Support Engineer: Francesc Martínez

Research Support Engineer: Francesco Benincasa

Research Support Engineer: Joana Aina Ortiz

Research Support Engineer: Luca Telloli

Research Support Engineer: Marc Guevara

Technical Project Support: Laura González

Technical Support: Kim Serradell

Visitor: Sylvain Mailler

Climate Change

Senior Researcher: **Maria Val**

Metereological Modelling

Metereological Modelling Group Manager: **Oriol Jorba**

Resident Student: Alba Badia

Resident Student: Michele Spada

HPC Europa Visitor: Mathias Ritter

Mineral Dust

Resident Student: Angel Alberto Rincón

Resident Student: Karsten Haustein

Resident Student: Sara Basart

HPC Europa Visitor: Italo Epicoco

HPC Europa Visitor: Silvia Mocavero

Life Sciences Department

Life Sciences Director: **Modesto Orozco**

Computational Genomics

Computational Genomics Group Manager: **David Torrents**

Senior Researcher: Bárbara Montserrat

Senior Researcher: Josep Maria Mercader

Researcher: Xavier Pastor

Junior Researcher: Santiago González

Resident Student: Elisa Duran

Resident Student: Leyden Fernández

Research Support Engineer: Montserrat Puiggrós

Research Support Engineer: Valentí Moncunill

Electronic and Atomic Protein Modelling

Electronic and Atomic Protein Modelling Group Manager: **Víctor Guallar**

Senior Researcher: Armin Madadkar

Researcher: Marcelo Puiatti

Researcher: Benjamin Philip Cossins

Researcher: Diego Fernando Masone

Researcher: Frank Heinrich

Researcher: Israel Cabeza de Vaca

Researcher: María de Fátima Assunção Lucas

Researcher: Suwipa Saen Oon

Resident Student: Evangelos Daskalakis

Resident Student: Max Von Vopelius

Resident Student: Ryoji Takahashi

Resident Student: Seyed Ali Hoseini

Resident Student: Víctor Alejandro Gil Sepúlveda

Research Support Engineer: Manuel Augusto Rivero

Visitor: Arturo Saliva

Visitor: James Valdés

INB-Computational Node 2

INB-Computational Node Group Manager: **Josep Lluís Gelpí**

Researcher: Dmitri Reptchevski

Researcher: Laia Codo Tarraubella

Resident Student: Alexis Torrano

Research Support Engineer: Jordi Camps

Research Support Engineer: Romina Royo

Molecular Modelling and Bioinformatics

Molecular Modelling and Bioinformatics Group Manager:
Modesto Orozco

Senior Researcher: Josep Ramon Goñi

Researcher::Alberto Pérez

Resident Student:Antonella Paladino

Resident Student: Ozgen Deniz

Research Support Engineer: Pau Andrio

Visitor: Kenneth Merz

Protein Interactions and Docking

Protein Interactions and Docking Group Manager:
Juan Fernández

Junior Researcher::Athi Narayanan

Resident Student:Albert Solernou

Resident Student: Brian Jiménez

Resident Student: Chiara Pallara

Resident Student: Laura Pérez

Resident Student: Mathias Pfeifer

Resident Student: Miguel Romero

Resident Student: Solène Grosdidier

Resident Student: Xavier Lucas Cabré

Research Support Engineer:Carles Pons

Visitor: Ida Fardi

Visitor: Jawon Song

Visitor: Jordi Triguero

Visitor: Samuel Flores

HPC Europa Visitor: Lykourgos Chinadis

Computer Applications in Science & Engineering Department

Computer Applications in e-Science and Engineering
Director: **José María Cela**

Associate Researcher: Carles Serrat

High Performance Computational Mechanics

High Performance Computational Mechanics Group
Manager: **Mariano Vázquez**

Senior Researcher:Alejandro Soba

Senior Researcher: Mauricio Gaspar Hanzich

Senior Researcher: Rogeli Grima

Researcher: Margarida Moragues

Researcher: Georg Huhs

Researcher: Hadrien Calmet

Researcher: Josep Fèlix Rubio

Researcher: Romain Mathieu Aubry

Researcher: Ruth Aris

Researcher: Xavier Rubio

Resident Student: Chiara Scaini

Resident Student: Cristina Montañola

Resident Student: Oscar Francisco Peredo

Resident Student: Pierre Lafortune

Visitor: Paula Villar

Visitor: Sujith Visalam Sukumaran

HPC Europa Visitor: Donald Taylor

HPC Europa Visitor: Felipe Cruz

HPC Europa Visitor: Rhodri Bevan

Physical and Numerical Modelling

Physical and Numerical Modelling Group Manager:
Guillaume Houzeaux

Senior Researcher:Angel Heriberto Coppola

Senior Researcher: José de La Puente Alvarez

Researcher:Albert Farrés

Researcher:Anne-Cécile Lesage

Researcher: Edgar Alejandro Bea

Researcher: Mauricio Andrés Araya

Researcher: Miquel Català

Researcher: Mohammed Jowkar

Researcher: Raúl De La Cruz

Researcher: Tano Varadinov

Researcher: Xavier Saez

Junior Researcher: Natalia Gutiérrez

Resident Student:Ane Beatriz Eguzkitza

Resident Student: Cristóbal Augusto Samaniego

Resident Student: Jelena Koldan

Visitor: Chantal Pic

Visitor: Benoit Ozell

Operations Department

Operations Director: **Sergi Girona**

Linux/ Unix Administrator: Guillermo Aguirre de Cárcer

Linux/Unix Administrator: Gabriele Carteni

Technical Res Project : Montserrat González

System Administration

Systems Group Manager: **Javier Bartolomé**

Helpdesk:Antonio Espinar

Helpdesk: Pedro Gómez

Helpdesk: Ferran Sellés

Network Administrator:Albert Benet

Performance Technician:Alejandro Lucero

Security And Networks: Juan Carlos Sánchez

System Administration: Carles Fenoy

System Administration: David Ocaña

System Administration: Jordi Valls

System Administration: Sergi Moré

User Support

User Support Group Manager: **David Vicente**

Support And Application Consultant: Jorge Rodríguez

User Support: Christian Simarro

User Support: Jorge Alberto Naranjo

User Support: Xavier Abellán

Visualitzation Technician: Carlos Tripiana

Web Graphic Designer: Jasmina Tomic

Web Graphic Designer:Valeria Azuriz

Webmaster: Nuria Montoya

Webmaster: Silvina Rusinek

Visitor Movilidad Española: Iñaki Silanes

Visitor Movilidad Española (ICTS): Raquel Alvarez

Facility Management

Facility Management Group Manager: **Ahmet Senata**

Maintenance Assistant:Albert Riera

Management Department

Management Director: **Ernest Quingles**

Finance and Business Administration

Administration, Finance and Human Resources Group

Manager: **Mercè Calvet**

Account Officer: M Cristina Calonge

Finance Assistant: Judit Soldevila

General Assistant: Gloria Alvarez

General Assistant: Laura Gutiérrez

General Assistant: Neus Jiménez

General Assistant: Núria Sirvent

Human Resources Officer:Ana Isabel Martín

Human Resources Officer: Lara Cejudo

Information System Developer:Toni Matas

Purchase Officer: Cristina Vargas

Purchase Officer: Elena Miró

Sap Technician: Rubén Ortiz

Technical Support For Economic Management Project:
Marina Utges

Travel Administrative Student:Aurora Rodríguez

Marketing and Communication

Communications Officer: María José Barroso

Communications Officer: Sara Ibáñez

ECRI Organisation Officer: Eva Comino

ECRI Organisation Officer: Ruth Pina

Marenostrum Visitors Manager: Oriol Riu

Marketing Assistant: Sonia Castel

Marketing Executive: Renata Giménez

Project Management

Research Project Group Manager: **Eugene Griffiths**

Research Project Manager:Anais González

Research Project Manager: Gina Alioto

Research Project Manager: Guadalupe Moreno

Research Project Manager: Pilar Callau

Research Project Manager: Maria Carreras

Research Project Manager: Marta Rosselló

Research Project Manager: Nuria Nadal

The financial accounts for 2010 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 2010 was composed of ordinary income derived from contributions by its patrons, as well as project income derived from competitive funding sources and agreements reached with private organisations. This income was then employed to cover expenses, including costs of operations and fulfilment of all financial obligations.

Income

The Consortium income of €15.939.527 recognised for fiscal year 2010 was derived from public administration contributions from the Ministry of Science and Innovation (MICINN), Generalitat de Catalunya (GdC) and European Commission (EC), as well as from agreements, contracts or other collaborative agreements with private organisations. Furthermore, the consolidated budget of the BSC-CNS included the assignment of internal resources carried over from the previous year's provisions.

INCOME	AMOUNT €
Ordinary Income	6.746.969
Ministerio de Ciencia e Innovación	4.335.320
Generalitat de Catalunya	2.411.649
Competitive Income	4.040.331
Ministerio de Ciencia e Innovación	804.086
Generalitat de Catalunya	254.245
European Commission	1.577.587
Private Companies	1.404.413
Other Income	7.704.873
Applied Previous Preserves	2.552.646
Strategic Investment	3.327.330
Overheads/Capital Transfers	1.824.897
TOTAL INCOME	18.492.173

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.

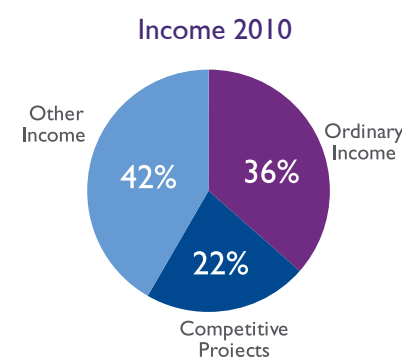
We not include as income for the period the advance competitive project funds receipt for future multi-year programs that are progressively applied over the lifetime of each project.

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.

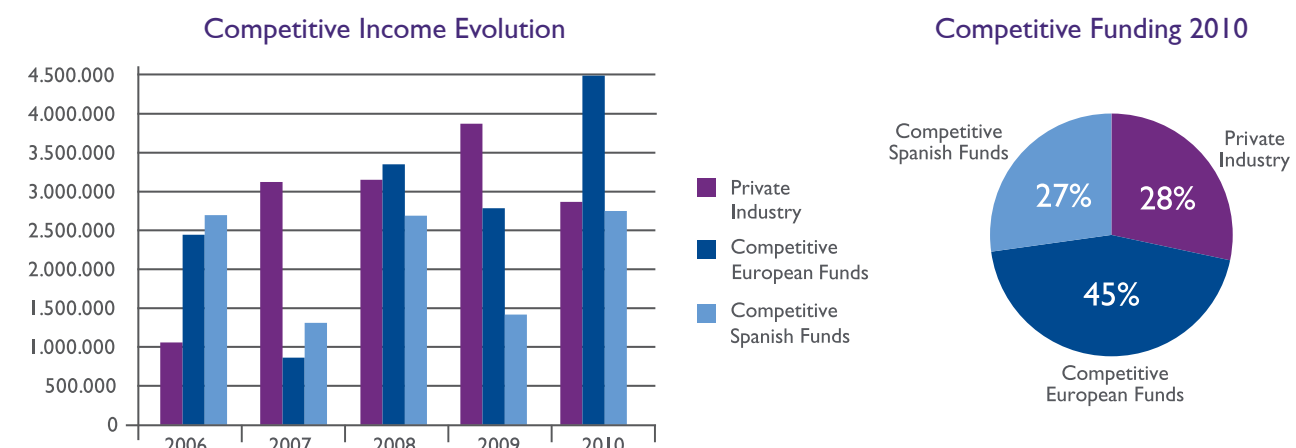
Overheads are incomes derived from ordinary projects, which according to the norms of the BSC/CNS are charged 10% to cover overhead expenses.

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

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



Expenses

The expenses of the BSC-CNS Consortium in the fiscal year 2010 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	4.384.366	3.762.544	8.146.909
Investments	3.973.237	136.179	4.109.417
Current Expenses	3.194.771	3.041.076	6.235.847
TOTAL EXPENSES	11.552.374	6.939.798	18.492.173

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.

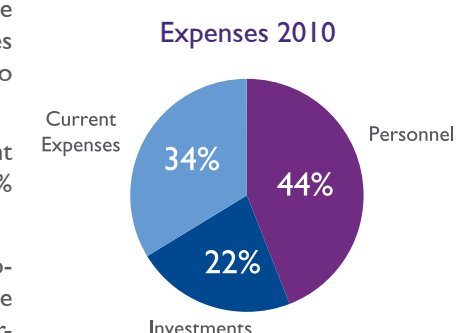
There was high growth of the center's staff related to the activity of current projects. The increase in personnel costs funded by project budget was 46% over the previous year.

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

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

In 2010, the BSC-CNS invited 10 public calls in order to accept 4 supply tenders, 5 services tenders and 1 works tender. 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. The works tender was held for the launching of the preparatory work for the land and demolition of UPC buildings, in order to start the construction of the new building of the BSC-CNS.

The BSC-CNS was the local organiser of the 6th European Conference on Research Infrastructures, ECRI2010, incurring costs to cover lodging and catering for the event. The funding granted for organising this conference was a total amount of 525,000€ by the MICINN and 170.000€ by the EC.



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 2010 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.

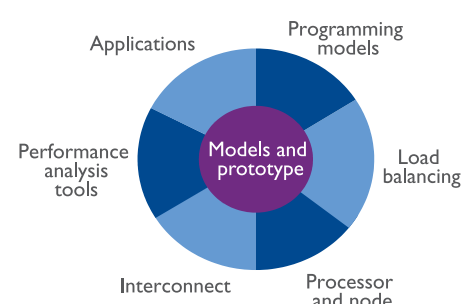
Joint collaborations with private industry are undertaken at both the system level, via direct collaborations with industry leaders such as IBM and Microsoft, and at the application level, where a significant research effort is dedicated to providing supercomputing based models for solving engineering problems in industrial sectors such as aerospace, transport, energy, medicine, geology, etc.

IBM MareIncognito



MareIncognito is a bilateral IBM-BSC research project to define the hardware and software components for the new generations of Petascale supercomputers, under the umbrella of a memorandum of understanding, led by Mateo Valero and Jesús Labarta. It encompasses research in several fields related to supercomputing, including: application porting and novel numerical methods, programming models and their runtime implementation, performance analysis and prediction tools, resource management layers, interconnection networks, and memory and processor architecture for novel multicore-based architectures. During 2010, the Project has been redefined in three major research areas: architecture, performance and workflows. A set of SOWs for specific work within each research area have been defined, and plan to start during 2011.

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 and Adrián Cristal, 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 presence of many- and multi-core processor computing architectures has made it possible to deliver enormous computational 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 are teamed up with computer scientists at Microsoft Research Cambridge (in the United Kingdom) and Redmond (in the United States) 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. Fundamental and applied research is being conducted in the following main topics: hardware/software transactional memory, runtime systems to support dataflow paradigms in novel architectures, OS/architectural support for managed programming languages and vector architectures for low-power media devices.

Nvidia-BSC CUDA Research Center



The BSC-CNS has been named by NVIDIA as a 2010 CUDA Research Center, the first one in Spain. The CUDA Research Center Program recognizes and fosters collaboration with research groups at universities and research institutes that are expanding the frontier of massively parallel computing. The Center, lead by Prof. Nacho Navarro, recognizes BSC-CNS's broad-based research success in leveraging the NVIDIA CUDA technology and GPU computing, both in major research initiatives such as Global Memory for Accelerators (GMAC) and in projects dealing with the optimisation of applications, such as Reverse Time Migration (RTM). The CUDA Research Center also recognises BSC's efforts in CUDA education, highlighted by means of the 2010 Summer School, “Programming and tuning Massively Parallel Systems (PUMPS),” offered in July on the Barcelona university campus. The event was co-sponsored by the University of Illinois, the HiPEAC NOE and NVIDIA, with distinguished faculty members Dr. David B. Kirk of NVIDIA and Prof. Wen-mei Hwu of the University of Illinois. PUMPS attracted more than 100 attendees from throughout the EU and beyond, from beginners to advanced faculty. The Center will promote the training in programming languages like CUDA, OpenCL, OpenMP, and StarSs, and the efficient optimisation of runtime environments and numerical methods.



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.



ITER Project

Goal: to provide computational resources, including 1 Million CPU-hours in MareNostrum, to ITER, the EU's hydrogen fusion reactor project.



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 characterisation 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 km² and 1 hour.



PRACE - Partnership for Advanced Computing in Europe



Background

The Partnership for Advanced Computing in Europe (PRACE) is a pan-European Research Infrastructure for High Performance Computing (HPC) and forms the top level of the European HPC ecosystem. The infrastructure consists of various tier-0 supercomputers distributed across the continent, with a centralised organisation which plans deployment and manages access to the computational resources. Through PRACE, European scientists and technologists are being provided with world-class supercomputers with capabilities comparable to those

available in the USA and Japan. These leadership class systems will help the continent's scientists and engineers to remain internationally competitive.

In June 2010, The PRACE Research Infrastructure was inaugurated at a ceremony held in Barcelona involving EC Deputy Director General Zoran Stancic and representatives of 20 nations (see map below). This ceremony was the culmination of many years work to create a distributed European supercomputing research infrastructure. Commission Vice-President for the Digital Agenda Neelie Kroes said: "I warmly welcome the launch of the PRACE supercomputer infrastructure as scientific computing is a key driver for the development of modern science and technology and for addressing the major challenges of our time like climate change, energy saving and the ageing population." The PRACE Research Infrastructure was created as an International Association (AISBL) with its headquarters in Brussels. In parallel, from June 2010 the PRACE First Implementation Phase Project continued providing support for the PRACE Research Infrastructure with the financial support of the EU's 7th Framework Programme.

A world class HPC Infrastructure has two unique characteristics which set it apart from other research infrastructures: it serves all scientific disciplines, and it needs to be continually upgraded in order to ensure global leadership. Four

Partners are responsible for hosting the PRACE supercomputers; these partners are Germany, France, Spain and Italy. At the end of 2010 the PRACE Research Infrastructure was operating with two of its Tier-0 nodes active (Germany and France). Spain and Italy will be deploying their systems in the next two-three years, and an aggressive upgrade program has been set by which each hosting partner will renew its resources on a 3-4 year cycle. The four Hosting Members have agreed to provide a sum total of 400 million Euros over the next 5 years for the PRACE Research Infrastructure. This funding will be complemented by up to 70 million Euros from the European Commission as well as contributions from the 16 Non Hosting Partners.



BSC-CNS and PRACE

The BSC-CNS played a key role in the creation of the PRACE Research Infrastructure at all levels, with Sergi Girona serving as Chairman of the Board of Directors, significant technical contributions, and leading the organisational design. This included the selection of the best legal form, the design of the governance structure, the funding and usage model, and the peer review process, resulting in the PRACE statutes and initial agreement which were signed in May 2010.

The BSC-CNS also designed, commissioned and constructed the Maricel prototype for PRACE. This machine uses the IBM Cell/B.E. architecture, has 1344 cores and a peak performance of more than 10 TFlops. In 2010 Maricel was used for performance analysis for various applications, and to develop the CellSs programming language (under the StarSs programming model). The BSC-CNS contributed to the development of the operation services that will be used in the PRACE Research Infrastructure for interconnecting and managing the different supercomputing nodes. The BSC was an active participant in STRATOS in 2010, the PRACE Advisory Group for strategic technologies, which involved more than 80 HPC stakeholders including vendors and academia. Extensive dissemination and training activities were also carried out by the BSC-CNS, including the organisation of the PRACE Autumn School.



In 2010, site preparations commenced for the construction of the new BSC-CNS building, which is scheduled to complete in 2013.



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. The new building 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 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 2013.

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



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 computer technology offers and application requirements, usually in collaboration with manufacturers.

Overview

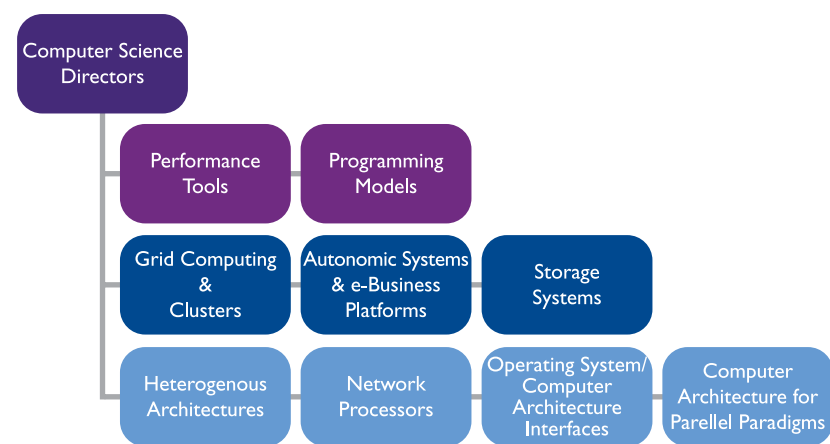
The Computer Sciences Department, led by Jesús Labarta and Eduard Ayguadé, is structured in 9 research Groups. Although each Group has its own specialised lines of research and unique projects, the teams often come together to collaborate on larger projects that require vertical integration, such as 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

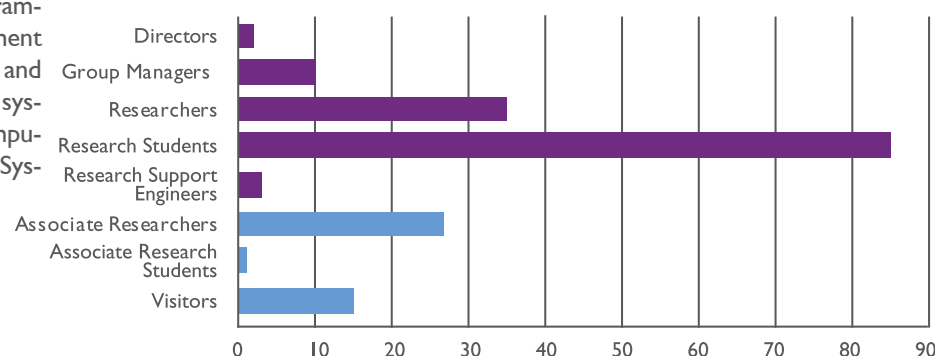
The combination of broad coverage of all facets of computer systems design and programming along with in-depth expertise in each area are somewhat unique amongst supercomputing centres. This unique strength of the BSC-CNS has attracted leading computing companies such as IBM and Microsoft to invest heavily in collaborative systems design R&D projects despite the relative youth of the Centre.

Organisational Structure

During 2010, some 135 staff and students, and further 43 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 programming and optimising 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).



Computer Science Department Staff & Collaborators 2010

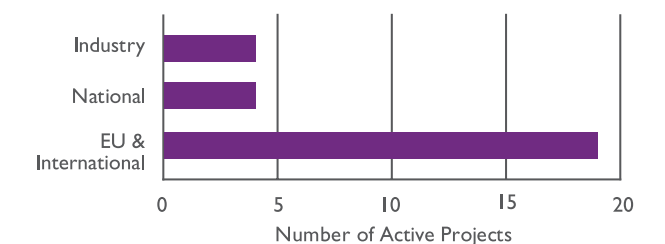


Key Projects & Networks

During 2010, the Computer Sciences Department participated in the following projects:

- ▶ 2 IST FP6 projects (SARC and XtreamOS) and 13 FP7 projects (EnCORE, IOlanes, IS-ENES, MERASA, OGF-Europe, OPTIMIS, PROARTIS, ScalaLife, SIENA, TERAFLUX, TEXT, VENUS-C and Velox);
- ▶ 2 networks of excellence (HiPEAC, and HPC-Europa);
- ▶ The SCALUS Marie Curie Initial Training network;
- ▶ The CUDA Research Center nominated by NVIDIA in 2010, which recognizes and fosters collaboration with research groups at universities and research institutes that are expanding the frontier of massively parallel computing;
- ▶ The IESP (International Exascale Software Project) and EESI (European Exascale Software Initiative);
- ▶ 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 through the MareIncognito project, Microsoft and Cisco Systems);
- ▶ The Spanish Consolider program "Supercomputing and eScience", coordinating the Basic Research in Supercomputing workpackage and the Plan Avanza2 NUBA project.

Computer Science Projects 2010



Scientific Output

Impacting the Future of Computing

In collaboration with market leaders such as IBM, Microsoft and Cisco Systems, as well as other international computing centres and standardisation efforts, the researchers of the Computer Sciences Department are involved in a range of projects covering the full spectrum of next generation computer design, from novel processor and multicore (homogeneous and heterogeneous) architectures, architectural support to the software stack (e.g. 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 2010

Publishing	
Journal Articles	25
Book Chapters	4
Conference Presentations	
International	66
National	2
Workshops	
Workshops	22
Education	
Theses Read	4

Heterogeneous Architectures Led by Alex Ramírez, this Group, in close interaction with the Programming Models Group, aims to design and evaluate the next generation of HPC systems based on heterogeneous components with a dual purpose: first, to develop the most energy efficient supercomputers; second, to focus the developments on the actual needs of the applications and the runtime system, and anticipate the needs of the runtime system for future architectures so that software can be ready when research trends become products. During 2010 the Group continued



its participation in a number of projects (SARC, MareIncognito, ENCORE and TERAFLUX) 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 (www.bscmsrc.eu) which focuses its research on lowering the programmability wall raised by new multicore architectures; research areas include Transactional Memory, hardware support for programming language runtimes and synchronization. During 2010, the Group added low-power vector processors to its core research area and explored the use of Transactional Memory for other research domains, such as reliability. In addition the Group participated in and coordinated the European VELOX project which ended in December 2010.



Operating System / Computer Architecture Interface Led by Francisco J. Cazorla, the Group focused on two main areas: hard real-time systems and operating systems for HPC systems. In the area of hard real-time systems two projects are the basis for the research activities in the area of multicore hard real-time architectures (MERA-SA, finished at the end of 2010) and architectures with random timing behaviour for hard-real time systems (PROARTIS, started in 2010). In



the area of operating systems for HPC, the research is conducted in collaboration with IBM. The Group also participated in the HiPEAC and ARTIST networks of excellence. New research activities in the area of fault-tolerant and energy-efficient hard real-time architectures were started during 2010.

Network Processors Led by Mario Nemirovsky, the Group is conducting research on the massive multithreaded architectures focused on network applications. Networks and their applications are a fundamental part of the Internet from its core to its edge. Additionally, the Network and its applications play a critical role in today's data centres and High Performance Systems (HPS). In these two directions, the Network Group concentrates in the study of these systems and the definition of new network architectures. During 2010 the Group was involved in research collaboration with Cisco Systems investigating analytical models to overcome the problems of simulating different realistic network processing scenarios.



Programming Models Led by Xavier Martorell, the Group explores new programming models and their efficient implementation for current and future architectures, ranging from multicore SMP architectures with support for accelerators (GPUs, FPGAs, ...) to clusters of SMPs, and exascale systems. This exploration is supported with the development of powerful compiler (Mercurium) and runtime (NANOS++) prototypes. In 2010, a big effort to join the programming models of OpenMP and StarSs (developed in the Grid Computing and Clusters Group) resulted in the joint OmpSs programming model that is currently the basis for future



developments and influencing standards, particularly in the framework of the joint BSC-IBM MareIncognito project. The Group also continued work on programming models for the cluster versions of OmpSs and NanosDSM, power modelling for multicore architectures and code transformations for processors with local memories. During 2010, the Group participated in several new EU projects (EnCORE, TERAFLUX and TEXT), and existing ones (HPC-Europa2 and SARC). The Group is coordinating the programming models cluster and applications taskforce in the HiPEAC2 Network of Excellence.

Performance Tools Led by Judit Giménez, the Group is working on the design of tools to instrument, analyze and predict the behaviour of parallel applications on parallel systems. The main goal of the Group is to provide technology to understand the issues that determine the actual performance of a parallel application or that contribute to its bottlenecks. This is extremely important both in novel homogeneous and heterogeneous multi-core architectures as well as in highly scalable cluster systems. During 2010 the activities of the Group focused on finishing the new Paraver GUI, extending the research modules (targeting automatic and on-line analysis and increasing detail level through sampling) and tools integration (including Eclipse and HPCST). The Group was also involved in ScalaLife, MareIncognito, DEISA2 and HPC-Europa2 projects.



Grid Computing & Clusters Led by Rosa M. Badia, this Group is researching new programming and execution models, and resource management for distributed computing. The team explores solutions in order to simplify application development, enable dynamic exploitation of parallelism at runtime and perform combined scheduling decisions at different levels. In this direction, the efforts of the Group have focussed in two projects: GRIDSS/COMPSs and SERA. In addition, the Group has participated in a number of EU projects (OPTIMIS, VENUS-C, SIENA, ScalaLife and IS-ENES), finished its participation in OGF-Europe and XtreamOS, and participated in the NUBA Spanish project. The Group has also continued the development of the StarSs programming model in cooperation with the Programming Models Group, specifically on the GPU and cluster versions of StarS, hybrid MPI/SMPs (TEXT EU project), support for array regions and transactional memory (TERAFLUX EU project) in SMPs.



Autonomic Systems and eBusiness Platforms Led by Jordi Torres, the 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 virtualised 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. In this scenario, the Group views the current workloads that must be handled are heterogeneous, including different types of jobs, not only CPU-intensive jobs, but also streaming, transactional, data-intensive, etc.



During 2010 the Group started two big EU projects, VENUS-C and OPTIMIS in the area of Cloud Computing. Also during 2010 the Group consolidated a new research line around workload management for MapReduce data analytics, including SLA management, resource management and energy consumption planning.

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 wide-area networks that solve the problems currently found (data location, replication and striping) and that will make these environments more efficient. In 2010 the Group focussed on three areas: file system scalability, Input/Output for wide-area systems, and file-system virtualisation. Within these, key efforts were the development understanding the data and metadata locality over long periods of time (more than 6 months), definition of policies to place data in large data centres merging randomized and deterministic approaches (work done as part of the SCALUS project), the application of COFS for composite file systems, using the advantages of multicore system to improve I/O within the IOlanes project, and a number of improvements in the XtreamOS project, in particular related to its file system XtreamFS.





José María Baldasano,
Director of the
Earth Sciences
Department

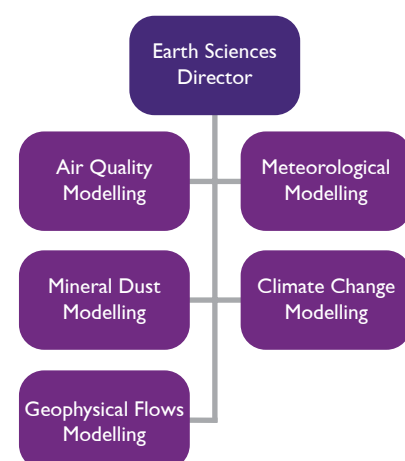
The Earth Sciences Department of the BSC-CNS has the aim of modelling and understanding the behaviour of the Earth System, focusing its research activities on atmospheric processes and climate change modelling.

Overview

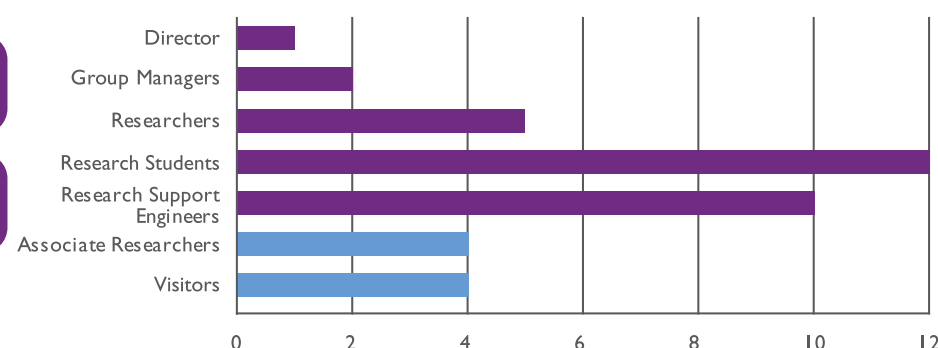
The high performance capabilities of MareNostrum enable the Earth Sciences Department to increase the spatial and temporal resolution of earth systems, in order to improve knowledge of dynamic patterns of air pollutants in complex terrains and interactions and feedbacks

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) under the umbrella of the CALIOPE project funded by the Spanish Ministry of the Environment; and mineral dust forecasts for the Euro-Mediterranean region and East Asia (www.bsc.es/projects/earthscience/DREAM). The Department also in collaboration with the World Meteorological Organization (WMO) and the Spanish Meteorological Agency (AEMet) have created the Regional Center for Sand and Dust Storm Warning System (SDS-WAS) covering Europe, northern Africa and the Middle-East. Other research activities involve the diagnosis of the behaviour of Earth System Modelling (ESFM) codes in a supercomputer framework and the improvement of parallel versions of atmospheric models to increase their horizontal and temporal resolution.

Organisational Structure



Earth Sciences Department Staff & Collaborators 2010



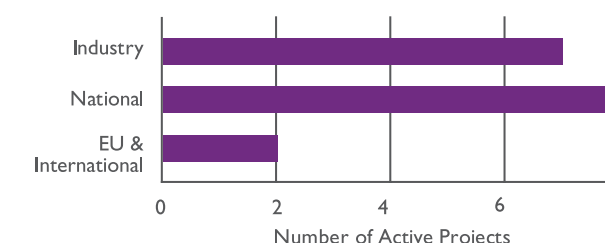
The Department is structured in five Groups that represent the main topics of Earth Sciences research: air quality modelling, mineral dust modelling, meteorological modelling, global and regional climate modelling and geophysical flows. These Groups are interrelated and work in a cooperative form. They 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 2010 some 38 staff, collaborators and visitors 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.

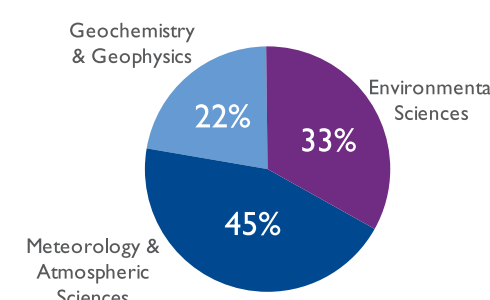
Earth Science Projects 2010



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 2010, such as the International Technical Meeting on Air Pollution and its Application supported by NATO, Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes; American Union Geophysical,

Journal Publications by Subject Category 2010



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 2010, and considerable augmentation of the number of ISI-JCR publications (from 3 in 2007 to 8 in 2010). The JCR publications in 2010 have an average quality of 3,6 (Average JCR Science Edition Impact Factor) that suppose an augment with regard to 2008 (2,4) and 2009 (2,9) and were distributed over a number of subject categories, as can be seen in the chart.

Communication & Dissemination 2010

Publishing	
Journal Articles	12
Book Chapters	6
Conference Presentations	
International	33
National	3
Workshops	
Workshops	4
Education	
Theses Read	0

Air Quality

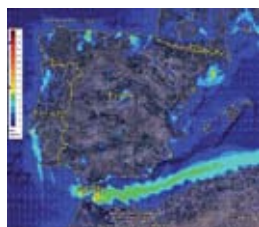


Figure 1 - Air quality modelling system (WRF-ARW/HERMES-EMEP/CMAQ/BSC-DREAM8b) forecast result for NO₂, visualized in Google Earth

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

In 2010 the activities of the Group 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, 1 hr) as well as to Europe (12 km x 12 km, 1 hr). 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 (taxis, 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 2010 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.

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 2010 the Group continued the development of the new on-line global/regional chemical weather prediction system (NMMB/BSC-CHEM) in collaboration with several research institutions (National Centers for Environmental Prediction, NASA Goddard Institute for Space Studies, International Research Institute for Climate and Society, and University of California, Irvine). All chemical processes are coupled on-line with the Nonhydrostatic Multiscale Meteorological Model on the

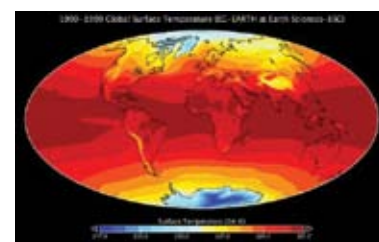


Figure 2 - Global surface temperature in 1990-1999 determined by EC-Earth v2.1

B grid (NMMB): anthropogenic and natural emissions, photolysis scheme, dry deposition, grid- and subgrid-scale wet deposition and the tropospheric chemical mechanism. Further developments are oriented to include the aerosol component within the chemistry. In the context of the CALIOPE project, the Group continues providing high-resolution meteorological forecasts as input for air quality modelling in the Barcelona area (1 km resolution), Andalusia region (2 km resolution), Canary Islands (2 km), Iberian Peninsula (4 km) and Europe (12 km). The model results are evaluated on a near-real time basis, and provide accurate information of the meteorological conditions over the regions of interest. Furthermore, such results were used to analyse and describe the main meteorological patterns that affected the Barcelona geographical area during the experimental campaign DAURE ("Determination of the sources of atmospheric Aerosols in Urban and Rural Environments in Spain") led by CSIC researchers.

The Group advances the exploration of new numerical techniques to better exploit massively parallel architectures for meteorological applications. The dry-atmosphere dynamical core tested provides successful results and the transport was implemented to allow the extension toward moist atmosphere cases.

Mineral Dust Modelling

The Mineral Dust Group provides daily operational forecasts of mineral dust for North Africa, Middle East, Europe and

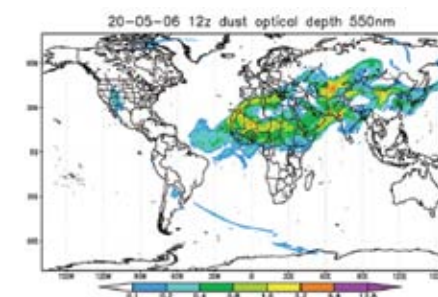


Figure 4 - First Simulations With the NMM/BSC-Dust Dust Modeling System on MareNostrum

East Asia based on the updated version of Dust Regional Atmospheric Model, BSC-DREAM8b. In 2010 the Group continued with the development of the new generation atmospheric mineral dust model (NMMb-BSC/Dust) coupled on-line to the new generation unified atmospheric model NMMb of the National Centers for Environmental Prediction (NCEP). The new modelling system is intended to be a powerful tool for research and to provide efficient global and regional chemical weather forecasts at sub-synoptic and mesoscale resolutions on MareNostrum supercomputer (Figure 4) including a physically-based dust emission scheme taking into account the effects of saltation and sandblasting, soil moisture and viscous diffusion close to the ground. 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, MétéoFrance, LISA, LSCE, IFT, EUMETSAT, CNR, AERONET/PHOTONS).

Geophysical Flows

The Geophysical Flows BSC-CNS Earth Science Department Group has worked on two main research areas, atmospheric dispersion of volcanic ash clouds and dispersion of pollutants at urban scale. The first line of research was of particular relevance as a consequence of the April-May 2010 Eyjafjallajökull volcano eruption in Iceland, which strongly disrupted the European air traffic when the ash clouds reached the continent. Scientific achievements from 3 research projects and a contract (see below) include:

- Operational implementation of the BSC-CNS FALL3D volcanic ash dispersal model at several institutions including the Buenos Aires Volcanic Ash Advisory Center (Argentina), Australian Geosciences International Facility for Disaster Reduction (Australia, Indonesia and Philippines), and members of the CENIZA international network (CYTED network 41ORT0392).
- Development and implementation of a volcanic ash wet aggregation model coupled with mesoscale weather forecasts furnishing atmospheric water contents.
- Ash cloud model validation using space-based remote sensing techniques based on TIR channel differences and ground-based instrumentation (EARLINET lidars, AERONET sun-photometers and ceilometers).
- Modelling of the Eyjafjallajökull volcano eruption in operational mode.
- Development and implementation in the ALYA code of a module for modelling atmospheric transport of passive substances. It includes a downscaling interpolator for the atmospheric boundary layer to furnish initial and boundary conditions from different mesoscale NWP models.

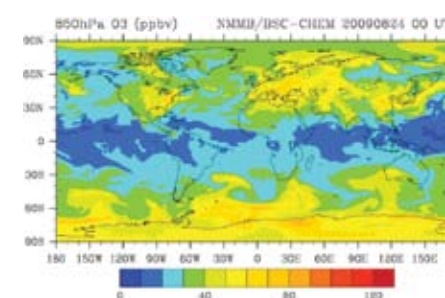


Figure 3 - NMMB/BSC-CHEM model results for ozone at 850 hPa

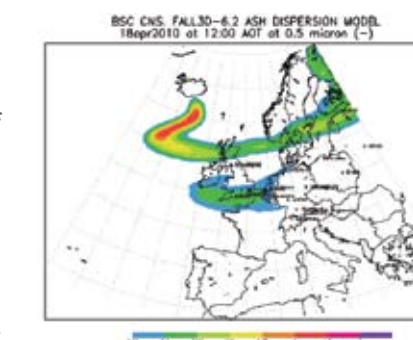


Figure 5 - simulation of the Eyjafjallajökull volcanic ash cloud aerosol optical depths. Results for 18 April 2010 at 12:00 UTC



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) 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

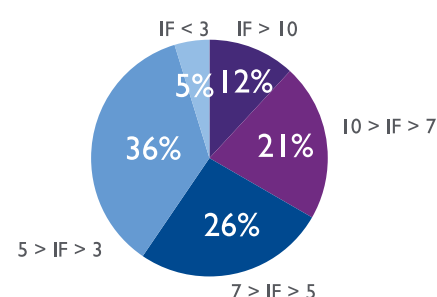


INSTITUTE
FOR RESEARCH
IN BIOMEDICINE

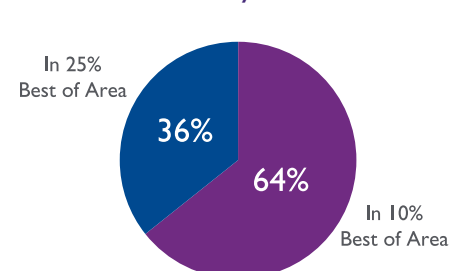
The Computational Biology Program was created as a joint venture between the BSC-CNS and the Institute for Research in Biomedicine (IRB Barcelona) with the mission to face the computational challenges in molecular biology. The Program coordinated by Modesto Orozco includes researchers from the Structural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

The group leaders involved in the Program are Victor Guallar (Electronic and Atomic Protein Modeling, BSC-CNS 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-CNS 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 €8.7M.

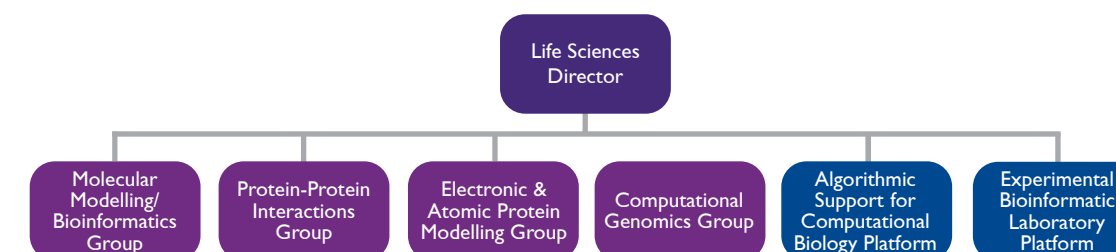
ISI Impact Factor of Articles
Published in 2010



Distribution of 2010 Scientific
Production by ISI IF Rank

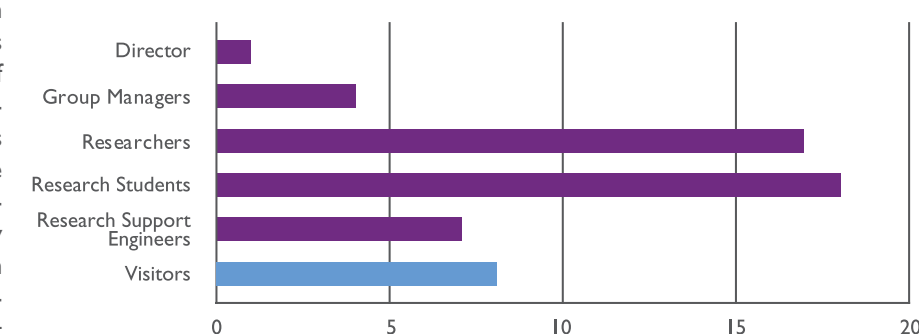


Organisational Structure



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 69 in 2008 to 79 in 2010, doubling in size since 2006.

Life Sciences Department Staff & Collaborators 2010

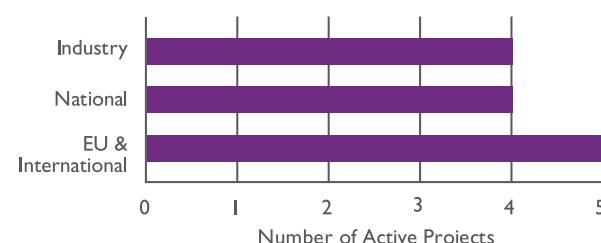


EU & National Projects

Key activities during 2010 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 – Construction and operation of a sustainable infrastructure for biological information in Europe to support life science research and its translation to medicine and the environment, the bio-industries and society. Funded by FP7.
- ▶ IMID-Kit - Development of a diagnostic kit for inflammatory diseases mediated by immune mechanisms. Funded by MICINN as a Singular Strategic Project.
- ▶ P.E.L.E (Protein Energy Landscape Exploration): a la carte drug design tools. ERC Advanced Grant
- ▶ Genetic Evolution in Vertebrates. Funded by CICYT, Spanish Government.
- ▶ Biochemical Modelling. Funded by CICYT, Spanish Government.
- ▶ Protein Docking Challenges. Funded by CICYT, Spanish Government.

Life Science Projects 2010



Scientific Output

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

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

Organised Events:

- ▶ ExaScale challenges in Computational Biology, Barcelona 2010.

Communication & Dissemination 2010	
Publishing	
Journal Articles	27
Book Chapters	1
Conference Presentations	
International	9
National	1
Workshops	
Workshops	0
Education	
Theses Read	1

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 characterisation of such complexes has enormous interest, both at an 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 optimisation 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 Atomic Protein Modeling Group

Led by Victor Guallar, the overall objective of this Group 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 2010 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.

INB Computational Bioinformatics Node Platform

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 who are assigned to the INB supported projects and help in the implementation and optimisation 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 creating and managing biological databases. During 2010 the ASU 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 2010 the Laboratory 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

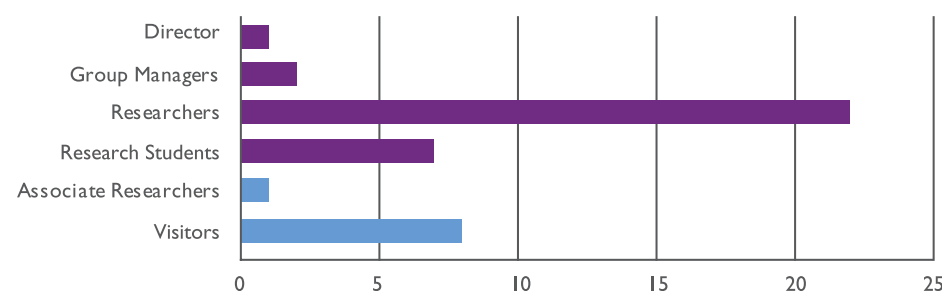
The applications developed by the CASE department are truly multidisciplinary, requiring depth of expertise in many fields. In order to successfully develop these applications, the skills of the CASE team in numerical methods and parallel programming must be complemented by experts in appropriate areas. 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 2010



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 2010, 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.
- ▶ W2PLASTICS: Magnetic Sorting and Ultrasound Sensor Technologies for Production of High Purity Secondary Polyolefins from Waste. Turbulent flow in complex geometries; particle tracing and collisions.
- ▶ 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.
- ▶ Scalable Parallel simulation for policy analysis.

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 designed 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, was 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.
- ▶ Cardiac simulation: Coupled electromechanical simulation of the heart. The project objective is to develop a simulator of the cardiac function considering the electrical activation potential and its coupling to the mechanical pumping action. Collaboration with UAB, Htal. St. Pau, Univ. Lleida, IMDEA Materiales.

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: FEF10 and ParCFD2010, SEG and EAGE conferences in Geophysics, International Conference on Mathematics and Continuum mechanics, as well as the International Conference on Computational & Mathematical Biomedical Engineering.

Case Projects 2010



Communication & Dissemination 2010

Publishing	
Journal Articles	12
Book Chapters	1
Conference Presentations	
International	15
National	0
Workshops	
Workshops	2
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:

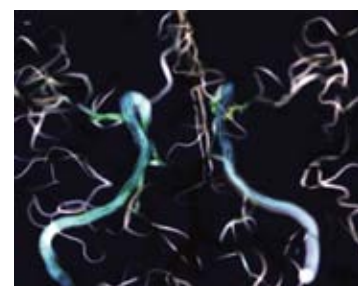
- ▶ Mathematical modelling of a given physical process.
- ▶ Numerical modelling of the mathematical equations - space and time discretisation: high order time integration schemes; variational multi-scale; finite element; domain decomposition (Chimera, non-overlapping meshes); turbulence models; PIC methods;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

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

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

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

Within these areas, in 2010 the PNM Group focused on the following activities:



Cerebral hemodynamics.

- ▶ Particle tracking: an immersed boundary condition for fluid-particle interactions.
- ▶ Particle collision: collision algorithm for particles of arbitrary shapes.
- ▶ A variational multiscale model for turbulent flows.
- ▶ Stabilisation algorithms for compressible flows for a wide range of Mach numbers.
- ▶ A Chimera method in Computational Mechanics: hole cutting and subdomain coupling via extension elements.
- ▶ Large-strain solid mechanics in the total Lagrangian formulation.



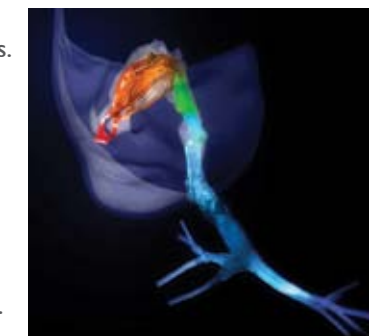
A Chimera method based on "Extension Elements".

High Performance Computational Mechanics (HPC)

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:

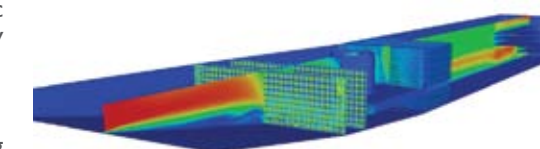
- ▶ Bio-mechanics: Hemodynamics, respiratory system air flow, cardiac simulations.
- ▶ Geophysics: seismic imaging and oil reservoir simulations.
- ▶ Plasma Physics.
- ▶ Atmospheric flows: mesoscale and urban environments.
- ▶ Energetically Efficient Building Design.
- ▶ Ab-initio DFT and TDDFT molecular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



Airflow in respiratory system.

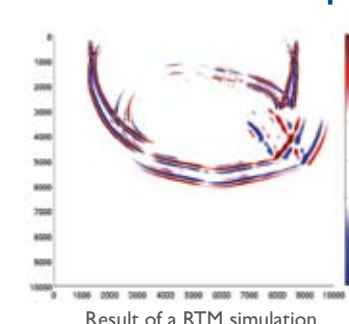
Within these fields, in 2010, the HPCM Group developed:

- ▶ 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 eigensolvers.
- ▶ Free surface parallel solver for sailing boats.



W2Plastics project: plastic separation device.

The Kaleidoscope Project: Seismic Imaging



Result of a RTM simulation.

The sediments below the deep and ultra-deep waters of the US Federal waters of the Gulf of Mexico shelter rich oil reserves, sometimes as much as 40,000 ft from the surface. Minerals Management Service (MMS), the federal agency in the U.S. Department of the Interior that manages the nation's oil, natural gas and other mineral resources on the outer continental shelf in federal offshore waters, estimates that the Gulf of Mexico holds 37 billion barrels of "undiscovered, conventionally recoverable" oil.

These reserves are very difficult to find and reach due to thick layers of salt that preclude the imaging and visualization of the oil-bearing sands underneath. The oil industry uses sophisticated technologies to locate and visualize these exploratory objectives. These technologies are computing intensive and the success to properly

"see underneath" depends largely on the power of the supercomputers used. It is remarkable that public benchmarks show that the Cell/BE Processors perform the computation of algorithms central to seismic imaging, 40 times faster than leading brand processors used in today's supercomputers. That increase in computer power makes feasible the application of imaging technologies that until today have been considered as a utopia in the oil industry, allowing more reliable exploration.

The Kaleidoscope Project seeks exploitation of Cell/BE unparalleled properties for the creation of the next generation seismic imaging technologies specifically tailored to the Processor for the visualization of the earth interior and the adaptation of existing imaging technologies used in oil exploration by exploiting the Cell/BE Processor unparalleled properties. The output from the Kaleidoscope Project will be faster tools, by several orders of magnitude, more reliable software to visualize below the thick layers of salt present in the Gulf of Mexico and therefore reducing significantly the exploration risks and making accessible oil reserves that otherwise would be invisible to the industry.

The Kaleidoscope Project is a "dream team" partnership of top geophysicists, computer scientists and organizations from around the world. It has been created by Repsol YPF, a Spanish integrated oil company with important assets in the US Gulf of Mexico, 3DGeo, a leader Houston-based imaging company formed by Stanford University professor and seismic imaging pioneer, Biondo Biondi, and the Barcelona Supercomputer Center (BSC-CNS). The BSC-CNS hosts the MareNostrum, powered by IBM, the third largest computer in Europe. 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 centers in the world developing libraries and codes for such processors.



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 on-line electronic applications, remote access, and porting of code; manage the environmental aspect of the BSC-CNS installations; manage the technical aspects of integration of the MareNostrum in the DEISA and European HPC

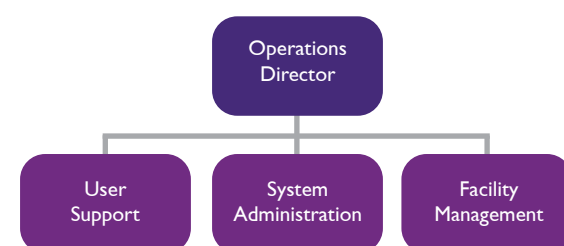
network grids; and ensure that RES staff receive appropriate training and skills development in order to be able to professionally carry out their duties in an environment of constant technological change and advancement.

Overview

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

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

Organisational Structure



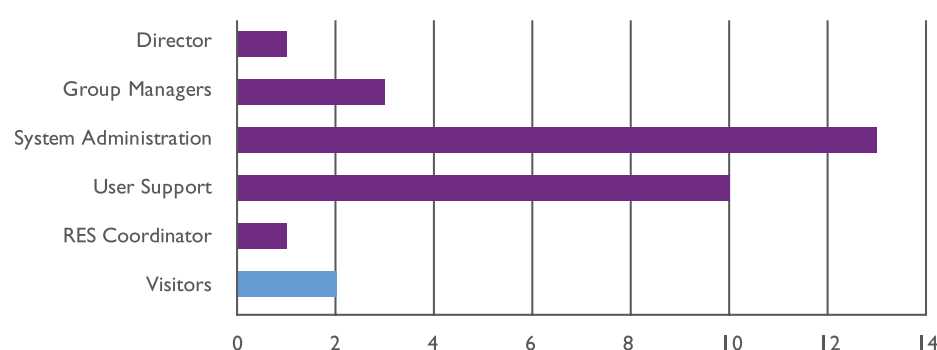
User Support is responsible for direct user support providing detailed knowledge of programming models, libraries, performance tools and applications, and also is responsible for management of the BSC website, and the management and support of 3D visualization equipment.

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

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

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

Operations Department Staff & Collaborators 2010



Key Projects

The Operations Department was involved in the following projects during 2010:

- ▶ RES (Red Española de Supercomputación): The Spanish Supercomputing Network offers coordinated HPC services to the Spanish scientific community. The Operations Department is responsible for the coordination of the network, including all support and administration services.
- ▶ DEISA2: the Distributed European Infrastructure for Supercomputing Applications is a consortium of leading national Supercomputing centres that aims to foster pan-European world-leading computational science research. The Operations Department is involved in most of the work packages, and coordinates the participation of the BSC-CNS in the project.
- ▶ PRACE PP : In the PRACE Preparation Phase, the Operations Department was involved in work packages WP4, WP5 and WP7.
- ▶ PRACE IIP: In the PRACE First Implementation Phase, the Operations Department is involved in WP6, WP7 and WP8, and coordinates the participation of the BSC-CNS in the project.
- ▶ HPC-EUROPA-2 : In the Pan-European Research Infrastructure on High Performance Computing, the Operations team is involved in work packages NA2 and JRA2, and coordinates the participation of the BSC-CNS in the project.
- ▶ HPC-WORLD: HPCW is a consortium of 6 key-players in High Performance Computing, all around the world, 5 Supercomputing Centers (CINECA, BSC, FZJ, SDSC and BlueFern) plus GENCI, the French national agency in charge of HPC coordination.
- ▶ EESI : The objective of this Support Action, co-funded by the European Commission, is to build a european vision and roadmap to address the challenges of the new generation of massively parallel systems composed of millions of heterogeneous cores which will provide multi-Petaflop performances in the next few years and Exaflop performances in 2020.

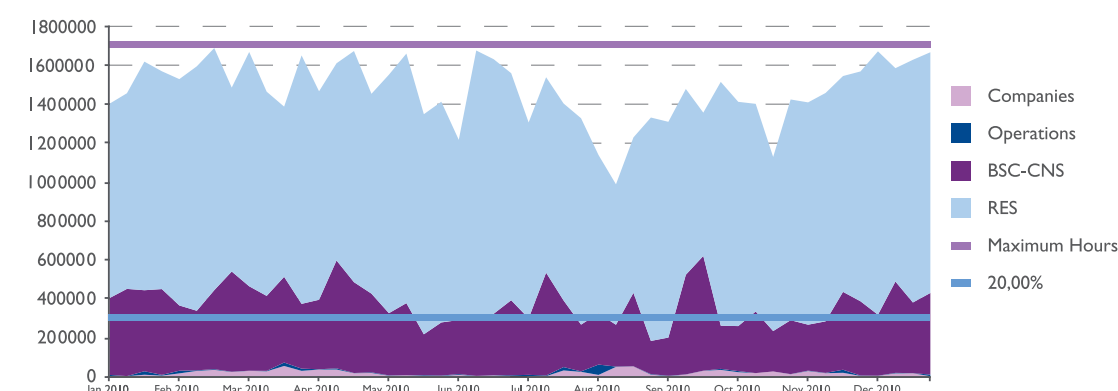
System Administration

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 2010

Weekly Use of the MareNostrum in 2010



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 85%. In addition to BSC-CNS internal groups, more than 279 external groups accessed to the MareNostrum system.

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

Training and Seminars

The Operations Department has been directly involved in the training program organised by the RES project during 2010. All the detailed information about the trainings scheduled is available in the RES section of this report.

HPC Storage Upgrade

BSC opened a tender to upgrade the MareNostrum storage system; the objective was not only a technological upgrade but a complete redesign of the original storage system. The most important change was the disassociation of the storage subsystem from the MareNostrum supercomputer. During recent years the BSC-CNS has increased the number and diversity of its HPC resources and so the need arose for a central disk to service them all. The new system addresses this need, and at the end of 2010 it was in the final stage of installation.

The new storage system will provide:

- ▶ 1.9 PB for user data storage
- ▶ 33.5 TB for metadata storage (inodes and internal filesystem data)
- ▶ Total aggregated performance of 15GB/s
- ▶ GPFS filesystems configured and optimized to be mounted on 3000 nodes



CNAG moved to production



In 2010 the Operations Department set up a production cluster and storage for the National Center for Genomic Analysis (Centro Nacional de Análisis Genómico, CNAG).

The production cluster consists of 104 R422E2 servers offering up to 832 cpus and 4.9 TB of memory with a peak performance of 9,52 TFlops in 2 racks. Each node includes a Xeon X5570 processor quad-core, 48 GB of DDR3 RAM memory, a 250 GB Hard Disk, 4 ethernet interfaces and 1 QDR Infiniband interface for MPI traffic.

The storage system offers up to 1 PB raw space composed of 600 2TB SATAII disks, and 29.5 TB for metadata storage in 66 SAS disks of 450 GB each. The parallel filesystem selected is Lustre, which is managed and served by 6 R423E2 servers.

Slurm was installed as the resource management system, configured with multiple queues and different priorities (according to CNAG production requirements).

An optimised transfer system was defined and implemented to move all sequencing information generated from the 13 sequencing machines to the central Lustre storage, so it can then be processed in the computing cluster. Several services, such as MySQL, have been installed for accessing all generated sequencing data.

The BSC-CNS is also providing remote backup service for CNAG data, and HPC user support and application enabling to optimise and parallelise CNAG applications.

User Support

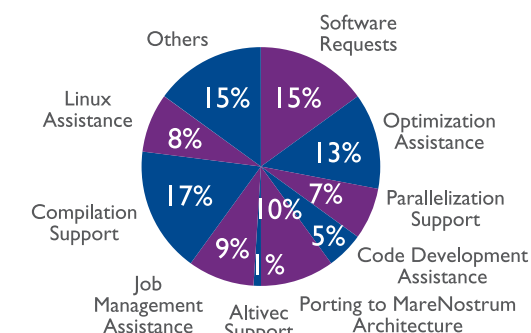
The User Support Group provides assistance with all aspects of scientific computing. This assistance includes general user support, code optimization and parallel model building support, and porting serial and parallel codes for supercomputers such as MareNostrum. The group is also involved in the creation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



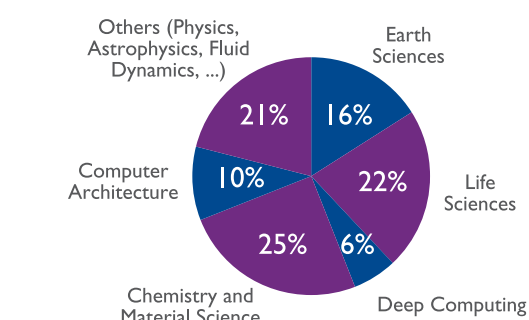
Support Requests in 2010

The number of support requests received in 2010 was 4643 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 2010



User Support Requested by Scientific Area 2010



3D visualisation system



A new powerful tool was built at the BSC-CNS in 2010; it is a VR-System configured like a stereo-wall and located in the foyer of the Chapel Building. The system is a stereoscopic visualisation device with a high-end BARCO projector which is able to project up to 120 Hz (60 frames per eye alternatively), giving professional-level 3D viewing. The image is projected over a big flat screen and viewers have to use active stereo glasses that are synchronised with the projector via infra-red emitters. The projection system is connected to a high-performance workstation which has stereoscopic native hardware.

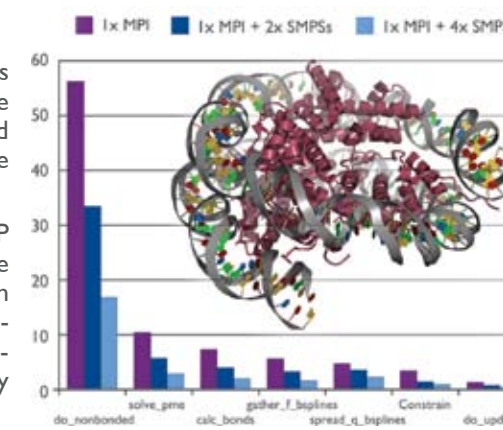
The VR-System was built with two main purposes, research and dissemination. Scientists will be provided specific software assistance in order to obtain a high quality visualisation from data resulting from MareNostrum simulations. For dissemination, researchers will be able to produce demonstrations of their results and disseminate their work to public audiences.

GROMACS optimization

In 2010 a hybrid parallelisation of a Molecular Dynamic Application was performed. GROMACS was chosen as this application is one of the most commonly used in Life Science HPC, and the one that consumed the most resources in MareNostrum during 2010. More than 7% of the hours granted by the Access Committee were used by GROMACS.

The parallelisation was constituted using the official MPI code plus SMP SuperScalar (programming model developed by the Computer Science Department at BSC-CNS). During the process, an intermediate version using OpenMP threads was developed and then the most intensive calculation parts of the code were ported to SMPs. With these improvements, the code is able to scale beyond 512 up to 2048 processors, by reducing the number of p2p and All-to-All communications.

This porting drove some interesting internal collaborations between Operations and Computer Science and helped strengthen relations with the GROMACS developers in Sweden. Part of the modifications are currently being analysed by the developers in order to include them in new releases of the code.



Facility Management

2010 Key Accomplishments

- ▶ Initiated planning and design of major projects such as MareIncognito*, Capacity expansion of MareNostrum*.
- ▶ Completed renovation and installation projects such as CNAG, 3D visualization system, refurbishment projects in Nexus I & Nexus II.
- ▶ Effectively completed over 233 work orders for maintenance.
- ▶ Updated and revised contracts for service suppliers to better reflect current business practices.
- ▶ Established a common folder which allows Facility Management and Administration departments to share documents.
- ▶ Developed detailed plans for the IT facilities of the new BSC-CNS building. Out of the total space, the IT installations will occupy an area of 1000 m², with a further 800 m² of related facilities.
- ▶ Revised systems to increase the number of racks in the Chapel, enabling racks with more power consumption, but maintaining or even improving the quality of the cooling system.





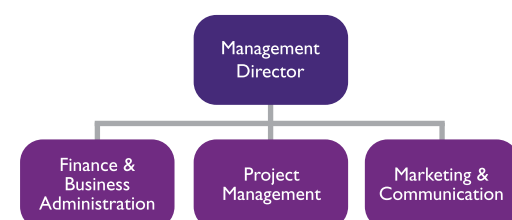
Ernest Quingles,
Management
Department
Director

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

Overview

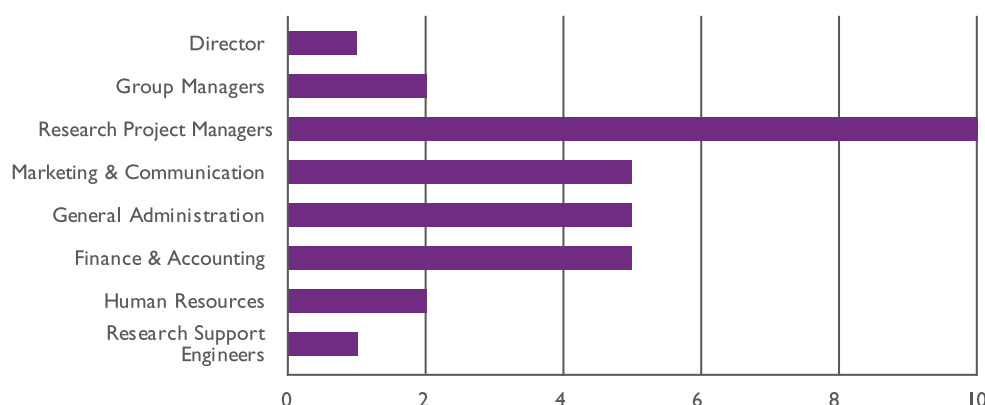
The Management Department, led by Ernest Quingles, aims to provide administrative and management services to all the other departments. It is responsible for the administration of finances, projects, human resources, communication and office management. Due to the continued growth of the BSC-CNS and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

Organisational Structure



The Management Department is structured in 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 super-computer, dissemination of activities and results to academia and industry and promoting science in society.

Management Department Staff & Collaborators 2010



Finance and Business Administration

Led by Mercè Calvet, the Finance & Business Administration Unit in 2010 improved internal management and reporting systems to support research projects and the increasing daily activity of the centre, and facilitated the integration of new staff and visitors from local universities, and national and international mobility programs.

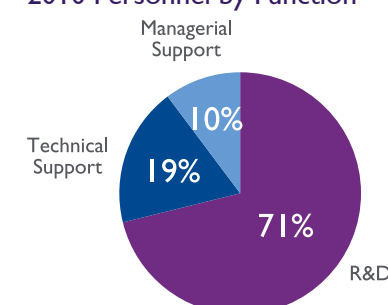
Finance & Accounting

The Finance & Accounting Group is responsible for the financial resources management of the BSC-CNS (expenses, budgets, audits, bank relations, suppliers, receiving payments and budget deviations). The Group also prepares the financial reporting for project audits, working closely with the Project Management Group, and the Marketing & Communication Group in preparing budgets. In 2010 the Group implemented the SAP BI tool to provide higher levels of fiscal control and better reporting capabilities.

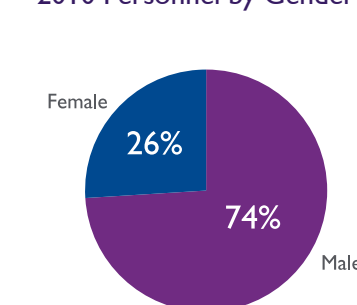
Human Resources

The Human Resources Group is responsible for managing selection processes, hiring and training, job descriptions, labour relations and collective bargaining, planning careers and internal promotion, and preventing work-related accidents. In 2010 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. The Human Resources Group support all personal contracts and scholarships/fellowships granted.

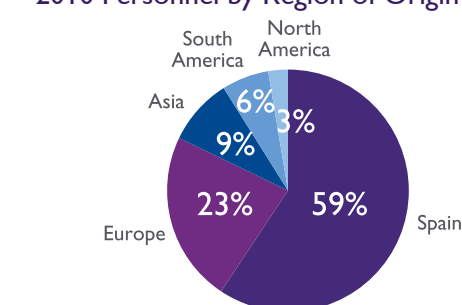
2010 Personnel by Function



2010 Personnel by Gender



2010 Personnel by Region of Origin



General Administration Support

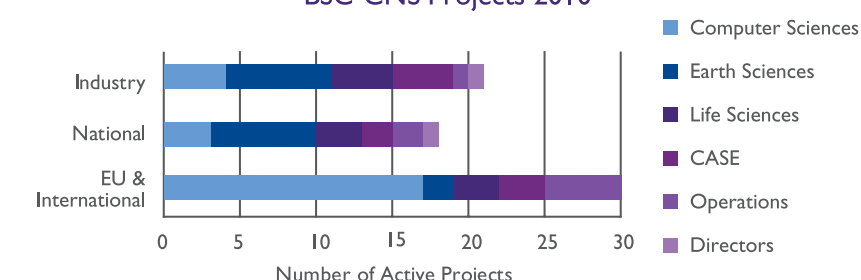
The General Administration Group is responsible for activities such as organisation of official meetings, including those of the Access Committee, the Executive Commission, the Board of Trustees and other events. The Group manages travel services, space allocation, supply orders and execution of public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

Project Management

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

In 2010, the BSC-CNS participated in 69 active projects, funded by national agencies, the European Commission and private industry. In addition to administering active projects, the Project Management Group assisted BSC-CNS researchers in submitting a large number of new project proposals during 2010 to help ensure continued funding for the BSC-CNS's research activities.

BSC-CNS Projects 2010



Marketing & Communication

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

Visitors

During the course of 2010, the BSC-CNS received a total of 7650 visitors from national and international centres, including universities, research centres, industry and non-profit organisations. This is an increase of 4% in respect to the the number of visits in 2009.

Visitors to the MareNostrum are given a tour of the supercomputer and view a specially prepared video describing the technology used in the centre and the applications resulting from research that uses the supercomputing capacity of the MareNostrum and other RES nodes. The visits are sometimes tailored depending on the target audience.

During 2010, the BSC-CNS received several official visits:

- September: Sr. Juan Tomás Hernani, Secretary of Innovation
- October: Artur Mas, Leader of the CiU
- November: Mariano Rajoy, President of Partido Popular, and Alicia Sánchez-Camacho, President of PP Cataluña

This year the Marketing and Communications Group organised for the first time an Open Day in collaboration with the City Council that opened relevant buildings in the city to the general public. Thanks to coverage of the event on the TV in the midday news, activity increased significantly in the afternoon, drawing over 300 visitors. This is another mechanism to disseminate BSC-CNS research results as well as familiarising the general public with supercomputing.

BSC-CNS in the Media

During 2010 the BSC-CNS was mentioned 171 times in national and international newspapers and magazines. Most coverage was received in the print media, with TV and online press in second place, followed by radio and lastly wires.

In total, the BSC-CNS sent out 11 press releases in Spanish, Catalan and English that were also posted to the Press section of the BSC-CNS website. All identified press impacts were also posted.

The press team also regularly updated the press dossiers of the BSC-CNS and the RES in English, Catalan and Spanish, as well as the press dossier of the BSC-Microsoft Research Center. This team also supported the production of various press releases of European Projects (VELOX, MERASA, Hipec, PRACE, HPC-EUROPA, etc.).

The BSC-CNS was the local host for the press of the ECRI conference (www.ecri2010.es), organising the European and National press tour to the different research institutes. The team coordinated the Spanish Ministry Press Department as well as the European Council press teams, providing required services to assist journalists during the conference.

Participation in Key Events, Seminars and Workshops

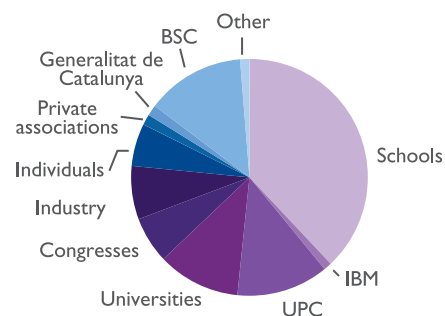
In 2010, BSC-CNS organised the following:

- Sixth European Conference on Research Infrastructures 2010, 22-24 March 2010
- Open e-IRG Workshop in Madrid, 17th June 2010
- DEISA- PRACE Symposium, 10-12 May 2010
- PRACE tutorial, 6-9 September 2010
- The Programming and Tuning Massively Parallel Systems Summer School (PUMPS), 5-9 July 2010
- PRACE Autumn school, 25-29 October 2010
- Jornada de Puertas Abiertas al BSC, 16 October 2010

The BSC-CNS also had a significant presence at:

- International Supercomputing Conference (ISC2009), Hamburg, June 2010
- Supercomputing (SC'09), November 2010

Visits to the MareNostrum 2010



Computer Sciences 2010 Publications

Journals

- » Alberto Sánchez, María S. Pérez, Jesús Montes, Toni Cortes, "A high performance suite of data services for grids". *Future Generation Computer Systems*, 1/4/2010
- » Alex Ramirez, Felipe Cabarcas, Ben Juurlink, Mauricio Alvarez Mesa, Friman Sanchez, Arnaldo Azevedo, Cor Meenderinck, Catalin Ciobanu, Sebastian Isaza, Georgi Gaydadjiev, "The SARC Architecture". *IEEE Micro*, vol. 30, no. 5, pp. 16-29, 1/9/2010
- » Andras Micsik, Jorge Ejarque, Rosa M. Badia, "A Semantic Toolkit for Scheduling in Cloud and Grid Platforms". *ERCIM News* 83, 14/10/2010
- » Eduard Ayguade, Rosa M. Badia, Pieter Bellens, Daniel Cabrera, Alejandro Duran, Marc Gonzalez, Francisco Igual, Daniel Jimenez-Gonzalez, Jesus Labarta, Luis Martinell, Xavier Martorell, Rafael Mayo, Jose M. Perez, Judit Planas and Enrique S. Quintana-Orti, "Extending OpenMP to Survive the Heterogeneous Multi-core Era". *International Journal of Parallel Programming*, vol. 38, nos: 5-6, pages: 440-459, 1/6/2010
- » Harm Munk, Eduard Ayguade, Cedric Bastoul, Paul Carpenter, Zbigniew Chamski, Albert Cohen, Marco Cornero, Philippe Dumont, Marc Duranton, Mohammed Fellahi, Roger Ferrer, Razya Ladelsky, Menno Lindwer, Xavier Martorell, Cupertino Miranda, Dorit Nuzman, Andrea Orstein, Antoniu Pop, Sebastian Pop, Louis-Noel Pouchet, Alex Ramirez, David Rodenas, Erven Rohou, Ira Rosen, Uzi Shvadrón, Konrad Trifunovic and Ayal Zaks, "ACOTES Project: Advanced Compiler Technologies for Embedded Streaming Harm Munk". *International Journal of Parallel Programming*, pp. 1-54, 20/4/2010
- » Hatem Ltaief, Jakub Kurzak, Jack Dongarra, Rosa M. Badia, "Scheduling Two-sided Transformations using Tile Algorithms on Multicore Architectures". *Scientific Programming*, vol. 18(1), pages 35-50, 1/1/2010
- » Isaac Gelado, John E. Stone, Javier Cabezas, Sanjay Patel, Nacho Navarro, Wen-mei W. Hwu, "An Asymmetric Distributed Shared Memory Model for Heterogeneous Parallel Systems". *ACM SIGARCH Computer Architecture News - ASPLOS'10*, 13/3/2010
- » J. Ejarque, M. de Palol, I. Goiri, F. Julià, J. Guitart, R. Badia, and J. Torres, "Exploiting Semantics and Virtualization for SLA-driven Resource Allocation in Service Providers". *Concurrency and Computation: Practice and Experience*, Vol. 22 (5), pp. 541-572, 1/4/2010
- » J. Guitart, J. Torres, and E. Ayguadé, "A Survey on Performance Management for Internet Applications". *Concurrency and Computation: Practice and Experience*, Vol. 22 (1), pp. 68-106, 1/1/2010
- » Jakub Kurzak, Hatem Ltaief, Jack Dongarra, Rosa M. Badia, "Scheduling dense linear algebra operations on multicore processors". *Concurrency and Computation: Practice and Experience*, volume 22, issue 1, 1/1/2010
- » Jesus Labarta, "MareIncognito: A Perspective towards Exascale". *Facing the Multicore-Challenge: Aspects of new Paradigms and Technologies in Parallel Computing. LNCS6310*, 18/3/2010
- » Jose María Cámara, Miquel Moretó, Enrique Vallejo, Ramón Beivide, Carmen Martínez, Jose Miguel-Alonso and Javier Navaridas, "Twisted Torus Topologies for Enhanced Interconnection Networks". *IEEE Transactions on Parallel and Distributed Systems*, 1/12/2010
- » M. Macías, O. Rana, G. Smith, J. Guitart, and J. Torres, "Maximizing Revenue in Grid Markets using an Economically Enhanced Resource Manager". *Concurrency and Computation: Practice and Experience*, Vol. 22 (14), pp. 1990-2011, 1/9/2010
- » Maja Etinski, Julita Corbalan, Jesus Labarta, Mateo Valero, "Utilization Driven Power-Aware Job Scheduling". *Computer Science - Research and Development*, Volume 25, Number 3-4, 1/9/2010
- » Marc Casas-Guix, Rosa M. Badia, Jesus Labarta, "Automatic Phase Detection and Structure Extraction of MPI Applications". *International Journal of High Performance Computing Applications*, Vol. 24, Number 3, pp. 335-360, 1/8/2010
- » Mateo Valero and Nacho Navarro, "Multicore, the View from Europe". *IEEE Micro Journal (special issue editors)*, 1/9/2010
- » Matthias Muller and Eduard Ayguade, "Guest Editors' Introduction". *International Journal of Parallel Programming (Special issue on OpenMPI)*, vol. 38, no. 5, pp. 339-340, 1/10/2010
- » Miquel Moretó, Francisco J. Cazorla, Alex Ramirez, Rizos Sakellariou and Mateo Valero, "FlexDCP: a QoS framework for CMP architectures". *ACM Operating Systems Review*, pp. 86-96, vol. 43, no. 2. Special Issue on the Interaction among the OS, Compilers, and Multicore Processors, 30/4/2010
- » Nikola Vujic, Felipe Cabarcas, Marc Gonzalez, Xavier Martorell, Alejandro Ramirez, Eduard Ayguade, "DMA++: On the Fly Data Realignment for On-Chip Memories". *IEEE transactions on computers*, 9/12/2010
- » Nikola Vujic, Marc Gonzalez, Xavier Martorell, Eduard Ayguade, "Automatic Prefetch and Modulo Scheduling Transformations for the Cell BE Architecture". *IEEE Transactions on Parallel and Distributed Systems*, vol. 21(4), pp.494-505, 15/4/2010
- » Ramon Bertran, Marc Gonzalez, Xavier Martorell, Nacho Navarro, Eduard Ayguade, "Local Memory Design Space Exploration for High-Performance Computing". *The Computer Journal*, vol. 53(3), 23/3/2010
- » Roger Ferrer, Pieter Bellens, Jae-Seung Yeom, Scott Schneider, Konstantinos Koukos, Michail Alvanos, Vicenç Beltran, Marc González, Xavier Martorell, Rosa M. Badia, Dimitrios S. Nikolopoulos, Angelos Bilas, Eduard Ayguadé, "Parallel Programming Models for Heterogeneous Multicore Architectures". *IEEE Micro*, vol. 30, no. 5, 1/9/2010
- » S. Reyes, C. Muñoz-Caro, A. Niño, R. Sirvent, R.M. Badia, "Monitoring and Steering Grid Applications with GRID superscalar". *Future Generation Computer Systems*, vol. 26 (4), pp. 645-653, 1/4/2010
- » Schwiegelshohn, U.; Badia, R.M.; Bubak, M.; Danelutto, M.; Dustdar, S.; Gagliardi, F.; Geiger, A.; Hluchy, L.; Kranzlmüller, D.; Laure, E.; Priol, T.; Reinefeld, A.; Resch, M.; Reuter, A.; Rienhoff, O.; Ruter, T.; Sloot, P.; Talia, D.; Ullmann, K.; Yahyap, "Perspectives on grid computing". *Future Generation Computer Systems*, Volume 26, Issue 8, October 2010, Pages 1104-1115, 1/10/2010
- » Yehuda Afek, Ulrich Drepper, Pascal Felber, Christof Fetzer, Vincent Gramoli, Michael Hohmuth, Etienne Riviere, Per Stenström, Osman S. Unsal, Walther Maldonado, Derin Harman, Patrick Marlier, Stephan Diestelhorst, Martin Pohlack, Adrián Cristal, Ibrahim Hur, Aleksandar Dragojevic, Rachid Guerraoui, Michal Kapalka, Sasa Tomic, Guy Korland, Nir Shavit, Martin Nowack, Torvald Riegel, "The Velox Transactional Memory Stack". *IEEE Micro* 30(5): 76-87, 1/9/2010

Book Chapters

- » Carlos Boneti, Roberto Gioiosa, Francisco J. Cazorla and Mateo Valero, "Using hardware resource allocation to balance HPC applications, Parallel and Distributed Computing". *Parallel and Distributed Computing*, 1/1/2010
- » Cecilia Gonzalez, Harald Servat, Daniel Cabrera, Xavier Aguilar, Carles Pons, Juan Fernandez and Daniel Jimenez, "Drug Design on the Cell BE". *Scientific Computing with Multicore and Accelerators*, pp 331-346, 23/12/2010

» Jesus Labarta, “New Analysis Techniques in the CEPBA-Tools Environment”. in Tools for High Performance Computing 2009. Springer. ISBN 978-3-642-11260-7, 1/1/2010

» Mateo Valero, “Computadores de Altas Prestaciones”. Memorias de la Real Academia de Ciencias y Artes de Barcelona. Vol. LXIV, no. 6, pp. 247-315., 1/1/2010

International Conferences

» Josep M Perez, Rosa M. Badia and Jesus Labarta, “Handling task dependencies under strided and aliased references”. Proceedings of the 24th ACM International Conference on Supercomputing, 4/6/2010

» Aislan G Foina, Rosa M Badia and Javier Ramirez-Fernandez, “G-means Improved for Cell BE Environment”. Facing the Multicore-Challenge, 17/3/2010

» Aislan G. Foina, Javier Ramirez-Fernandez, and Rosa M. Badia, “Cell BE and Bluetooth applied to Digital TV”. proceedings of 12th IEEE/IFIP Network Operations and Management Symposium (NOMS 2010), 19/4/2010

» Aislan Gomide Foina, Francisco Javier Ramirez-Fernandez, Ahmed El-Deeb, Rosa M Badia, “Player Tracker - A Tool to Analyze Sport Players using RFID”. proceedings of 8th IEEE International Conference on Pervasive Computing and Communications PerCom 2010, 29/3/2010

» Alejandro Rico, Jeff H. Derby, Robert K. Montoyo, Timothy H. Heil, Chen-Yong Cher, Pradip Bose, “Performance and Power Evaluation of an In-line Accelerator”. Proceedings of the 2010 ACM International Conference on Computing Frontiers, 1/5/2010

» Alessandro Cilardo, Luigi Esposito, Antonio Veniero, Antonino Mazzeo, Vicenç Beltran and Eduard Ayguadé, “A CellBE-based HPC Application for the Analysis of Vulnerabilities in Cryptographic Hash Functions”. Melbourne, Australia, 1/9/2010

» Alessandro Morari, Francesco Piermaria, Emiliano Betti, Roberto Gioiosa, Marco Cesati, “Analyzing OS noise for HPC systems”. The 6th ACACES 2010 (Advanced Computer Architecture and Compilation for High-Performance and Embedded Systems), 12/7/2010

» Alvaro Martínez, Santiago Prieto, Noé Gallego, Ramon Nou, Jacobo Giralt, Toni Cortes, “XtreemOS-MD: Grid computing from mobile devices”. Mobilware 2010, 30/6/2010

» Bhavishya Goel, Sally A. McKee, Roberto Gioiosa, Karan Singh, Major Bhadauria and Marco Cesati, “Portable, Scalable, per-Core Power Estimation for Intelligent Resource Management”. Green Computing Conference, 2010 International, 16/8/2010

» Enric Tejedor, Rosa M. Badia, Romina Royo and Josep L. Gelpi, “Enabling HMMER for the Grid with COMP Superscalar”. Proceedings of the International Conference on Computational Science 2010, 31/5/2010

» Enrique Vallejo, Ramón Beivide, Adrián Cristal, Tim Harris, Fernando Vallejo, Osman Unsal, Mateo Valero, “Architectural support for Fair Reader-Writer Locking”. 43rd International Symposium on Microarchitecture (Micro-43), 18/12/2010

» Ernest Artiaga and Toni Cortes, “Using File System Virtualization to Avoid Metadata Bottlenecks”. Design, Automation and Test in Europe (DATE 2010), 8/3/2010

» Felipe Cabarcas, Alejandro Rico, Yoav Etsion, Alex Ramirez, “Interleaving Granularity on High Bandwidth Memory Architecture for CMPs”. In Intl. Conf. on Embedded Computer Systems: Architectures, Modeling, and Simulation (SAMOS), 2/7/2010

» Ferad Zylkyarov, Srdjan Stipic, Tim Harris, Osman Unsal, Adrián Cristal, Ibrahim Hur, Mateo Valero, “Discovering and Understanding Performance Bottlenecks in Transactional Applications”. 19th International Conference on Parallel Architectures and Compilation Techniques PACT2010, 18/9/2010

» Ferad Zylkyarov, Tim Harris, Adrian Cristal, Osman S. Unsal, Mateo Valero, “Debugging Programs that use Atomic Blocks and Transactional Memory”. 15th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (PPoPP’10), 18/1/2010

» Friman Sánchez, Felipe Cabarcas, Alex Ramirez, Mateo Valero, “Long DNA Sequence Comparison on Multicore Architectures”. Proceedings of the 16th international Euro-Par conference on Parallel processing, 1/9/2010

» G. Reig, J. Alonso, and J. Guitart, “Prediction of Job Resource Requirements for Deadline Schedulers to Manage High-Level SLAs on the Cloud”. 9th IEEE International Symposium on Network Computing and Applications (NCA’10), Cambridge, Massachusetts, USA, pp. 162-167 (Short Paper), 15/7/2010

» German Llort, Juan Gonzalez, Harald Servat, Judit Gimenez, and Jesus Labarta, “On-line Detection of Large-scale Parallel Application’s Structure”. 24th IEEE International Parallel and Distributed Processing Symposium (IPDPS’2010), 1/5/2010

» I. Goiri, F. Julià, J. Guitart, and J. Torres, “Checkpoint-based Fault-tolerant Infrastructure for Virtualized Service Providers”. 12th IEEE/IFIP Network Operations and Management Symposium (NOMS’10), Osaka, Japan, pp. 455-462, 19/4/2010

» I. Goiri, F. Julià, R. Nou, J. L. Berral, J. Guitart, and J. Torres, “Energy-aware Scheduling in Virtualized Datacenters”. 12th IEEE International Conference on Cluster Computing (Cluster’10), Heraklion, Crete, Greece, pp. 58-67, 20/9/2010

» I. Goiri, J. Guitart, and J. Torres, “Characterizing Cloud Federation for Enhancing Providers’ Profit”. 3rd IEEE International Conference on Cloud Computing (CLOUD’10), Miami, Florida, USA, pp. 123-130, 5/7/2010

» I. Goiri, J. O. Fitó, F. Julià, R. Nou, J. L. Berral, J. Guitart, and J. Torres, “Multifaceted Resource Management for Dealing with Heterogeneous Workloads in Virtualized Data Centers”. 11th International Conference on Grid Computing (Grid’10), Brussels, Belgium, pp. 25-32, 25/10/2010

» J. L. Gonzalez, Toni Cortes, Jaime Delgado-Meraz, Ana Piedad Rubio, “HRaidTools: An on-line Suite of Simulation Tools for Heterogeneous RAID systems”. Third International Conference on Simulation Tools and Techniques (SIMUTools 2010), 15/3/2010

» J. L. Berral, I. Goiri, R. Nou, F. Julià, J. Guitart, R. Gavalda, and J. Torres, “Towards Energy-aware Scheduling in Data Centers using Machine Learning”. 1st International Conference on Energy-Efficient Computing and Networking (e-Energy’10), University of Passau, Germany, pp. 215-224, 13/4/2010

» J. O. Fitó, I. Goiri, and J. Guitart, “SLA-driven Elastic Cloud Hosting Provider”. 18th Euromicro Conference on Parallel, Distributed and Network-based Processing (PDP’10), Pisa, Italy, pp. 111-118, 17/2/2010

» J. O. Fitó, M. Macías, and J. Guitart, “Toward Business-driven Risk Management for Cloud Computing”. 6th IEEE/IFIP International Conference on Network and Service Management (CNSM’10), Niagara Falls, Canada, pp. 238-241 (Short Paper), 25/10/2010

» Javier Bueno, Xavier Martorell, Juan José Costa, Toni Cortés, Eduard Ayguadé, Guansong Zhang, Christopher Barton and Raul Silvera, “Reducing Data Access Latency in SDSM Systems using Runtime Optimizations”. Proc. of the CAS Conference (CASCON’10), pp. 160-173, 1/11/2010

» Javier Díaz., Sebastián Reyes, Rosa M. Badia, Alfonso Niño, Camelia Muñoz-Caro, “A General Model for the Generation and Scheduling of Parameter Sweep Experiments in Computational Grid Environments”. proceedings of the International Conference on Computational Science 2010, ICCS2010, 31/5/2010

» Jordà Polo, David Carrera, Yolanda Becerra, Jordi Torres, Eduard Ayguadé, Malgorzata Steinder, Ian Whalley, “Performance-Driven Task Co-Scheduling for MapReduce Environments”. 2010 IEEE/IFIP Network Operations and Management Symposium (NOMS2010), 19/4/2010

» Jorge Ejarque, Andras Micsik, Raül Sirvent, Peter Pallinger, Laszlo Kovacs and Rosa M. Badia, “Semantic Resource Allocation with Historical Data Based Predictions”. The First International Conference on Cloud Computing, GRIDs, and Virtualization, 23/11/2010

» Jorge Ejarque, Enric Tejedor, Daniele Lezzi, Raül Sirvent, Rosa M. Badia, “Supporting Parallel Tasks with GRID superscalar”. 4th Iberian Grid Infrastructure Conference, 27/5/2010

» Jorge Ejarque, Raül Sirvent and Rosa M. Badia, “A Multi-Agent Approach for Semantic Resource Allocation”. 2nd IEEE International Conference on Cloud Computing Technology and Science, 23/11/2010

» Josep M. Perez, “An overview of StarSs”. DEISA-TeraGrid Summer School, Catania, Italy, 26/10/2010

» Juan Gonzalez, Judit Gimenez, and Jesus Labarta, “Performance Data Extrapolation in Parallel Codes”. ICPADS’10: Proceedings of the 16th International Conference on Parallel and Distributed Systems, 1/12/2010

» Juan José Costa, Toni Cortes, Xavier Martorell, Javier Bueno-Hedo and Eduard Ayguadé, “Transient Congestion Avoidance in Software Distributed Shared Memory Systems”. 11th International Conference on Parallel and Distributed Computing, Applications and Technologies (PDCAT-10), pp. 357-364, 8/12/2010

» K. Huck and J. Labarta, “Detailed load balance analysis of large scale parallel applications”. 39th International Conference on Parallel Processing (ICPP 2010), 1/9/2010

» Kamil Kedzierski, Miquel Moreto, Francisco J. Cazorla and Mateo Valero, “Adapting Cache Partitioning Algorithms to Real pseudo-LRU Replacement Policies”. In 24th IEEE International Parallel & Distributed Processing Symposium (IPDPS), Atlanta, Georgia, 19/4/2010

» M. Macías and J. Guitart, “Using Resource-level Information into Nonadditive Negotiation Models for Cloud Market Environments”. 12th IEEE/IFIP Network Operations and Management Symposium (NOMS’10), Osaka, Japan, pp. 325-332, 19/4/2010

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» Mauricio Álvarez, Alex Ramirez, Mateo Valero, Arnaldo Azevedo, Cor Meenderinck and Ben Juurlink, “Performance Evaluation of Macrobloc-level Parallelization of H.264 Decoding on a cc-NUMA Multiprocessor Architecture”. In 4CCC. 4th Colombian Computing Conference, Bucaramanga (Colombia), 1/4/2010

» Mehmet Kayaalp, O uz Ergin, Osman Ünsal, Mateo Valero, “Exploiting Inactive Rename Slots for Detecting Soft Errors”. 23th Conference on Architecture of Computing Systems (ARCS’10), 18/2/2010

» Miquel Moreto, Francisco Javier Cazorla, Rizos Sakellariou and Mateo Valero, “Load Balancing Using Dynamic Cache Allocation”. ACM International Conference on Computing Frontiers (CF), 18/5/2010

» Nicolas Poggi, David Carrera, Ricard Gavalda, Jordi Torres and Eduard Ayguadé, “Characterization of Workload and Resource Consumption for an Online Travel and Booking Site”. 2010 IEEE International Symposium on Workload Characterization (IISWC-2010), 2/12/2010

» Nikola Vujic, Marc González, Eduard Ayguadé, Xavier Martorell, Alex Ramirez and Felipe Cabarcas, “DMA++: On the Fly Data Realignment for On-Chip Memories”. In 16th IEEE International Symposium on High-Performance Computer Architecture, Bangalore (India), 1/1/2010

» Paul Carpenter, Alex Ramirez and Eduard Ayguadé, “Buffer sizing for self-timed stream programs on heterogeneous distributed memory multiprocessors”. In International conference on High-Performance Embedded Architectures and Compilers (HiPEAC) 2010, Pisa (Italy), 1/1/2010

» Paul M. Carpenter, Alex Ramirez, Eduard Ayguade, “Starsscheck: a tool to find errors in task-based parallel programs”. Proceedings of the 16th international Euro-Par conference on Parallel processing, 1/9/2010

» Petar Radojkovic, Vladimir Cakarevic, Javier Verdu, Alex Pajuelo, Francisco J. Cazorla, Mario Nemirovsky and Mateo Valero, “Thread to Strand Binding of Parallel Network Applications in Massive Multi-Threaded Systems”. In 15th ACM SIGPLAN Annual Symposium on Principles and Practice of Parallel Programming, Bangalore, India, 9/1/2010

» Pilar González-Férez, Juan Piernas, and Toni Cortes, “Simultaneous Evaluation of Multiple I/O Strategies”. 22nd International Symposium on Computer Architecture and High Performance Computing, 25/10/2010

» Ramon Bertran, Marc Gonzalez, Xavier Martorell, Nacho Navarro, and Eduard Ayguade, “Decomposable and Responsive Power Models for Multicore Processors using Performance Counters”. Proc. of the 24th ACM Int. Conf. on Supercomputing, pp. 147-158, 1/6/2010

» Ramon Bertran, Marc González, Yolanda Becerra, David Carrera, Vicenç Beltran, Xavier Martorell, Jordi Torres, Eduard Ayguadé, “Accurate Energy Accounting for Shared Virtualized Environments using PMC-based Power Modeling Techniques”. 11th ACM/IEEE International Conference on Grid Computing (Grid 2010), 25/10/2010

» Ramón Nou, Jacobo Giralt, Julita Corbalan, Enric Tejedor, J. Oriol Fitó, Josep M. Pérez, Toni Cortes, “XtreemOS Application Execution Management: A scalable approach”. 11th ACM/IEEE International Conference on Grid Computing (Grid 2010), 25/10/2010

» Roberto Gioiosa, “Towards sustainable exascale computing”. The 18th IEEE/IFIP VLSI System on Chip Conference (VLSI-SoC), 27/9/2010

» Roberto Gioiosa, Sally A. McKee, Mateo Valero , “Designing OS for HPC Applications: Scheduling”. The 2010 IEEE International Conference on Cluster Computing (CLUSTER), 20/9/2010

» Roger Ferrer, Vicenç Beltran, Marc González, Xavier Martorell and Eduard Ayguadé, “Analysis of Task Offloading for Accelerators”. Proc. of the 5th International Conference, HiPEAC 2010, Pisa, Italy, January 25- 27, 2010, 25/1/2010

» Sebastian Isaza, Friman Sanchez, Georgi Gaydadjiev, Alex Ramirez, Mateo Valero, “Scalability Analysis of Progressive Alignment on a Multicore”. Proceedings of the 2010 International Conference on Complex, Intelligent and Software Intensive Systems (CISIS’10), 1/7/2010

» T. Cortes, “Implications of Exascale Computing for Storage Systems Research”. IEEE International Conference on Cluster Computing, 22/9/2010

- » Tanauus Ramirez, Oliverio Santana, Alejandro Pajuelo and Mateo Valero, “Efficient runahead threads”. PACT 2010. International Conference on Parallel Architectures and Compiler Techniques, 1/9/2010
- » Tim Harris, Adrian Cristal, Sasa Tomic, Osman Unsal, “Dynamic Filtering: Multi-purpose Architecture Support for Language Runtime Systems”. In the 15th International Conference on Architectural Support for Programming Languages and Operating Systems (ASPLOS XV), 18/3/2010
- » Victor Jimenez, Carlos Boneti, Francisco Cazorla, Roberto Gioiosa, Eren Kursun, Chen-Yong Cher, Canturk Isci, Alper Buyuktosunoglu, Pradip Bose, Mateo Valero, “Power and Thermal Characterization of POWER6 System”. The 19th International Conference on Parallel Architectures and Compilation Techniques (PACT), 13/9/2010
- » Victor Jimenez, Roberto Gioiosa, Eren Kursun, Francisco Cazorla, Chen-Yong Cher, Alper Buyuktosunoglu, Pradip Bose, Mateo Valero, “Trends and techniques for energy efficient architectures”. The 18th IEEE/IFIPVLSI System on Chip Conference (VLSI-SoC), 28/9/2010
- » Vladimir Marjanovic, Jesús Labarta, Eduard Ayguadé and Mateo Valero, “Effective Communication and Computation Overlap with Hybrid MPI/ SMPs”. 15th ACM SIGPLAN Annual Symposium on Principles and Practice of Parallel Programming (PPoPP), 10/1/2010
- » Vladimir Subotic, Jesus Labarta and Mateo Valero, “Simulation environment to study overlapping of communication and computation”. IEEE International Symposium on Performance Analysis of Systems and Software, 1/3/2010
- » Vladimir Subotic, Jose Carlos Sancho, Jesus Labarta and Mateo Valero , “A simulation framework to automatically analyze the communication-computation overlap in scientific applications”. IEEE International Conference on Cluster Computing, 1/9/2010
- » Yoav Etsion, Felipe Cabarcas, Alejandro Rico, Alex Ramirez, Rosa M. Badia, Eduard Ayguade, Jesus Labarta, Mateo Valero, “Task Superscalar: An Out-of-Order Task Pipeline”. IEEE/ACM Intl. Symp. on Microarchitecture (MICRO-43), 6/12/2010

National Conferences

- » Adrian Jackson, Adam Carter, Joachim Hein, Jan Westerholm, Mats Aspnäs, Matti Ropo, and Alejandro Soba, “EUFORIA HPC: Massive Parallelisation for Fusion Community”. PDP,
- » Daniel Jimenez, Raul Sanchez, Carlos Alvarez, Julian Morillo-Pozo, Daniel Cabrera, Xavier Martorell and Eduard Ayguade, “GPPPGA: entorno para la generación automática de códigos HDL portables entre FPGAs”. X Jornadas de Computación Reconfigurable y Aplicaciones (JCRA’10), pp. 19-26, 10/9/2010

Workshops

- » Alejandro Duran, Roger Ferrer, Michael Klemm, Bronis R. de Supinski and Eduard Ayguade, “A Proposal for User-defined Reductions in OpenMP”. 6th International Workshop on OpenMP (IWOMP 2010), 14/6/2010
- » Augusto Vega, Alejandro Rico, Felipe Cabarcas, Alex Ramirez, Mateo Valero, “Comparing last-level cache designs for CMP architectures”. IFMT ‘10: International Forum on Next-Generation Multicore/Manycore Technologies, 1/6/2010
- » Eduard Ayguade, James Beyer, Alejandro Duran, Roger Ferrer, Grant Haab, Kelvin Li and Federico Massaioli, “An extension to improve OpenMP tasking control”. 6th International Workshop on OpenMP (IWOMP 2010), 14/6/2010
- » Gulay Yalcin, Osman Unsal, Ibrahim Hur, Adrian Cristal, Mateo Valero, “FaulTM: Fault-Tolerance Using Hardware Transactional Memory”. he 3nd Workshop on Parallel Execution of Sequential Programs on Multi-core Architectures (PESMA 2010), 18/6/2010
- » I. Goiri, F. Julià, J.O. Fitó, M. Macías, and J. Guitart, “Resource-level QoS Metric for CPU-based Guarantees in Cloud Providers”. 7th International Workshop on Economics of Grids, Clouds, Systems, and Trace Services (GECON 2010), Ischia, Italy, 31/8/2010
- » Jacobo Girarlt, Christine Morin, Yvon Jegu, “Easing Application Execution in Grids with XtreamOS Operating System”. 2nd XtreamOS summit, 30/8/2010
- » Jesus Labarta, “Programming Models and Scalability”. Scalable Algorithms for Large-Scale Systems@ SC’10, 15/11/2010
- » Jesus Labarta, “On the route to Exascale”. ATOMIC AND MOLECULAR SIMULATIONS : CHALLENGES FOR THE NEXT DECADE. ZCAM Launching meeting, 28/5/2010
- » Judit Giménez, Jesús Labarta, F. Xavier Pegenaute, Hui-Fang Wen, David Klepacki, I-Hsin Chung,, Guojing Cong, Felix Voigtlaender and Bernd Moht, “Guided Performance Analysis Combining Profile and Trace Tools”. PROPER2010, 30/8/2010
- » Kamil Kedzierski, Francisco Cazorla, Roberto Gioiosa, Alper Buyuktosunoglu, Mateo Valero. , “Power and Performance Aware Reconfigurable Cache for CMPs”. Workshop on Next Generation Multicore/Manycore Technologies (IFMT), in conjunction with ISCA, 7/6/2010
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- » Nebojša Mileti , Vesna Smiljkovi , Cristian Perfumo, Tim Harris, Adrián Cristal, Ibrahim Hur, Osman Unsal, Mateo Valero, “Transactification of a real-world system library”. Fifth ACM SIGPLAN Workshop on Transactional Computing TRANSACT, 18/4/2010
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- » Roger Ferrer, Alejandro Duran, Xavier Martorell, Eduard Ayguadé, “Harmonizing serial optimizations with OpenMP”. 15th Workshop on Compilers for Parallel Computing (CPC-2010), 7/7/2010
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- » Scollo S.; Folch, A.; Coltelli, M.; Realmuto, V.J, “Volcanic aerosol dispersal: a comparison between MISR data and numerical simulations”. Journal of Geophysical Research, 115, D24210, 21/12/2010
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- » Baldasano J.M.; A. Soret; O. Jorba; E. López, “Metodología para la Evaluación del Impacto Ambiental sobre la Atmósfera de Plantas de Valorización Energética”. Evaluación ambiental: cooperación, desarrollo y sostenibilidad. Libro de actas del V congreso. V CONEIA. Ed. Ministerio Agric Pesca Alimen: 179-185, 11/3/2010
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- » Piot M.; M.T. Pay; O. Jorba; P. Jimenez-Guerrero; E. Lopez; S. Gasso; J.M. Baldasano, “Annual Dynamics and Statistical Evaluation of an Air Quality Forecasting System (CALIOPE) with High Resolution for Europe”. Air Pollution Modeling and its Application XX. Editors: Down G. Steyn and S.T. Rao. Springer: 241-245, 1/1/2010

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- » Baldasano J.M, “HPC & Earth Sciences Research at the Barcelona Supercomputing Center”. IS_ENES 1st Gral. Assembly, Barcelona, 26/5/2010

- » Baldasano J.M., “Earth System Modeling Framework: Computation+Data”. DEISA PRACE Symposium 2010, Barcelona, 11/5/2010
- » Baldasano J.M., “L’aprofitament energètic”. Jornada “El futur de la gestió dels residus municipals a Catalunya”. Diputació de Barcelona-Fundación Forum Ambiental, Barcelona, 27/4/2010
- » Baldasano J.M., “CALIOPE-CAN: Sistema de Modelización de la Calidad del Aire en Canarias”. I Jornadas sobre Calidad del Aire y Meteorología Ambiental en Canarias, Santa Cruz de Tenerife, 17/3/2010
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- » Baldasano J.M., “Evidencias del Actual Cambio Climático”. Universitat de Girona, Girona, España, 24/2/2010
- » Baldasano J.M. y A. Soret, “Balanços de carboni–Emissions”. Grup d’Experts sobre Canvi Climàtic de Catalunya, Monestir de les Avellanes, Lleida, 11/11/2010
- » Baldasano J.M.; O. Jorba, “CALIOPE: Sistema de Información para el Pronóstico y Vigilancia de la Calidad del Aire en Andalucía”. Jornadas Técnicas de Participación-Evaluación de la Calidad del Aire en Andalucía, Sevilla-Málaga, 3/12/2010
- » Barsotti, S.; M. Coltelli; A. Costa; A. Folch; G. Macedonio; L. Nannipieri; A. Neri; M. Prestifilippo; S. Scollo; G. Spata, “Investigation of the model-dependent uncertainty of volcanic ash dispersal forecasts”. 28th IUGG Conference on Mathematical Geophysics, Pisa, Italy, 7/6/2010
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- » Folch, A., “Forum on the assessment of volcanic ash threat: learning and considerations from the 2010 Eyjafjallajökull eruption”. Cities on Volcanoes 6, Tenerife, 4/6/2010
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- » Sulpizio, R.; A. Folch, “Far-range Volcanic Ash Hazard from Somma-Vesuvius. Consequences for Civil Aviation over the Central Mediterranean Area”. Cities on Volcanoes 6, Tenerife, 4/6/2010
- » Terradellas E.; J.M. Baldasano; E. Cuevas; M.Á. Martínez, “Current and planned activities of the WMO SDS-WAS Regional Center for Northern Africa, Middle East and Europe”. EUMETSAT Meteorological Satellite Conference. Cordoba (España), 20/9/2010

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- » Fernando Martín; Alberto González Ortiz; Enrique Bailly-Baillière; Rafael Borge; Rosa Soler; José María Baldasano; Jose Luis Palau; Roberto San José; Elena Agirre; José Antonio Souto; Marivi Alvizu; Eva Pérez; Antonio Lozano; Eloy Piernagorda; Cecilia Soriano; David Cartelle; J.A. García-Moya; Pedro Jiménez-Guerrero; Carlos G. Giralda; Marta G. Vivanco; I. Palomino; Oscar Hernanz, “Red Temática de Modelización de la Contaminación Atmosférica”. 10 Congreso Nacional de Medio Ambiente. CONAMA 10. Madrid, España, 22/11/2010
- » Jorba O., C. Pérez, K. Haustein, D. Dabdub, J. M. Baldasano, A. Badia, M. Spada, “Development of an integrated chemical weather prediction system for environmental applications at meso to global scales: NMMB/BSC-CHEM”. Segones Jornades de Meteorologia i Climatologia de la Mediterrània Occidental, Valencia, 11/3/2010
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- » Baldasano J.M.; M. Piot; O. Jorba; M. Goncalves; M.T. Pay; S. Basart; P. Jiménez and S. Gassó, “CALIOPE: an Operational Air Quality Forecasting System for Europe and Spain”. Mesoscale Modelling For Air Pollution Applications: Achievements And Challenges (COST 728 Final Workshop), Organisers: COST 728, WMO/GURME and MEGAPOLI, Geneva, 25/2/2010
- » Baldasano J.M.; M.T. Pay; O. Jorba; J. Ortiz; M. Gonçalves; S. Gassó; P. Jiménez-Guerrero, “Evaluation of the Spanish Operational Air quality Forecasting System: Diagnostic and Near Real-Time”. International Workshop on Air Quality Forecasting Research (IWAQFR). Org. WMO-NOAA, Quebec (Canada), 16/11/2010
- » Folch, A.; A. Costa, “Modeling volcanic ash transport using FALL3D: model description, validation results and future perspectives”. The 5th MWO International Workshop on Volcanic Ash, Santiago de Chile, Chile, 22/3/2010
- » J. M. Baldasano; M.T. Pay; O. Jorba; J. Ortiz; M. Gonçalves; S. Basart; S. Gassó; P. Jiménez-Guerrero, “Evaluation of the Spanish operational air quality forecasting system: diagnostic and near real time”. International Workshop on Air Quality Forecasting Research. Québec, Canada, 16/11/2010

Theses

- » Marc Casas, “Spectral Analysis of Executions of Computer Programs and its Applications on Performance Analysis”. March 2010. Advisor Rosa M. Badia and Jesús Labarta.
- » Miquel Moretó, “Improving Cache Behavior in CMP Architectures through Cache Partitioning Techniques”. March 2010. Advisor Mateo Valero and Francisco J. Cazorla.
- » Tanausú Ramírez, “Runahead Threads”. April 2010. Advisor Mateo Valero, Alex Pajuelo and Oliverio J. Santana.
- » Isaac Gelado, “On the Programmability of Heterogeneous Massively-Parallel Computing Systems”. July 2010. Advisor Nacho Navarro and Wen-mei W. Hwu.

Life Sciences 2010 Publications

Journals

- » Alías, M., Ayuso-Tejedor, S., Fernández-Recio, J., Cativiela, C., Sancho, J., “Helix propensities of conformationally restricted amino acids. Non-natural substitutes for helix breaking proline and helix forming alanine.”. Org. Biomol. Chem. 8, 788-792., 22/4/2010
- » Banás, P.; Hollas, D.; Zgarbová, Jurecka, P.; Orozco, M.; Cheatham, T.E.; Spomer, J.; Otyepka, M., “Performance of molecular mechanics force-fields for RNA simulations. Stability of UUCG and GNRA hairpins”. J. Chem. Theory Comput., 2010, 6 (12), pp 3836–3849, 9/11/2010
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- » Curr. Opin. Struct. Biol. 20, 139-141., “Protein docking by Rotation-Based Uniform Sampling (RotBUS) with fast computing of intermolecular contact distance and residue desolvation”. BMC Bioinformatics 11, 352, 22/9/2010
- » E.M. Novoa, L. Ribas de Pouplana, X. Barril and M. Orozco., “Ensemble docking from homology models”. J. Chem. Theory Comput., 2010, 6 (8), pp 2547–2557, 16/7/2010
- » Eliahoo, E., Ben Yosef, R., Pérez-Cano, L., Fernández-Recio, J., Glaser, F., Manor, H., “Mapping of interaction sites of the Schizosaccharomyces pombe protein Translin with nucleic acids and proteins: a combined molecular genetics and bioinformatics study.”. Nucleic Acids Res. 38, 2975-2989., 22/1/2010
- » F. Raimondi, M. Orozco and F. Fanelli, “Deciphering the deformation modes associated with function retention and specialization in members of the Ras Superfamily”. Structure. (2010), 18, 402-414, 10/3/2010
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- » Fernández-Recio, J., Verma, C., “Theory and simulation: integrating models into experimental scenarios.”. Curr. Opin. Struct. Biol. 20, 139-141., 22/1/2010
- » Frank Wallrapp, Alexander Voityuk, and Victor Guallar, “Temperature Effects on Donor-Acceptor Couplings in Peptides. A Combined Quantum Mechanics and Molecular Dynamics Study”. Journal of Chemical Theory and Computation, 10:3341-3348, 1/10/2010
- » G. Portella and M. Orozco., “Multiple routes characterize the folding of a small DNA hairpin”. Angew. Chem. Int. Ed. Eng. (2010), 49, 7673-7676., 15/9/2010
- » I. Faustino, A. Pérez and M. Orozco., “Towards a Consensus view of duplex RNA flexibility”. Biophysical Journal. (2010), 99, 1876-1885., 22/9/2010
- » I. Soteras, M. Orozco and F. J. Luque, “Performance of the IEF-MST solvation continuum model in the SAMPL2 blind test prediction of hydration and tautomerization free energies”. J. Computer Aided Mol. Design. (2010), 24, 281-291., 19/3/2010

- » Kenneth Borrelli, Benjamin Cossins, and Victor Guallar, “Exploring hierarchical refinement techniques for induced fit docking with protein and ligand flexibility”. J. Comp. Chem, 1: 1224-35, 1/4/2010
- » L.Orellana, M.Rueda, C.Ferrer-Costa, J.R.López-Blanco, P.Chacón and M.Orozco., “Approaching elastic network models to atomistic molecular dynamics”. J. Chem.Theory Comput., 2010, 6 (9), pp 2910–2923, 20/8/2010
- » Pérez-Cano, Fernández-Recio, J., “Dissection and prediction of RNA-binding sites on proteins”. BioMol Concepts, 1, 345–355, 7/12/2010
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- » Pons, C., Solernou, A., Pérez-Cano, L., Grosdidier, S., Fernández-Recio, J., “Optimization of pyDock for the new CAPRI challenges: Docking of homology-based models, domain-domain assembly and protein-RNA binding”. Proteins 78, 3182-3188, 22/5/2010
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- » A.Pérez and M.Orozco, “Real time atomistic description of DNA unfolding”. Angew. Chem. Int. Ed. Eng. (2010), 49, 4805-4808., 17/5/2010

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- » Frank Wallrapp and Victor Guallar, “M/MM e-pathway: mapping Electron transfer processes in proteins”. ACS National Meeting “San Francisco(USA), 2/5/2010
- » M.Orozco, “Datamining in cancer genome projects.Why a supercomputer center is needed”. III International Symposium on * Biomedical Informatics in Europe, 17/11/2010
- » M.Orozco, “Biomolecular simulations. An overview”. IV Spanish Portuguese Biophysical Congress, 7/7/2010
- » M.Orozco, “Challenges in molecular dynamics of macromolecules”. EMBO Course on Molecular Modeling, 26/6/2010
- » M.Orozco, “Exploring DNA folding and unfolding from molecular dynamics simulations”. Symposium on nucleic acid chemistry, structure and interactions, 29/5/2010
- » M.Orozco, “Computational challenges in Life Sciences”. HPC-Prace meeting, 20/4/2010
- » M.Orozco, “New computational challenges in Biology”. EGEE’10 User Conference, 12/4/2010
- » Pérez-Cano, L., Solernou, A., Pons, C., Fernández-Recio, J., “Structural prediction of protein-RNA interaction by computational docking with propensity-based statistical potentials”. 15th Pacific Symposium on Biocomputing. Kohala Coast HI (USA), 23/3/2010

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- » Fernández-Recio, J., “Constraints in protein-ligand and protein-protein docking”. ZCAM Workshop on Constraints in Molecular Simulation. Zaragoza (Spain), 23/10/2010

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- » Par Strand, Bernard Guillerminet, Isabel Campos Plasencia, Jose Maria Cela, Rui Coelho, David Coster, Lars-Goran Eriksson, Matthieu Haefele, Francesco Iannone, Frederic Imbeaux, Adrian Jackson, Gabriele Manduchi, Michal Owsiak, Marcin Plociennik, Alejandro Soba, Eric Sonnendrücker, and Jan Westerholm, “A European Infrastructure for Fusion Simulations”. PDP,
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- » Xavier Sáez, Alejandro Soba, Edilberto Sánchez, Ralf Kleiber, Francisco Castejón, and José M. Cela, “Improvements of the particle-in-cell code EUTERPE for petascaling machines”. Computer Physics Communications,

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- » Carlos Sanz-Navarro, Rogeli Grima, Alberto Garcia, Edgar Bea, Alejandro Soba, Jose Maria Cela, and Pablo Ordejon, “An efficient implementation of a QM-MM method in SIESTA”. Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta),

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- » A.C. Lesage, G. Houzeaux, M.Vázquez, and H. Coppola-Owen, “A High-Performance Parallel Incompressible Navier-Stokes Two-Phase Flow Solver using the Level Set Method for Hydrodynamics design”. 5th European Conference on Computational Fluid Dynamics, Lisbon (Portugal), 14/6/2010
- » F.Mut, R.Aubry, J. Cebal, R. Lohner, and G. Houzeaux, “Deflated Preconditioned Conjugate Gradient Solvers: Extension and Improvements”. AIAA Conference, Orlando (USA), 4/1/2010
- » G. Houzeaux, R. Aubry, M. Vázquez, and J.M. Cela, “Extension of fractional step techniques for incompressible flows on Parallel Architectures”. PARCFD2010, Kaohsiung (Taiwan), 17/5/2010
- » G. Houzeaux, R. de la Cruz, M.Vázquez, José Maria Cela, and Herbert Owen, “Implementation issues in Alya, a Parallel Computational Mechanics Code”. Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA), New Orleans (USA), 14/11/2010
- » M.Vázquez and G. Houzeaux, “Towards the Homo-Computationalis: High Performance Computational Bio-Mechanics”. PARCFD2010, Kaohsiung (Taiwan), 17/5/2010
- » M.Vázquez, R.Aris, G. Houzeaux, P.Villar, P. Lafortune, C. Labarta, D. Gil, J. Garcia-Barnes, M. Ballester, and F. Carreras, “A massively parallel electro-mechanical model of the heart for large-scale simulations”. IV European Conference on Computational Mechanics (ECCM), 17/5/2010
- » M.Vázquez, R. Aris, P. Lafortune, P.Villar, G. Houzeaux, D. Gil., and J. Garcia -Barnés., “Massively Parallel Electromechanical Model of the Heart”. 9th International Symposium on Computer Methods in Biomechanics and Biomedical Engineering (CMBBE2010), Valencia (Spain), 24/2/2010
- » M.Vázquez, S. Marras, M. Moragues, O. Jorba, G. Houzeaux, and R.Aubry., “A Massive Parallel Variational Multiscale FEM Scheme Applied to Non-hydrostatic Atmospheric Dynamics”. EGU Annual Meeting, number EGU2010-9060, Vienna (Austria), 4/5/2010
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- » Mohammad Jowkar, Raúl de la Cruz and José M. Cela, “Exploring a Novel Gathering Method for Finite Element Codes on the Cell/B.E. Architecture”. In Proceedings of the 2010 ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis, SC’10, 13/11/2010
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- » S. Marras, M. Vázquez, O. Jorba, R. Aubry, G. Houzeaux, and J.M. Baldasano, “Application of a Galerkin Finite Element Scheme to Atmospheric Buoyant and Gravity Driven Flows”. AIAA Conference, number AIAA 2010-690, Orlando (USA), 22/2/2010
- » S.Onggo, C. Montañola-Sales, J. Casanovas-García, “Performance analysis of parallel demographic simulation”. Proceedings of the 2010 European Simulation and Modeling Conference, 25/10/2010
- » Simone Marras, Mariano Vázquez, Oriol Jorba, Guillaume Houzeaux, Romain Aubry, and Arnau Folch. , “Massively parallel finite element applications to atmospheric dynamics”. Model and Data Hierarchies for Simulating and Understanding Climate, Los Angeles (USA). Institute of Pure and Applied Mathematics, UCLA, 22/6/2010
- » X. Rubio, José Ma. Cela, “Large-scale agent-based simulation in archaeology: an approach using High-performance computing”. Computer Applications in Archaeology, 8/4/2010

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- » J. Agustí, X. Rubio, “Neandertal extinction dynamics”. II mini-workshop of Working Group 4 “Evolution and Co-evolution” of COST Action MP0801 “Physics of Competition and Conflict”, 24/2/2010
- » X. Rubio, “Simulating Societies: Large-Scale agent-based modelling in archaeology”. Interdisciplinary Workshop: Peopling, Resources and Environment in Northern Gujarat (India) during the Holocene. New perspectives for simulating landscape change using High Performance Computing, 22/2/2010





Throughout 2010 the RES continued to offer high value services to the Spanish scientific community, organising training sessions and seminars to improve dissemination of scientific results obtained by RES users and to improve the knowledge base of both technicians and researchers. Continuing the trend of previous years, 2010 saw the demand for access to RES services continue to increase, exceeding by almost 200% the time available for allocation. More than 100 projects utilised RES resources during 2010, taking the total number of scientific projects supported since the creation of the RES to more than 1300, highlighting the importance and urgent need of access to supercomputing facilities in Spain.

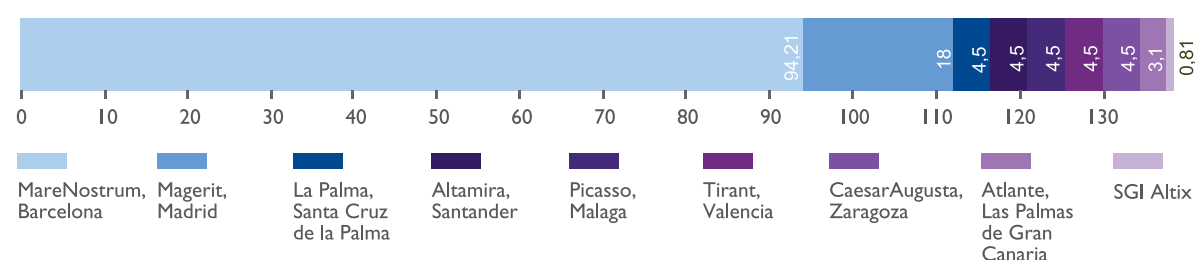


Nodes of the Spanish Supercomputing Network (RES)

RES main goals, resources and members

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

RES Processing Power in TFLOP/s



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

The total processing capacity of the RES is 138,5 TFLOP/s (138,5 trillion floating point operations per second) and 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 the aspects related with the user support.

Access protocol and allocations in the RES during 2010

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

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 formed by prestigious scientists external to the BSC-CNS. The four Expert Panels are defined according to the classification established by the Spanish Foundation of Science and Technology (FECYT).

The Expert Panels

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

Access Committee Core Team 2010

- ▶ 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

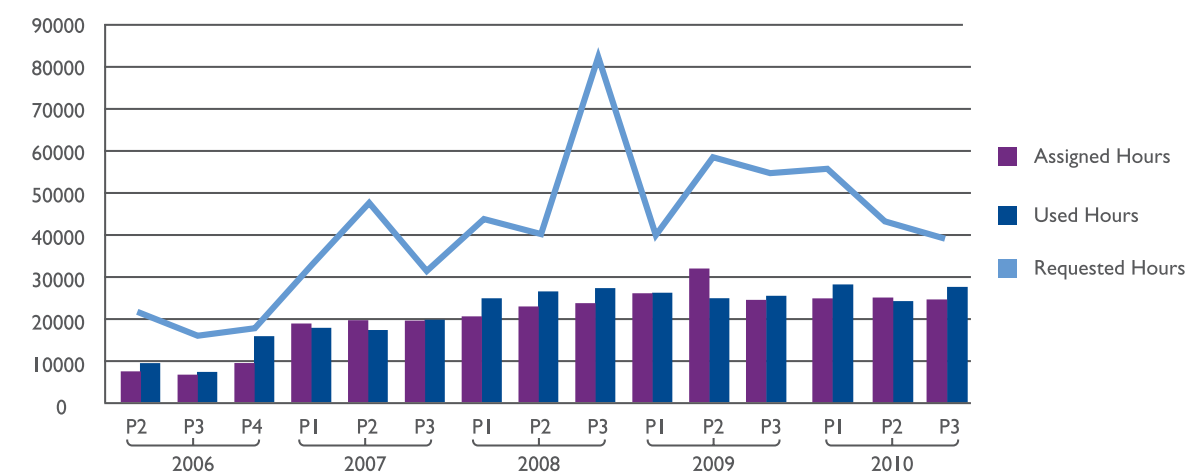
The Access Committee allocates to both Spanish and international researchers more than 25 million computational hours every four months. In addition to internal research groups, over 150 external activities made use of the RES system in 2010. It is important to note that many scientific projects often request numerous periods of access to the RES in order to perform different work activities (new activities or continuation activities). As specified in the Access Protocol, 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 2010

Once the Access Committee has published its four monthly list of successful applicants and the number of computing hours that each one has been granted and allocated, the Operations Department of BSC-CNS takes over the logistical processes of scheduling the users, preparing their software for loading and running the software and ensuring the users have access to 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 (light blue), assigned hours (violet) and used hours (dark blue) over the last four years.

Number of RES Hours



In the five years since the MareNostrum commenced operation, the MareNostrum and other RES nodes have collectively provided more than 310 million hours of computation. Over the same period 628 million hours were requested, indicating that the demand is more than double the hours that RES can provide to the scientific community.

RES Users' Committee (CURES)

On the 9th February 2010, a new committee called CURES (Committee of the Users of the Spanish Supercomputing Network) was established. The purpose of this new committee is to provide advice and feedback to management and technicians on the current state and future delivery of RES resources and services.

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

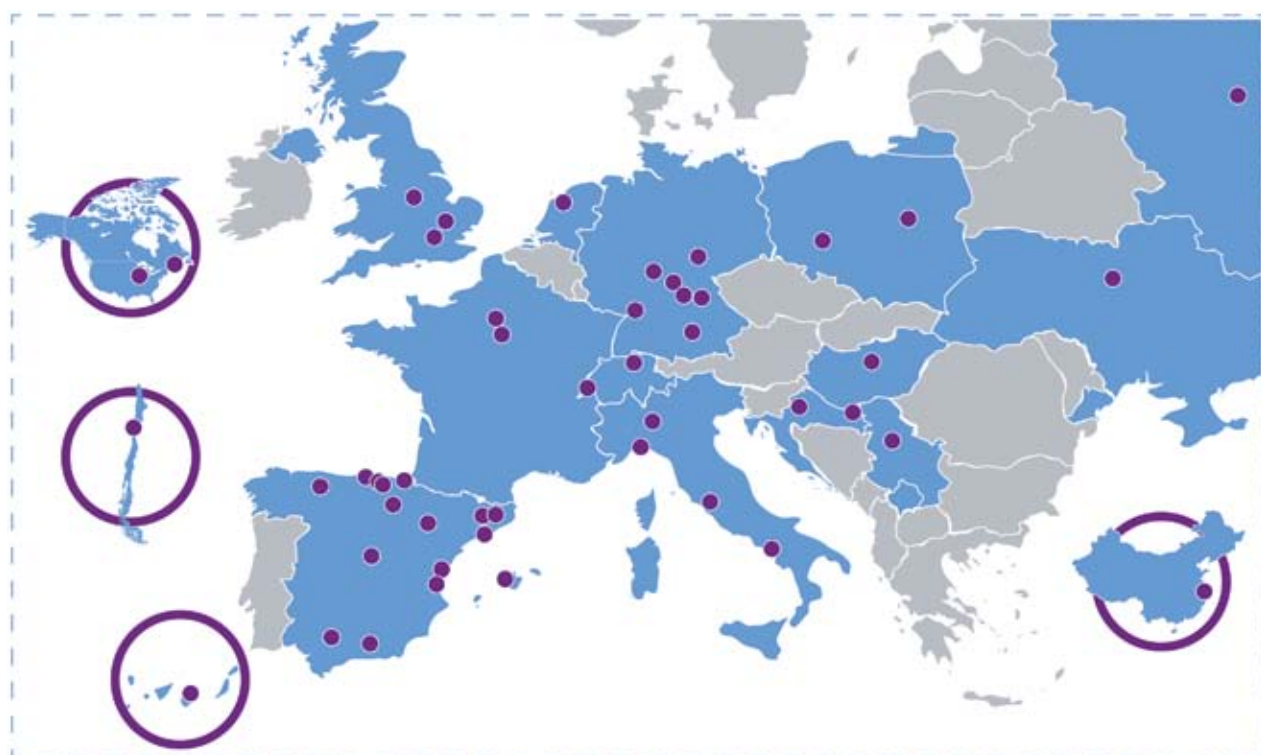
The members of the CURES committee elect amongst themselves the Chair and Vice-Chair, who act as representatives on behalf of the whole committee. Each member may hold office a maximum of two years, with half the members of the committee renewed every year. Chair and Vice-Chair are replaced alternately with the Vice-Chair assuming the Chair's role, thereby ensuring continuity.

The CURES members

- ▶ Eight scientists who are users of RES - two per scientific area of the Expert Panels and chosen by the Coordinators of the Access Committee.
- ▶ One RES representative chosen by the RES members.

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 since 2006. More than 150 R&D activities took advantage of the RES infrastructure in 2010, led by the most prominent researchers from institutions in over 40 cities in Spain, Europe and overseas.

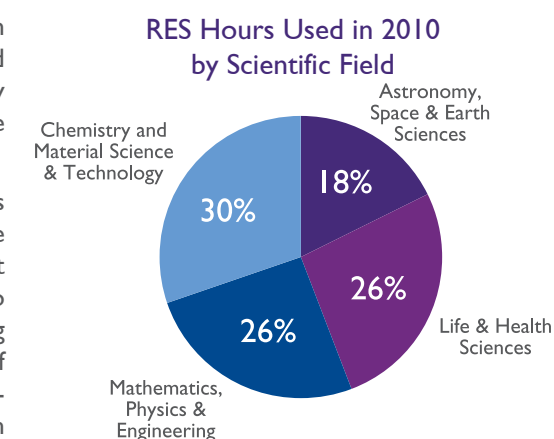


Cities of Origin of RES Users, 2010

The different research activities carried out on RES supercomputers during 2010 cover a huge range of scientific fields, from ocean models to protein definition, nanotechnology, and the study of subatomic interactions, among others. The results of these studies were disseminated in seminars and conferences all over the world and some led to published articles in the most prestigious scientific journals.

Many of these results would have been impossible to obtain in such short timeframes using traditional computers, that would take many years to complete such intensive computations. Only the powerful computing capability offered by the RES makes these research projects feasible.

In addition to traditional channels of dissemination, the RES teams organised both general and field-specific seminars to disseminate scientific findings, and also held training sessions to inform current and potential RES users on available tools and the key issues to consider during project execution to maximise the benefit of using RES facilities. A key objective is to more widely inform sectors of the scientific community who have not traditionally used supercomputers on how to access RES resources. Additionally, in-depth technical training sessions were held for the teams that manage each RES node and any scientific users interested in the subject.



RES Users Conferences in 2010

Two user conferences were held in 2010. The 3rd RES Users Conference took place on July 1st in Zaragoza and the 4th RES Users Conference took place on December 15th in Madrid.

The aim of the conferences is to disseminate the results obtained via use of RES supercomputing facilities by different research groups in each of the four scientific areas. The meetings thereby provide a forum for numerous distinguished researchers to present their work and results.

At each meeting the Access Committee and its operation were presented, and special attention was devoted to the newly created Users Committee, outlining its operation and allowing the audience (more than 70 attendees in both conferences) to participate in formulating proposals for improving its performance.

Finally, an introduction to the PRACE (Partnership for Advanced Supercomputing in Europe) initiative was presented in order to ensure the Spanish scientific community is kept abreast of the different resources that will become available in the future.



Opening of the 3rd RES Users Conference

RES Scientific Seminars 2010



RES Scientific Seminar on Parallel Simulations

The BSC-CNS in collaboration with UZ (University of Zaragoza) and BIFI (Institute of Biocomputing and Physics of Complex Systems) organised the RES Scientific Seminar on Parallel Simulations in the Network on November 30th, 2010.

The aim of these seminars is to educate scientists on how to improve the efficacy of their simulations. The discretisation of space (and even time) greatly reduces the degrees of freedom and significantly speeds up simulations. Furthermore, an appropriate discretisation in problems where the interaction is relatively local allows the parallelisation of tasks in a highly efficient way, enabling parallel simulations to be applied to different research areas such as Molecular Dynamics of condensed matter or Monte Carlo simulations of magnetic systems, among many others. The development of numerical and computational algorithms can further improve model efficiencies.

In the seminar, users learnt the basics of various methods that can be applied in order to develop parallel processes in their simulations and thereby dramatically improve their algorithms.

RES Users Trainings in 2010



RES Users Seminar on Programming Models (STARs)

The RES held two user trainings during 2010 with a very favorable response from the more than 50 attendants.

The RES User's Seminar on Programming Models (STARs) took place in Barcelona from 20 - 21st September 2010, conducted by experts from the Computer Science Department of the BSC-CNS. The seminar was focused on providing an introduction in programming models such as GRIDSs, COMPSs, MPI, SMPs and STARs to scientific and technical developers in order to improve the code of the applications they develop to run on RES resources.

The BSC-CNS in collaboration with IFCA (Institute of Physics of Cantabria) and the UC (University of Cantabria), also organised in Santander on November 5th, 2010 the RES Users Seminar on Parallel Computing. This seminar, taught by UC and BSC-CNS staff, focused

on presenting the efficient use of I/O parallel libraries (e.g. Parallel-HDF5, PNETCDF), MPI2 focused on parallel I/O, parallel file systems and parallel code debugging, to RES users, researchers and students interested in parallel computing.

RES Technical Seminars in 2010

All the RES nodes share the desire to provide the best possible services to the Spanish scientific community. A key element in achieving this goal is to provide ongoing training and professional development for their technical staff.

During 2010, a total of four technical seminars were held. Two were held in Santander from 18 - 20th May, organised by the BSC-CNS in collaboration with IFCA (Institute of Physics of Cantabria), one focused on the implementation of ITIL in supercomputing centers and one centered on Energy Management and Cooling of a Data Processing Center. Then in Barcelona on 14th and 15th September, the BSC-CNS organised a technical training on Storage Management in the RES, and another technical training on the Function and Application of Perfminer.



Some attendants of the RES Technical Seminars



Overview



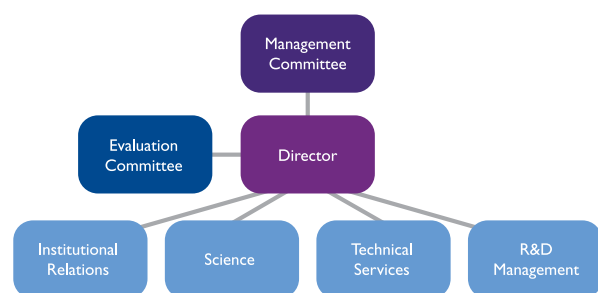
The MAGERIT Supercomputer

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 Infrastructures 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



During 2010 the organisation of the CeSViMa changed radically: new management structure, new position within the UPM's organisational structure... In late 2010, a new management group took over control of CeSViMa.



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

Technical and Scientific Highlights 2010

In 2010 the Magerit supercomputer achieved an average load of more than 80% with 24x7 availability. This represents a provision of 20,480,000 CPU hours. Projects allocated via the RES access committee used near 13,000,000 CPU hours (63.5% of the total provisioned hours) while the rest were assigned by local access committee. Local activities ranged from studies of nuclear fusion, physical properties of polymers, to analysis of behaviour of liquid and air flows. For a list of key scientific outputs during 2010, please consult the online version of this report.

Key Projects 2010

In addition to computing time dedicated to the RES, Magerit also provided support to numerous local research projects during 2010:

Blue brain project, José María Peña Sánchez (CeSViMa)

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

Computational and experimental Aero-Aoustics for prediction and control of noise (ACE-PCOR), Eusebio Valero Sánchez (UPM)

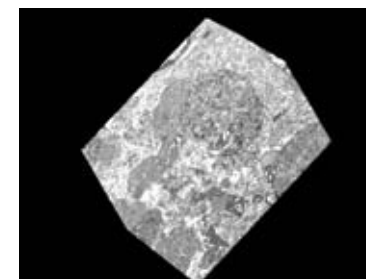
CRP on analytical and experimental benchmark analyses of accelerator driven systems (ADS), Alberto Abánades Velasco, Vassilis Theofilis (UPM)

Development and formalisation of monitoring techniques for 3D images with application to the analysis of CT/MRI hepatic images, Carlos Platero Dueñas (UPM)

Advanced multiscale nucleo-cellular methods in tridimensional and multigroup geometries for calculations of light water reactors, Carolina Ahnert Iglesias (UPM)

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

SEALS, Asunción Gómez Pérez (UPM)



Brain affected by Alzheimer's (image: CajalBBP)

Evolution and explosion of electrically charged fluid masses, Ultano Kindelán Bustelo (UPM)

Development of a regional climate model with atmospheric-oceanic coupling and optimisation of code for massively parallel computers, Antonio García Dopico (UPM) Fernando Cuartero Gómez, Clemente Gallardo Andrés (UCLM)

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

Development of indicators of chaos for analysis of the dynamics of Hamiltonian systems of three degrees of freedom, Juan Carlos Losada González (UPM)

Development of algorithms for parallel simulation of dynamic problems of deformable solids with disparate time scales, Ignacio Romero Olleros (UPM)

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

Characterisation of magnetic nanostructures obtained by cathodic pulverisation and nanolithography by electron beam, Marco César Maicas Ramos (UPM)

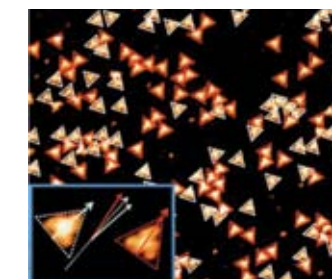
Mechanoquantum calculations in mesoscopic systems, Vicente Martín Ayuso (UPM)

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

Homeland security: technologies for integral security in public spaces and infrastructures (HESPERIA), Pedro Gómez Vilda (UPM)

Operational system for air quality prediction for the european continent (MM5-CMAQ-EMIMO): Regional information systems, Roberto San José (UPM)

Development of numerical algorithms for the simulation of multiscale mechanical systems in distributed calculation platforms, Ignacio Romero Olleros (UPM)



STM image of the C60H30 PAHs deposited on a Pt(111) surface. Inset: STM image showing a detail of two molecules. The white arrow indicates the [1-10] surface crystallographic direction. Bias voltage and tunnel current are 750 mV and 0.2 nA, respectively. (image: Gonzalo Otero, et al)

Modeling of Synthetic and Biological Macromolecules Through a Hierarchical Multiscale Approach, Nikolaos Karayiannis (UPM)

Design, synthesis and characterisation of advanced high efficiency photovoltaic materials, Perla Wahnón Benarroch (UPM)

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

Modelling shock wave propagation in advanced materials and nanostructures, Santiago Cuesta López (UPM)

Determination of the stress-optical coefficient and plateau modulus from atomistic simulations of polyethylene melts, Vicente Lorenzo (UPM)

Method of integration of public and private, heterogeneous data sources, oriented at recompilation, Víctor Manuel Maojo García (UPM)

QUINFOG, Juan José García Ripoll (QUITEMAD)

MIC, David Pérez García (QUITEMAD)

GICC-UPM, Vicente Martín Ayuso (QUITEMAD)

Cryptography, computation and simulation, Miguel Ángel Martín Delgado (QUITEMAD)

Proximity Microscopes: transport, reactivity and manipulation in nanostructures, Rubén Pérez (UAM)

Transport in nanostructures and proximity microscopes, Rubén Pérez (UAM)

Mechanical-quantum study of the photochemistry and control of molecules on metal oxide surfaces, María Pilar de Lara Castells (CSIC)

Dynamics, molecular compatibility and nanostructures of new generation polyolefins, Javier Martínez de Salazar Bascuñana (CSIC)

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 User Support. Ángel de Vicente Garrido (Engineer), User Support. Victor Plasencia Darias (Operator), User Support.



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

Technical and Scientific Highlights 2010

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.

Local research activities are primarily focused on astrophysics and studies of the sun. For a list of key scientific outputs during 2010, please consult the online version of this report.

Key Projects 2010

Aside from the projects assigned by the RES, which utilise approximately 80% of LaPalma's capacity, during 2010 the IAC executed its own scientific projects, among which highlights are:

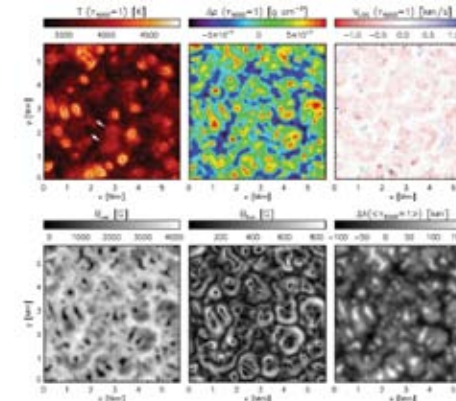
Magneto-convection simulations of stellar atmospheres: the new era of chemical abundances (P.I.: Damian Fabbian)

The research project encompasses magnetohydrodynamic simulations of the Sun and stars using the stagger-code of A. Nordlund (Copenhagen University). This effort is part of the solar physics European network SOLAIRE (<http://www.solaireretwork.net/>). Running simulations on the LaPalma supercomputer helps test the performance of the latest version of the code. Previous versions of this code were proven to perform well on different systems, with a good speed-

up when increasing the number of CPUs used. The simulations cover a few hours of solar time. The output snapshots will be used to synthesize spectra in order to study the line formation in detail (Kiselman & Nordlund 1995) and compare with results from other theoretical studies and from observations. This is of extremely high interest for the astronomical community, in particular for the solar and stellar groups working at IAC. The aim is to allow the determination of stellar chemical composition to a higher degree of precision than ever before, thus unravelling crucial clues on our sun, and enabling to put tighter constraints on galactic evolution models via stellar studies. The analysis work is now well-tested, with initial results being very promising in the sense of an effect of magnetic fields on the chemical abundance derived.

3D MHD radiation convection simulations with Muram (P.I.: Hector Socas Navarro)

In this project the Muram code was used to produce realistic 3D models of the solar photosphere, including non-grey radiative transfer. These simulations were used to produce synthetic Stokes profiles comparable to those observed in order to test new abundance determination schemes (such as the novel method introduced by Centeno and Socas-Navarro 2008 for the determination of the O abundance) and to compare with other determinations based on 3D models (e.g., those from Asplund et al 2001; or the CO5BOLD group).



Sections through a snapshot of a simulated sunspot umbra. Upper row: temperature (left, arrows show two examples of decaying umbral dots), deviation from the local mean density (center) and line of sight velocity (right). Lower row: vertical (left) and horizontal (center) component of the magnetic field vector, and differential Wilson depression (right). All quantities are shown at constant optical depth unity.

An accurate description of the cosmological recombination: the ionization history and the cosmic microwave background frequency spectrum (P.I.: Jose Alberto Rubino Martin)

In the last twenty years, many experiments have been devoted to the study of the cosmic microwave background (CMB). Results of the WMAP satellite in conjunction with other data sets (observations of Type Ia supernovae or galaxy surveys) give us the most precise determinations of the cosmological parameters describing our Universe, and constitute one of the most important confirmations of the hot Big Bang theory. With upcoming experiments, as the Planck satellite (launched May 2009), we expect to reach unprecedented accuracies in the description of the underlying cosmological parameters. However, in order to maximise the knowledge gained from this high-resolution experiment, it is important that theoretical calculations are equally precise. Currently, uncertainty in the ionisation history of the universe around redshift $z=1000$ remains one of the major factors limiting the accuracy of power spectrum calculations. The project produced a very accurate code which describes the detailed physics of recombination in the Universe, and also computes the recombinational spectrum. It involves the simultaneous evolution of hundreds or thousands of differential equations for the occupation numbers of the individual levels of the hydrogen and helium atoms. However, the simultaneous and self-consistent inclusion of all the physical processes makes the computations very difficult and ti-

me-consuming. To solve this issue, the Group presented RICO (<http://cosmos.astro.uiuc.edu/rico>), a framework for using a highly accurate but computationally-intensive cosmological recombination code together with the machine learning algorithm Pico (<http://cosmos.astro.uiuc.edu/pico>) to allow high precision cosmological parameter estimation at the level required for the Planck satellite.

Propagation of magnetoacoustic waves in magnetic structures (P.I.: Tobias Felipe Garcia)

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.

Galaxy transformations through interactions, mergers and accretion (P.I.: Marc Balcells Comas)

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 (P.I.: Artemio Herrero Davo)

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.



Composite color image of the Local Group galaxy IC1613. The zone of intense star formations are clearly seen through the bright stars and the surrounding nebosity. The Genetic Algorithm has been used on the La Palma node for the determination of stellar parameters of some of the youngest and most massive stars in the galaxy

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 of two engineers from ITC (Yeray Gutiérrez Cedrés and María Belén Esteban Sánchez), who are responsible for system management and user support, and a group manager (Juan 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.



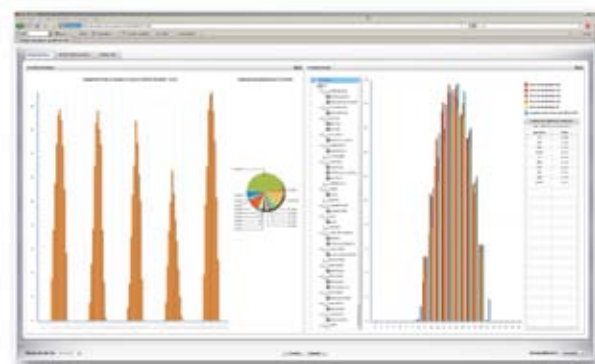
The Atlante Supercomputer Team:
M^a Belén Esteban Sánchez (right, User Support)
Yeray Gutiérrez Cedrés (left, System Administrator)

Technical and Scientific Highlights 2010

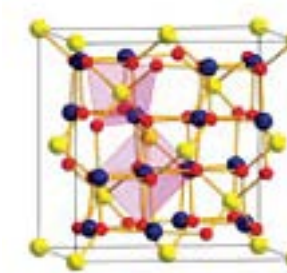
Although new, the Atlante node is already highly productive, providing computing time for RES users as well as local researchers. These local activities covered numerous disciplines, most prominently physics and chemistry resulting in a number of highly regarded publications and numerous conference presentations. For a list of key scientific outputs during 2010, please consult the online version of this report.

Key Projects 2010

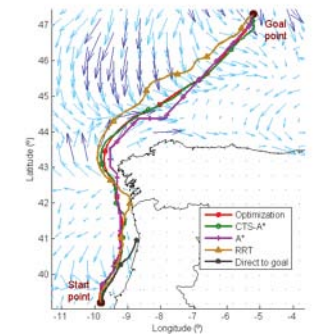
Photovoltaic Systems Simulator The project deals with meteorological data processing to estimate the amount of energy that Photovoltaic Systems allocated in Canary Islands would be able to generate according to the expected weather conditions, which are estimated using Numerical Weather Prediction models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



Simulation of Photovoltaic Energy in Gran Canaria



Estructural, electronic and dynamical properties under extreme conditions



Trajectories found with different path planning strategies in the North-Atlantic coast of Spain using the ESEOAT region of the ESEO's Regional Ocean Model.

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

CAIBEX The CAIBEX project aims the interdisciplinary study of the The Cape Ghir Upwelling Filament located at the Northwest African Coast. This study includes the continued development of a numerical model started in 2008 in order to study the dynamics that govern the generation of the filament. During 2010 new numerical experiments were developed and improved the climatologically forcing and initialisation of the model. As suggested by earlier experiments new results indicate that the generation of the filament is controlled by the wind curl and the potential vorticity balance (Beta-effect). Model results are being compared with observation obtained during CAIBEX III Cruise (August 2009), in particular the generation of a subsurface anticyclonic eddy related with the Filament.

SLAM The problem of Simultaneous Localization and Mapping (SLAM) addresses the issue of a mobile robot moving through an environment of which no map is available a priori. The goal of SLAM is to reconstruct a map of the world and the path taken by the robot, being a key prerequisite to truly autonomous robots. This project is concerned with the cooperative and integrated use of vision and range sensors to map and localise a robot in indoor environments. Solving the general SLAM problem is noticeably time consuming due to the high dimensionality of the problem, with a 6DOF state space, and the temporal dynamics. Even a simplification of the problem, taken some assumptions, is still computationally demanding when targeting online real-time performance.

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.

Overview



The ALTAMIRA Supercomputer

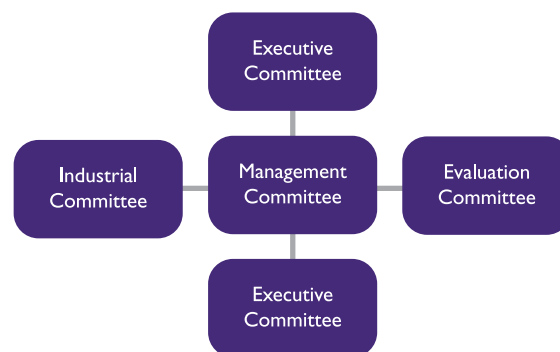
The ALTAMIRA node of the RES at the University of Cantabria is located in the Juan Jorda Building and is jointly managed by the IFCA Distributed Computing Team and the Computer Architecture Group (ATC) of the University of Cantabria.

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 and Miguel Angel Nuñez

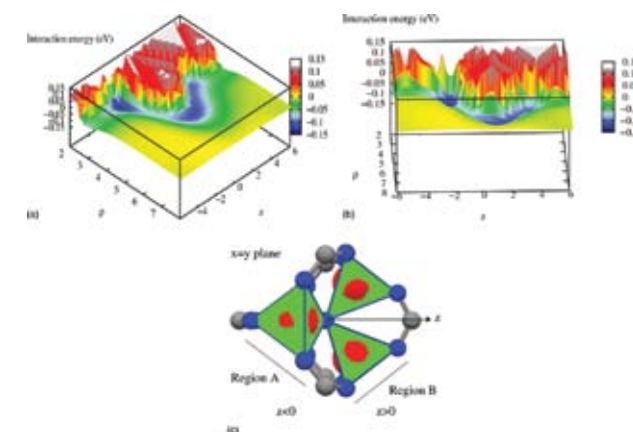
Technical and Scientific Highlights 2010

In 2010 the Altamira node provided more than 1 million hours of CPU time, with some 20% dedicated to executing applications corresponding to local users at the University of Cantabria. Of particular note were the outputs publications and conference presentations relating to HPC algorithms and architecture. For a list of key scientific outputs during 2010, please consult the online version of this report.

Key Projects 2010

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.

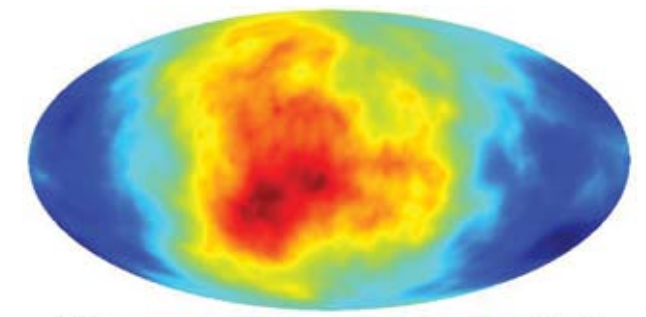


Location of the oxide core of the MOF-5 Material

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.

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 Sachs-Wolfe effect using N-body program

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

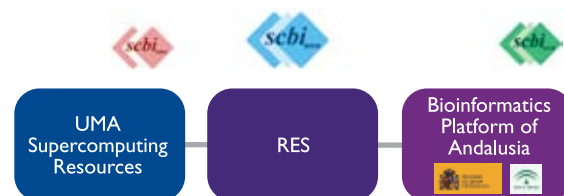


The Picasso Supercomputer

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

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

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

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

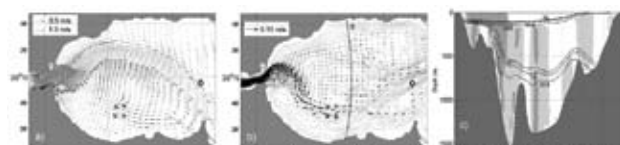


SCBI team at Málaga (left to right):
Darío Guerrero Fernández (sysadmin)
Guillermo Pérez Trabado (manager)
Rafael Larrosa Jiménez (sysadmin)

Technical and Scientific Highlights 2010

In 2010, 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. This local work resulted in a number of scientific publications, covering topics as diverse as genetics, radioactivity, geography and solid state physics. For a list of key scientific outputs during 2010, please consult the online version of this report.

Key Projects 2010



Gibraltar Strait and Alboran Sea

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

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

of deep/bottom waters. The different forces driving the exchange and its variability are investigated within this research line, which is funded by the Spanish Government (Ministerio de Ciencia e Innovación) under the INGRES projects. One concrete research shows how the meso-scale circulation in the Alboran sea influences the exchange flow through the Strait of Gibraltar, as can be seen in the figure on the right, consisting of three panels: (a) Modeled surface velocity in the Western Alboran Sea. (b) Same as a) at $z=500$ m depth. Isobaths $z=100, 200, \dots, 2000$ m are given by gray lines (c) Cross section S, (panel b) of temperature and zonal velocity. Light contours are for negative velocities. Darker contours indicate velocities below -0.02 m/s.

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

Parallel programming models and compilers Computer Architecture Department of the University of Málaga.

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.

The Group also 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.

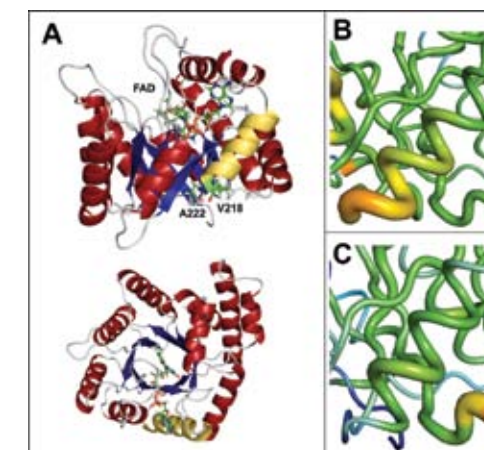
Andalusian platform for genomics, proteomics, and bioinformatics research Bioinformatics Platform of Andalusia

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.

Bioinformatics and information technologies Group INB (Instituto Nacional de Bioinformática) (National Bioinformatics Institute).

The Group's main focus the application of information technologies to bioinformatics. It has developed a new parallel algorithm to do large microarray quantile normalisation.



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 $\alpha 5$ 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.

Molecular modelling in rare diseases Department of Molecular Biology and Biochemistry of the University of Málaga.

The Group belongs 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.

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

Statistical physics and dispersed media Department of Applied Physics of the University of Málaga.

The Group develops models and numerical simulations to study the collective behavior of many-particles systems.

The behaviour of ensembles of magnetic nanoparticles and molecular magnets is investigated, exploring the physical limits of information storage in magnetic devices.

As an example, the figure at the right shows a phase diagram of a diluted system of dipoles placed on a 3D single cubic lattice. X is a fraction of sites of the lattice that contains dipoles, T is the transition temperature between phases, AF and SG shows an antiferromagnetic phase and another of spin-glass.

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.

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 catalan 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 Universitat 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.

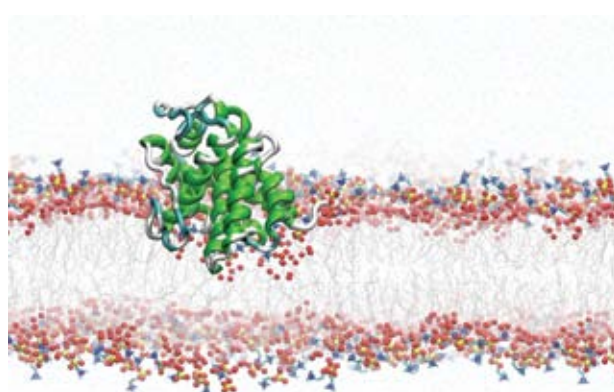


From the left: Jose María González - Operator, Alejandro Soriano - System Analyst, Gabriel Aparicio - System Analyst, Josep Vicent Sala - System Analyst, Salvador Roca - IT Group Director

Technical and Scientific Highlights 2010

In 2010, Tirant offered 4,42 million CPU hours of which some 2,61 million hours 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. This work resulted in numerous scientific papers, posters and oral presentations. For a list of key scientific outputs during 2010, please consult the online version of this report.

Key Projects 2010



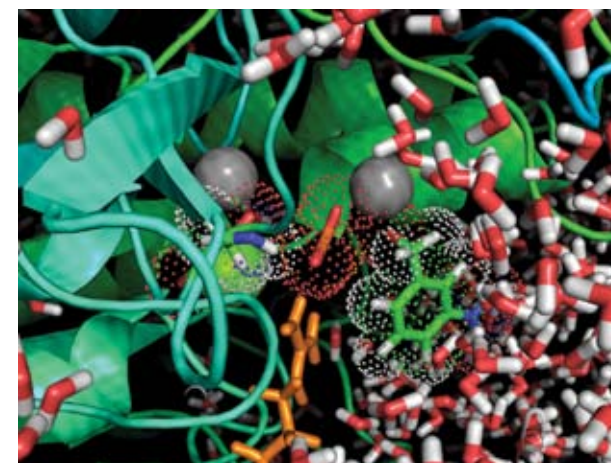
The protein Bax at the interface of a hydrated DMPC lipid bilayer

Coupling of gold catalysed 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 specialised 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.

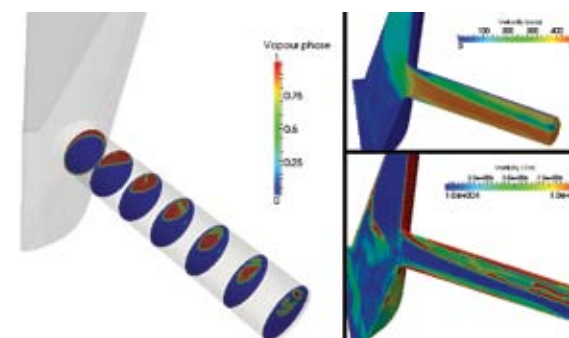
Numerical simulations of hadron properties Led by Vicent Giménez Gómez the main goal is to quantitatively describe and predict, using numerical simulations of the Quantum Chromodynamics (QCD), the properties of hadrons, mesons and baryons, like the proton and the neutron which form the nucleus of all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



Microquasar Jets With RATPENAT (3D Simulations)

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.

Large eddy Simulation for internal flow in diesel injectors The work developed by the Group led by R. Payri involved the simulation of the internal flow of diesel injectors, commonly used in passenger cars, using the Large Eddy Simulation (LES) technique. The main code was developed by OpenSource Ltd for OpenFOAM, and the authors have introduced additional expressions in order to calculate particular variables. Two main activities were developed in Tirant: the first was the application of the technique to critical operating conditions in diesel engines, such as very low temperatures; the second was dedicated to improving the solver code in order to calculate liquid flows with density variations.



Microquasar Jets With RATPENAT (3D Simulations)

Study of the cavitation phenomena in diesel injector nozzles Under the injection conditions in modern diesel engines (where injection pressure can reach up 180 MPa) cavitation often occurs in fuel injector nozzles, having a strong impact on the spray and its atomisation, and therefore in the efficiency of the combustion process.

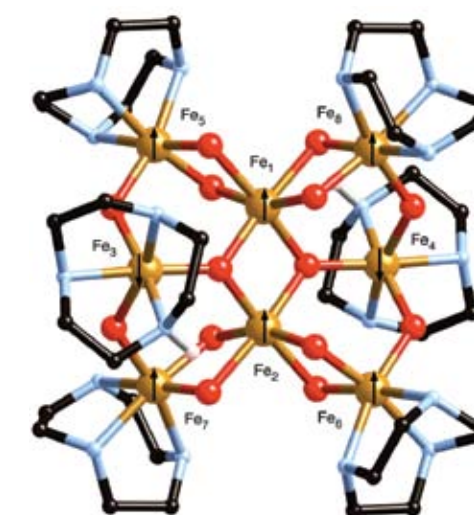
Large eddies simulations have been performed allowing to advance the knowledge of the cavitation phenomena to understand the injection and combustion process and solve a large number of problems related with this phenomenon.

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.

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 thermodynamics and optics, of high-nuclearity spin clusters.



Molecular structure of Fe₈ compound showing electronic spin orientation in fundamental state

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. The Group investigates 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 (Spanish Supercomputing Network). It is managed by the Supercomputing Area of the Institute for Biocomputation and Physics of Complex Systems (BIFI).

BIFI is a research institute that promotes interdisciplinarity to develop competitive research in computation applied to physics of complex systems and biological systems. Despite its youth, the Institute has already developed intensive research activity in several fields of computation: cluster, grid computing, 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 are coordinated with the BSC-CNS operations department.

There is also a local Access Committee which manages the 20% of the CPU time which is at the disposal of the University of Zaragoza. This time is assigned by the Committee after evaluating the applications received for each four-month period (coinciding with RES schedule). During 2010, 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)

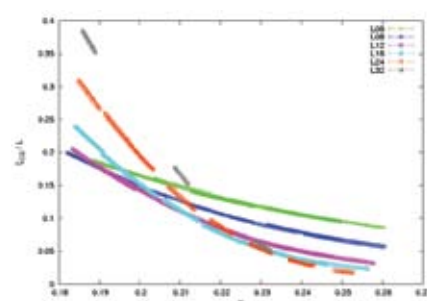


CAESARAUGUSTA Operations Team
(from left to right):
Javier Alcázar Luque (BIFI's sysadmin),
Arturo Giner (BIFI's sysadmin), Guillermo
Losilla (BIFI's computing manager), Alfonso
Tarancón (BIFI's secretary professor &
Head of the Computing Area)

Technical and Scientific Highlights 2010

2010 was a great year for CAESARAUGUSTA with a total of 13 local projects accepted by the local Access Committee utilising 950.000 hours of CPU time. These activities have produced numerous scientific results and publications, including invited oral presentations at conferences in South Korea, Ireland and France. For a list of key scientific outputs during 2010, please consult the online version of this report.

Key Projects 2010



For all our system sizes and temperatures simulated, we show the Chiral Glass Correlation Length in units of the lattice size as a function of the temperature. Each data patch corresponds to an independent simulation, in which the reweighting method was used to extrapolate to contiguous temperatures.

Critical properties of the anisotropic heisenberg spin-glasses in three dimensions Led by Victor Martín Mayor (BIFI, Theoretical Physics Department UCM), the Project studies the critical behaviour of the Heisenberg Spin Glass model in three dimensions in the presence of a weak anisotropy. The phase diagram of the Heisenberg spin glass, in the ideal limit of purely isotropic interactions, has been the subject of lively debate in recent years. However, no real material is faithfully represented by purely isotropic models.

The project considers the effects of these small anisotropies, by means of Monte Carlo simulations on very large lattices (size up to $L=32$). The large computing power of the Caesar Augusta cluster was crucial to obtaining results, which showed that, no matter how small, anisotro-

pies are a relevant perturbation. This means that anisotropic interactions dominate the physics once close enough to the phase transition. The data strongly suggests that chiral ordering sets up at a higher temperature than the spin-glass ordering, and that the difference in the ordering temperatures is sizable. This is certainly surprising, and unexpected from a theoretical point of view, but is also something that can be experimentally investigated.

These results have been reported in a manuscript (<http://arxiv.org/abs/1101.2509>) which is currently under review in a research journal.

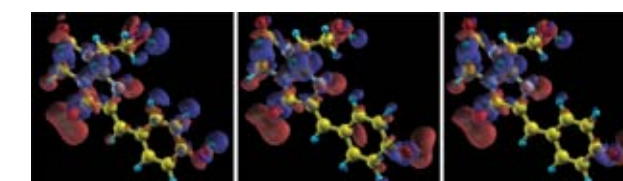
Calculation of the bootstrap current profile in TJII stellarator with NEOMC Led by José Luis Velasco (LNF, Ciemat & BIFI). The control of the bootstrap current, and thus of the total parallel current, may lead to the possibility of continuous operation in tokamak overdense plasmas and the control of the rotational transform profile in stellarators, with access to improved confinement regimes. The precise calculation of the bootstrap current is a numerical challenge. A new code, NEO-MC, was developed at TU Graz in order to overcome this problem. It combines the standard delta-f method with an algorithm employing constant particle weights and re-discretisations of the test particle distribution. This makes it possible, for the very first time, to calculate the bootstrap current at TJ-II, a stellarator device located at Madrid. Even with this optimisation, large amounts of CPU time were required, and therefore the resources from CAESARAUGUSTA were of great value.

A stepwise algorithm for combining diagnostic tests Led by Luis Mariano Esteban (Escuela Universitaria Politécnica La Almunia. UZ), the working Group continued development of the Project to build models that achieve a greater ability to discriminate between different disease states. A non parametric approach to building linear models which combine multiple markers was used for this purpose; this is a step by step algorithm that has been implemented in R language. The various simulations carried out allowed the study of the behaviour of these models for different simulated clinicopathological variables or biomarkers, each of them based on 1000 or 1000 simulation runs. The Project also examined new measures to identify genetic markers that are statistically significant in prostate cancer recurrence. The use of these new measures can be effective to build Risk Scores that combine genetic markers in order to improve the predictiveness of models based only in clinicopathological variables.

4D Edwards-Anderson Spin Glass in Magnetic Field Led by Alfonso Tarancón (BIFI, Theoretical Physics Department, UZ). The replica symmetry breaking (RSB) theory, holding in the mean field regime for spin glasses, predicts a thermodynamic finite-temperature transition, even in the presence of an external magnetic field, h . According to this scenario, there exists a transition line, called the de Almeida-Thouless line, which separates the paramagnetic phase at high temperatures and fields from a spin-glass phase at lower fields and temperatures. In the droplet and TNT frameworks, instead, any infinitesimal external field is expected to destroy the SG phase. In order to study the existence of an AT line in finite di-

mensions and below the upper critical dimension of the model, the project discusses different observables, such as spin glass susceptibilities, cumulants of the overlap probability density, and Fourier transforms of the overlap correlation function.

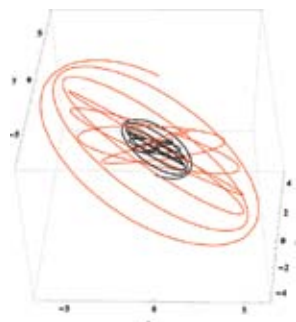
TDDFT simulations of fluorescent proteins Led by José Luis Alonso (BIFI, Theoretical Physics Department UZ). At present, biological molecules are studied with increasing interest due to both their theoretical interest and their huge applications. The Green Fluorescent Protein (GFP) is especially important, as the 2008 Nobel Prize in Chemistry confirms. The Project's aim is to develop computational and theoretical tools which enable the project to tackle such complex systems and simulate them accurately. In the frame of Time-dependent Density Functional Theory, the Project is checking different conformations of GFP and studying the influence of both the number of atoms and the environment of the GFP chromophore on the accuracy of the ground state energy and the absorption spectrum of the molecule. The results point that quantum regions can be reduced in size if such an environment is modelled as a set of classical point charges.



Comparison of electronic densities in the GFP-wt, displayed as the subtraction of density when considering classical environment minus density not considering it. A (left), B (centre) and I (right) conformations.

Numerical simulation of unsteady free surface flows Shallow water model is widely used to simulate surface geophysical flows. These situations usually involve large size domains and long time scales. Practical applications require a compromise between spatial accuracy and computational efficiency. In order to achieve the necessary spatial resolution, rather fine grids become necessary in many cases thus requiring more data storage, increasing proportionally the number of operations and reducing the allowable time step size for explicit calculations. To construct an efficient parallel implementation there are two requirements: the computational load assigned to each processor must be balanced and the communication between processors must be minimised. In the case of explicit numerical schemes this can be easily done using domain decomposition strategies. When dealing with transient inundation flows, the computational domain in the model changes during the simulation since only wet cells are included. This makes necessary a dynamic work assignment to the processors in order to keep balanced their work load. At the same time, the method used to control the correct numerical modelling of the wetting/drying fronts involves a correction step that is not fully local. This is an additional difficulty for the parallelisation structure.

Coalescence of Black Hole Binary system, Sascha Husa, Universitat de les Illes Balears



Orbital tracks of a precessing binary with mass ratio 1:3.

Abstract In this project the Group numerically solves Einstein's equations, which describe gravitation in general relativity, to study black holes and gravitational waves. The latter are generated as massive bodies that dynamically distort the surrounding space-time. The energy loss due to wave emission makes black holes in a binary system spiral together and eventually coalesce in a burst of gravitational waves. An international network of interferometric detectors that targets the detection of such signals has recently started to operate and is currently being upgraded. First gravitational wave observations are expected once upgraded detectors become operational in about five years. Optimal detection sensitivity and signal interpretation rely on being able to accurately model the orbital dynamics and gravitational wave signal, which is the goal of the Group's work.

Results Until 2005 modeling the inspiral and coalescence of black hole binaries had to rely on perturbative methods, which are known to not converge and to break down before merger. Only in recent years has it become possible to solve the Einstein equations numerically without further approximations. Numerical results like those produced by the Group are now rapidly transforming gravitational wave data analysis by adding information from the last orbits up to the merger, which occurs when the gravitational field and wave signal are strongest and represents the best chance to find entirely new physics. In recent work the Group has compared standard perturbative results for spinning binaries with numerical data; studied the accuracy of glueing together perturbative and numerical waveforms for a complete description of the coalescence process; and presented a first complete model of non-precessing spinning binaries, which is already in use to search for signals in the LIGO and Virgo gravitational wave detectors. In the Group's most recent paper it has developed a simple method to bring the complicated signals from precessing binaries into a simple normal form, paving the way for parameter studies of black hole binaries.

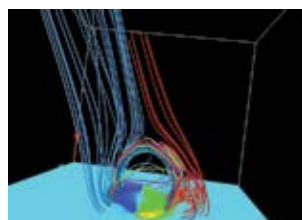
Publications Mark Hannam, Sascha Husa, Frank Ohme, P. Ajith, "Length requirements for numerical-relativity waveforms", *Phys. Rev. D* 82, 124052, December 2010.; Mark Hannam, Sascha Husa, Frank Ohme, Doreen Mueller, Bernd Bruegmann, "Black-hole binaries with non-precessing spins", *Phys. Rev. D* 82, 124008, December 2010.; Lucia Santamaria et al., "Matching post-Newtonian and numerical relativity waveforms: systematic errors and a new phenomenological model for non-precessing black hole binaries", *Phys. Rev. D* 82, 064016, September 2010.; Denis Pollney, Christian Reisswig, "Gravitational memory in binary black hole merger", accepted for publication in *Astrophysical Journal Letters*, 2010.; Patricia Schmidt, Mark Hannam, Sascha Husa, P. Ajith, "Tracking the precession of compact binaries from their gravitational-wave signal", submitted to *Phys. Rev. D*, Dec. 2010.; Ajith Parameswaran et al., "Inspiral-merger-ringdown waveforms for black-hole binaries with non-precessing spins", submitted to *Phys. Rev. Letts.*, June 2010.; Christian Reisswig, Denis Pollney, "Notes on the integration of numerical relativity waveforms, submitted to *Classical Quantum Gravity*, June 2010.

Eruptive phenomena in the atmosphere of the Sun and cool stars, Fernando Moreno-Insertis, Instituto de Astrofísica de Canarias

Abstract The global objective of this activity is to model and understand the physics of eruptive processes in the atmosphere of the Sun and cool stars via numerical experiments and computer simulations with massive parallel magnetohydrodynamical computer codes. Eruptive processes take place continually in the Sun and active cool stars; they belong to the least understood processes in stellar physics. Knowledge of these processes is essential in understanding the structure and life of the star and its effects on planets like the Earth. Two different aspects that will be studied are: (a) the process of emergence of magnetised plasma into the atmosphere in interaction with the radiation field, along with other relevant magnetohydrodynamical aspects. (b) the interaction between rising magnetised plasma and the pre-existing coronal magnetic field.

Results Results have been obtained concerning the structural properties and the time evolution of X-ray jets in the solar corona, which is the hot and extended region of the solar atmosphere in which the Sun's spectacular large-scale eruptions take place. The focus was set on jets in coronal holes, i.e., regions with open magnetic field directly linked to the interplanetary medium. The jets are launched through the collision of magnetized regions rising from the solar interior with the preexisting magnetized plasma in the coronal hole, leading to intense electric currents at the interface, field line reconnection, large temperature increase (resulting temperatures of up to 10 million degrees) and ejection of matter with velocities of order 100 km / sec. We have used coronal hole regions of different densities and studied the velocity, temperature and density of the jet, the topology of the surrounding magnetic field and the formation of plasmoids in the reconnection site. In a separate study within this activity, we have obtained the geometry of the magnetic field above convection cells using vector magnetograms obtained with the IMAx detector aboard the SUNRISE mission.

Publications Yelles Chaouche, L. Moreno-Insertis, F. et al, *The Astrophysical Journal Letters*, vol 727, L30, (2011).; Moreno-Insertis, F. & Galsgaard, K., The structure and evolution of X-ray jets in the Sun, to be submitted to *The Astrophysical Journal* in May 2011.

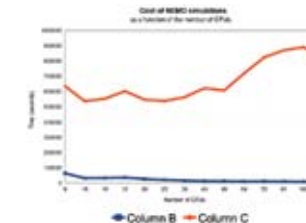


Magnetic structure of an X-ray jet following from an episode of flux emergence. The jet field lines, a plasmoid at the reconnection site, and a number of resulting hot loops are visible.

Evaluation of a global ocean simulation performance in a massively parallel system, Joaquim Ballabrera, ICM/CSIC

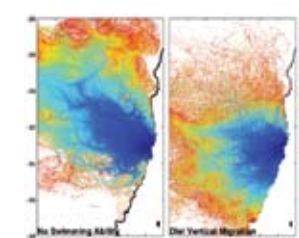
Abstract Thermohaline ocean circulation and its variability requires global ocean models rather than regional models because meridional heat and masses fluxes in regional simulations are strongly modulated by the conditions imposed at the open boundaries. Moreover, when interested in the variability of geophysical parameters, such as surface temperature or salinity, global simulations have the advantage of simultaneously investigating regions with low and high temporal variability. The aim of this Project is to evaluate the computational cost of a global simulation with a $1/2$ -degree horizontal resolution and 46 vertical levels in the RES. The Project also plans to identify the optimal use of the computational resources to allow the largest number of sensitivity studies of the model outputs to key physical parameters.

Results The main result obtained from this test activity is that the performance of the model being used strongly depends on the number of processors and the amount of data being written to disk. The results are based on a series of four-month simulations of the $1/2$ -degree horizontal resolution. The model grid is $722 \times 511 \times 76$. The simulations are identical except for the number of CPUs used by each different simulation. The number of CPUs has ranged from 9 to 121. For some of them various parallel-domain configurations are compared (e.g. 8×2 , 4×4 , and 2×8) to identify their impact on the time required by each simulation. The main result is that, without data output (only the final state is saved) the better configuration uses 25 CPUs (5×5). When data is saved every 5 days, the best configuration uses 16 CPUs (4×4). The time of each simulation is obtained by multiplying the number of processors by the difference of time between the last and first files written by the model (this assumes that the model has not be put on hold during the simulation). The results obtained seem robust and well identified minima have been obtained.



Cost of the simulation by number of CPUs. Shown is the cost of the simulation (blue), which reduces as the number of CPU increases. Also shown is the total cost (simulation length multiplied by the number of CPUs), which has an optimum at 16.

High resolution simulations of the biophysical response to climate change in the south east Pacific, Christopher Aiken, LincGLOBAL, Pontificia Universidad Católica de Chile



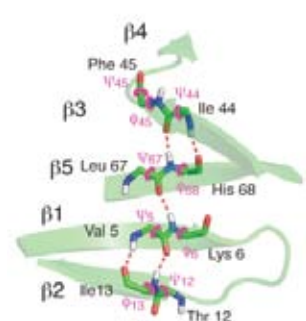
Distribution of larval positions at varying Pelagic Larval Durations (PLD) for passive (left) and vertically migrating (right) larvae released from Las Cruces, Chile.

Abstract The life history of many marine species contains a larval dispersal phase during which their fate is determined to varying degrees by the local ocean circulation. The on-going survival of such species requires that sufficient young manage to return to the population, and as a result these populations can display high sensitivity to ocean conditions. Hence the large-scale ocean circulation changes that may accompany climate change could potentially alter the viability and distribution of species along the coast. In this project we produce extended high resolution simulations of the present and possible future ocean circulation on the central Chilean coast using a state-of-the-art numerical ocean model. This will allow us to investigate the changes in larval dispersal patterns that may accompany climate change in this region.

Results Potential changes in larval dispersal patterns were determined from high resolution simulations of the coastal circulation under both present day and projected future conditions. The hydrodynamic simulations revealed that the upwelling circulation along the Chilean coast is likely to spin up over the coming century, producing an intensification of the overturning upwelling circulation and a relative reduction in coastal sea surface temperatures. The consequence of these circulation changes for coastal organisms was found to be sensitive to the larval behavior in the water column. Larvae that are advected passively were found to be less likely to return to shore under future conditions, while those that are able to vary their vertical position experienced increased rates of arrival to shore. This implies that organisms with a vertical larval migration capacity may be favored in the future at the expense of those that disperse passively. This suggests that a reorganisation in the coastal marine ecosystem of central Chile may take place over the coming century, bringing consequences for the many artisan fishermen whose livelihoods depend on coastal marine resources.

Publications Aiken CM, Navarrete SA, Pelegri JL, "Projected changes to the circulation and along-shore connectivity on the central Chilean coast", in preparation.

“Determination of native ensembles for proteins using ensemble restrained simulations, Xavier Salvatella, Institute for Research in Biomedicine (IRB)



Channel of residues responsible for the collective motion that allows ubiquitin to bind a wide range of partners

Abstract A description of the relationship between the structure and the function of proteins is not complete without a thorough understanding of dynamics. Methods are available for the characterization 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 our research is to develop procedures for the generation of such ensembles using ensemble molecular simulations restrained by the results of Nuclear Magnetic Resonance (NMR) experiments.

Results In 2010 we developed methods to characterize the dynamics of globular, multi-domain and intrinsically disordered proteins (IDPs). For each of these we chose representative systems and wrote algorithms to generate ensembles. Ubiquitin is recognized by the protein degradation machinery to target proteins for degradation. Using a method developed in 2009 we analyzed the motions of ubiquitin and found that its surface undergoes collective conformational changes that allow it to adapt to different binding partners. T4 Lysozyme is a two-domain protein. It is well-known that

its inter-domain motions are key for ligand access but no method can characterize such motions. In 2010 we developed one such method and showed that it represents the inter-domain orientations sampled in solution. Alpha synuclein is an IDP involved in Parkinson's disease. It forms neurotoxic aggregates. In 2009 we developed a method to determine ensembles of conformations that represent disordered proteins; in 2010 we used it to determine an ensemble for this protein that we will use in the fight against Parkinson's disease.

Publications Esteban-Martin S., Fenwick R. B., Adén J., Cossins B., Wolf-Watz M., Guallar V. and Salvatella X. (2011) "Direct characterization of structural heterogeneity in multi-domain proteins using NMR" under review; Fenwick R. B., Esteban-Martin S., Richter B., Lee D., Walter K. F. A., Milovanovic D., Becker S., Lakomek N. A., Griesinger C. and Salvatella X. (2011) "Long-range correlated motions in a surface patch of ubiquitin involved in molecular recognition" under review; Fenwick R. B., Esteban-Martin S. and Salvatella X. (2010) "Influence of experimental uncertainties on the properties of ensembles derived from NMR residual dipolar couplings" *J Phys Chem Lett* 1, 3438-3441.; Esteban-Martin S, Fenwick R. B. and Salvatella X. (2010) "Refinement of ensembles describing unstructured proteins" *J Am Chem Soc* 132, 4626-4632.

“Maximum-likelihood refinement of electron microscopy data, Jose María Carazo, Centro Nacional de Biotecnología - CSIC

Abstract We have developed several, unsupervised maximum-likelihood classification algorithms for structurally heterogeneous cryo-electron microscopy data sets. The co-existence of macromolecular complexes in distinct conformational states is a major problem in 3D electron microscopy, as the inability to separate them limits the resolution obtained and loses the (often functional) information that resided in these conformational differences. Applications of our methods to experimental cases have shed new lights on several biological systems, like protein synthesis by the ribosome, protein degradation by the 26S proteasome, assisted protein folding by the chaperonin CCT, and ATP synthesis by the V-ATPase motor.

Results Many vital processes in the living cell are performed by large and flexible macromolecular complexes that consist of multiple protein, RNA or smaller molecules. These complexes have been called molecular machines because just like machines invented by humans, they employ highly coordinated movements of separate parts to fulfill their often complicated tasks. Understanding how these complexes work is a strategic goal in modern biology.

However, the intrinsic flexibility of molecular machines complicates their structural characterization. Cryo-electron microscopy holds great potentials to study these machines, as individual copies that are free to adopt any conformational state may be visualized. Thereby, provided that images of different states may be separated in the computer, 3D-EM could provide structural information about multiple functional states of these machines.

The methods developed in this project allow this type of image separation, and provide the unique opportunity to visualize a range of "snapshots" along the functional cycle of these machines, which will greatly improve our understanding of how they work.

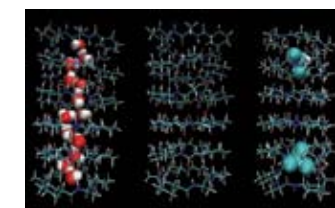
Publications K. Cheng, N. Ivanova, S.H.W. Scheres, M.Y. Pavlov, J.M. Carazo, H. Hebert, M. Ehrenberg & Martin Lindahl (2010). "tmRNA-SmpB complex mimics native aminoacyl-tRNAs in the A site of stalled ribosomes". *J. Struc. Biol.*, 169, 342-348



Two functional states of a protein folding machinery (groEL-groES), as separated using the methods developed in this project

“Study of the transport properties of nanotubes in solution and lipid bilayers, Rebeca García Fandiño, Universidad de Santiago de Compostela

Abstract Self-assembling peptide nanotubes (SPNs) made from ALPHA,GAMMA cyclic peptide nanotubes, consisting of alternating (1R,3S)-3-aminocyclohexane- or cyclopentane- carboxylic acid (GAMMA-Ach/Acp-OH) and D-ALPHA-amino acid, have structural and functional properties that may be suitable for various applications in biology and materials science. The results obtained in the group support that heterodimerization between GAMMA-Ach-based and GAMMA-Acp-based ALPHA,GAMMA CPs is not only possible, but is favoured over homodimerization for the compounds prepared. NMR and FTIR spectroscopy and X-ray diffraction data showed that cyclic ALPHA,GAMMA hexapeptides containing three GAMMA-Acp units can form stable cylindrical dimers in which antiparallel peptide rings are linked by a BETA-sheet- like set of six hydrogen bonds. Even greater stability was shown by the heterodimers of these GAMMA-Acp ALPHA,GAMMA CPs with GAMMA-Ach ALPHA,GAMMA CPs. From the structures obtained from X-ray crystallography, it is planned to construct models of peptide nanotubes to be investigated through Molecular Dynamics calculations (NAMD/AMBER). Molecular modelling method will permit the investigation of the stability, adsorption and transport of these interesting and promising systems.



Final snapshots for the simulations of hexameric SPNs in water, methanol and chloroform.

Results The structural and dynamical behaviour of a promising class of self-assembling peptide nanotubes (SPN) composed of alternating D-alpha-amino acids and (1S,3S)-3-aminocyclohexane (or pentane)carboxylic acids, has been analyzed using molecular dynamic (MD) simulations in water, MeOH and CHCl₃ with the Gromacs software package. The SPN structure is always well preserved (, mostly due to formation of a complete network of inter cyclopeptide Hbonds), but solvent-dependent dynamic alterations are evident. Such flexibility allows the generation of Hbonds with the solvent and, hence, the creation of a partial hydrophilic interior in the SPN, which explains the surprisingly good ability of the interior of the nanotube to coordinate water and also the quite slow kinetics of its transfer process. These transport properties combined with the high stability of the channel in different solvents (including very apolar ones) suggest that these nanotubes can act as good channels for transporting small polar molecules across biological membranes. On the contrary, in the presence of apolar molecules the interior remains fully hydrophobic and becomes an excellent container for apolar solvents like CHCl₃, which displays a low kon, to enter into the channel but, once inside, resides inside for long periods of time. We have also started to extend our investigations to SPNs with larger diameters of the pore, which will open the possibility of transporting bigger molecules and ions through these channels. The size of these systems implies the need to employ the power of Marenostrum to make possible such calculations in a reasonably, not-eternal, period of time.

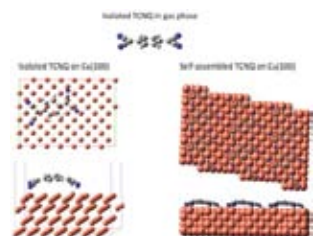
Publications R. García Fandiño, J. R. Granja, M. D'Abramo, and M. Orozco "Theoretical characterization of the dynamical behavior and transport properties of alpha,gamma-peptide nanotubes in solution", 7th Flash Conference on Bioinspired Chemistry, Book of Abstracts, page 74. Santiago de Compostela, 24-27 October 2010; A. Guerra, M. J. Pérez-Alvite, R. J. Brea, R. García-Fandiño and J. R. Granja "Covalent-Linked Self-Assembled a,g-Cyclic Peptides", 7th Flash Conference on Bioinspired Chemistry. Book of Abstracts, page 79, Santiago de Compostela Fecha: 24-27 October 2010; Rebeca García-Fandiño, Luis Castedo, Juan R. Granja, and Saulo A. Vazquez "Interaction and Dimerization Energies in Methyl-Blocked ,gamma-Peptide Nanotube Segments" *J. Phys. Chem. B*, 2010, 114 (15), pp 4973-4983; Rebeca García-Fandiño, Juan R. Granja, Marco D'Abramo, and Modesto Orozco "Theoretical Characterization of the Dynamical Behavior and Transport Properties of alpha,gamma-Peptide Nanotubes in Solution". Book of Abstracts: Expanding the frontiers of molecular dynamics simulations in biology. BSC-IRB Joint Conference. Page 29.; R. García Fandiño, J. R. Granja, M. D'Abramo, and M. Orozco "Theoretical characterization of the dynamical behavior and transport properties of alpha,gamma-peptide nanotubes in solution", 7th Flash Conference on Bioinspired Chemistry, Book of Abstracts, page 74. Santiago de Compostela, 24-27 October 2010

“The molecular bases of the transport cycle of APC antiporters, Manuel Palacín Prieto, University of Barcelona and Institute for Research in Biomedicine (IRB)

Abstract We plan to decipher the mechanistic clues determining amino acid transport (particularly Arg) across AdiC antiporter embedded in prokaryotic membranes. A combination of coarse-grained and atomistic molecular dynamics simulations will be used to determine the connection between protein movements and ligand transport. The simulations will provide important clues on the functioning of this transport, which could be experimentally verified in our laboratory by determining transport and binding of substrate in relevant AdiC mutants reconstituted in artificial proteoliposomes.

Publications Lukasz Kowalczyk, Mercè Ratera, Antonella Paladino, Paola Bartoccioni, Ekaitz Errasti-Murugarren, Eva Valencia, Guillem Portella, Susanna Bial, Antonio Zorzano, Ignacio Fita, Modesto Orozco, Xavier Carpena, José Luis Vázquez-Ibar and Manuel Palacín, "Molecular basis of substrate-induced permeation by an amino acid antiporter", PNAS published ahead of print February 22, 2011, doi:10.1073/pnas.1018081108; Molecular basis of substrate-induced permeation by an amino acid antiporter, *Proc. Natl. Acad. Sci. USA*, in press. (*, first co-authors)

Clusters as building blocks in nanotechnology: fragmentation and self assembling, Manuel Alcamí Pertejo, UAM



Structure of TCNQ (tetracyano-p-quinodimethane) in gas phase and deposited on the Cu(100) surface.

Abstract The project has two objectives: to study the fragmentation of clusters and molecules impacted by highly charged ions and to study the self-assembly of molecules on surfaces. Fragmentation has been studied in charged systems bonded either through weak interactions (water and fullerene clusters) or strong bonds (uracil and fullerenes). The study of the self-assembly of electron donors/acceptors (C60 derivatives, TTF, Thiolates...) on surfaces, aims to determine the factors that govern the process.

Self assembly of donors/acceptors can be a mechanism to improve the efficiency of organic solar cells and in collision of highly charged ions with C60 clusters new fullerenes of higher sizes and potential use in nanotechnology are formed. Fragmentation dynamics has also application in another field: to elucidate the mechanism of radiation damage.

Results In the study of fragmentation of clusters and molecules we have obtained results that are important in two different fields: nanotechnology and radiation damage. We have found that collision of ions with C60 clusters induce fullerene growing and the formation of new fullerenes. We have also studied the dynamics of fragmentation of water clusters and uracil when two electrons are removed from inner shells, a key mechanism in radiation damage and modern cancer therapies with swift heavy ions. These ultrafast dynamics can be only treated by simultaneously taking into account the electronic and nuclear movements; a formidable task that can be only achieved by using supercomputers.

In the study of the self-assembly of molecules on surfaces, we have explained the mechanism of self-assembly of PCBM on gold surfaces, where two different patterns are observed, described the structure of different molecules when deposited on a surface and shown in the case of TCNQ on Cu(100) surfaces, that the surface-molecule interactions can induce a extremely large modification of both the molecule and the substrate. In both topics the work has been done in close collaboration with experimental teams.

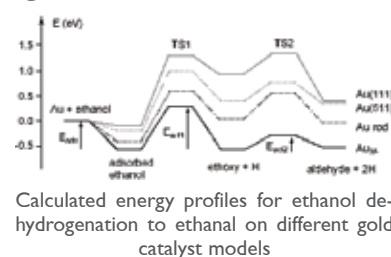
Publications T.-C. Tseng, C. Urban, Y. Wang, R. Otero, S.L. Tait, M. Alcamí, D. Ecija, M. Trelka, J.M. Gallego, N. Lin, M. Konuma, U. Starke, M.A. Herranz, F. Martín, N. Martín, K. Kern and R. Miranda, Charge Transfer-induced Structural Rearrangements at Both Sides of Organic/Metal Interfaces, *Nature Chemistry* 2, 374-379 (2010); A "News and Views" on this article has also appeared in *Nature Chemistry*. C. Santato and F. Rosei "Organic/metal interfaces: Seeing both sides" *Nature Chemistry* 2, 344-345 (2010); C. Urban, D. Ecija, Y. Wang, M. Trelka, I. Preda, A. Vollmer, N. Llorente, A. Arnau, M. Alcamí, L. Soriano, N. Martín, F. Martín, R. Otero, J.M. Gallego and R. Miranda, Growth and structure of self-assembled monolayers of a TTF derivative on Au(111), *J. Phys. Chem. C* 114, 6503-6510 (2010); J. G. Solano Canchaya, Y. Wang, M. Alcamí, F. Martín and H. F. Busnengo, Study of the interaction between short alkanethiols from ab initio calculations, *Phys. Chem. Chem. Phys.* (accepted).

Coupling of gold catalyzed hydrogenations and oxidations in single-pot processes, Avelino Corma Canós, Instituto de Tecnología Química UPV-CSIC

Abstract Gold nanoparticles supported on titanium dioxide have shown extraordinary catalytic properties in the selective oxidation of alcohols to carbonyl compounds and in the chemoselective hydrogenation of substituted nitroaromatics. Since it has been suggested that both reactions involve a common gold hydride Au-H intermediate, the possibility of coupling the two reactions in one single process will be explored. In this way, the hydrogen dissociation and oxygen activation steps could be avoided and the catalyst might be simplified. Following the same coupling philosophy, the mechanism of oxidation of anilines, which are obtained by hydrogenation of nitrocompounds in a very fast process, with molecular O₂ will be investigated in order to find the catalyst able to stop the reaction at the formation of the valuable azo compound intermediates.

Results The mechanism of selective alcohol oxidation to aldehydes on several models of gold catalysts was investigated using DFT methods. Surface reactivity increases with decreasing Au coordination number, suggesting that alcohol dehydrogenation on gold catalysts might be a structure sensitive reaction and that real gold catalysts might have heterogeneous surfaces, with Au atoms in different coordination state showing different reactivity. This hypothesis emerging from the theoretical study was experimentally confirmed by measuring the kinetics of benzyl alcohol oxidation on a series of Au/MgO catalysts having different particle diameter and therefore different concentration and distribution of low coordinated Au sites. Moreover, the interaction of the ethoxy radical formed in the first step of the mechanism with the (111), (100), (511) and (310) surfaces of Cu, Pd, Ag and Au was studied and it was found that the adsorption energy may change up to 40% on going from the (111) surface with highly coordinated atoms to the stepped (310) surface, suggesting the possibility to tune the interaction energy by surface engineering.

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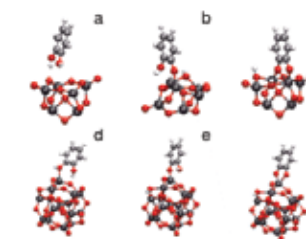
Calculated energy profiles for ethanol dehydrogenation to ethanal on different gold catalyst models

Dye-sensitized solar cells: model quantum simulations of the electrode structure and dye-electrode interactions, Javier Fdez Sanz, Universidad de Sevilla

Abstract Dye Sensitized Solar Cells (DSSC) based on organic dyes have attracted considerable attention for clean and sustainable energy. Dyes with different geometries and electronic structures show important differences as sensitizers and they can even present different mechanisms for electronic injection into the semiconductor conduction band. In this work computational simulations of TiO₂ supported dyes (catechol, alizarine, coumarin...) are reported. The electronic structure and the optical response of different dyes, free and bound to TiO₂ (one of the most common semiconductors used in DSSC) have been analysed and compared using time dependent density functional theory (TD-DFT) performed both in real time and frequency domains. Results illustrate those characteristic aspects of each sensitizer to follow different electron injection mechanisms.

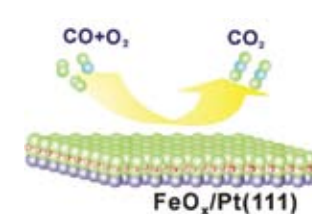
Results The electronic absorption spectrum of free alizarin shows a first band centred at 2.67 eV that upon adsorption red shifts by 0.28 eV, which is consistent with a Type I electron injection mechanism. In contrast, catechol spectrum shows a new wide band at low energy when the dye is adsorbed to TiO₂ nanoparticles, while bands of free molecule spectrum remain almost unaltered. As we step in the sequence: catechol, 2,3-naphthalenediol, C343, alizarin and NKX-2311 the electron injection moves from a purely direct mechanism to a purely indirect mechanism. Alizarin and C343 represent the intermediate behaviour in which both injections regimes are present. The electronic coupling between semiconductor conduction band and dye molecule strongly influences the electron injection mechanism. Direct mechanism requires a strong electronic coupling while weak electronic coupling favours indirect mechanism. To theoretically determine or analyse the kind of injection mechanism for a particular dye, it is necessary to include the effect of the semiconductor explicitly in the model. Computational design of more efficient dyes (and hopefully more efficient solar cells) is currently in progress.

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Adsorption of catechol on two TiO₂ model clusters: U6 (top) and U15 (bottom). Three different adsorption modes: molecular, monodentate and bidentate complexes (from left to right).

Metal clusters on oxide ultra-thin films: the way towards new materials with unprecedented properties, Gianfranco Pacchioni, Università Milano Bicocca



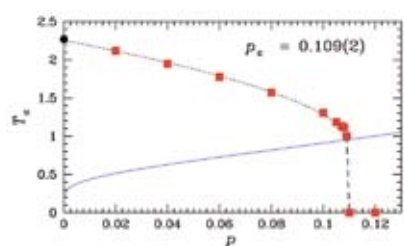
By interacting with a ultrathin FeO film on Pt under oxygen pressure CO molecules are efficiently converted into harmful CO₂

Abstract The activity is aimed at the identification of the mechanisms of nucleation, growth, and reactivity of metal nanoclusters supported on oxides surfaces and thin films. Combining theory with experiment we hope to be able to identify new practical ways to modify and functionalise thin oxide films, in order to direct the growth of the metal particles in one specific direction (e.g. flat, two-dimensional or round, three-dimensional; neutral or charged; magnetic or nonmagnetic etc.). The results can be of interest and importance in various fields, from nanocatalysis to molecular electronics.

Results A joint experimental-theoretical study on ultrathin oxide films (FeO grown on Pt) have shown that under pressure of oxygen and carbon monoxide, CO, the system behaves as an efficient catalyst which converts the CO molecules into harmful carbon dioxide, CO₂. The calculations have helped to elucidate the mechanism of the reaction. Under oxygen pressure the chemically inert FeO film transforms into a catalytically very active FeO₂ phase. This demonstrates the high structural flexibility of oxide ultrathin films which makes these materials of great interest for applications in catalysis. The work has also shown the potential of ultrathin films to stabilise nanoclusters and activate adsorbed species, relevant phenomena for the design of new catalysts.

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



“\$p\$-\$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\$”.

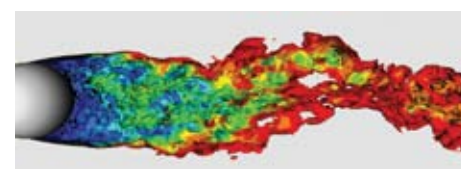
Abstract Quantum technologies, including topological quantum computation (TQC), are emerging technologies which have the potential to revolutionise computing and science. However, sensitivity to quantum noise or decoherence makes most of the current quantum computing schemes prone to error and nonscalable. 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.

Direct Numerical Simulation of turbulent natural convection flows in enclosed cavities, Assensi Oliva Llena, Universitat Politècnica de Catalunya

Abstract The Direct Numerical Simulation (DNS) of a flow past a sphere at $Re=10000$ is investigated. As the three-dimensional and time depending flow behaviour demand the use of fine grids and large integration times, there is still a lack of detailed information about turbulent statistics in the wake of the sphere. Previous DNS carried out have allowed the validation of the numerical methodology used and the CFD code developed. In this sense, the main objectives of the present project are: (i) to investigate the characteristics of turbulent flow over the sphere and the vortical structures associated and, (ii) to provide useful information about turbulent statistics for the assessment of turbulence models. The latter is of relevance for the prediction of flows with massive separation in many engineering and industrial applications.



Instantaneous velocity contours in the wake of the sphere

Results Numerical simulations of the flow over a sphere have been performed at $Re=10000$. This is the first DNS carried out for the flow past a sphere at this Reynolds number. Solutions are obtained in a cylindrical computational domain of dimensions $x=[-5D, 20D]$; $r=[0, 7D]$; $\theta=[0, 2\pi]$. The governing equations are discretised on an unstructured mesh generated by the constant-step rotation around the axis of a two-dimensional unstructured grid. The final grid simulated is about 18.2MCVs (142254x128planes). It is worth to highlight that the methodology developed for solving bodies of revolutions using unstructured grids has allowed to accurately solve the flow in the wake of the sphere with good results. The computational cost of the present computations is relatively small for the computational grids used, which is encouraging for carrying out DNS at higher Reynolds numbers with a reasonable cost of CPU time and computational resources. One of the outcomes of this projects is to give new insights into the physics of turbulence and will provide statistical data for future progresses on turbulence modelling.

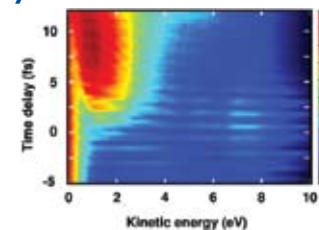
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Nuclear And Electronic Dynamics In One- And Multi-photon Ionization Of Atoms And Molecules By Ultrashort Pulses And Synchrotron Radiation, Fernando Martín García, UAM

Abstract The advent of laser technology has led to time-resolved images of ultrafast molecular phenomena, whose interpretation requires the support of accurate theoretical descriptions. Our group is pioneer in developing and applying robust theoretical methods that provide a realistic description of the dynamics of molecules subject to ultrashort laser pulses. In particular, we have worked in detailed studies on autoionising states of hydrogen molecule, describing the photoelectron emission upon autoionisation pumped by attosecond XUV pulse and recorded in the presence of a weak IR field. This work has pioneered the analysis of attosecond autoionisation dynamics in the presence of weak IR fields, leading to the understanding of the novel physics that is responsible for the striking asymmetries observed in the photoelectron spectra.

Results Ab initio time-dependent calculations with the full dimensionality of the problem were carried out to understand pump-probe experiments on H₂. This implies a high computational effort and has been feasible thanks to a parallel implementation of our codes. The MPI software and related libraries, as PETSC, and the computational support available in Mare Nostrum have been indispensable in these works: - XUV pump-IR probe experiments on autoionising states of H₂. The localization of the electronic charge distribution within the molecule has been analysed – with attosecond time-resolution – as a function of time delay; - XUV pump-XUV probe experiments. XUV pulses of 4 fs or longer lead to asymmetries in the molecular frame photoelectron angular distributions (MFPAD); whereas shorter pulses lead to symmetric ones. We have found that the combination of two pulses (attosecond pulse train) with controlled time delays still leads to asymmetric MFPADs; - XUV pump-XUV probe in double ionization of H₂. First results obtained within an independent-electron two-step model.

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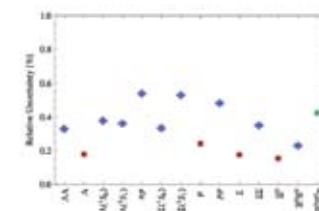
Calculated H⁺ kinetic energy distributions for the formation of H⁺ ions in two-color XUV+IR dissociative ionization of H₂ as functions of the delay between the attosecond pulse and the infrared pulse.

Study of subatomic interactions through lattice quantum chromo dynamics on MareNostrum (SAIL), Assumpta Parreno García, University of Barcelona

Abstract Quantum Chromodynamics (QCD) is the underlying theory governing the interaction between quarks and gluons, the strong force, and therefore, responsible for all the states of matter in the Universe. Analytical solutions of QCD in the low energy regime cannot be obtained due to the complexity of the quark-gluon dynamics. The only known non-perturbative method that systematically implements QCD from first principles is its formulation on a discretised space-time, lattice QCD. This numerical simulation of the theory consists in a Monte Carlo evaluation of a functional integral. Our goal is to extract information on hadronic interactions through Lattice QCD using the enormous computing capabilities that the most modern supercomputers, as Mare Nostrum, offer us, especially on those sectors where experiments are difficult to perform.

Results During the last year, we completed a series of high-statistics calculations of multi-hadron systems in four lattice volumes at a pion mass of around 390 MeV, and at a spatial lattice spacing on 0.123 fm. We obtained precise baryon masses with uncertainties at the 0.2 % -level, that have allowed for precise infinite-volume extrapolations of the masses. We found that in order for the exponentially suppressed finite-volume contributions to the baryon masses to be much smaller than the scale of nuclear binding, it is necessary to have $m(\pi) L > 2 \pi$. One exciting result that emerged from this set of calculations is the evidence for a bound H-dibaryon at this pion mass. The state in the channel with the quantum numbers of two Lambda hyperons was negatively shifted in energy in all four lattice volumes, and the analysis of the largest two lattice volumes indicated the state to be on the bound-state branch of Lüscher’s energy-eigenvalue relation. Soon after our paper was arXived, the HALQCD collaboration arXived a paper suggesting that the H-dibaryon is bound at a heavier pion mass, of around 700 MeV.

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In the figure, the relative uncertainties in the extraction of one-, two- and three-baryon ground state energies obtained in Refs. *Phys. Rev. D* 79, 114502 (2009); 80, 074501 (2009) and *Phys. Rev. D* 81, 054505 (2010) are shown.

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