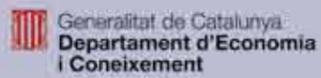


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BSC-CNS Patrons



BSC-CNS gratefully acknowledges the support of:



(10)

The 2014 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.

2014 // Annual Report





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

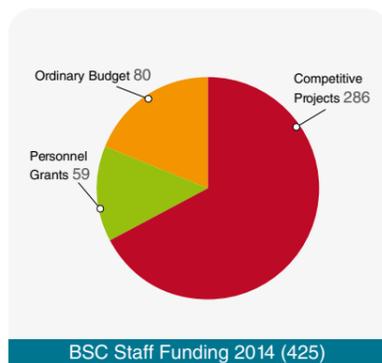
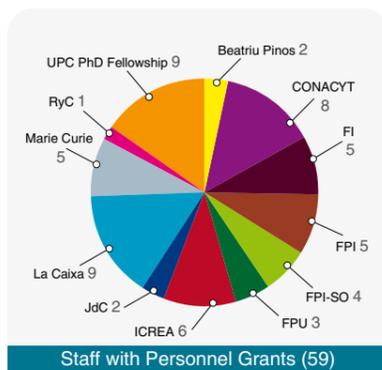


We are very proud to say that 2014 was another year of strong growth and development at BSC-CNS, with excellent scientific results from all research departments, strong growth in project activity and increased diversity of industrial collaborations.

Mission

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

The work carried out by the scientists at BSC-CNS resulted in over 155 journals, books and book chapter publications, and some 205 key conference presentations. Additionally, BSC-CNS researchers presented numerous workshops at both national and international levels, and the Centre hosted a number of key international events.



World Map of Countries of Origin

BSC-CNS has established its international profile as a leader in both HPC research and interaction with leading industry, as evidenced by its ever-increasing capacity to attract international talent from around the world for both fundamental and applied research activities. During 2014, some 513 people performed research or provided support at the Centre. Some 37% of staff are of foreign nationality, with over 48 countries represented including: Argentina, Austria, Bangladesh, Belgium, Bosnia-Herzegovina, Brazil, Bulgaria, Canada, China, Colombia, Denmark, Ecuador, Finland, France, Germany, Greece, Hungary, Iceland, India, Iran, Iraq, Ireland, Italy, Japan, Lebanon, Lithuania, Mexico, New Zealand, Pakistan, Panama, Peru, Poland, Portugal, Romania, Russian Fed., Serbia, Slovakia, South Korea, Switzerland, Syria, Taiwan, Tunisia, Turkey, Ukraine, United Kingdom, USA, Venezuela, Vietnam and Spain. As can be seen in the charts to the right, the vast majority of BSC-CNS staff are funded by competitive projects or prestigious personal fellowships such as ICREA, Marie Curie, Ramón y Cajal, and many others. That BSC-CNS has grown so strongly through competitive funding of research staff during the economic crisis of recent years is testament to the relevance and excellence of its research programs to European, national and industrial research priorities, and to the quality of its people. Highlights in this area include the three Advanced ERC Grants held by senior researchers at BSC-CNS. ERC grants are considered amongst the most distinguished and competitive of European grants, and the three projects are recognition of their groundbreaking research activities. Of

particular note is BSC-CNS's first ERC Proof-of-Concept grant, awarded to Dr. Víctor Guallar to facilitate the translation of his research results into a commercial product.

In 2014, BSC-CNS participated in one hundred and twelve externally-funded projects, with a total BSC-CNS grant of over thirty-nine million euros. Forty-six projects were funded by the extremely Seventh competitive Framework Programme of the European Commission (FP7) and the Centre began its first project funded by the Horizon 2020 programme. Five of the FP7 projects were led by BSC-CNS, in which the Centre coordinated partners based all around Europe. One project was funded

BSC-CNS Achieves HR Excellence in Research Award

As a direct result of actions initiated as part of the Severo Ochoa Programme, in 2014 BSC-CNS achieved the HR Excellence in Research Award, bestowed by the European Commission in recognition of the Centre's progress in aligning human resource policies with the principles set out in the European Charter and Code for Researchers, and providing a stimulating and favourable working environment where researchers can expect fair and transparent recruitment practices and appraisal procedures.

by the Artemis Joint Technology Initiative on embedded computing. Twenty-five projects were funded by Spanish National or Catalan funds including the Centre's Severo Ochoa award and its Consolider projects. Of the other projects, twenty-four were research activities funded by private companies, eight were funded by Spanish and international public bodies, including the UN, Barcelona City Council, Fusion for Energy and ITER, and four were funded by the European Space Agency (ESA). The Marató funding program, which supports scientific research into diseases which are currently incurable, financed two of the projects through donations from the public. The Centre also managed numerous personnel grants funded by ICREA, la Caixa, and CONACYT, among many others.

The year also saw further hardware and systems development of MareNostrum III, the main supercomputer at BSC-CNS. These include a new server to perform specific pre-and post-processing analysis that requiring large shared memory systems, upgraded nodes to accommodate memory-bound parallel applications, two new servers based on the cutting-edge Power8 processor technology to perform research in Big Data, computer architecture and parallel application development, security enhancements for access, and a BigData infrastructure to receive and store all MareNostrum III jobs information. A new User Portal interface was launched, enabling users to better understand the behaviour of their applications and the resources used during their execution. MareNostrum III is one of only six nodes in four countries that together form the pan-European PRACE (European HPC Infrastructure Initiative) Tier-0 network, which provides world-class supercomputing services to European scientists, and as such 70% of its capacity is dedicated to PRACE. A further 24% of MareNostrum III capacity, along with capacities provided by other nodes in the Spanish Supercomputing Network (RES), is available for public access via the Spanish (RES) Access Protocol, thus guaranteeing Spanish scientists access to first-class supercomputing services. The final 6% capacity is reserved for use by BSC-CNS scientists.

Efficient Computing

A major achievement of MareNostrum III has been its power efficiency. Two full years of operation of MareNostrum III have delivered a 10-fold increase in computing power over the previous MareNostrum II, with an increased power consumption of only 10%. This significant achievement is due to the advanced technologies developed and deployed by BSC-CNS and the diligent management of the facility by the BSC-CNS Operations Department.

A total of 237 activities were run on RES nodes during 2014. This brings to more than 2,380 the number of different projects awarded computing time on the RES network since its establishment in 2006. Despite large increases in computing capacities in previous years, demand continues to exceed supply with an increasingly diverse array of scientists requesting access. In 2014, BSC-CNS increased dissemination and training events in order to support both users and RES node technicians.



BSC-CNS Patronage

Patrons of BSC-CNS

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

The income of BSC-CNS in 2014 was €25 M, of which €13.7 M corresponded to ordinary budget and strategic investments funded by the patrons of BSC-CNS, the Spanish and Catalan Governments; and €11.2 M from competitive projects (up from €10.1 M in the previous year), just under a third of which was derived from projects with private companies.

Since its inception, BSC-CNS has collaborated with many of the world's leading IT companies. Industrial collaborations have grown year on year, and now include many major IT companies (IBM, Intel, Microsoft, NVIDIA and SAMSUNG), as well as major multinationals from the energy sector (Repsol and Iberdrola), space technologies with the European Space Agency, applications in Life sciences with multinational biotech and pharmaceutical companies (Astrzeneca, Novozymes and Schrödinger), and major global public agencies relating to climate and air pollution modelling (WMO, NOAA and UNEP). A total of 32 private projects with industry and public agencies were active in 2014. Technology transfer at BSC-CNS reached a new milestone in 2014 with the Board approving the formation of the Centre's first spin-off company, **Nostrum Biodiscovery**, to offer chemical computational services (principally drug discovery). BSC-CNS is developing technologies in a broad range of industrially-relevant areas, including IT hardware and software (programming models, performance tools, energy efficient hardware, middleware and system software); bioinformatics tools for target and drug discovery; embedded electronics for improving safety in time-critical applications; air quality, weather and climate modelling products; and simulations of complex problems.

HPC and Big Data

BSC-CNS is focusing very strongly on developing HPC technologies for Big Data applications. Big Data problems requiring rapid processing of massive amounts of data are increasing in importance in many scientific and technological fields, including biomedicine, environment, smart cities, mining and resources, engineering and even social sciences. BSC-CNS has been working for many years on improving HPC capabilities for these sorts of applications, from energy-efficient hardware to user-friendly programming models and performance tools. Boosted by the Severo Ochoa programme and participation in major Big Data projects such as PanCancer, the International Cancer Genome Consortium, TransPLANT, Human Brain Flagship, and multi-scale dust and pollution modelling for Europe and North Africa, the increasing convergence of HPC and Big Data was a major feature of BSC-CNS research in 2014.

JLESC - Joint Laboratory on Extreme Scale Computing

In 2014, the University of Illinois at Urbana-Champaign, INRIA, Argonne National Laboratory, Jülich Supercomputing Centre, Riken AICS and BSC-CNS came together to form the Joint Laboratory on Extreme Scale Computing (JLESC). The Joint Laboratory focuses on software challenges found in extreme scale high-performance computers. Research areas include:

- Scientific applications (Big Compute and Big Data).
- Modelling and optimising numerical libraries, which are at the heart of many scientific applications.
- Novel programming models and runtime systems to take full advantage of extreme-scale supercomputers.
- Resilience and fault-tolerance research, which reduces the negative impact when processors, disk drives, or memory fail in supercomputers.
- I/O and visualisation for numerical simulations and data analytics.
- HPC Clouds.

At the European level, BSC-CNS plays a very active role in the HPC Technology Platform and PRACE, which respectively define and implement the vision for the future of HPC infrastructure for R&D in Europe. Senior BSC-CNS staff regularly participate in committees, roadmapping forums, and international liaison activities, while BSC-CNS and its patrons remain committed to maintaining Tier-0 status as a key node in the PRACE network servicing scientists throughout Europe and beyond. During 2014, BSC-CNS developed and participated in a record number of project proposals under the European H2020 framework. This reflects the broad range of HPC related disciplines developed at BSC-CNS, including Big Data, Extreme Scale Computing, Open MP, alternative architectures, performance tools and grid computing, to name a few. In addition to research excellence, BSC-CNS places great importance on training at all levels. The appointment in recent years of dedicated edu-

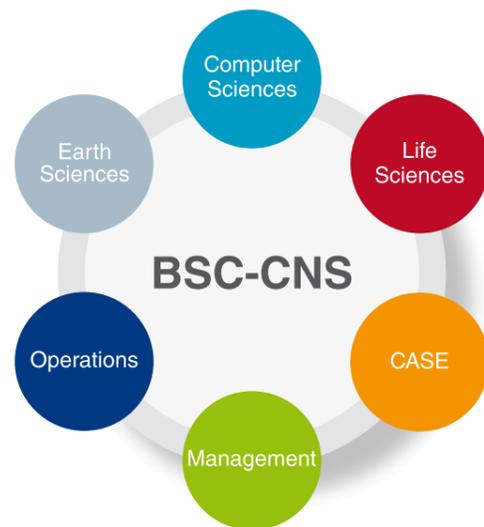
cation and training staff is bearing fruit with a range of new training initiatives underway, including professional training programs (PRACE, RES and CUDA courses), research seminars, joint activities with universities (MSc in HPC, scholarships and internships), scientific workshops and renowned summer schools.

At the international level, BSC-CNS is driving the establishment of the RISC network (Iberoamerican Supercomputing Network) via CYTED (Iberoamerican Program for Science and Technology Development). Involving Argentina, Brazil, Belgium, Chile, Colombia, Italy, México, Portugal and Spain, RISC aims to deepen strategic R&D cooperation between Europe and Latin America in HPC by building a multinational and multi-stakeholder community, including researchers, policy makers and users.

Support and Research

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

The 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 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 **Computer Sciences Department** continued its strong research in all areas of HPC development and its deep collaborations with industry leaders, including Intel, NVIDIA, Microsoft, IBM, Samsung, Xilinx, and Qualcomm, amongst others. In addition to continued expansion of international collaborations with other leading HPC centres, in particular through the JLESC network, the Department is increasingly interacting with the other research departments of BSC-CNS on multi-disciplinary projects. This is due in large part to the Severo Ochoa program.

Highlights of 2014 include the Department's participation in some 27 European FP7 projects, two ERC grants, ongoing participation in key networks such as ETP4HPC, HiPEAC-3, and the SCALUS Marie Curie training network, the ever-broadening array of industrial collaborations, and projects with the European Space Agency.

The **Earth Sciences Department** experienced a major change in November 2014 with the retirement of director José María Baldasano after almost 10 years at the helm, and the appointment of Francisco J. Doblas-Reyes as the new director, with Prof. Baldasano remaining at BSC-CNS as a research fellow. ICREA Prof. Doblas-Reyes joins BSC-CNS from the Catalan Institute of Climate Sciences (IC3) where his main research focused on climate variability, modelling and prediction for the development of climate services on time scales ranging from one month to several years.

The Department continued its extensive activities in modelling atmospheric dust and pollution, including running the daily high-resolution operational air quality forecasts for Europe and Spain under the umbrella of the CALIOPE project, and also mineral dust forecasts for the Euro-Mediterranean region and East Asia. A highlight of the year was the creation in February of the Barcelona Dust Forecast Center, the first Regional Specialized Meteorological Center with activity specialisation on Atmospheric Sand and Dust Forecast (RSMC-ASDF). It operationally generates and distributes predictions for Northern Africa, Middle East and Europe.

The **Life Sciences Department** also saw new developments in 2014 with the integration of researchers from the Centre for Genomic Regulation (CRG) into the Joint IRB-BSC Research Program on Computational Biology. The Department worked in a diverse range of European projects and industrial collaborations, producing a number of notable scientific discoveries in structural biology and genomics. The Centre's first spin-off company was approved to commercialise a number of drug discovery tools developed by the Department, and an ERC Proof-of-Concept grant helped refine the Department's PELE platform for drug design for more commercial applications.

The **CASE Department** underwent a restructure during 2014 to better support the increasing diversity of the Department's industrial collaborations. The new structure consists of three horizontal groups that develop core components and tools, which are used by the other three vertical groups who develop complete solutions to problems in Environmental, Geoscience and Computational Mechanics fields. Work continued on long-term projects with Repsol and Iberdrola, while a number of international collaborations in the biomedical field (cardiovascular and respiratory simulations) achieved significant progress thanks to support by the Severo Ochoa program.

The **Operations Department** performed further upgrades of BSC-CNS's HPC installations, and launched a new interface for users providing them with better understanding of the performance of their applications. The acquisition of IBM's server business by Lenovo gave new impetus to the Department's plans for future developments of the MareNostrum supercomputer, which is based on IBM hardware. The

Department also participated in a number of strategic projects at European level, such as PRACE 2nd and 3rd Implementations, EESI2 to develop a vision of future European Petaflop machines, EUDAT to provide a pan-European solution for research data, and RDA Europe to conduct cross-infrastructure experiments on global interoperability.

Directors' Office

The Directors' Office is a small cadre of multidisciplinary individuals who manage a variety of strategic actions directly promoted by the BSC-CNS Director and Associate Director. These include the Directors' personal assistants, the co-ordinator of the Severo Ochoa programme, the coordinators for European Relations and Latin American Relations, the Education and Training team, and the coordinator of Media Relations and Protocol.



Summing up, 2014 saw BSC-CNS continue to provide world-class supercomputing services to scientists throughout Spain and Europe, while continuing strong growth in research activities in areas of high relevance to a range of industrial and societal needs. The challenges posed by the new European H2020 funding program were met head-on, with the Centre demonstrating its capacity for adaptability combined with long-term strategic vision to emerge as a strong leader at national and European levels in key research consortia and networks. The sustained growth of the Centre over many years has created new challenges in areas such as human resources and other support services. The Severo Ochoa program has been critical in helping BSC-CNS step up to the next level, as evidenced by the HR Excellence in Research award and other key achievements of the Centre's support departments.

The Directors wish to extend their profound thanks to all BSC-CNS staff, students, and collaborators, and in particular recognise the continued strong support of the BSC-CNS patrons, MINECO, DECO and UPC, and other key funding and support agencies such as the European Commission, Repsol, ICREA, CSIC and the European Research Council. It is thanks to the dedication, effort and commitment of the whole team that this very positive report on 2014 has been achieved.

Mateo Valero, Director

Francesc Subirada, Associate Director

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

As at 31 December 2014, the core staff of BSC-CNS included 87 permanent positions, 196 staff dedicated to specific projects and 97 scholarship students. These numbers were significantly augmented by additional staff who participated in BSC-CNS via a number of programmes.

Total personnel who worked at BSC-CNS throughout the year increased from 464 during 2013 to 513 during 2014, mainly through new temporary and shared staff, resident students and collaborating and visiting researchers.

Shared Staff and Human Resources Programmes

In addition to its own staff, BSC-CNS hosts shared staff from other public institutions such as the Universitat Politècnica de Catalunya (UPC), Fundació Bosch i Gimera (UB), the Institute for Research in Biomedicine (IRB) and the Consejo Superior de Investigaciones Científicas (CSIC). In 2014, BSC-CNS also welcomed high level scientific personnel from special human resources public programmes such as the Ramón y Cajal Programme, the ICREA Programme and other personnel training research programmes sponsored by various Spanish ministries.

The BSC-CNS Fellowship Programme

The BSC-CNS Fellowship programme 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 2014, BSC-CNS hosted 109 student researchers associated with several research projects.

ICREA

Created in 2001, the Catalan Institution for Research and Advanced Studies (ICREA) is a foundation supported by the Government of Catalonia and governed by a Board of Trustees. Its aim is to promote research in any field of knowledge, facilitating the consolidation of collective research and the retention of talented research staff within the Catalan university and research centre system. ICREA, through a selection process based on scientific talent, hires senior scientists from around the world to work in and cooperate with local universities and research centres. BSC-CNS was proud to host 6 ICREA professors during 2014.



CSIC

The Spanish National Research Council (CSIC) is the largest public institution dedicated to research in Spain and the third largest in Europe. Belonging to the Spanish Ministry of Economy and Competitiveness through the Secretary of State for Research, Development and Innovation, its main objective is to develop and promote research that will help bring about scientific and technological progress, and it collaborates with Spanish and foreign entities in order to achieve this aim. BSC-CNS was proud to host 4 CSIC researchers during 2014.



UPC

The Universitat Politècnica de Catalunya · BarcelonaTech (UPC) is a public institution dedicated to higher education and research, specialised in the fields of engineering, architecture and science. As a leading member of international networks of excellence, the UPC has a privileged relationship with global scientific and educational organisations and therefore is well positioned for attracting international talent. UPC participates in the governing Board of BSC-CNS, and in 2014 assigned 17 researchers and professors to BSC-CNS.



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Ernest Quingles, Manager.

Commission Secretaries

Ramón Fernández Calvo, State lawyer.

Sue de Antonio Calvo, State lawyer.

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Mateo Valero, Director.

Francesc Subirada, Associate Director.

Ernest Quingles, Manager.

Commission Secretaries

Ramón Fernández Calvo, State lawyer.

Sue de Antonio Calvo, State lawyer.



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Prof. Janet Thornton, Director European Bioinformatics Institute, United Kingdom.

Dr. Satoshi Matsuoka, Professor of the High Performance Computing Systems Group Tokyo Institute of Technology, Japan.

Dr. Thomas Zacharia, Executive Vice President of Research & Development, Qatar Foundation.

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

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

Prof. Leonard Barrie, Bolin Centre for Climate Research Stockholm University.

Management Board

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Mateo Valero, Director.

Management Board Vice-Chairman

Francesc Subirada, Associate Director.

Members

Jesús Labarta, Computer Sciences Director.

Eduard Ayguadé, Computer Sciences Associate Director.

José María Baldasano, **Francisco J. Doblas-Reyes**, Earth Sciences Director.

Modesto Orozco, Life Sciences Director.

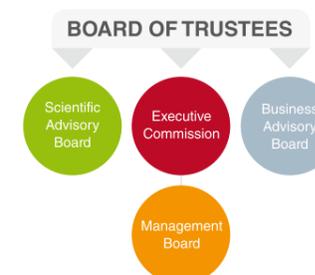
Sergi Girona, Operations Director.

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

Ernest Quingles, Management Director.

Strong Governance

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



Access Committee

Core Team

Julio Bravo, Agencia Nacional de Evaluación y Prospectiva.

Alfonso Tarancón, Universidad de Cantabria.

Joaquín Serrano, Ministerio de Ciencia e Innovación.

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

Biomedicine and Health Sciences Expert Panel

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

Assistant: **Andrés Aguilera**, Universidad de Sevilla.

Chemistry and Material Sciences Expert Panel

Coordinator: **Elvira Guardia**, Universitat Politècnica de Catalunya.

Assistant: **Mariona Sodupe**, Universitat Autònoma de Barcelona.

Physics and Engineering Expert Panel

Coordinator: **Francisco Domínguez-Adame**, Universidad Complutense de Madrid.

Assistant: **Francisco Castejón**, CIEMAT.

Astronomy, Space and Earth Sciences Expert Panel

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

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

RES Users Committee (CURES)

Physics and Engineering (FI) representatives

Javier Jiménez Sendín, **Fernando Martín García**.

Chemistry and Material Sciences (QCTM) representatives

Rubén Pérez, **Núria López**

Biomedicine and Health Sciences (BCV) representatives

Carme Rovira, **Francisco Javier Luque**.

Astronomy, Space and Earth Sciences (AECT) representatives

Jordi Torra, **Miguel Ángel Aloy**.

BSC-CNS Staff and Collaborators during 2014

Directors Office

Director: **Mateo Valero Cortés**.

Associate Director: **Francesc Subirada Curcó**.

Director Assistant: **Lourdes Cortada Agustí**.

Associate Director Assistant: **Judith Camba Alvariño**.

Research Fellow: **José María Baldasano Recio** (UPC).

European Relations Senior Advisor: **Fabrizio Gagliardi**.

Latin America Relations Coordinator: **Ulises Cortés García** (UPC).

Severo Ochoa Program Coordinator: **Josep Casanovas** (UPC).

Associate Researcher: **Anna Ripoll Aracil**.

Associate Researcher: **Fermín Sánchez Carracedo**.

Visiting Collaborator: **Daniel Jiménez**.

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RES Technical and Training Coordinator: **Montserrat González Ferreiro**.

Professional HPC Training: **Evguenia Stoilova Alexandrova**.

Visiting Collaborator: **Darío Casaburi**.

Press & Protocol

Press and Protocol Relations Manager: **Gemma Ribas Maspoch**.

Computer Sciences Department

Computer Sciences Director: **Jesús Labarta Mancho**.

Computer Sciences Associate Director: **Eduard Ayguadé Parra**.

Computer Sciences Director Assistant: **Núria Sirvent Pardell**.

PhD Student: **Dario García Gasulla**.

Accelerators for High Performance Computing

Accelerators for High Performance Computing Group Manager: **Nacho Navarro**.

Junior Researcher: **Javier Cabezas Rodríguez**.

PhD Student: **Diego Marrón Vida**.

PhD Student: **Ivan Tanasic**.

PhD Student: **Marc Jorda Peroliu**.

PhD Student: **Víctor García Flores** (BECA UPC).

Master Student: **Pau Farré González**.

Autonomic Systems and e-business Platforms

Autonomic Systems and e-Business Platforms Group Manager: **Jordi Torres Viñals** (UPC).

Senior Researcher: **David Carrera Pérez** (UPC).

Senior Researcher: **Jordi Guitart Fernández** (UPC).

Senior Researcher: **Yolanda Becerra** (UPC).

Postdoctoral Researcher: **Jordà Polo Bardes**.

Postdoctoral Researcher: **Josep Lluís Berral García**.

Postdoctoral Researcher: **Mario Macías Lloret**.

Postdoctoral Researcher: Nicolás Poggi Mastrokalo.
 Junior Developer: Álvaro Villalba Navarro.
 Junior Developer: Cesare Cugnasco.
 Junior Developer: David Ortiz López.
 Junior Developer: Jordi Aranda Flores.
 Junior Developer: Josep Subirats Castell.
 Junior Developer: Juan Luis Pérez Rico.
 Junior Developer: Mauro Canuto.
 PhD Student: José Alejandro Cordero Rama (La Caixa).
 PhD Student: Marcelo Carneiro do Amaral.
 PhD Student: Nesrine Khouzami.
 Associate Researcher: Jordi Nin Guerrero (UPC).
 Associate Researcher: Rubén Tous Liesa (UPC).
 Trainee Developer: Aaron Call Barreiro.
 Trainee Developer: Guillem Alomar Sitjes.
 Trainee Developer: Roger Hernández Domingo.
 Undergraduate Student: Josep Cugat Prieto.
 Visiting Collaborator: Daniel Cea.

Computer Architecture / OS Interface (CAOS)

Computer Architecture / OS Interface (CAOS) Group Manager: Francisco Javier Cazorla Almeida (CSIC - UPC).
 Senior Researcher: Eduardo Quiñones Moreno.
 Senior Researcher: Jaume Abella Ferrer.
 Postdoctoral Researcher: Carles Hernández Luz.
 Junior Developer: David Morales Sáez.
 Junior Developer: Mikel Fernández Oreja.
 PhD Student: Javier Jalle Ibarra.
 PhD Student: José Carlos Ruíz Luque.
 PhD Student: Leonidas Kosmidis (FPU-UPC).
 PhD Student: Milos Panic (FPU-BSC).
 PhD Student: Mladen Slijepcevic (La Caixa).
 PhD Student: Phuong Tran Gia.
 PhD Student: Qixiao Liu.
 PhD Student: Roberto Vargas Caballero.
 Associate Researcher: Kamil Kedzierski.
 Master Student: David Prat Robles.
 Master Student: David Trilla Rodríguez.
 Master Student: Gabriel Fernández Díaz.
 Master Student: Maria Aston Serrano Gracia.
 Master Student: Suzana Milutinovic.
 Undergraduate Student: Francesc Gispert Sánchez.
 Visiting Collaborator: Calvin Bulla.
 Visiting Collaborator: Enrique Díaz.
 Visiting Collaborator: Jaume Espinosa.

Computer Architecture / OS Interface (CAOS) - Runtime Aware Architectures

Senior Researcher: Marc Casas Guix (Beatriu Pinos)
 Senior Researcher: Miquel Moretó Planas
 Junior Developer: César Allande Álvarez
 PhD Student: Dimitrios Chasapis (FPI-SO)
 PhD Student: luc Jaulmes (FPU-BSC)
 PhD Student: Paul Caheny
 Master Student: Cristóbal Ortega Carrasco
 Master Student: Iulian Brumar
 Master Student: Vladimir Dimic
 Undergraduate Student: Raúl Vidal Ortiz

Computer Architecture for Parallel Paradigms

Computer Architecture for Parallel Paradigms Group Manager: Adrián Cristal Kestelman (CSIC - UPC).

Computer Architecture for Parallel Paradigms Group Manager: Osman Unsal (RyC).
 Postdoctoral Researcher: Adrià Armejach Sanosa.
 Postdoctoral Researcher: Ferad Hasanov Zyulkyarov.
 Postdoctoral Researcher: Georgios Passas.
 Postdoctoral Researcher: Nehir Sonmez.
 Postdoctoral Researcher: Óscar Palomar Pérez (UPC).
 Postdoctoral Researcher: Santhosh Kumar Rethinagiri.
 Junior Developer: Francisco Javier Arias Moreno.
 PhD Student: Azam Seyedi.
 PhD Student: Behzad Salami.
 PhD Student: Daniel Nemirovsky.
 PhD Student: Gulay Yalcin.
 PhD Student: Ivan Ratkovic (FPU-UPC).
 PhD Student: Milan Stanic (FI-BSC).
 PhD Student: Milovan Duric.
 PhD Student: Nikola Markovic (FPI-UPC).
 PhD Student: Omer Subasi (FI-UPC).
 PhD Student: Oriol Arcas Abella.
 PhD Student: Srdjan Stipic.
 PhD Student: Tassadaq Hussain.
 PhD Student: Timothy Hayes (FPU-UPC).
 PhD Student: Vasileios Karakostas (FPU).
 PhD Student: Vesna Nowack.
 PhD Student: Vladimir Gajinov.
 Associate Researcher: José Ruben Titos.
 Visiting Collaborator: Abhari Morteza Biglari.
 Visiting Collaborator: Abraham Josafat Ruiz Ramírez.
 Visiting Collaborator: Cristóbal Ramírez.
 Visiting Collaborator: Eduardo Ramírez.
 Visiting Collaborator: Furkan Ayar.
 Visiting Collaborator: Gorke Alp Malazgirt.
 Visiting Collaborator: Hamzeh Ahangari.
 Visiting Collaborator: Rasha Faqeh.
 Visiting Collaborator: Sanketh Nalli.
 Visiting Collaborator: Serhat Gesoglu.
 Visiting Collaborator: Tatiana Martsinkevich.

Extreme Computing

Extreme Computing Group Manager: Vassil Nikolov Alexandrov (ICREA).
 Postdoctoral Fellow: Oscar Alejandro Esquivel Flores (CONACYT).
 Visiting Collaborator: Dobromir Georgiev.
 Visiting Collaborator: Florian Urmetzer.
 Visiting Collaborator: Jean Michel Sellier.
 Visiting Collaborator: Qi zhi Quan.
 Visiting Collaborator: Sofiya Ivanovska.
 Visiting Collaborator: Tzvetan Tomov Ostromsky.

Grid Computing and Clusters

Grid Computing Group Manager: Rosa Maria Badia Sala (CSIC - UPC).
 Senior Researcher: Daniele Lezzi.
 Senior Researcher: Raúl Sirvent Pardell
 Postdoctoral Fellow: Fredy Juárez Pérez (CONACYT).
 Postdoctoral Researcher: Enric Tejedor.
 Postdoctoral Researcher: Pieter Bellens.
 Junior Researcher: Jorge Ejarque Artigas.
 Junior Researcher: José María Pérez Cáncer.
 Research Support Technician: Judit Planas Carbonell.

Junior Developer: Carlos Díaz Suárez.
 Junior Developer: Kalliopi Chronaki.
 PhD Student: Francesc Lordan Gomis (FPI-UPC).
 PhD Student: Jan Ciesko.
 PhD Student: Marta García Gasulla.
 PhD Student: Rahul Gayatri.
 PhD Student: Sicong Zhuang.
 PhD Student: Tomasz Patejko.
 PhD Student: Vinoth Krishnan Elangovan.
 Master Student: Cristian Ramon-Cortés Vilarrodona.
 Master Student: Pedro Benedicte Illescas.
 Trainee Developer: Javier Álvarez Cid-fuentes.
 Trainee Developer: Roger Rafanell Mas.

Heterogeneous Architectures

Heterogeneous Architectures Group Manager: Álex Ramírez Bellido.
 Associate Researcher: Agustin Fernández Jiménez.
 Associate Researcher: Julio Ramón Beivide Palacio.
 Visiting Collaborator: Hyunsung Shin.

Heterogeneous Architectures - Architecture Simulation Environments

Senior Researcher: Alejandro Rico Carro.
 Junior Developer: Francesc Martínez Palau.
 PhD Student: Nikola Rajovic.
 PhD Student: Thomas Grass (FI-UPC).
 PhD Student: Ugljesa Milic (FPI-UPC).
 Master Student: Constantino Gómez Crespo.

Heterogeneous Architectures - Memory Technologies

Postdoctoral Researcher: Petar Radojkovic.
 PhD Student: Darko Zivanovic.
 PhD Student: Kazi Asifuzzaman.
 PhD Student: Milan Pavlovic.
 PhD Student: Milan Radulovic.

Heterogeneous Architectures - Microserver Architectures & System Software

Senior Researcher: Paul Matthew Carpenter.
 Junior Developer: Vishal Mehta.
 PhD Student: Branimir Dickov.
 PhD Student: Karthikeyan Palavedu Saravanan (FI).
 PhD Student: Luis Ángel Garrido Platero.
 PhD Student: Renan Fischer e Silva.

Heterogeneous Architectures - Mobile and Embedded-Based HPC

Postdoctoral Researcher: Filippo Mantovani.
 Undergraduate Student: Alice Valentini.
 Undergraduate Student: Daniel Ruiz Muñoz.
 Undergraduate Student: Josep Oriol Vilarrubí Barri.
 Undergraduate Student: Luna Backes Drault.

Performance Tools

Performance Tools Group Manager: Judit Giménez Lucas (UPC).
 Senior Researcher: José Carlos Sancho Pitarch (RyC).
 Postdoctoral Researcher: Claudia Andreina Rosas Mendoza.
 Postdoctoral Researcher: Estanislao Mercadal Melia.
 Postdoctoral Researcher: Steluta Iordache.
 Postdoctoral Researcher: Vladimir Subotic.
 Junior Researcher: Francesc Xavier Pegenaute Bresme.
 Junior Researcher: German Lloret Sánchez.

Junior Researcher: Harald Servat Gelabert.
 Junior Researcher: Hugo Daniel Meyer.
 Junior Researcher: Juan González García.
 Junior Developer: Eloy Martínez Hortelano.
 Junior Developer: Laura Auton García.
 Junior Developer: Pedro Antonio González Navarro.
 PhD Student: Ana Jokanovic.
 Master Student: Arturo San Emeterio Campos.
 Undergraduate Student: Alejandro Velasco Jiménez.
 Visiting Collaborator: Hans Christian Hoppe.

Programming Models

Programming Models Group Manager: Xavier Martorell Bofill (UPC).
 Senior Researcher: Isaac Juan Rudomin.
 Senior Researcher: Vicenç Beltran Querol.
 Postdoctoral Fellow: Benjamín Hernández Arreguin (CONACYT).
 Senior Developer: Julián David Morillo Pozo.
 Junior Researcher: Javier Teruel García.
 Junior Researcher: Roger Ferrer Ibáñez.
 Junior Developer: Bence Kodaj.
 PhD Student: Alejandro Fernández Suárez.
 PhD Student: Antonio Filgueras Izquierdo.
 PhD Student: Diego Caballero de Gea (FI).
 PhD Student: Diego Nieto Muñoz.
 PhD Student: Fahimed Yazdanpanah Ahmada.
 PhD Student: Guray Ozen.
 PhD Student: Javier Bueno Hedo.
 PhD Student: Lluc Álvarez Martí.
 PhD Student: Lluís Vilanova García.
 PhD Student: Rajiv Nishtala.
 PhD Student: Sara Royuela.
 PhD Student: Vasileios Koutsoumpos.
 PhD Student: Víctor Hugo Pérez Váldez (CONACYT).
 PhD Student: Xubin Tan.
 Associate Researcher: Carlos Álvarez.
 Associate Researcher: Daniel Jiménez.
 Associate Researcher: Guillermo Miranda.
 Associate Researcher: Julita Corbalán González.
 Associate Researcher: Marc González Tallada.
 Associate Researcher: Marisa Gil.
 Associate Researcher: Montserrat Farreras.
 Master Student: Albert Segura.
 Trainee Developer: Florentino Sainz Manteca.
 Trainee Developer: Jorge Bellón Castro.
 Trainee Developer: Marçal Solà Vélez.
 Trainee Developer: Sergi Mateo Bellido.
 Trainee Developer: Víctor López Herrero.
 Undergraduate Student: David Guillen Huerga.
 Undergraduate Student: Marcos del Amo.
 Undergraduate Student: Marcos Maroñas Bravo.
 Visiting Collaborator: Robert Briggs.
 Visiting Collaborator: Robert Eduard Strzodka.
 Visiting Collaborator: Yale Patt.

Storage Systems

Storage Systems Group Manager: Antonio Cortés Rosselló (UPC).
 Senior Researcher: Anna Queral Calafat.
 Senior Researcher: Ramón Nou Castell.
 Junior Researcher: Alberto Miranda Bueno.

Junior Researcher: Ernest Artiaga Amouroux.
 Junior Researcher: Jonathan Martí Fraiz.
 Junior Researcher: Juan José Costa Prats.
 Trainee Developer: Alex Barceló Cuerda.
 Trainee Developer: Daniel Gasull Moreira.
 Visiting Collaborator: Christos Filippidis.
 Visiting Collaborator: Luis Carlos Erpen de Dona.
 Visiting Collaborator: Pablo Andrés.
 Visiting Collaborator: Pablo Pessolani.

Unconventional Computer Architecture and Networks

Unconventional Computer Architecture and Networks Group Manager: Mario Nemirovsky (ICREA).
 Postdoctoral Fellow: Alexandro Castellanos Mier (CONACYT).
 PhD Student: Damian Roca Marí (La Caixa).
 PhD Student: Francesco Ciaccia.

Earth Sciences Department

Earth Sciences Director: **Jose María Baldasano Recio**.
Francisco J. Doblas-Reyes.

Visiting Collaborator: Julian Jaramillo.

Air Quality

Earth Sciences Associate Director: Santiago Gassó Domingo.
 Senior Researcher: Antonios Gkikas.
 Senior Researcher: Gustavo Arévalo Roa.
 Postdoctoral Fellow: Sergio Natan González Rocha (CONACYT).
 Postdoctoral Researcher: Maria Teresa Pay (Beatriu Pinos).
 Postdoctoral Researcher: Valentina Sicardi.
 Research Support Coordinator Technician: Kim Serradell Maronda.
 Junior Researcher: Marc Guevara Vilardell.
 Research Support Technician: Albert Soret Miravet.
 Research Support Technician: David Carrió Díaz.
 Junior Developer: Miguel Castrillo Melguizo.
 PhD Student: Alba Badia i Moragas.
 PhD Student: Lluís Vendrell Miguel (La Caixa).
 PhD Student: Lola Guerreiro Pérez.
 PhD Student: Lorenzo Fileni.
 PhD Student: Víctor Manuel Valverde Morales.
 Master Student: José Suárez Repiso.
 Visiting Collaborator: Ioannis Binietoglou.
 Visiting Collaborator: Neamah Al-Datla.
 Visiting Collaborator: Sama K. Mohammed Aldabbagh.

Atmospheric Modelling

Atmospheric Modelling Group Manager: Oriol Jorba Casellas.
 Postdoctoral Researcher: Enza di Tomaso.
 Senior Developer: Georgios Markomanolis.
 PhD Student: Michele Spada.
 PhD Student: Vincenzo Obiso (FPI-SO).
 Visiting Collaborator: Joana Raquel Alves Antunes.

Climate Change

Associate Researcher: Maria Gonçalves.

Climate Modelling

Visiting Collaborator: Vicente Pastor.

Mineral Dust

Postdoctoral Researcher: Sara Basart Alpuente.
 Research Support Technician: Francesco Benincasa.

Associate Researcher: Carlos Pérez García-Pando.
 Associate Researcher: Enric Terradellas.

Life Sciences Department

Life Science Director: **Modesto Orozco López (Fundació Bosch Gimpera)**

Computational Genomics

Computational Genomics Group Manager: David Torrents Arenales (ICREA).
 Postdoctoral Researcher: Josep Maria Mercader.
 Research Support Technician: Ana Milovanovic.
 Research Support Technician: Friman Sánchez Castaño.
 Research Support Technician: Montserrat Puiggros Maldonado.
 Research Support Technician: Valenti Moncunill González.
 PhD Student: Bernardo Rodríguez Martín (La Caixa).
 PhD Student: Marta Guindo Martínez.
 PhD Student: Marta Munar Ortiz.
 PhD Student: Mercè Planas Fèlix (La Caixa).
 PhD Student: Santiago González Rosado.
 PhD Student: Sílvia Bonàs Guarch (FI).
 Master Student: Elias Rodríguez Fos.
 Visiting Collaborator: Jordi Deus Pons.
 Visiting Collaborator: Jordi Valls Margarit.

Electronic and Atomic Protein Modelling

Electronic and Atomic Protein Modelling Group Manager: Víctor Guallar Tasies (ICREA).
 Senior Researcher: Armin Madadkar Sobhani.
 Postdoctoral Researcher: Maria de Fatima Assunção Lucas.
 Postdoctoral Researcher: Martin Ivanov Kotev.
 Postdoctoral Researcher: Ryoji Takahashi.
 Research Support Technician: Manuel Augusto Rivero González.
 Research Support Technician: Pedro Riera Martorell.
 Junior Developer: Jorge Estrada Collado.
 Junior Developer: Suwipa Saen Oon.
 PhD Student: Daniel Lecina Casas (FPI).
 PhD Student: Emanuele Monza (FI).
 PhD Student: Israel Cabeza de Vaca López.
 PhD Student: Pedro Hermosilla Casajus.
 PhD Student: Sandra Acebes Serrano (FPI).
 PhD Student: Seyed Ali Hoseini.
 PhD Student: Victor Gil Sepúlveda.
 Visiting Collaborator: Antonella di Pizzio.
 Visiting Collaborator: Cristopher Grebner.
 Visiting Collaborator: Ferrán Sancho Jodar.
 Visiting Collaborator: Gudrun Gygli.
 Visiting Collaborator: James Valdés.
 Visiting Collaborator: Marc Noguera Julián.
 Visiting Collaborator: Marina Canellas.

INB-Computational Node 2

INB - Computational Group Manager: Josep Gelpí (Fundació Bosch Gimpera).
 Research Support Technician: Dmitry Reptchevski.
 Research Support Technician: Laia Codó Tarraubella.
 Research Support Technician: Pau Andrio Balado.
 Research Support Technician: Romina Royo Garrido.
 PhD Student: Víctor López Ferrando (LA CAIXA).

Molecular Modelling and Bioinformatics

Senior Researcher: Josep Ramón Goñi Macia (PTA).
 Postdoctoral Researcher: Robert Soliva.
 Research Support Technician: Carles Fenollosa.
 Research Support Technician: Jorge Cortés de la Fuente.
 Research Support Technician: Nuria Villegas Forn.
 Junior Developer: Ivan Navarro Parreño.
 Master Student: Gerard Santiago Morcillo.
 Associate Research Student: Alexandra Emilia Balaceanu.
 Associate Research Student: Diana Camila Buitrago.
 Undergraduate Student: Cristian García Montilla.
 Undergraduate Student: Ricard Illa.

Protein Interactions and Docking

Protein Interactions and Docking Group Manager: Juan Fernández Recio (I3 - RYC).
 Postdoctoral Fellow: Sergio Mares Samano (CONACYT).
 Postdoctoral Researcher: Iain Moal (Marie Curie).
 Postdoctoral Researcher: Santiago Esteban Martín
 Postdoctoral Researcher: Lucía Díaz Bueno.
 PhD Student: Brian Jiménez García (FPI).
 PhD Student: Chiara Pallara.
 PhD Student: Didier Barradas (CONACYT).
 PhD Student: Miguel Romero Durana.
 PhD Student: Mireia Rosell Oliveras (FPI-SO).
 Visiting Collaborator: Justas Capkunas.
 Visiting Collaborator: Luis Ángel Rodríguez.

Computer Applications in Science & Engineering Department

Computer Applications in Science and Engineering Director: **José María Cela Espín (UPC)**.
 CASE Director Assistant: Beatriz López Gómez.
 CASE Director Assistant: Laura Gutiérrez Salamero.
 Senior Developer: Georg Huhs.
 Junior Developer: Luis Beltrán Súcar Segarra.
 Associate Research Student: Cristina Montanola.

Data Pre&Post Processing

Data Pre&Post Processing Group Manager: Fernando Martin Cucchiatti.
 Postdoctoral Researcher: Mohammad Jowkar.
 Visualisation Technician: Guillermo Marín Getino.
 Junior Developer: Abel Gargallo Peiro.
 Junior Developer: David García Povedano.
 Junior Developer: Luz Calvo Flores.
 Visiting Collaborator: Diana Fernanda Vélez.
 Visiting Collaborator: Diana Vélez García.
 Visiting Collaborator: Juan Carlos Nava.

Environmental Simulations

Environmental Simulations Group Manager: Arnau Folch Duran (RYC).
 Postdoctoral Researcher: Ángel Coppola Owen.
 Postdoctoral Researcher: Matías Oscar Ávila Salinas.
 Junior Researcher: Raúl de la Cruz Martínez.
 Junior Developer: Oddur Oskar Kjartansson.
 PhD Student: Alejandro Martí Donati (Marie Curie).
 PhD Student: Chiara Scaini.
 PhD Student: Georgios Chrysokentis (FPI).
 PhD Student: Jordi Barcons Roca.

Visiting Collaborator: Deepak Garg.
 Visiting Collaborator: Francisco Javier Delgado Vences.

Fusion

Senior Researcher: Mervi Johanna Mantsinen (ICREA).
 Postdoctoral Researcher: Shimpei Futatani.
 Junior Researcher: Xavier Sáez Pous.
 Master Student: Daniel Gallart Escola.

Geosciences Applications

Geosciences Applications Group Manager: Josep de la Puente Álvarez.
 Senior Researcher: Jean Antoine Kormann.
 Senior Researcher: Volodymyr Puzyrov.
 Junior Researcher: Yevgeniy Gruver.
 Junior Developer: Miguel Ferrer Ávila.

High Performance Computational Mechanics

High Performance Computational Mechanics Group Manager: Mariano Vázquez (CSIC - UPC).
 Senior Researcher: Mohammad Kouhi.
 Postdoctoral Researcher: Daniel Mira Martínez.
 Postdoctoral Researcher: Jazmin Aguado Sierra.
 Senior Developer: Rogeli Grima Torres.
 PhD Student: Alfonso Santiago.
 PhD Student: Margarida Moragues Ginard.
 PhD Student: Mariña López Yunta (FPI-SO).
 PhD Student: Matías Ignacio Rivero (FPI).
 PhD Student: Miguel Zavala Ake (Marie Curie).
 PhD Student: Ruth Aris Sánchez.
 Undergraduate Student: Gabriel Bernardino Pérez.
 Visiting Collaborator: Mónica Zoppè.
 Visiting Collaborator: Xavier de Bergua Domingo.

HPC Software Engineering

HPC Software Engineering Group Manager: Mauricio Hanzich.
 Senior Developer: Albert Farrés Coma.
 Junior Researcher: Fèlix Rubio Dalmau.
 Junior Developer: Juan Esteban Rodríguez Rodríguez.
 Junior Developer: Natalia Gutiérrez Navarro.
 Junior Developer: Samuel Rodríguez Bernabéu.

Physical and Numerical Modelling

Physical and Numerical Modelling Group Manager: Guillaume Houzeaux (I3).
 Postdoctoral Fellow: Juan Carlos Cajas García (CONACYT).
 Postdoctoral Researcher: Alberto Gambaruto (Marie Curie).
 Postdoctoral Researcher: Beatriz Eguzkitza.
 Postdoctoral Researcher: Eva Casoni Rero.
 Senior Developer: Antoni Artigues Barceló.
 Junior Developer: Cadrien Calmet.
 Junior Developer: Genis Aguilar López.
 PhD Student: Cristóbal Augusto Samaniego.
 PhD Student: Edgar Olivares Mañas (La Caixa).
 PhD Student: Paula Córdoba Pañella.
 Visiting Collaborator: Benjamin Uekermann.
 Visiting Collaborator: Benoit Ozell.
 Visiting Collaborator: Florencia Reckziegel.
 Visiting Collaborator: Raul Cetto.
 Visiting Collaborator: Ruslan Gabbasov.

Smarter City Initiative

Senior Researcher: Jorge García Vidal (UPC).
 Postdoctoral Researcher: María Cristina Marinescu.

Senior Developer: Mónica Marrero Llinares.
Junior Developer: Sergio Mendoza Fariña.

Social Simulation

Postdoctoral Researcher: Xavier Rubio Campillo.
Postdoctoral Researcher: Jean Marc Montanier.
Junior Developer: Guillem Laborda Cabo.
Junior Developer: Jorge Caro Saiz.
PhD Student: Alexis Torrano Martínez.

Operations Department

Operations Director: **Sergi Girona**.
Operations Director Assistant: Núria Saavedra Hernández.

Facility Management

Facility Management Consultant: Ramón Pallisa.
Maintenance Technician: Albert Riera Muñoz.
Maintenance Technician: Miguel Armenta Sánchez.

System Administration

Systems Group Manager: Javier Bartolomé Rodríguez.
IT Security & Networks Engineer: Marcel Malet Abuli.
Network Technician: Albert Benet Vila.
Performance Technician: Alejandro Lucero Palau.
Performance Technician: Alejandro Sánchez Graells.
Performance Technician: Carles Fenoy García.
System Administrator: Felip Moll Marques.
System Administrator: Aníbal Moreno Gil.
System Administrator: David Ocaña Labrador.
System Administrator: Jordi Valls Pérez.
System Administrator: Marc López de Mantaras.
System Administrator: Sergi Moré Codina.
Helpdesk Technician: Antonio Espinar Sallares.
Helpdesk Technician: Ferran Sellés Mompert.
Helpdesk Technician: Pedro Gómez Bretones.
Visiting Collaborator: Alejandro Flores Méndez.
Visiting Collaborator: Daniel Ortiz Gutiérrez.

User Support

User Support Group Manager: David Vicente Dorca.
First Level User Support: Borja Arias Navarro.
First Level User Support: Miguel Bernabéu Díaz.
PRACE Support: Janko Strassburg.
Support Applications Consultant: Christian Simarro.
Support Applications Consultant: Jorge Rodríguez Rey.
Support Applications Consultant: Pablo Ródenas Barquero.
Visualisation Technician: Carlos Tripiana Montes.
Web Graphical Designer: Jasmina Tomic
Web Graphical Designer: Laura Bermúdez Guerrero.
Webmaster: Silvina Rusinek Milner.

Management Department

Management Director: **Ernest Quingles**.

Administration

General Assistant: Aurora Rodríguez Velasco.
General Assistant: Lisandra Souza do Nascimento.
Purchasing Officer: Cristina Vargas Cambilhon.
Support Purchasing Officer: Neus Jiménez Ferrer.
Receptionist: Carola Torra Miró.

Business Administration

Administration, Finances and Human Resources Group
Manager: Mercè Calvet Gómez.

Communication

Communications Officer: Estefanía de la Torre.
Communications Officer: Eva Alloza Anguiano.
Communications Officer: Maria José Barroso Sáez.
Communications Officer: Sara Ibáñez Leciñena.
Marketing Officer: Nuria Masdeu Font.
Marketing Officer: Renata Giménez Binder.
Dissemination Project Officer: Madeleine Gray.
Dissemination Project Officer: Nagham Salman.
MareNostrum Visits Manager: Oriol Riu.

Finance and Accounting

Accounting Manager: Cristina Calonge Cortés.
Economic Management Project Technical Support: Laia Traveset Solé.
Economic Management Project Technical Support: Laura Viñas Alcoz.
Support Accounting Technician: Alba Deldos Miret.
Support Accounting Technician: Irene Belda Jañez.
Support Accounting Technician: Judit Soldevila García.

Human Resources

Head of Human Resources: Marc González Vidal.
HR Officer: Anna Martín Balbuena.
HR Officer: Georgina Reig Mestres.
HR Officer: Julio Gómez Navarro.
HR Officer: Lara Cejudo García.
HR Junior Officer: Carla Santamaria Giménez.

Information Systems & Services

Information System Developer: Sergi Carrere Bach.
Information System Developer: Toni Matas Figueras.

Projects and Technology Transfer

Business Development Group Manager: Eugene Griffiths.
Technology Transfer Manager : Anna Escoda Sabater.
Project Manager: Emma Torrella Amador.
Project Manager: Francesca Arcara.
Project Manager: Guadalupe Moreno Beltran.
Project Manager: Marina Azor Alastuey.
Project Manager: Marta Rosselló Vallés.
Project Manager: Pilar Callau Uson.
Project Manager: Xavier Salazar Forn.

Strategy Support

Strategic Projects Senior Coordinator: Gina Michelle Alioto.
Business Analyst: Marcin Ostasz.
PRACE Project Manager: Carlos David Mérida Campos.
PRACE Project Manager: Oriol Pineda Martínez.

The mission of the Education and Training Team is to coordinate training and education activities and to research and develop opportunities for collaboration with other leading High Performance Computing (HPC) and Supercomputing centres in the areas of education, training and mobility.

Activities

There is a long-standing tradition of BSC-CNS leadership at national and European levels regarding training initiatives due to BSC-CNS's strategic commitment to offer education and training to students, researchers and industry. The BSC-CNS training programme derives significant benefit from the unique role of BSC-CNS as both an HPC provider and R&D Centre in Computer, Life, Earth & Physical Sciences.

Fostering Collaboration with Universities and Industry

The relationship with the Polytechnic University of Catalonia (UPC), and in particular with Barcelona School of Informatics, was further developed during 2014 through the extensive PATC programme offered to students at Master and PhD levels, particularly to those enrolled in the MIRI MSc course, who can take PATC courses as credited seminars.

BSC-CNS was closely involved in the design and delivery of the HPC Stream of the MIRI Master programme and offered six new MSc Scholarships under the BSC-CNS Severo Ochoa project, in addition to the four previously awarded Masters scholarships whose holders are now in their 2nd year.

BSC-CNS also led the proposal of an Erasmus+ JMD MSc in HPC. The aim of this request was to foster the development of education and training in HPC while promoting cooperation between universities, research centres and industrial partners.

Mobility as a key success factor for education

The BSC-CNS mobility programme is available to staff researchers, post-doctoral researchers and PhD students at BSC-CNS as well as researchers from institutions collaborating with BSC-CNS. This programme supports collaboration and short-term visits worldwide in leading research and academic institutions and provides grants for visitors collaborating with BSC-CNS research groups. The programme is currently funded through the Severo Ochoa project. In the four mobility calls held to date, grants totalling nearly 70.000€ were awarded, benefiting 36 researchers from BSC-CNS and other institutions.

Training Courses

BSC-CNS is a PRACE Advanced Training Centre (PATC) and delivered 13 courses with more than 300 attendees in the 2013-2014 academic year. By organising the training events at a post-graduate level of understanding and marketing them across diverse communities, BSC-CNS built the events into a meeting place for scientists of different disciplines but with similar levels of capability, thus intensifying cross-disciplinary collaboration. BSC-CNS courses were very highly rated by the attendees, placing BSC-CNS in a leading position among the other PATC centres in Europe.

Summer Schools

PUMPS Summer School, organised and delivered by the specialists from the CUDA Center of Excellence awarded by NVIDIA to BSC-CNS in association with UPC, held its fifth edition in 2014 with more than 90 attendees. The training was aimed at enriching the skills of researchers, graduate students and teachers with cutting-edge techniques and hands-on experiences in developing applications for many-core processors with massively parallel computing resources, such as GPU accelerators.

The E2SCMS2 European Earth System and Climate Modelling summer school, hosted by BSC-CNS in 2014, was launched by the European Network for Earth System Modelling (ENES) with support of the FP7 project IS-ENES2. It merges two very successful summer schools: the Earth System Modelling School by MPI for Meteorology, and the Climate Modelling Summer School of the British National Centre for Atmospheric Science (NCAS).

Workshops

The Education and Training team organised three workshops in 2014:

- Best Practices for HPC Training on SC14. Some topics addressed were: methods of delivery, development of curricula, optimising duration, surveys and evaluations, metrics and determining success.
- BRIDGE: Bridging the Talent Gap with Computational Science Methods, Workshop in ICCS 2014.
- Simulation Methods Used for the In-flight Icing Certification of Aircraft, Rotorcraft and Jet Engines.

Research Seminar Series & Doctoral Symposium

The Research Seminar program is an initiative to improve communication, professional training and mobility of BSC-CNS staff and increase visibility of incoming mobility; this is aligned with the main objective of promoting collaborative research. During the 2013-14 academic year, 17 research seminars were held. The Book of Abstracts is available at <https://upcommons.upc.edu/revistes/bitstream/2099/15530/1/so-boa-201314.pdf>

The first BSC-CNS Doctoral Symposium was held in 2014. The aim of the Doctoral Symposium is twofold; on the one hand it aims to provide a framework to share research results of the theses developed by PhD students at BSC-CNS, and on the other hand to offer training sessions on topics and skills that may be useful to future researchers and professionals. A total of 17 presentations were given and 10 posters were exhibited. The Book of Abstracts can be downloaded at <https://upcommons.upc.edu/revistes/bitstream/2099/15063/1/~5651762.pdf>

Communication & Dissemination 2014

Conference Presentations

International

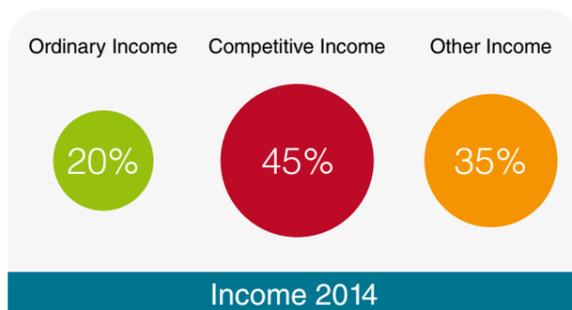
6

The financial accounts for 2014 presented here were drawn up following the accounting principles laid out in the General Plan of Public Accounting. The operating budget of BSC-CNS for the fiscal year 2014 was composed of ordinary income derived from contributions by its patrons, as well as project income derived from competitive funding sources and agreements reached with private organisations. This income was then employed to cover expenses, including costs of operations and fulfilment of all financial obligations.

Income

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

INCOME 2014	AMOUNT €
Ordinary Income	5.092.200,00
Ministry of Science and Innovation	4.288.320,00
Generalitat of Catalonia	803.880,00
Competitive Income	11.199.028,73
Spanish Government	1.630.819,55
Generalitat of Catalonia	132.432,43
European Commission	6.156.028,01
Private Companies	2.717.876,90
Other Institutions	561.871,84
Other Income	8.680.899,46
Applied Previous Reserves	2.361.564,41
Strategic Investment	5.275.461,00
Overheads/Capital transfers	1.043.874,05
TOTAL INCOME	24.972.128,19



Other Income includes strategic investments, overheads and capital transfers.

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

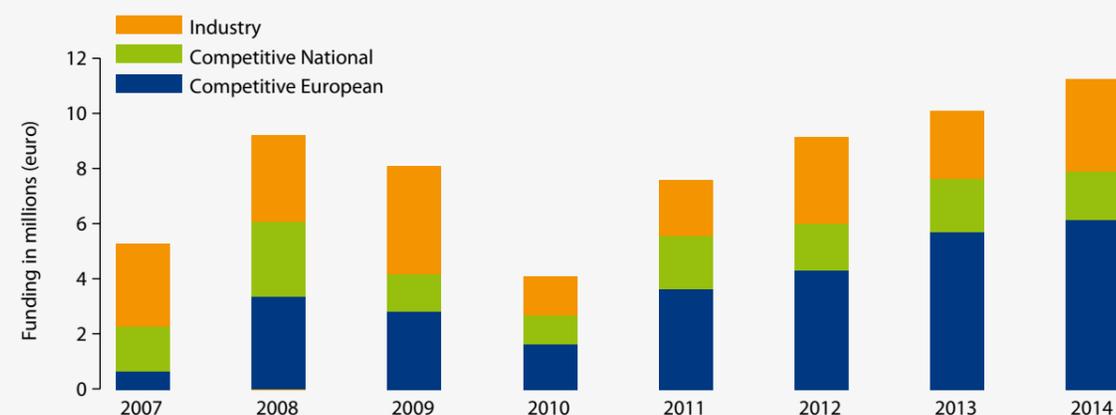
Overheads are incomes derived from ordinary projects, which according to the norms of BSC-CNS are charged 10% to cover overhead expenses.

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

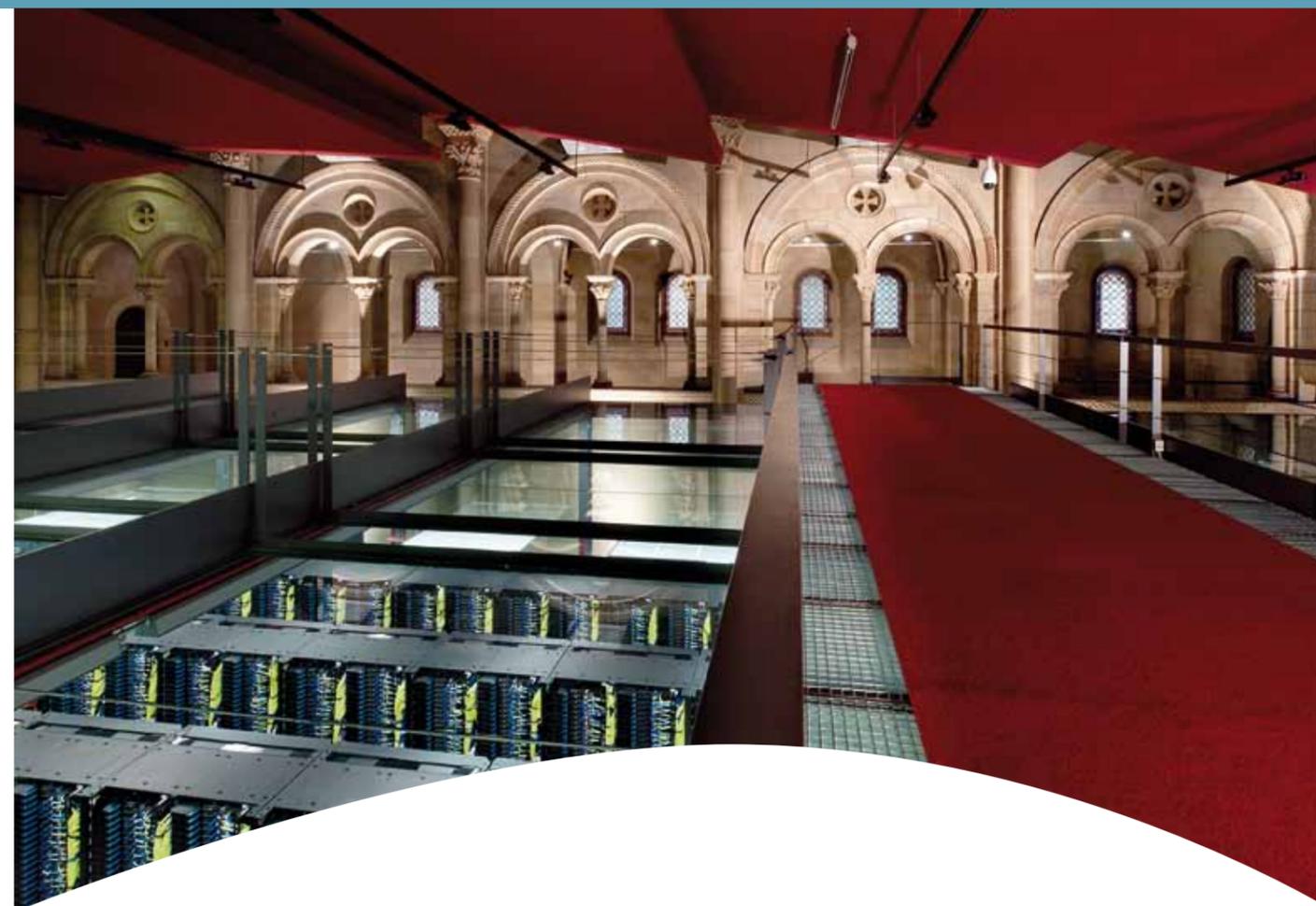
Competitive Income represents the funds derived from competitive project grants from various Ministries, the European Commission and R&D projects sponsored by private companies. Note that competitive project funds received in advance for future multi-year programs, that are progressively applied over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

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.



BSC Competitive and Industry Funding 2007-2014



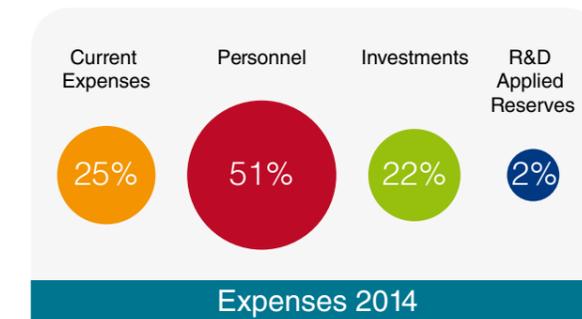
Expenses

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

All major acquisitions were made following the legal procedures established by the law regulating contracting in public administrations, and all contracts were open to public tenders. A total of 11 public tender contracts were signed during the year.

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

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



EXPENSES	AMOUNT €			
	Ordinary Budget	Strategic Budget	Projects Budget	Total
Personnel	3.995.690	397.153	8.422.998	12.815.841
Investments	167.431	4.455.858	924.667	5.547.956
Current Expenses	3.068.293	422.450	2.756.904	6.247.648
R&D Applied Reserves	360.683	-	-	360.683
TOTAL EXPENSES	7.592.098	5.275.461	12.104.570	24.972.128

BSC-CNS - Severo Ochoa Center of Excellence

BSC-CNS received the "Severo Ochoa Center of Excellence" support and accreditation in the 2011 call, a programme of the Secretary of State for Research, Development and Innovation of the Ministry of Economy and Competitiveness that aims to promote excellence in scientific research in Spain. The award confirmed BSC-CNS's reputation as one of the world's leading centres applying and doing research on supercomputing technologies. The programme commenced in January 2012 with an ambitious research programme: to design novel hardware and software technologies to address the computational and Big Data requirements of three challenging applications in personalised medicine, biomechanics and high-resolution air quality climate modelling.

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

The BSC-CNS Severo Ochoa Project

The BSC-CNS Severo Ochoa research programme takes as its starting point the fact that Exascale supercomputers will be crucial in tackling major societal problems in areas such as human health and the environment. The computational requirements of the numerical simulations in these scientific fields will go together with new requirements in terms of data management and storage, to so called Big Data. However, attaining Exascale and Big Data poses significant challenges, due to requirements on system hardware and software design, of which energy consumption is one of the main factors.

2014 was a year of consolidation of various important developments of the programme, such as the deployment of improvement mechanisms in the management of Human Resources in Research, the empowerment of and networking between young researchers, conducting 12 sessions of Severo Ochoa Research Seminars (SORS), the celebration of the first BSC-CNS doctoral Symposium, the Amber, E2SCMS2 and PUMPS Summer Schools, as well as the mobility programme and MIRI scholarships for MSc in HPC at the UPC. Finally, the continued promotion of the BSC-CNS communication and outreach programmes aimed at engaging society with BSC-CNS activities.



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



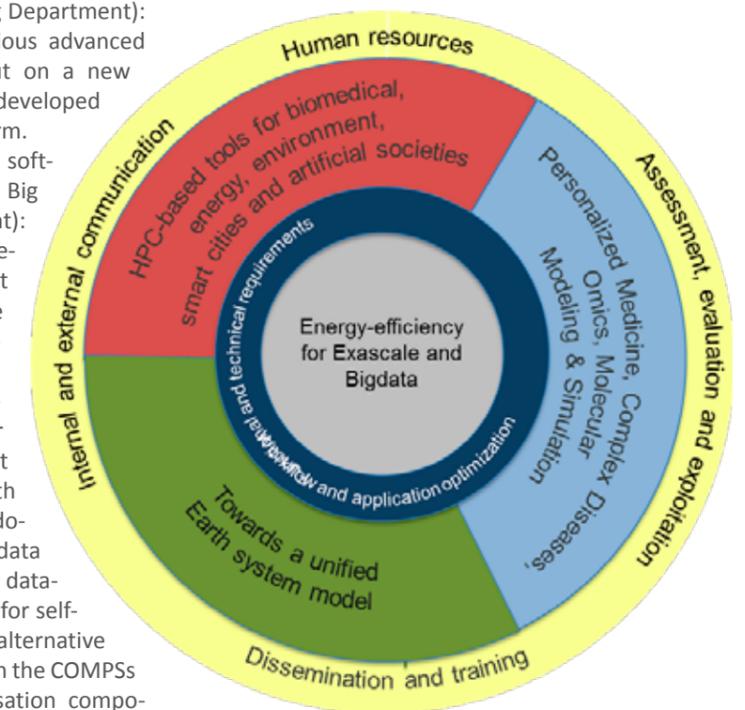
Severo Ochoa Retreat - interdisciplinary team building and brainstorming.



Specific activities within the main scientific pillars of the Severo Ochoa programme included:

- Personalised medicine (Life Sciences Department): The combination of genomics, proteomics and transcriptomics analysis with computer simulation is being explored to create models capable of predicting certain diseases or the effects of drugs on patients before a pathology starts.
- Multi-scale air quality climate modelling (Earth Sciences Department): Further developments were made on a high-resolution modelling system for short- and long-term applications, as well as new methodologies to run high-resolution models on exascale machines and methodologies to handle big amounts of data produced by complex high-resolution models.
- Computational biomechanics--Alya Red (Computer Applications in Science and Engineering Department): Implementation and validation of various advanced physiological models were carried out on a new Cardiac Computational Model (CCM) developed using the BSC-CNS Alya software platform.
- Novel components in the hardware and software stacks to achieve the Exascale and Big Data (Computer Sciences Department): During 2014 the Computer Sciences Department continued the development of novel technologies to facilitate the implementation of the applications developed by the scientific departments, including: 1) the adaptation of the BSC-CNS's OmpSs programming mode for energy-efficiency and the development of PyCOMPSS workflow applications with BigData demands; 2) design of methodologies and technologies to support data organisation in key/value non-relational databases; 3) development of a new library for self-contained objects (dataClay), as an alternative to the use of files and its integration with the COMPSS programming model and data organisation components; and 4) design of Domain Specific Languages (DSL) for accelerator-based clustered architectures.

The image below summarizes the BSC-CNS Severo Ochoa programme, which is made up of four main scientific sub-projects: the proposal and development of novel models in three application domains which rotate around novel components in the hardware and software stacks to achieve the Exascale and Big Data. In the following paragraphs the applications and achievements during 2014 are described.



A picture is worth 1000 words: BSC-CNS's Severo Ochoa programme



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



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



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

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

During 2014, more than 450 IT and senior executives from over 400 companies of different types and sizes visited BSC-CNS facilities, and were given presentations with examples of usage of HPC in their respective sectors. A total of 24 sectorial visits were organised. Some of the industrial sectors covered were: aeronautics, automotive, telecommunications, robotics, pharma, logistics, textile, and governmental IT related organisations.

European Space Agency



In 2014, the collaboration with the European Space Agency (ESA) was structured around four projects: 1)

ESA NPI (Architectural solutions for the timing predictability of next-generation multi-core processors), where a number of memory controller and bus architectures were trialled to enable a Worst Case Execution Time (WCET) analysis of time-critical space applications in a multi-core execution environment such as the New Generation Multi-Core Processor (NGMP) while attaining tight WCET estimates for critical tasks and high average performance for non-critical ones; 2) ESA PROARTIS for SPACE, integrating software-randomisation techniques onto real space setups (i.e. operating system, application and hardware) used by ESA and its system providers; 3) ESA HAIR, developing several timing models that will be integrated as part of a virtual machine for the NGMP; and 4) ESA PMCs (Multi-Core Architectures - Cache Structure Optimisation for better RT Performance), focused on the analysis and proposal of a new performance monitoring counter support for the NGMP with the goal of better capturing how tasks interact and are delayed when accessing NGMP's hardware shared resources.

Fundación Botín



The Botín Foundation is helping to establish a spin-off company, NOSTRUM DRUG DISCOVERY, to commercialise technologies developed by the Life Sciences department. The company aims to develop a drug-design simulation platform to reduce the need for clinical trials of new drugs.

Iberdrola-BSC Research Collaboration



IBERDROLA and BSC-CNS are jointly developing a major R&D&I initiative known as the 'SEDAR Project (High Resolution Wind Simulation)'. SE-

DAR is an innovative project aimed at developing a new computer model to improve estimates of electrical energy production in wind farms before their construction. Current models have a significant limitation in their calculation times and the resolution of physical models, and this project seeks to overcome these

shortcomings through the use of supercomputing techniques.

The software developments in SEDAR are based on the Alya software platform developed at BSC-CNS. Current work focuses on introducing more complexity in the physical models simulated by Alya, with the objective to obtain a robust short-term power production forecast tool.

IBM-BSC Research Collaboration



During 2014, the 3-year collaboration with IBM established in 2013 was continued. A number of Joint Study Agreements were executed with the Watson Research laboratory: High-performance in-memory databases, Software-defined environments for HPC workloads, Adaptive resource management for Power, OmpSs @ P8/GPU, Resilience compiler support and Performance API for OpenMP, and Smart cities. Further JSAs with the Zurich Research Laboratory were also conducted: OmpSs programming model for asynchronous applications and Applicable research to interconnection networks.

Intel-BSC Exascale Laboratory



The main objective of the Intel-BSC Exascale Laboratory is to conduct research activities on novel programming models and prediction tools that will be needed to exploit extraordinary levels of parallelism in future Intel-architecture based supercomputers, consisting of millions of cores. During 2014 the collaboration mainly focussed on performance analysis and prediction for HPC code targeting these future exascale systems, transparent support for heterogeneity in the OmpSs programming model, dynamic load balancing (DLB) in hybrid MPI/OmpSs applications and fault tolerance transparently managed by highly scalable parallel run-time systems (OmpSs).

Microsoft-BSC Research Centre



Since 2014, the Microsoft-BSC Research Centre targets BigData topics, and in particular, the

development of performance models for large scale data analytics frameworks, initially focusing on Hadoop ecosystems. With this objective in mind, researchers at BSC-CNS have teamed up with computer scientists at Microsoft Corporation and Microsoft Research in Redmond (US) to develop automated

optimisation for the performance of Hadoop infrastructure deployments. The goal is to explore upcoming hardware architectures for Big Data processing and to reduce the TCO of running Hadoop clusters, by creating the most comprehensive open public Hadoop benchmarking repository. The research compares not only software configuration parameters, but also contrasts current and newly available hardware including SSDs, InfiniBand networks, and Cloud services, while at the same time evaluating the TCO of each possible setup along with the running time to offer a recommendation. This analysis serves as a reference guide for designing new Hadoop clusters, exploring parameter relationships as well as reducing the TCO for existing data processing infrastructures. Ultimately, the Centre will develop automated learning mechanisms for providing cost-effective characterisation of Hadoop workloads. In other activities in 2014, centre researchers worked on low-power vector architectures and finalising research on Transactional Memory.

NVIDIA-BSC/UPC Research Collaboration



BSC-CNS, in association with the Universitat Politècnica de Catalunya (UPC), was awarded by NVIDIA as CUDA Center of Excellence (CCoE) in 2011. The Center acknowledges the broad-based research success of BSC-CNS in leveraging the NVIDIA CUDA technology and GPU computing. As part of the CCoE training, during 2014 several courses were offered in graduate and master programs at UPC, and as part of the PRACE Advanced Training Center (PATC). In addition, the renowned Programming and Tuning Massively Parallel Systems (PUMPS) Summer School is held each year in Barcelona since 2010. During 2014 the research activities at the CCoE focussed in the following areas: 1) Use of low-power GPUs in platforms oriented to high-performance computing; 2) Optimisation of applications in different domains in conjunction with the CASE, Life and Earth Sciences departments; 3) Facial recognition and security video surveillance with the UPC start-up company HERTA Security; 4) Development of software infrastructures to ease the development on multi-GPU systems, and mechanisms and policies for scheduling multiprogrammed workloads; and 5) Task-parallel simulation and visualization of crowds in hybrid GPU/CPU platforms.

Repsol-BSC Research Center



In 2010, and following the success of the Kaleidoscope project, both BSC-CNS and Repsol decide to create a joint research centre: the Repsol-BSC Research Center (RBRC). The aim of the Center is to tackle geophysical problems and a broad spectrum of other HPC challenges of interest for Repsol. RBRC is an interdisciplinary group of engineers and researchers from the geophysics, IT and telecommunication fields from the CASE Department. The geophysical and computational developments at the RBRC have resulted in a unique software platform called Barcelona Subsurface Imaging Tools (BSIT). BSIT has enabled the development of a whole set of imaging applications which include

state-of-the-art solutions for the most challenging problems in exploration geophysics. The platform includes different packages for processing seismic data: Forward Modelling, Reverse Time Migration and Full Waveform Inversion. In addition, the software supports different rheologies including: acoustic, acoustic with variable density, elastic and viscoelastic. Moreover, several levels of anisotropy are supported: VTI/HTI, Orthorhombic, TTI and arbitrary anisotropy (for elastic and viscoelastic rheologies). In recent years new capabilities have been added to simulate electromagnetic wave problems, including modelling and inversion.

In 2014, the AURORA project was launched in order to obtain a 3D joint full waveform inversion of elastic and electromagnetic waves able to be applied to real problems.

SAMSUNG Collaboration



In 2014, the collaboration with Samsung Co., Ltd. focused on memory systems for high-performance computing. The collaboration targets three areas: 1) the analysis of application memory requirements in terms of capacity and bandwidth, analysing the impact of main memory latency on the overall performance; 2) the study of DRAM errors in production HPC workloads running on the MareNostrum supercomputer. In addition to the detection of DRAM errors, the system logs and correlates a number of statistics of interest such as the error type, time-stamp, physical position of errors, and the DIMM manufacturer; 3) analysis of the suitability of STT-MRAM for main memory of HPC systems, simulating HPC systems with the STT-MRAM main memory and the conventional DRAM, and comparing their performance on a set of production HPC applications.

Xilinx-BSC Research Collaboration



During 2014, the Programming Models Group continued its collaboration with Xilinx towards easy programmability of the Xilinx Zynq platform. Using the OmpSs infrastructure ported to Zynq during the previous period, the Group evaluated the benchmarks Cholesky, Covariance and Matrix Multiplication. The results were jointly published in the FPGA conference. The Group also developed a performance estimator to overcome the large FPGA synthesis times. The performance estimator is based on traces obtained from the serial execution of the applications, annotated with OmpSs tasks. The tool does a design space exploration by mapping the tasks onto the FPGA or the SMP cores, and it uses simulation to estimate which mapping will deliver better performance. Following the indications of the tool, the user can then select the proper tasks to be synthesised for the FPGA for the final application binary generation.

1.7 PRACE: Supercomputing Research Infrastructure for Europe



Other Industry and Institutional Collaborations

In addition to the above described long-term major industrial collaborations, BSC-CNS conducts a wide range of collaborative research activities with many local and international companies, as can be seen by their logos above.

Amongst the many collaborations with companies, BSC-CNS has specific focus areas, namely in Life Sciences (computational biology) and Earth Sciences (air quality forecasting):

Life Sciences

Collaborates with more than 50 biomedical companies on projects related to computational biology ranging from bioinformatics for genomics to computational biochemistry and drug discovery. Some important collaborations include:

AstraZeneca www.astraeneca.com BSC-CNS collaborates with AstraZeneca in the frame of their new (2014) internal postdoctoral program to develop and use PELE ("Novel in silico approaches using PELE for modeling the dynamic nature of proteins"), and in research studies in nuclear hormone receptors. AstraZeneca is also an industrial partner in the BSC-CNS ERC Proof of Concept grant.

Novozymes www.novozymes.com BSC-CNS is working with Novozymes in the INDOX (FP7-KB-BE-2013-7-613549) consortium for the development of improved oxidoreductases.

SCHRÖDINGER www.schrodinger.com BSC-CNS is a beta tester of all Schrödinger software and contributes to its development. In 2014, BSC-CNS conducted teaching seminars using Schrödinger software in Israel and Spain.

The BSC-CNS Life Sciences department has patented two biotechnological tools related with computational genomics, EDMD and SMUFFIN. One of them is being transferred to a spin off company.

Earth Sciences

Also of particular note are the development of operational air quality forecasting and assessment services for various regional governments throughout Spain and international public bodies, and the analysis of impacts on air quality for power generation and other industries:

World Meteorological Organization (WMO): BSC-CNS, together with AEMET, coordinates a Regional WMO SDS-WAS Center in Barcelona for Northern Africa, Middle East and Europe. BSC-CNS also hosts the WMO Barcelona Dust Forecast Center.

AEMET (The State Meteorological Agency): BSC-CNS has ongoing activities with AEMET to implement, disseminate and validate the operational prediction of the North African dust transport in the Iberian Peninsula.

Environment and Water Agency of Andalusia: BSC-CNS is developing 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.

International Research Institute for Climate and Society: BSC-CNS is collaborating with IRI in connecting climate, atmospheric aerosols and health.

National Oceanic and Atmospheric Administration - National Centers for Environmental Predictions and Environmental Modeling Center: BSC-CNS is working with NOAA in developing new chemical weather prediction and chemical transport models intended to be a powerful tool for research and to provide experimental efficient global and regional chemical weather forecast.

UNEP (SDS-WAS West Asia): following the success of the SDS-WAS node hosted at BSC-CNS, a similar node is being proposed for the West Asian region.

Barcelona City Council: BSC-CNS is conducting a study on backup energy plants.

The Partnership for Advanced Computing in Europe (PRACE) is a pan-European Research Infrastructure for High Performance Computing (HPC) and forms the top level of the European HPC ecosystem. The infrastructure consists of several Tier-0 supercomputers (including one at BSC-CNS) distributed across the continent, providing outstanding computing services to enable world-class research on world-class systems. The systems are installed at centres in France, Germany, Italy and Spain. Through PRACE, scientists and technologists from Europe and around the world are provided access to world-class supercomputers with capabilities comparable to those available in the USA and Japan. These leadership class systems will help the continent's scientists and engineers to remain internationally competitive. BSC-CNS played a key role in the creation of the PRACE Research Infrastructure at all levels, with Sergi Girona serving as Chairman of the Board of Directors, significant technical contributions, and leadership of the organisational design. This included the selection of the best legal form, design of the governance structure, funding and usage models, and the peer review process, resulting in the PRACE statutes and initial agreement which were signed in May 2010. From that date, PRACE has operated as a Belgium-based legal entity (AISBL-Association Internationale Sans But Lucratif) in parallel to the supporting European projects.



techniques. Finally, within the 3rd Implementation Project, BSC-CNS continued many of the PRACE 1st implementation phase PRACE activities including research on organisational aspects and the development of an impact assessment framework.

Within the framework of the PRACE Implementation Phase projects, BSC-CNS first deployed a 16-node cluster of hybrid ARM + CUDA GPU compute nodes to serve as a software development vehicle, and then deployed the first large-scale cluster using ARM processors driving the high-end NVIDIA Tesla accelerator. BSC-CNS also led and coordinated activities in four key research areas: auto-tuned and automatic techniques to be applied in parallel programming models, scalable numerical algorithms, performance tools, and file systems. BSC-CNS also significantly contributed to Community codes work in the fields of engineering and materials science with the most outstanding improvements achieved for Alya and SIESTA codes. The work for Alya consisted of parallelizing the partitioning of input meshes with PARMETIS. For SIESTA a solver was developed that reduces computational complexity without loss of accuracy. This was successfully tested on systems with tens of thousands of atoms, making new classes of physical problems accessible to first principle calculations.

BSC-CNS and PRACE

In May 2014, BSC-CNS hosted the first of the series of PRACE-days, the annual Scientific and Industrial conference of PRACE. The conference was addressed to scientists, industrial users, policy makers and HPC managers, for a better and common understanding of the needs, requirements and benefits of HPC for research, innovation and society.

BSC-CNS continues to operate as one of the six selected PRACE Advanced Training Centres (PATC). Each of the sites coordinates and executes training and education activities enabling the European research community to utilise the computational infrastructure available through PRACE. BSC-CNS is amongst the best performing PATC centers and in the 2013-14 academic year developed new courses based on tools and programming models developed at BSC-CNS.

Following completion of the PRACE 1st Implementation Phase project, another two European funded projects supporting implementation of the PRACE Research Infrastructure were run in parallel during 2014, all with a significant level of involvement of BSC-CNS. In the 2nd Implementation Project, BSC-CNS evaluated the latest hardware components installed in the previously selected prototypes, extended the community code enabling support, and continued research on best practice for HPC system commissioning and novel programming

Spanish participation in PRACE

Spanish scientists were very successful in participating in important research projects that were awarded with computing time on the various PRACE nodes.

Some of the projects with Spanish participation are:

- *Direct Numerical Simulation of Equilibrium Adverse Pressure Gradient Turbulent Boundary Layers*, Prof. Javier Jiménez Sendín (UPM), 17 million hours on SuperMUC@LRZ@GCS
- *Large-scale radiation damage cascades from first principles*, Prof. Emilio Artacho (CIC nanoGUNE), 36 million hours on Hermit@HLRS@GCS
- *INFLUM2 - Effects of selective mutations on the ligand binding and unbinding to the M2 proton channel of influenza virus*, Prof F. Javier Luque (UB), 22 million hours on MareNostrum@BSC
- *NEMERTE - Numerical Experiment on the Mediterranean model response to Enhanced Resolution and Tide*, with the participation of IMEDEA, 17 million hours on Fermi@CINECA
- *Identification of somatic variations in PanCancer genomes using SMUFIN*, a reference-free approach. Prof. David Torrents, 6 million hours on MareNostrum@BSC
- *Protein-DNA binding allostery*, Prof. Modesto Orozco (IRB), 29 Million hours on MareNostrum@BSC
- *EXCOMM - Extreme scale domain decomposition solvers for COMPUTATIONAL MECHANICS*, Prof. Santiago Badia (CIMNE-UPC), 10 million hours on Fermi@CINECA



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

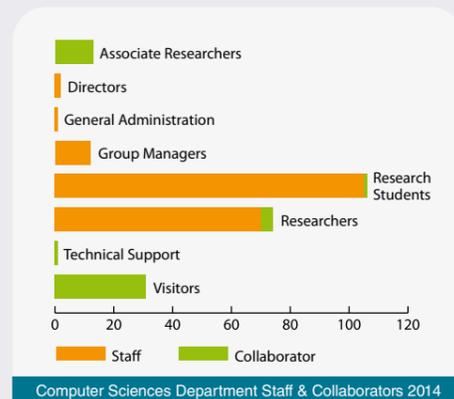


The scientific mission of the Computer Sciences Department is to influence the way computing machines are built, programmed and used. This is done through ideas, cooperation with manufacturers as technology transfer activities and “product-quality” open source developments that are usable by the scientific community. The Department includes researchers with a holistic and vertical background and vision and combines both stable and exploratory research paths, always with a co-design approach in mind, which covers from computer architecture, to resource management, performance tools, programming environments and algorithms, targeting not only supercomputer architectures but also BigData, realtime, embedded and mobile platforms. Performance, productivity, power/energy and reliability are the factors that drive our co-design approach.

The Computer Sciences Department, led by Jesús Labarta and Eduard Ayguadé, is structured in 11 research groups. Although each group has its own specialised lines of research, the teams often come together to collaborate on projects that require vertical integration, such as the Exascale EU projects Mont-Blanc/Mont-Blanc2 and DEEP/DEEP-ER, the ERC RoMoL award, the Human Brain Project (HPB) flagship and the national Severo Ochoa program. 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.

The combination of broad coverage of all facets of computer systems design and programming, along with in-depth expertise in each area, are somewhat unique amongst supercomputing centres. This unique strength of the Computer Sciences Department has continued attracting leading computing companies to invest during 2014 in collaborative systems design R&D projects.

During 2014, some 190 staff and students and 50 collaborating researchers worked within the Department, organised in 11 research Groups; 4 focused on Computer Architecture (Heterogeneous Architectures, Computer Architecture for Parallel Paradigms, Operating System/Computer Architecture Interfaces and Unconventional Computer Architecture and Networks), 3 focused on improving productivity when programming and optimising parallel applications on large scale parallel systems (Programming Models, Performance Tools and Accelerators for HPC), 3 focused on APIs and resource management middleware for distributed heterogeneous architectures (Storage Systems, Grid Computing and Clusters, Autonomic Systems and e-Business Platforms) and one on novel scalable mathematical methods and algorithms for large scale systems (Extreme Computing).



Scientific Output

For additional information, please see the Detailed Report of Research Activities 2014 for the Computer Sciences Department on the BSC-CNS website.

Impacting the Future of Computing

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

The research results of the Department were published in the proceedings of high quality conferences in the area (A* and A in CORE2013 conference ranking, www.core.edu.au/coreportal), including International Symposium on Computer Architecture (ISCA), International Conference on Parallel Architectures and Compilation Techniques (PACT), Annual Design Automation Conference (DAC), International Conference on Supercomputing (ICS), International Parallel & Distributed Processing Symposium (IPDPS), Design, Automation, and Test in Europe (DATE) conference, International Conference on Computing Frontiers (CF), International Conference on Hardware/Software Codesign and System Synthesis (CODES+ISSS), International Conference on Application Specific Systems, Architectures, and Processors (ASAP), Symposium on Principles and Practice of Parallel Programming (PPoPP), International Conference on Parallel Processing (ICPP), International Symposium on Cluster Computing and the Grid (CCGrid) and International Conference on Cluster Computing (CLUSTER).

Communication & Dissemination 2014

Publishing	
Journal Articles	48
Books	1
Book Chapters	1
Conference Presentations	
International	107
Education	
PhD Theses Read	16
Masters Theses Read	1

In addition, other more consolidated research results have been published in prestigious journals in the area, including IEEE Transactions on Computers, IEEE Micro, IEEE Transactions on Parallel and Distributed Systems, IEEE Transactions on Very Large Scale Integration Systems, ACM Transactions on Architecture and Code Optimization, ACM Transactions on Design Automation of Electronic Systems, Future Generation Computing Systems, Concurrency and Computation: Practice and Experience, Parallel Computing, Journal of Parallel and Distributed Computing, International Journal of Parallel Programming and Information Systems Frontiers.

Nine PhD thesis were defended during 2014 in the Computer Architecture Department at the Universitat Politècnica de Catalunya (UPC-BarcelonaTECH).

Key Projects and Networks

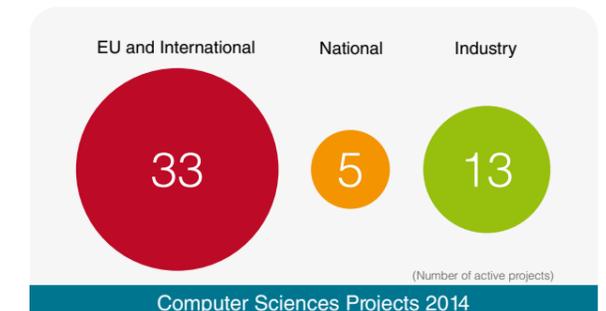
During 2014, the Computer Sciences Department participated in the following:

EU projects:

- 23 FP7 projects: ASCETIC, AXLE, COMPOSE, DEEP, DEEP-ER, EESI2, EUBrazil CloudConnect, EuroServer, HOPSA-EU, Human Brain Project HBP, Lightness, Mont-Blanc, Mont-Blanc2, P-Socrates, ParaDIME, parMERASA, PROXIMA, ReNewIT, RETHINK Big, SECURED, TERAFLUX, TransPLANT and ARTEMIS VeTeSS;
- RoMoL (Riding on Moore's Law) ERC grant (Mateo Valero);
- Hi-EST (Holistic Integration of Emerging Supercomputing Technologies) ERC grant (David Carrera);
- The Second Implementation Phase in the PRACE EU FP7 project: FTI and energy-efficient prototype;
- The HiPEAC-3 network of excellence;
- The European Technology Platform for HPC (ETP4HPC);
- The SCALUS Marie Curie Initial Training network.

Collaborations with IT companies:

- Intel Corporation with a multi-year agreement Intel-BSC Exascale Lab, on topics related to analysis of applications and performance prediction tools and programming models;
- NVIDIA through the CUDA Center Of Excellence (CCoE), in association with the Universitat Politècnica de Catalunya (UPC-BarcelonaTECH);
- Microsoft Research through the BSC-Microsoft Research Centre agreement, on topics related to low-power vector architectures, architectural support for programming languages and analysis of Hadoop for MapReduce workloads;
- IBM Research through the following Joint Study Agreements: High-performance in-memory databases, Software-defined environments for HPC workloads, Adaptive resource management for Power, OmpSs @ P8/GPU, OmpSs programming model for asynchronous applications, Resilience compiler support, Performance API for OpenMP and Applicable research to interconnection networks;
- Samsung to evaluate memory behavior of HPC production applications and frequency and locality of memory errors;
- Xilinx Ireland to research on OmpSs support for FPGA accelerators;
- Qualcomm to port BSC's instrumentation packages to their DragonBoard development kit;
- The European Space Agency (ESA), with the "Multicore OS benchmark" and "Architectural solutions for the timing predictability of next-generation multi-core processors" project;



National projects:

- The BSC-CNS Severo Ochoa program, where the Department is developing a novel platform to support interactive simulation and computational workflows with Big Data requirements, to be applied to the three challenging applications in the project from Life and Earth Sciences and CASE Departments.



Programming Models

Led by Xavier Martorell, the Group explores new programming models and their efficient implementation for current and future architectures, from manycore SMPs with support for accelerators (GPUs, MIC, FPGAs), to clusters of SMPs with accelerators, to exascale systems. The research is supported by two powerful tools: the Mercurium compiler, used to prototype new programming model approaches, and Nanos++, the runtime library supporting the variety of hardware resources under consideration. During 2014, the Group improved the support for GPUs with CUDA and OpenCL, with the use of an asynchronous thread to deal with the GPU operations. The Group also worked on the support for FPGAs and developed a preliminary implementation on OmpSs using the hStream model for the MIC processor. The Group also continued the development of DLB (Dynamic Load Balancing) techniques and providing a better interoperability solutions between MPI and OmpSs, and OpenMP. The Group developed DSL (Domain Specific Languages) extensions for solving partial differential equations as part of the collaboration with Repsol. The Group continued the work on power modelling for multicore architectures and code transformations for processors with local memories. During 2014, the Group also continued the participation in the EU FP7 projects Mont-Blanc (I and II), DEEP, DEEP-ER, the Human Brain Project (HBP) and TERAFLUX (finalized), as well as in the HiPEAC-3 network of excellence and the research collaborations with Intel, IBM and Xilinx Research Labs in Dublin. Finally, the Group successfully applied for a H2020 project, AXIOM, on research on new software/hardware architectures for Cyber-Physical Systems.

Heterogeneous Architectures



This Group aims to design and evaluate the next generation of HPC systems capable of achieving the energy efficiency required by future Exaflop supercomputers. The Group believes that components coming from the embedded and mobile device markets will replace current HPC components coming from the PC and server markets, due to their larger unit count, lower unit price, rapid evolution, and higher energy efficiency. To that end, during 2014, the Group performed Tracked the evolution of ARM-based chips from either the mobile market, or the server market and successfully installed the first chassis of the Mont-Blanc prototype consisting of 135 compute nodes based on Samsung Exynos 5 dual SoC interconnected through gigabit ethernet with a total power consumption below 3 kWatts. The group also participated in the FP7 EuroServer project, evaluating the use of energy-efficient technologies from the mobile market for BigData processing, and continued the collaboration with Samsung Co., Ltd. in the field of memory systems for high-performance computing (HPC). Finally, the Group developed performance and power modeling tools for next-generation HPC systems with a special focus at the node level with the objective of predicting the impact of architectural enhancements in the compute units. The Group was lead by Alex Ramirez during the first half of the year; since then the Group is managed by the Department Directors.

Unconventional Computer Architecture and Networks

Led by Mario Nemirovsky, UCAN group is conducting research on Internet of Things (IoT), Fog computing, Big Data, simulation techniques, and processor architectures. In this direction, the group has been positioning as a referent in platforms for IoT. Areas such as security, virtualization, and infrastructure are under study, proposing new solutions to break the silos problem while maintaining real-time constraints. The group is also working on new processor architectures and algorithms that can take advantage of Wireless Network-on-Chip (NoC), by using antennas at core-level to enable a natural broadcast network to communicate the cores. Additionally, UCAN group is consolidating new simulation techniques based on queue models, allowing faster simulations with an excellent accuracy.



Computer Architecture for Parallel Paradigms



Led by Adrián Cristal and Osman Unsal, the Group focuses its research on the architectural support for novel programming models and execution environments for future multicore architectures. The Group focuses its research on lowering the programmability wall raised by multicore architectures; research areas include low-power vector processors, transactional memory, reliability and hardware for big data. During 2014, the group continued its work in five FP7 projects (ParaDIME, AXLE, RETHINK big, ICT-Energy and Mont Blanc). The group finalized their work on reliability as part of the Intel-BSC Laboratory and the G8 Enabling Climate Simulation at Extreme Scale project. In April 2014, the group also finalized their work in the BSC-Microsoft Research Centre, and passed the baton to the BSC Autonomic Systems and eBusiness Platforms research group to continue the center activities.

Operating System / Computer Architecture Interface

The CAOS Group has focused its research on embedded real-time and high-performance systems. During 2014, in the area of real-time systems the group successfully completed the EU FP7 parMERASA project, started three projects with the European Space Agency and continued its participation in the EU FP7 PROXIMA, P-SOCRATES and ARTEMIS VeTeSS projects. In the area of high-performance systems, the group continued its work on energy and CPU accounting and on adaptive prefetching techniques as part of a Joint Study Agreement with IBM. Researchers of the Group constitute the core of the research activities in the RoMOL ERC grant.



Performance Tools



This Group, led by Judit Giménez, works on the design of tools to measure, analyze and predict the behavior of parallel applications on parallel systems. The main goal of the Group aims at providing technologies to understand the issues that determine the actual performance of a parallel application or contribute to the application bottlenecks. This knowledge is extremely important in both novel homogeneous and heterogeneous multicore architectures as well as in highly scalable cluster systems. During 2014, the activities developed within the Group evolved the research lines targeting performance analytics and models as well as improving the tools infrastructures and their integration. The Group also participated in the EU exascale projects Mont-Blanc/Mont-Blanc2 and DEEP/DEEP-ER. With respect to projects with private companies, the group is highly involved in the joint Intel-BSC Exascale Laboratory and during this year we also had a project with IBM. We have established an international collaboration with RIKEN (K-Computer) as well as contributed to the JLESC activities.

Storage Systems



Led by Toni Cortés, this Group explores appropriate solutions to the scalability of parallel storage systems in large installations (in which very large volumes of data need to be generated and accessed), new file-system approaches to increase their performance, and new approaches to store and manage Big Data. In 2014, the Group focussed on increasing the performance and scalability of parallel file systems by applying de ideas of guided IO (hints by the programmer) and extending the direct look up file system designed in 2012 to support new key-value devices. In addition, the group has continued the development a new storage abstraction based on self-contained objects. During 2014 the research activities of the Group have been supported by the Severo Ochoa programme, the Mont-Blanc, PRACE and HBP EU projects.

Extreme Computing

Led by Vassil Alexandrov, this Group focuses on development of novel scalable mathematical methods and algorithms for large scale systems and applying these to solving problems with uncertainty on such systems. The Group's main expertise is in the area of computational science, novel scalable mathematical methods and algorithms for large scale systems and exascale computing paradigm. In particular, scalable Monte Carlo and hybrid algorithms are developed for linear algebra, optimisation, computational finance, environmental models, computational biology, etc. In addition the research focuses on scalable, fault-tolerant and resilient algorithms for extreme scale (peta and exa scale) computing. During 2014 the Group has been recognised as emerging research group in Extreme Scale Computing by Catalan Government.



Autonomic Systems and eBusiness Platforms

Led by Jordi Torres, this Group performs high-level research in eBusiness applications and platforms executing on high-productivity multiprocessor architectures as well as distributed environments. The aim of this group is to research autonomic and intelligent resource management techniques for today's business applications. The objective is to create new components at the middleware level that provides holistic solutions for some of the new IT challenges in the industry: Cloud computing, Big Data, Data Analytics, high-performance computing or sustainable computing. The Group is also researching new architectural proposals for the memory/storage hierarchy including processing-in-memory techniques and novel key-value storage models to support Big Data workloads. The research is supported by the EU FP7 COMPOSE and LIGHTNESS projects, the Severo Ochoa program and the two collaborations with IBM Research. Three new EU FP7 projects (RenewIT, ASCETiC and EuroServer) started by the end of 2013 as well as the participation in the HBP EU project.



Grid Computing & Clusters

Led by Rosa M. Badia, this Group is researching new programming and execution models and resource management techniques for distributed computing. The Group explores solutions in order to simplify application development, to enable dynamic exploitation of parallelism at runtime, and to perform combined scheduling decisions at different levels. In these directions, the efforts of the Group during 2014 focused on further development of the COMPSs programming model, specially in the Python binding, the completion of the graphical IDE to support application developers, support to multiple task versions, new implementation of the support to tasks' constraints, and other updates. The Group has also continued with the integration of COMPSs with novel storage technologies, like the dataClay self-contained objects layer or the Hecuba layer for Cassandra databases, both in development as part of the Severo Ochoa programme). The Group is also researching new technologies for low-cost energy efficient microservers. Finally, the Group has continued its participation in several EU FP7 projects (transPLANT, HBP, ASCETiC, EuroServer and EUBrazil CloudConnect) as well as in the Severo Ochoa center of Excellence, all of them related with extensions of COMPSs and porting of applications.



José María Baldasano, Director of the Earth Sciences Department →



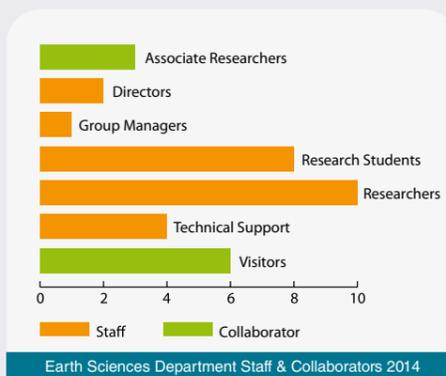
The Earth Sciences Department of BSC-CNS has the aim of modelling and understanding the behaviour of the Earth System, focusing its research activities on atmospheric processes and climate change modelling.

The goal of Earth Sciences is to apply the latest advances of High Performance Computing (HPC) and Big Data on Earth system modelling, putting the department at the forefront of the emerging problem of environmental forecasting. This very broad and ambitious objective is divided into four specific goals:

- Develop a modelling capability including the modelling of combined atmospheric processes, from urban to global scales, along with their impacts on weather, air quality, climate, health and ecosystems.
- Implement the most efficient climate prediction system to cover time scales ranging from a month to a few decades (subseasonal-to-decadal climate prediction) at global and regional spatial scales, while expanding at the same time our understanding of the climate system.
- Research the impact of weather, atmospheric chemistry, and climate on socio-economic sectors through the development of user-oriented services that ensure the transfer of developed technologies, and facilitate societal adaptation to a rapidly changing environment, especially for highly vulnerable communities.
- Use cutting-edge HPC and big data technologies to increase the efficiency, portability, and user-friendliness of the Earth system models, including pre-processing and post-processing of weather, atmospheric chemistry and climate data.

Currently, the Group maintains daily high-resolution operational air quality forecasts for Europe and Spain[1] under the umbrella of the CALIOPE project; and also mineral dust forecasts for the Euro-Mediterranean region and East Asia[2]. The Department, in collaboration with the World Meteorological Organization (WMO) and the Spanish Meteorological Agency (AEMET), created the Regional Centre for Sand and Dust Storm Warning System (SDS-WAS) covering Europe, northern Africa and the Middle-East [3] and the first WMO regional meteorological centre specialized in atmospheric sand and dust forecast, the Barcelona Dust Forecast Centre (BDFC) [4].

The Department is structured in four groups that represent the main topics of Earth Sciences research: air quality modelling, mineral dust modelling, atmospheric modelling, and global and regional climate modelling. These groups are interrelated and work in a cooperative form. They are each 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 2014 some 46 staff, collaborators and visitors worked with the Department.



Scientific Output

For additional information, please see the Detailed Report of Research Activities 2014 for the Earth Sciences Department on the BSC-CNS website.

The dissemination of research results obtained by the Earth Sciences Department is significant. These results were presented in numerous ISI-JCR journals, European and international congresses and symposia organised during 2014, such as the Annual CMAS Conf., Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes;

American Union Geophysical, European Geosciences Union General Assembly Meeting and other congresses organised by the European Meteorology Society (EMS), GLOREAM Conf., International Workshop on Air Quality Forecasting and Research.

Communication & Dissemination 2014

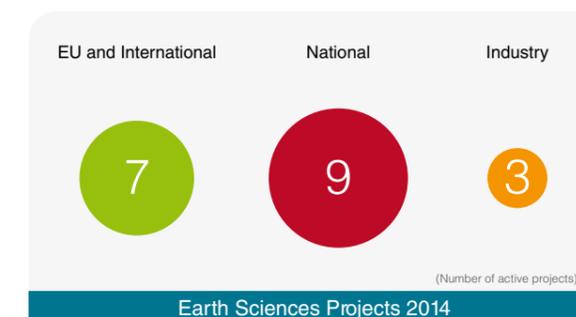
Publishing	
Journal Articles	31
Book Chapters	1
Conference Presentations	
International	38
National	8
Workshops	
Workshops	8
Education	
PhD Theses Read	3

Key Projects and Networks

- Continued IS-ENES2 project Infrastructure for the European Network for Earth System modelling - Phase 2, an FP7 Integrating Activity in the Capacities Programme;
- Continued the MACC-III (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;
- Continued the APPRAISAL project. Air Pollution Policies for Assessment of Integrated Strategies At regional and Local scales, an FP7 Environment project;
- Initiated the CICYT project: Aerosol forecasting and assessment of radiative forcing on weather and climate applications with the online NMMB/BSC-CTM model. Funded by MINECO;
- Participated in the COST Action ES1004. European framework for online integrated air quality and meteorology modelling (EuMetChem) - focusing on a new generation of online integrated Atmospheric Chemical Transport (ACT) and Meteorology (Numerical Weather Prediction and Climate) modelling with two-way interactions between different atmospheric processes including chemistry (both gases and aerosols), clouds, radiation, boundary layer, emissions, meteorology and climate;
- Participated in the European Aerosol Research Lidar Network: EARLINET. The dataset generated is used to validate and improve models that predict the future state of the atmosphere and its dependence on different scenarios;
- Participated in AERONET (AErosol RObotic NETwork), an optical ground based aerosol monitoring network and data archive supported by NASA's Earth Observing System and expanded by federation with many non-NASA institutions;
- Hosted the World Meteorological Organization (WMO) SDS-WAS Northern Africa-Middle East-Europe (NA-ME-E) Regional Centre. The SDS-WAS mission is to enhance the ability of

countries to deliver timely and quality sand and dust storm forecasts, observations, information and knowledge;

- Hosted the first WMO Regional Meteorological Centre Specialized on Atmospheric Sand and Dust Forecast, the Barcelona Dust Forecast Centre (BDFC; <http://dust.aemet.es/>). This centre will build and maintain a web portal to provide forecast products, related information, verification results and services on the internet; it is supported by the WMO;
- Participated in international initiatives such as the International Cooperative on Aerosol Prediction (ICAP) initiative, the Chemistry-Aerosol Mediterranean Experiment (ChArMEx), Air Quality Modelling Evaluation International Initiative (AQ-MEII), and the EURODELTA phase III;
- Participated in the Desert-dust Impact on Air quality through model - Predictions and Advanced Sensors Observations (Diapason) Project from Institute for Atmospheric Science and Climate of the National Research Council of Italy (CNR-ISA; LIFE+ 2010 ENV/IT/391);
- Participated in a European modelling exercise to explore the impact of using finer grid horizontal resolution for policy support applications of the European Monitoring and Evaluation Programme (EMEP) model within the Convention on Long-Range Transboundary Air Pollution (CLRTAP) convention;



- Participated in the The Forum for Air quality Modelling (FAIR-MODE) a joint response initiative of the European Environment Agency and the European Commission Joint Research Centre. It aims to bring together air quality modellers and users in order to promote and support the harmonized use of models by European Member States, with emphasis on model application under the European Air Quality Directive;
- Initiated the Marie Curie project: Effects of Mediterranean desert dust outbreaks on radiation, atmospheric dynamics and forecasting accuracy of a numerical mesoscale model (MDRAF);

Air Quality

The Air Quality Group focuses its research on understanding the physico-chemical processes in the atmosphere that contribute to improvement of the air quality, and analyses the interactions between air pollutants and atmospheric processes, with the aim of obtaining a precise estimation of the air pollution through high-resolution modelling, especially the relation between emissions, atmospheric transport, chemistry and deposition. For that purpose, an air quality modelling system with high spatial and temporal resolution (1 km – 4 km and 1 hour) is under development, implementation and evaluation using 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 2014 the activities of the Group were mainly related to maintaining and improving the daily operational air quality forecast of the CALIOPE system. It encompasses an operational high resolution air quality forecasting system, namely WRF-ARW/HERMES/CMAQ/BSC-DREAM8b, being applied to Europe as a mother domain: 12 km×12 km, 1 h as well as to Spain as the nested domain: 4 km×4 km, 1 h, and with higher detail for some hot spot areas like Andalusia, Barcelona and Madrid, (<http://www.bsc.es/caliope>). Figure 1 shows the improvement in NO₂ emission (top panel) and concentration (bottom panel) when increasing resolution from 4 to 1 km. Such high resolution of the modelling system is made

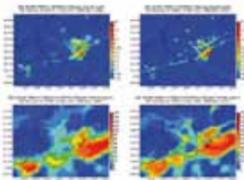


Figure 1

possible by its implementation on the MareNostrum supercomputer hosted by BSC-CNS. In parallel, CALIOPE was involved in a model intercomparison exercise to explore the impact of using finer grid horizontal resolution for policy support applications of the European Monitoring and Evaluation Programme (EMEP) model within the Convention on Long-Range Transboundary Air Pollution

(CLRTAP) convention.

The CALIOPE website and app (web application) for mobiles and tablets devices were maintained and updated with a new products during 2014; the number of people exposed to contamination above air quality limit values by administrative region, and the hourly emission forecast by pollutant and SNAP sector in Spain and by administrative region.

Within the CALIOPE system, the meteorological model was updated to version 3.5.1, and a more accurate land use database (CORINE Land Cover V16) replaced the default database (USGS). WRF meteorological forecasting was improved by using the high resolution digital elevation data base from NASA at 90m.

Regarding emissions, HERMESv2 was updated to use the revised European inventory based on 2011. In order to increase the confidence on the emission model, HERMESv2.0 was intercompared with the TNO-MACC-II emission dataset which is a widely used inventory in Europe. Both emission datasets were implemented inside the CALIOPE system, and intercompared in terms of air quality concentrations over Spain and compared with ground-based observations. The exercise showed significant advantages of the HERMESv2.0 because it uses local information from Spain, meanwhile TNO-MACC-II uses less accurate European databases.

The chemical transport model CMAQ was updated to version 5.0.2 which is more efficient in terms of computational time. To improve predictions of high polluted plumes coming from power plants and refineries, the hourly plume rise calculations over Spain in terms of vertical emission allocations and modelled air quality concentrations for point source were implemented.

CALIOPE was used in many in different studies, including assessment of the dynamic of air pollution in the Iberian Peninsula as a function of representative climatic synoptic circulations, as a management tool to study air quality impact of urban management strategies such as the implementation of electric vehicle fleet in the urban areas of Barcelona and Madrid, and to assess air pollution effects on health in Spain.

Climate Modelling

In the framework of the IS-ENES2 project, the 2nd European Earth System and Climate Modelling Summer School (<https://verc.enes.org/community/schools/2nd-e2scms>) was jointly organised in Barcelona in summer 2014 by the German Max Planck Institute for Meteorology (MPI-M), the English National Centre for Atmospheric Research (NCAR), and the Earth Sciences Department of BSC-CNS. It trained 30 international students during two weeks, including theoretical and practical assignments, which were developed both in MareNostrum III and the MPI-M computational facilities. Invited speakers from different institutions shared their expertise in atmospheric, ocean, chemistry, biogeochemistry and land processes and its implementation within Earth System Models. The Earth Sciences Department acted as the summer school host, contributing to the selection of candidates, the definition of the program, the selection of experts to be appointed to the different talks and support activities, the preparation of the practical exercises, and the assessment of the outcomes. BSC-CNS staff also provided technical and scientific support.

Regional climate activities during 2014 focused on dynamic downscaling of global projections for the Mediterranean area and its analysis. The results of the ESCAT project, which aims to provide high resolution climate projections for Catalonia, were further exploited. Two scientific articles were published on this analysis, one focusing on mean climatic trends (Gonçalves et al., 2014) and the other on extreme events (Barrera-Escoda et al., 2014) for temperature and precipitation. These work results were also presented in multiple international and national conferences on the geosciences field. Additionally, ESCAT wind projections were analysed to assess the capabilities of regional climate models (RCMs) for providing relevant information for final users (in this case, the wind energy industry). RCMs are able to define wind patterns and as such, they could be used to study the suitability of the preferential areas for the location of wind farms over a region when applied at high resolution. The group also participated in networking activities at the Catalan level, such as the Climate Change Experts Group of Catalonia (GECCC) annual meeting.

The group was also involved in COordinated Regional Downscaling Experiment (CORDEX) of the World Climate Research Programme (WCRP). Our goal was to contribute to the ensemble that was being generated for the Mediterranean area (MedCORDEX) with a new member: the NMMB/BSC-CTM model. First steps included an assessment of the NMMB/BSC-CTM capabilities to perform long-term climate runs at high resolution, in which an evaluation performed using ERA-Interim reanalysis as a driver was tested. Preliminary results regarding the computational time and the model assessment against observations are promising, however a deeper analysis and ongoing work on this subject are required.

Atmospheric Modelling

The research group continued the developments of its main modelling tool, the NMMB/BSC-Chemical Transport Model (NMMB/BSC-CTM). During 2014, the system was enhanced with a computationally efficient complete aerosol chemical mechanism. State-of-the-art parametrisations for secondary organic aerosols and inorganic chemistry are now included in the system. Aerosols affect the radiative transfer across the atmosphere by scattering and absorbing solar radiation. An explicit treatment of the scattering and absorption of aerosols was implemented in NMMB/BSC-CTM to address the impact of the direct effect of aerosols on meteorology.

In the framework of the Severo-Ochoa project, the Group continued collaboration with the Computer Sciences Department to improve and extend the computing performance of the NMMB/BSC-CTM system. The model was prepared to use the OmpSs programming model. Performance improvements of specific parts of the model were achieved using tasks provided by OmpSs. Three study cases were addressed; im-

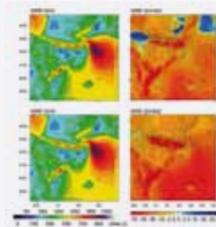


Figure 2

proving computation routines, overlapping communication with computation, and combining tasks with computation and communication. Moreover, the use of multithread MPI was investigated in order to improve a specific code that had been identified as having strong potential for executing MPI calls at the same moment from different threads. The NMMB/BSC-CTM was ported and tested to the MontBlanc prototype hosted by BSC-CNS.

Collaboration with the Geophysical Flows group was established to implement the ash aerosol module of the model Fall-3D within the NMMB/BSC-CTM model. The main objective of the work is to study the effects of ash dispersal and sulphate formation from volcanic eruptions on the radiative budget and meteorology.

An additional development of the Group's chemical transport model was in the field of data assimilation, a statistical framework for combining model simulations and observations to estimate the optimal state of the atmosphere (also known as analysis). Following what is the state-of-art in the field, the dust module of the NMMB/BSC-CTM was coupled with an ensemble-based data assimilation scheme called Local Ensemble Transform Kalman Filter (LETKF). The LETKF scheme requires an ensemble of model runs whose spread around the mean represents the model background uncertainty and is a technique particularly suited for high-performance computing applications: the execution of an ensemble of independent model integrations is highly parallel, while the analysis calculations are explicitly parallelised in the code (the analysis can be performed locally in the model grid). As uncertainty in the emission term is particularly high for mineral dust, an ensemble was chosen according to perturbations in the model's dust emission. The system was tested on the assimilation of Aerosol Optical Depth (AOD) retrievals from the U.S. Naval Research Laboratory (NRL) MODIS product and from the MODIS Deep Blue product. The MODIS Deep Blue product provides information over dust source regions which is unique in the family of aerosol satellite retrievals. Observations were carefully preprocessed for dust with the use of other satellite products and underwent quality control during the assimilation process according to their departures from the model background. The assimilation of satellite retrievals showed a relevant impact on the characterisation of the atmospheric dust load by the NMMB/BSC-CTM model (see Figure 3).

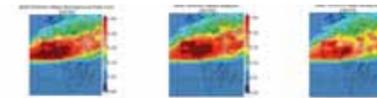


Figure 3

Mineral Dust Modelling

The Mineral Dust Group provides daily operational forecasts of mineral dust for North Africa, Middle East, Europe and East Asia based on the updated version of BSC-DREAM8b. The model is participating in the Sand and Dust Storm Warning and Assessment and Advisory System (SDS-WAS) Regional Centre for Northern Africa, Middle East and Europe. Also BSC-DREAM8b is offline coupled to the CALIOPE air quality forecasting system, thereby enabling CALIOPE to offer a unique operational forecasting air quality system over Europe including the contribution of Saharan dust on an hourly basis.

In 2014 the Group continued development of the NMMB/BSC-Dust model. This is the mineral dust module of the NMMB/BSC-Chemical Transport Model (NMMB/BSC-CTM) which is on-line coupled to the new generation unified atmospheric model NMMB of the National Centres 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 in the framework of the NMMB/BSC-CTM project. NMMB/BSC-Dust includes a physically-based dust emission scheme taking into account the effects of saltation and sandblasting, soil moisture and viscous diffusion close to the ground. In this period, the NMMB/BSC-Dust model is in operational status and provides operational dust forecasts over North Africa-Middle East-Europe and global re-



Figure 4

gions. The dust forecasts are published daily and evaluated (against ground-based and satellite observations) in the website of the model (<http://www.bsc.es/projects/earth-science/NMMB-BSC-DUST/>).

The NMMB/BSC-Dust model provides operational dust forecasts to the first WMO Regional Meteorological Centre Specialized on Atmospheric Sand and Dust Forecast and the Barcelona Dust Forecast Centre (BDFC; <http://dust.aemet.es/>). The Centre operationally generates and distributes predictions for the NAMEE region. Moreover, the NMMB/BSC-Dust model is participating in the International Cooperative on Aerosol Prediction (ICAP) model inter-comparison initiative (<http://www.nrlmry.navy.mil/aerosol/icap.1087.php>) as well as in SDS WAS Regional Centre for Northern Africa, Middle East and Europe.

The dust forecasts of both the BSC-DREAM8b and NMMB/BSC-Dust models are accessible from the new new graphical interface implemented in the BSC-CNS website (<http://www.bsc.es/earth-sciences/mineral-dust/>).

In 2014, the MDRAF project started with the objective to describe the 3D structure of Mediterranean desert dust outbreaks and study their effects on radiation and atmospheric dynamics by means of numerical modelling (NMMB/BSC-CTM). The study region covers the broader Mediterranean basin and the analysis extends over the period of 2002-2012.

WMO SDS-WAS NAMEE Regional Center

Activities in the framework of World Meteorological Organization (WMO) Sand and Dust Storm Warning and Assessment and Advisory System (SDS-WAS) Regional Centre for Northern Africa, Middle East and Europe (NA-ME-E), hosted by AEMET and BSC-CNS, were also undertaken. The web portal of the NA-ME-E Regional Centre (<http://sds-was.aemet.es/>) provides National Meteorological and Hydrological Services with the necessary information to issue operational predictions and warning advisories related to the dust content in the atmosphere. During 2014, 2 new operational systems were added to the list of 9 already existing operational dust forecast systems (BSC-DREAM8b, DREAM8-NMME-MACC, MACC, NMMB/BSC-Dust, MetUM, GEOS-5, NGAC, EMA RegCM and DREAMABOL) and were also included in the daily activities of NA-ME-E Regional Centre. In addition to AERONET observations, the dust forecast evaluation was expanded to include MODIS aerosol product (Figure 5).



Figure 5

In 2014, the Regional Centre organised, coordinated and participated in: Cours sur l'utilisation des produits satellitaires aux applications agrometeorologiques held in Ouagadougou, Burkina Faso, 5-9 May 2014.

The 4th Training course on WMO SDS-WAS products held in Casablanca, Morocco, 17-20 November 2014.

World Health Organisation (WHO) Regional Consultation on Air Quality and Health held in Amman, Jordan, 10-11 December 2014.

The experience acquired by the management in coordination with Spanish Weather Agency (AEMET) of the WMO SDS-WAS NA-ME-E Regional Centre and the demand of many national meteorological services led to the deployment of operational dust forecast services to the creation of the first WMO Regional Meteorological Centre specialized on Atmospheric Sand and Dust Forecast, the Barcelona Dust Forecast Centre (BDFC; <http://dust.aemet.es/>), which was publicly presented in June 2014. The Centre operationally generates and distributes predictions for the NAMEE region. The dust forecasts are based on the NMMB/BSC-Dust model developed at BSC-CNS.

Modesto Orozco, Director of the Life Sciences Department →



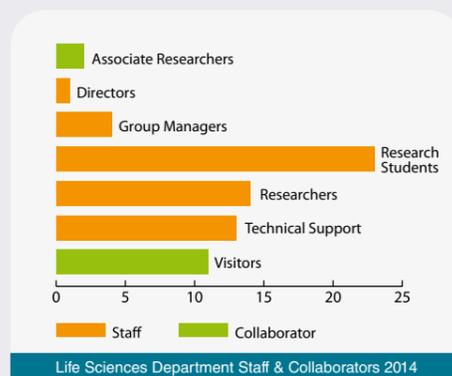
The aim of the scientists in the Life Sciences Department is to understand the molecular biology and evolution of living organisms using theoretical models and simulation algorithms.

The Department benefits greatly from its unique situation in a major supercomputer centre, and also exists within a large and active environment of research in experimental biology. Its research line is tightly integrated in a collaborative effort with the Institute for Research in Biomedicine (IRB Barcelona) under the Joint IRB-BSC Research Program on Computational Biology, with an extension signed in December 2013 to also include research groups from the Centre for Genomic Regulation (CRG), which commenced in 2014. The Department also has strong collaborations with ICREA and the National Institute of Bioinformatics (INB). Major areas of research include Molecular Modelling, Structural Bioinformatics, Computational Genomics, Network Medicine, Subatomic Study of Protein Functions, and Protein-Protein Docking.

Developments of note in 2014 include the identification of the first structural basis for the interaction between the catalytic light subunit and the heavy subunit of a human Heteromeric Aminoacid Transporter (Rossell et al PNAS 2014) and the discovery of one of the mechanisms by which Legionella infect human cells (Lucas et al PNAS 2014). In the genomics field Department researchers developed an innovative method to determine somatic mutations (SMUFIN; Moncunill et al Nature Methods 2014), identified new asthma genetic markers (Bonnelykke et al Nature Genetics 2014), and studied the genetic factors of auto-immune diseases (Alonso et al. Gastroenterology 2014; Julià et al Human molecular genetics 2014).

The structure of the Department and the technology platforms enables coverage of the entire field of computational biology, from atomistic detail to holistic views of the entire ecosystem. The Groups integrate different independent researchers, led by senior scientists who work in different aspects of computational biology. The Department is composed of 4 research groups and 2 research platforms.

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



Joint IRB-BSC-CRG Program on Computational Biology

The Computational Biology Program is a joint venture between BSC-CNS, IRB Barcelona and CRG with the mission to address the computational challenges in molecular biology. The Program, coordinated by Modesto Orozco, includes researchers from the Structural and Computational Biology, and the Chemistry and Molecular Pharmacology Programs at IRB, and from the Life Science Department of BSC-CNS:

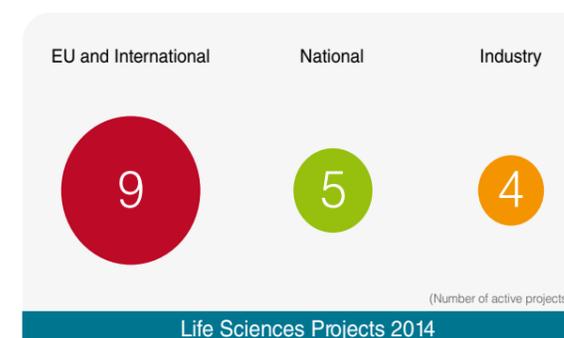


- Dr. Patrick Aloy, Group Leader, IRB Barcelona
- Dr. Xavier Salvatella, Group Leader, IRB Barcelona
- Dr. Juan Fernández Recio, Group Leader, Barcelona Supercomputing Center
- Dr. Victor Guallar, Group Leader, Barcelona Supercomputing Center
- Dr. David Torrents, Group Leader, Barcelona Supercomputing Center
- Dr. Roderic Guigó, Group Leader, CRG
- Dr. Cedric Notredame, Group Leader, CRG
- Dr. Yogi Jaeger, Group Leader, CRG
- Dr. Gian Gaetano Tartaglia, Group Leader, CRG



EU & National Projects

Highlights among 2014 projects include:



- ERC Advanced Grant PELE, a project to develop a software platform for "a la carte" drug design
- Collaboration with CETEMMSA to design bio-ink
- TransPLANT, an European project to develop a trans-national infrastructure for plant genomics
- ProCoGen, a European project to study confiner genomics
- BLUEPRINT, a European initiative to study haematopoietic epigenomes
- eDRUG: the ERC market Proof-of-Concept for PELE
- INDOX, a collaboration with Anaxomics to improve the design of industrial enzymes
- Marató TV3, to discover new inhibitors of the glutamate transporter

Scientific Output

For additional information, please see the Detailed Report of Research Activities 2014 for the Life Sciences Department on the BSC-CNS website.

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

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

Communication & Dissemination 2014

Publishing

Journal Articles	41
Book Chapters	1

Conference Presentations

International	7
National	1

Education

PhD Theses Read	1
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Organised Events:

In 2014 the Department organised the Amber Workshop in collaboration with Prof Ross Walker (UCSD) and Prof Adrian Roitberg (U Florida) and with the support of NVIDIA and the BSC Severo Ochoa Centre of Excellence program. Together with CRG and IRB Barcelona, the Department organised the Joint Programme retreat and the DNA retreat.



Protein Interaction and Docking (PID) Group

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



Molecular Modelling and Bioinformatics (MMB) Group

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



Electronic and Atomic Protein Modelling (EAPM) Group

The Electronic and Atomic Protein Modelling Laboratory is devoted to the development of computational algorithms to advance in the understanding of protein's biochemistry and biophysics. For these purposes, the Group applies and develops two different sets of techniques: classical and quantum simulations.



INB-BSC-CNS

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

Experimental Bioinformatics Laboratory (EBL) Platform

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



Computational Genomics (CG) Group

The aim of the Computational Genomics Group is to investigate different processes of the biology of genomes and to contribute to the understanding of how the sequence and the structure of these macromolecules determine their basic functions. The research lines focus on deciphering the code and the mechanisms that control when and where genes are expressing their function in the cell. The Group has developed tools and strategies for the identification and classification of gene regulatory regions to study their function, their evolution and their role in the adaptation of organisms to their environment. The Group is also interested in determining how modifications and alterations of the sequence are directly responsible or confer susceptibility to certain diseases. This is done through the application of systems biology approaches and sequence analysis strategies involving large DNA sequencing efforts to understand the causes and the evolution of complex pathological processes, such as type 2 diabetes, anaemia, and even the immunological rejection of transplanted liver. Simultaneously, the Group is developing tools for the analysis of the cancer genome in the context of the Cancer Genome Project to identify somatic mutations, with particular interest in those affecting regulatory regions. The Group also engages in collaborative efforts within high impact projects related to the assembly and the primary analysis of genomes and metagenomes.

José María Cela, Director of the CASE Department →



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

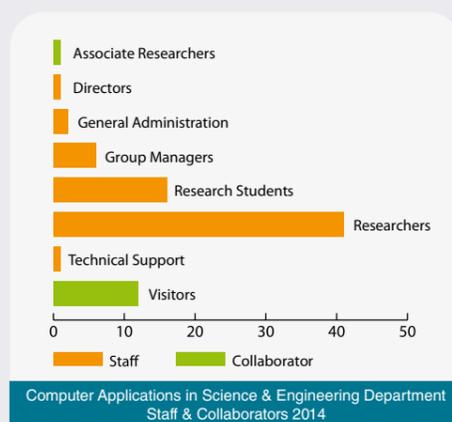
The applications developed by the CASE department are truly multidisciplinary, requiring a deep level of expertise in many fields. In order to successfully develop these applications, the skills of the CASE team in numerical methods and parallel programming must be complemented by experts in the appropriate areas. The Department therefore develops collaborations with other scientific groups in all areas of science and technology. Examples of Spanish institutions with strong research links with CASE include CIEMAT, CSIC, IAC, ICFO, IMDEA and different universities. CASE also collaborates with institutions abroad like Imperial College, Oxford University, STFC in the UK, EDF and Ecole Centrale de Paris in France, and George Mason University and Jackson State University in the USA. This is complemented with strong links with industrial partners in need of advanced simulations of complex technology problems, such as REPSOL or Iberdrola.

The main research field of CASE is High Performance Computational Mechanics, which requires a deep background in Computer Science, Physics and Numerical Methods. Major research areas are Computational Fluid Dynamics and Solid Mechanics, Ab-initio DFT and TD-DFT molecular dynamics, Seismic Imaging and Parallel Programming. Major application areas are Aerospace, Fusion Physics (plasma core and edge transport, plasma instabilities), Biomechanics (Cardiovascular and Respiratory systems), Geophysics and Atmospheric flows. CASE also has a group working in large scale social simulations and smart cities. Finally, CASE has a group devoted to visualisation tools and techniques, which are critical to extract full benefit from numerical simulations.

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

- Alya: HPCM system. Fluid mechanics, Solid mechanics, Electric propagation, Combustion, etc.
- FALL3D: Volcanic ash transport. Operational at the Buenos Aires Volcanic Ash Center (VAAC)
- BSIT (Barcelona Subsurface Imaging Tools): Acoustic/Elastic/EM waves, Forward Modelling, RTM, FWI. Promoted by Repsol.
- SIESTA: Ab-initio molecular dynamics. CASE is a co-developer of this code.
- Pandora: An HPC Agent-Based Modelling framework for social simulation.

The CASE Department is led by José María Cela. The research lines fall naturally in six main groups: Physical & Numerical Modeling (PNM), High Performance Computational Mechanics (HPCM), Environmental Simulations (ES), Geosciences Applications (GA), HPC Software Engineering (HPCSE), and Data Pre & Post Processing (DPPP). Each Group consists of around 10 people, comprising several senior scientists, post and pre-doctoral students and visiting scientists. PNM, HPCSE and DPPP research lines are horizontal, in the sense that they develop core components and tools used by other groups. HPCM, ES and GA lines are vertical, in the sense that they develop applications tailor-made to meet specific project needs. Due to the multidisciplinary character of CASE research activities several groups are often involved in each project.



Scientific Output

For additional information, please see the Detailed Report of Research Activities 2014 for the CASE Department.

Communication & Dissemination 2014

Publishing

Journal Articles	26
Books	1
Book Chapters	3

Conference Presentations

International	35
National	3

Education

PhD Theses Read	3
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Except for work that is private and confidential and cannot be published, research results of the CASE Department were presented in congresses and conference lectures as well as a number of scientific publications, including:

- Development and optimization of a solid mechanics module in Alya.
- Implementation of coupling strategies in a distributed memory environment (FSI).
- Coupling of Alya and Code_Saturne, the CFD code developed at EDF, France.
- Development of an implicit VMS compressible solver and preconditioning techniques.
- 3D Seismic inversion for large data sets using FWI from BSIT.
- Development of electromagnetic modelling (CSEM) on BSIT.
- BSIT kernel optimization for both Intel Sandy Bridge processors and Intel Xeon Phi co-processors.

Key Projects

In 2014, the CASE Department carried out work under the scope of the following projects:

- EU-funded projects:

CASE was actively involved in PRACE3IP and PRACE 4IP projects, mainly concerning the optimisation on massively parallel supercomputers of Alya code, which is part of the European Unified Benchmark Suite. Also, important contributions were made to applications work packages of DEEP and DEEP-ER.

- Enterprise-funded projects:

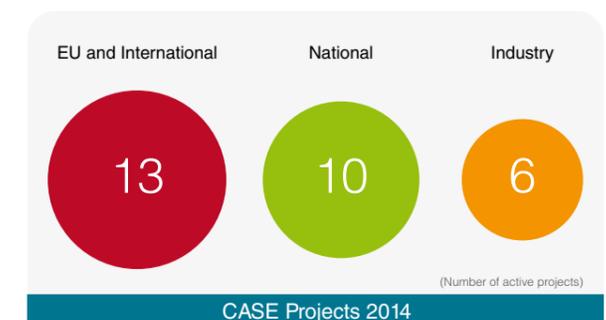
Iberdrola and Repsol are CASE's main industrial collaboration partners in the energy sector. Also, CASE actively participates in the Exascale Lab funded by Intel on topics related to Geophysics

- Nationally funded projects:

CASE was involved in the S4E (Supercomputing for Energy) project, which aims to develop high performance simulation codes in the area of energy, namely wind energy and oil and gas.

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

CASE has established strong national and international collaborations, all of them fostered by the Severo Ochoa Programme. In summary: A CASE post doctoral researcher spent nine months as resident researcher at the Mount Sinai Hospital in New York, starting a research line on carotids simulations; an MOU was signed with the National Centre for Cardiology Research (CNIC) to work on ventricular arrhythmias, with a BSC-CNS PhD student co-supervised by CNIC; CASE is performing full cardiovascular simulations from the heart up to the cerebral arteries by coupling Alya with ADAN, the arterial network created at the LNCC in Brazil; a collaboration with Imperial College and St Mary's hospital (UK) conducted respiration and sniff simulations with an unprecedented degree of accuracy; a collaboration with Jackson State University coupled real patient large airways to generic models for small airways, in order to carry out simulation of the almost complete respiratory system.



- Other collaborations:

The department is collaborating in various topics with the following institutions:

- CINES, France: asynchronous and dynamically load balanced code coupling.
- Technical University of München, Germany: multi-code coupling strategies.
- STFC, UK: multi-code coupling strategies.
- EDF, France: multi-code coupling strategies.
- NCSA, USA: performance studies of Alya code on Blue Waters supercomputer and scalability of direct solvers.

Physical and Numerical Modelling (PNM)

Computational Mechanics

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

- Mathematical modelling of a given physical process.
- Numerical modelling of the mathematical equations.
- Numerical algorithms to solve the discrete equations efficiently, or to couple a set of algorithms to solve complex physical problems.
- Efficient implementation in a computational mechanics code.
- Chimera method applied to the structure dynamics of a neurone using the HERMESH method
- Code performance analysis and optimisation.

Due to the installation of new large scale supercomputers in Europe during recent years, the Group dedicated a lot of resource to upgrade the Alya high performance computational mechanics (HPCM) code, including:

- Solvers.
- Sparse direct solver.
- Implementation of the restricted Additive Schwarz preconditioner.
- A parallel version of SIESTA code with better load balancing and sparse iterative eigensolvers.
- Speed up tests were carried out on the main European supercomputers on up to 22528 CPUs.

Computational Social Sciences

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

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

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

High Performance Computational Mechanics (HPCM)

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

Activities 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:



- Alya applications:
 - Biomechanics: hemodynamics, respiratory system air flow, cardiac simulations.
 - Building, energy and environment: mesoscale, urban environments, wind farms, plastics recycling.
 - Vehicle dynamics: cars, racing yachts, high speed trains.
 - Simulation of chemical reactions in biodiesels inside batch reactors, coupling with mixing blades, transfer of chemical species through the interfaces of immiscible liquids.
 - Combustion chamber simulation in gas turbines, both for aerospace and energy production.
- Fall3D applications:
 - Atmosphere science: Volcanic ash transport.
- SIESTA Applications:
 - Ab-initio DFT and TDDFT molecular dynamic simulations.
- Other applications:
 - Plasma physics.

HPC Software Engineering (HPCSE)

The HPC Software Engineering team is responsible for the good performance of the different codes developed by CASE. This group designs the applications software architecture and performs fine tuning of these codes on different hardware architectures. The applications are designed in such a way that all possible levels of parallelism are exploited and aspects such as fault tolerance are taken into account. For the software tuning this group collaborates with hardware manufacturers to obtain roofline analysis of the codes and other performance metrics. Aspects like documentation, testing, etc, are also responsibility of this group.

Environmental Simulations (ES)

Atmospheric Transport

Modelling of atmospheric transport, with particular emphasis on volcanic ash. Research lines include:

- Volcanic Ash Transport and Dispersal Models (VATDMs), including model validation, ensemble forecast and operational implementation.
- Development of theoretical models for ash aggregation, dynamics of volcanic plumes, gravity currents, and resuspension of ash by wind.
- Assessment of hazard and impact of volcanic ash fallout on local communities and of volcanic ash clouds on civil aviation.
- Study the feedback effects of large-magnitude eruptions on regional

meteorology. This is done in collaboration with the Earth Science Department and using FALL3D-NMMB/BSC-CTM, an on-line multi-scale meteorological model coupling the dispersion and sedimentation functionality of FALL3D with the powerful NMMB/BSC-CTM weather forecasts from global to mesoscale domains.

- Code optimisation. Implementation of transport models in multi-purpose frameworks and porting of parallel software to different architectures.

Meteorological Modelling

Research lines include:

- Mesoscale Numerical Weather Prediction (NWP).
- Data assimilation and downscaling from mesoscale NWP models to local-scale.
- High-resolution wind field modelling in complex terrains using CFD, with Alya.
- Modelling of the atmospheric boundary layer including turbulence and thermal effects.

Wind energy

Numerical modelling of wind farms is a crucial aspect in terms of both wind farm design and management. Applications using ALYA Green for high-resolution wind field modelling include:

- Modelling of on-shore and off-shore wind farms considering all aspects affecting surface layer atmospheric flows such as topographic variations, heterogeneities in the roughness of the terrain, and the downwind wake effects of rotors.
- Modelling of wind turbines using actuator disks and the HERMESH method. This method allows efficient local mesh refinements.
- Wind resource assessment.
- Forecast of short-term wind farm power production.
- Tailored modelling postprocess using GoogleEarth to facilitate visualization and standard data interchange.



Geosciences Applications (GA)



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

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

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

The final objective is to merge all developments in the BSIT geophysical imaging toolkit (www.bsc.es/bsit).

Data Pre & Post Processing (DPPP)

The DPPP team, comprising scientists, programmers, and visual communication and interaction experts, works on the visual representation of HPC simulation data for three main communicative situations:

- Data exploration as a tool for scientists.
- Outreach to the community at large.
- Publication of results from a scientist to other experts in the field.

Achievements and work during 2014:

The DPPP team collaborated with the international music festival Sónar to produce and showcase a general information visualisation webpage, A.Track.Tion (<http://www.bsc.es/atraction/>), around the topic of music. The web showcased an interactive visualisation of the popularity of music genres since 1954, as well as the influence between them. Apart from the visualisation and interaction design, the team also obtained and analysed the data behind the application, creating and using automatic web crawlers and parsers to gather genre information from unstructured text sources like Wikipedia.

A multiyear collaboration was initiated with the Life Sciences department for designing and producing a graphical interface for the PELE molecular dynamics simulation software.

Within the frame of the European CONSOLIDER project SyEC, in February 2014 the Team released the short film documentary "Supercomputers" (youtu.be/b5bQdTLOwAg).

Snapshot of the shortfilm documentary "Supercomputers" Through high-end render visualisations and interviews the film explains the impact of high performance computing on science, technology, and society. "Supercomputers" received the following awards at international film festivals:

- Winner, Academia Film Olomouc International Festival of Science Documentary Films (Czech Republic),
- Winner, 2014 Ronda International Scientific Film Biennial (Spain),
- Winner, Daroca&Prisión Film Festival (Spain)
- Official Selection, Science Film Festival (Southeast Asia)
- Winner, Festival Internacional de Cortometrajes de Torrelavega (Spain)

The audience reached through the festival screenings exceeds half a million a people.

The team also produced numerous short videos and static images for scientists of BSC-CNS and the RES for use in scientific publications and webpages.



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 and PRACE. Further core objectives are to manage upgrades to the MareNostrum and other RES nodes; facilitate access to RES facilities, including online electronic applications, remote access, and porting of code; manage the environmental aspect of the BSC-CNS installations; manage the technical aspects of integration of the MareNostrum in the PRACE, EUDAT and European HPC network ; 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.

Led by Sergi Girona, the Operations Department ensures the continuous daily functioning of RES supercomputers and remote access by users, both within Spain and internationally. In addition to all the routine maintenance and operations tasks, 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-2 and EUDAT. The constant upgrading and utilisation of cutting edge technology implies that staff within the Department, liaison staff at the RES and PRACE 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.

The continuous growth of the BSC-CNS team requires a constant remodelling of premises to accommodate the new employees, and to facilitate the development of their research. Until the BSC-CNS headquarters building is ready to be used, maintenance and extension of current computer rooms, office space and meeting rooms requires an intensive effort.

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 BSC-CNS and related facilities.

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

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



Key Projects

The Operations Department was involved in the following projects during 2014 :

- RES (Red Española de Supercomputación): The Spanish Supercomputing Network offers coordinated HPC services to the Spanish scientific community. The Operations Department is responsible for the coordination of the network, including all support and administration services.
- PRACE 2IP: In the PRACE Second Implementation Phase, the Operations Department is involved in WP2, WP5, WP6, WP7 and WP10, and coordinates the participation of BSC-CNS in the project.
- PRACE 3IP: In the PRACE Third Implementation Phase, the Operations Department is involved in WP2, WP5, WP6 and WP7, and coordinates the participation of BSC-CNS in the project.
- EESI2: The objective of this Support Action, co-funded by the European Commission, is to build a European vision and roadmap to address the challenges of the new generation of massively parallel systems composed of millions of heterogeneous cores which will provide multi-Petaflop performances in the next few years and Exaflop performances in 2020.
- EUDAT: The EUDAT project aims to contribute to the production of a Collaborative Data Infrastructure (CDI). The project's target is to provide a pan-European solution to the challenge of data proliferation in Europe's scientific and research communities.
- RDA-EUROPE: The RDA-EUROPE is a project focuses on coordinating a series of cross-infrastructure experiments on global interoperability with a selected group of projects and communities. One of its main functions is support of the RDA initiative.



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.

Gateway hardware updated

During October 2014 the platform to access BSC-CNS resources from internal and external networks was upgraded to enhance security. The technology used is SSL VPN which first performs a user authentication followed by host checking to determine the level of reliability of the client machine. Depending on this level one of two roles will be offered to the user:

- 1) BSC-CNS Basic external access where only web access is permitted
- 2) BSC-CNS VPN external access: In addition to the web services this role allows the establishment of a VPN connection to internal BSC-CNS resources.

Performance monitoring improvements

A BigData infrastructure was deployed to receive and store all MareNostrum3 jobs information. This SaaS receives a continuous stream of information as jobs are being executed in the supercomputer and provides dynamic accounting and several graphical tools to help the Operations team analyse usage distribution providing a wider understanding of the overall system behaviour.

In addition to the graphic interface, this platform provides back-end information for Support's team public reporting tools.

New HPC machines

During 2014, three new installations and upgrades were performed on BSC-CNS HPC resources:

First, an IBM x3850X5 shared memory multiprocessor composed of 80 cores and 2 TB of main memory was installed and completely integrated as a node inside MareNostrum3. This server allows researchers to perform specific pre and post-processing analysis that require large shared memory systems.

Second, 256 MareNostrum nodes were upgraded to accommodate memory-bound parallel applications, half of those nodes had their memory quadrupled from from 32GB to 128GB, and the other 128 nodes had their memory improved from 32GB to 64GB. These special nodes can be requested using a specific key in the jobs description.

Finally, two new servers based on the cutting-edge Power8 processors technology were installed. Each server has:

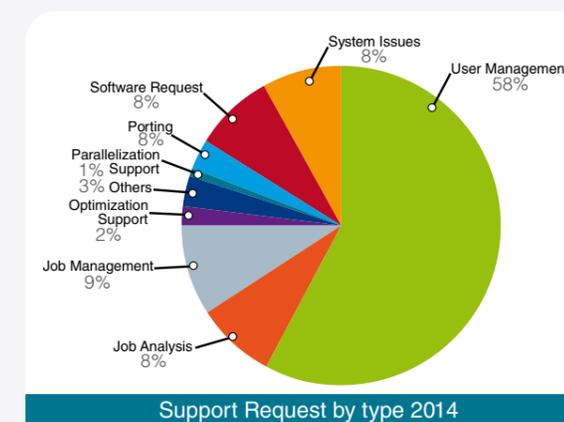
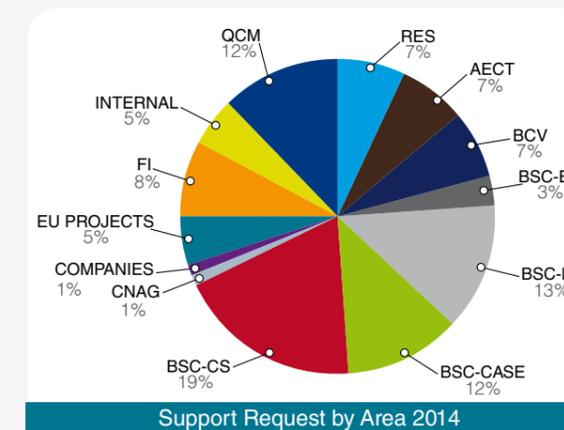
- 4 Sockets Power8 12-core at 3 GHz (8 threads per core)- 1 TB main memory- 2 NVIDIA Tesla K40m
- These servers will help to perform research in Big Data, Computer architecture and parallel application development based on this new technology.



User Support

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

Some 7403 support requests were received in 2014 as presented in the figures below, split by support request area and by type.



Highlighted Projects

UserPortal

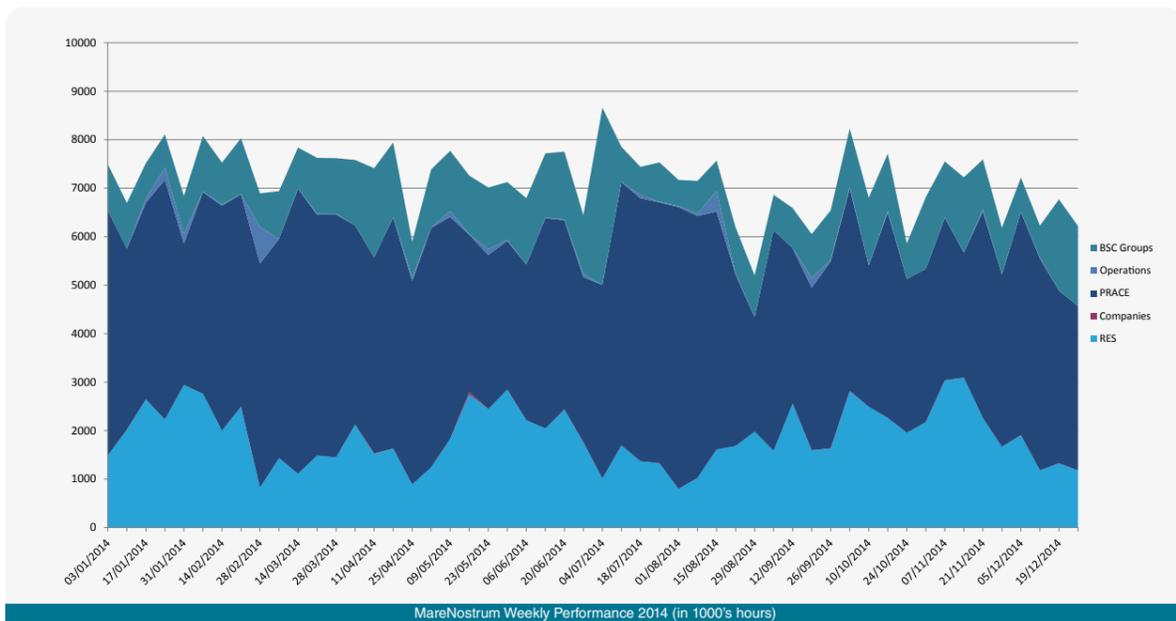
During 2014 the User Support Team put into production the UserPortal interface. This service provides the end user, in a single entry point, with a collection of the most relevant monitoring information gathered by BSC-CNS monitoring tools. This service uses the BSC-CNS central authentication service for security. Users will now be able to better understand the behaviour of their applications and the resources used during their execution.



MareNostrum Performance 2014

MareNostrum was in full production during the entire year with a total of 48128 cores. The observed system utilisation was approximately 88%. In addition to BSC-CNS internal groups, more than 207 external groups accessed the MareNostrum system during 2014.

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



Facility Management

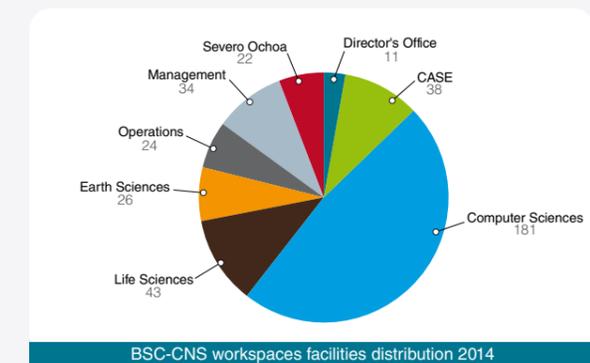
The mission of Facility Management (FM) is to keep BSC-CNS facilities under its purview in a safe and efficient working condition.

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

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

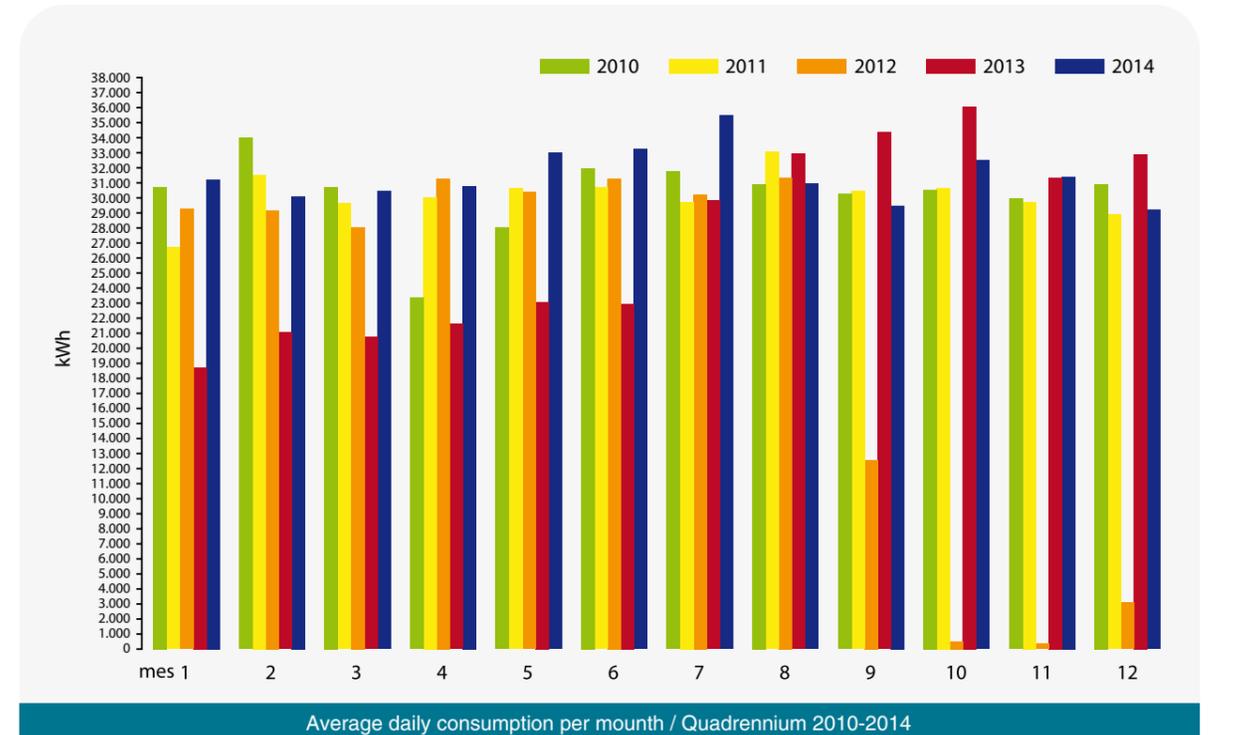
BSC-CNS workspaces facilities distribution 2014

Facility management group includes in its tasks the preparation of the office space for all departments at BSC-CNS. Since 2004, different buildings and office space have been set for those departments, with a continuous and significant growth.



MareNostrum3, reducing power consumption

In September 2012 MareNostrum2 finished its services. MareNostrum3 started operations in January 2013. The full system capacity was reached in July 2013. At that point, by using the best practices, an intensive work to reduce the total power consumption of MareNostrum3 and all cooling facilities was initiated. The upgrade to MareNostrum3 increased the computational capacity 10 times, but the total power consumption increased only by 10%.



Ernest Quingles, Management Department Director →



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

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

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



Finance and Business Administration

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

Finance & Accounting

The Finance & Accounting Group is responsible for the financial resources management of all activities at BSC-CNS (expenses, budgets, audits, bank relations, suppliers, receiving payments and control budget deviations). According to existing financial legislation and accounting norms, it manages and safeguards acquired patrimony with the support of the Administration group. The Group also prepares financial reports for project audits in coordination with the project office and principal researchers.

In 2014, due to the difficult economic environment and public funding delays, the role of controller was reinforced. The unit also worked on the automation of data analysis and exploitation processes, and also introduced the semiannual follow-up of key financial indicators. The SAP B1 Tool was upgraded for better reporting capabilities.



Information System & Services

The Business Administration area strengthened the information management service by creating a new Technical Support unit, in order to develop and improve the SAP management program and other new management software tools installed for the exploitation, control, and reporting of business activity.

Human Resources

The Human Resources Group is responsible for managing selection processes, hiring and training, job descriptions, labour relations and collective bargaining, compensation and benefits, development programmes, planning careers and internal promotions, and health & safety.

In 2014, the Group continued working on a professional development system for all BSC-CNS staff. The new web tool, which was implemented in 2013, helped manage the BSC-CNS Staff Professional Development Plan. The tool facilitated the annual staff evaluation, monitoring the Plan's development, and keeping it aligned with annual goals of the department as well as of the entire Centre.

This year the HR team hired a new Head of Human Resources and a Specialist in HR Development, allowing a restructuring of the Department into specialised areas to give better focus on the BSC-CNS vision that both researchers (at all levels) as well as support staff, are essential contributors and key players in the success of the Centre. BSC-CNS wants to promote a challenging work environment where equal opportunities, ethics & integrity, work-life balance, career prospects and the best work conditions are met.

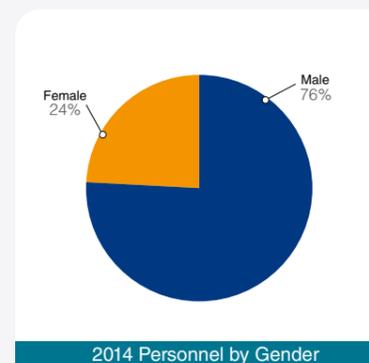
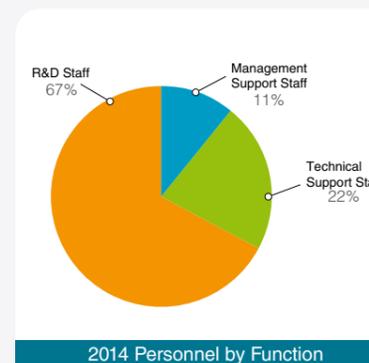
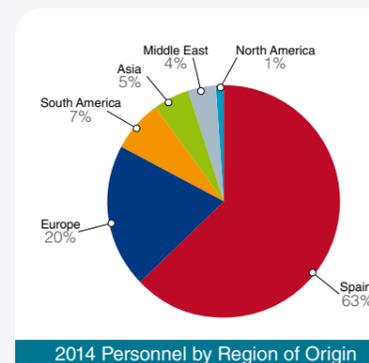
During 2014, BSC-CNS committed to implement and apply the principles of the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers, and to work towards an award of Excellence in Human Resources and management policies (HRS4R), with the aim of promoting transparency, accessibility, and equity in the recruitment and promotion of researchers. BSC-CNS set up a working group that helped to define an action plan to be presented in 2015 to European Commission covering these areas:

- the creation of advisory committees,
- boosting equal opportunities and gender policies,
- strengthening activities in outreach and public engagement,
- maintenance of our career development system.

BSC-CNS also became a member of Euraxess.

BSC-CNS continues to attract researchers from all over the world and currently 37% of its staff is from abroad (from a total of 40 countries). In 2014, 19 BSC-CNS postdoctoral researchers had external fellowships or contractual funding.

The BSC-CNS International PhD Programme continued to attract a lot of young talent from all over the world, supported by internal and external competitive funding and the "la Caixa" International PhD Fellowship Programme. The four candidates selected in the "la Caixa" call 2014 started their PhD thesis in September, after a highly competitive selection process involving significantly number of applicants (126 candidates from over 22 countries).



General Administration

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

In 2014 the administrative support was restructured to increase efficiency and adapt to the growing needs of the Centre and requirements of new projects. New dedicated reception and secretarial services were established for most departments.

During the year, BSC-CNS invited 12 public calls in order to accept 4 supply tenders, 7 service tenders and 1 work tender. The total number of administration contracts signed during the year was 76. Work tenders were held for the continuation of the 2nd phase construction of the new BSC-CNS building.

Project Management

Project Management Office

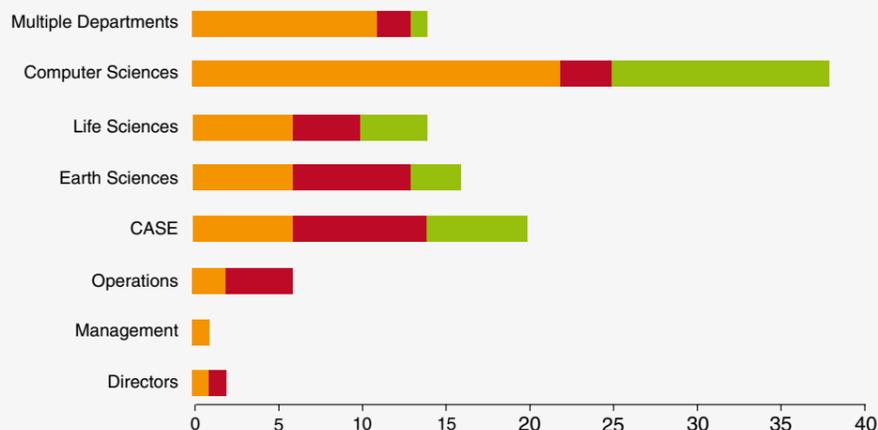
The BSC-CNS Project Management Office (PMO) is staffed by eight experienced project managers, who work closely with the centre's Principal Investigators. PMO is responsible for detecting and communicating research funding opportunities; coordinating and contributing to project proposals; managing contract negotiations and managing legal, financial and administrative aspects of contracts and projects. This includes both publicly funded projects as well as collaborations with private industry. PMO also maintains a comprehensive database of project information which it uses to generate reports on the Centre's performance in various areas.

PMO is responsible for tracking and anticipating developments in relevant funding programmes and helping the Centre adapt to changing requirements. 2014 was the first year of the European Union's Horizon 2020 funding program and the Centre's project managers played a key role in helping the researchers understand and fulfill the program's requirements thus increasing BSC-CNS's capacity to effectively leverage competitive funding.

In 2014, BSC-CNS participated in 111 projects (excluding personnel grants), with a total BSC grant of over thirty-nine million euros. Some 48 projects were funded by the extremely competitive FP7 and H2020 programs of the European Commission. Eight of these European projects were led by BSC-CNS, in which the Centre coordinated partners based throughout Europe and overseas. Four projects were funded by the European Space Agency, and 25 projects were funded by Spanish National or Catalan funds. A total of 32 research projects were funded by private companies, representing total financing of over 12 million euros.

In addition to managing active projects, the Project Management Office assists BSC-CNS researchers in submitting new project proposals for research projects and personnel grants to help ensure continued funding future funding of BSC-CNS activities.

BSC-CNS Projects 2014



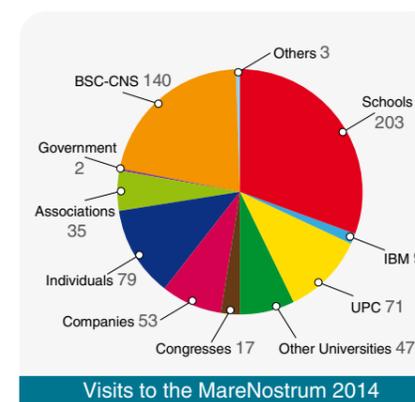
Strategy Support

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



Communication Area

The BSC-CNS Communications team is in charge of increasing awareness of the Centre and disseminating information about research activities both in the scientific and industrial communities, as well as society in general.



Visits

During the course of 2014, BSC-CNS received a total of 9.702 visitors from national and international groups, including schools, universities, research centres, industry and non-profit organisations. Visitors to the MareNostrum are given a tour of the supercomputer and a talk about the Centre, its technology and its research lines. Most visits are tailored depending on the target audience and often incorporate videos and a visit to the BSC-CNS collection of "antique" supercomputers.

BSC-CNS in the Media

BSC-CNS sent out 14 press releases in Spanish, Catalan and English, and identified 440 unique media impacts, all posted on the "BSC in the media" section of the BSC-CNS website. Efforts are made to promote and track BSC-CNS appearances in local, international, general, specialized, on and off line media.

Web and Social Media

In 2014 the Communication team made a major effort to strengthen BSC-CNS's web presence and social media networks. The website had more than 1,375,000 visits. 85 articles were published on the corporate website and 1,618 posts were made on Facebook (437) and Twitter (1,181, tweets and retweets included). The number of Facebook fans increased by more than 100% and the number of Twitter followers, by 100%. The Youtube Channel had almost 400 subscribers and more than 32,000 views in 2014.

Internal Communication

The BSC-CNS Newsletter was launched in 2014 and is published every four months. The team also coordinated the development of the BSC-CNS social plan, managed the BSC-CNS welcome guide in coordination with the HR department, and promoted the creation of an internal repository to share and disseminate information and documentation. The Communication team also:

- provides internal support to Education & Training actions
- organises the annual BSC-CNS meeting and management retreat
- is responsible for organising the photo competition
- disseminates internally information of interest for BSC-CNS staff
- collaborates with HR in preparing the Education Protocol

Events, Seminars and Workshops

In 2014, BSC-CNS hosted and organised the following events: • PRACE days, 20-22 May • CSW & Block Review Barcelona, 12-26 May • Second European Earth System and Climate Modeling School 2nd E2SCMS, June 9-20 • PUMPS Summer School, July 7-11 • PARMERASA dissemination event, 22-23 September • PRACE Council meeting, October 16-17 • Transcardio14, 13-14 November

Participation in International Supercomputing Conferences

The Communications team prepared and supported the BSC-CNS presence at the exhibitions of the International Supercomputing Conference 2014 and SuperComputing14, and the exhibition of the SEG Annual Meeting, 26-31 October 2014.

Dissemination of European and National Projects

The Communications team also carried out BSC-CNS dissemination tasks for 42 European and National projects. PRACE, Mont-Blanc, EUDAT, Paradime and RethinkBig were the projects with most dissemination time assigned to BSC-CNS in 2014.



Computer Sciences 2014 Publications

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- » Gladys Utrera, Julita Corbalán, Jesús Labarta, "Scheduling parallel jobs on multicore clusters using CPU oversubscription", *Journal of Supercomputing*, 68, 1113–1140, 2014
- » Gulay Yalcin, Oguz Ergin, Emrah Islek, Osman Unsal, Adrián Cristal, "Exploiting Existing Comparators for Fine-Grained Low-Cost Error Detection", *ACM Transactions on Architecture and Code Optimization*, 11, 32–32, 2014
- » Isaac Rudomin, Jorge Ramirez, Christian Arzate, "Método Robusto para Detectar Dedos Usando Profundidad", *Research in Computing Science*, 64,

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- » Jordi Balasch-Masoliver, Victor Muntés, Jordi Nin, "Using genetic algorithms for attribute grouping in multivariate microaggregation", *Intelligence Data Analysis*, 8, 819–836, 2014
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- » E. Terradellas, "The dust cycle and impacts", 4th Training Course on WMO SDS-WAS products, Casablanca, Morocco, 17-20 November, 2014
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Life Sciences 2014 Publications

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- » Arcas A, Fern ndez-Capetillo O, Cases I, Rojas AM, "Emergence and evolutionary analysis of the human DDR network: Implications in comparative genomics and downstream analyses", Molecular Biology and Evolution, 31, 4, 940-61, 2014
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- » Dans, Pablo Daniel, Faustino, Ignacio, Battistini, Federica, Zakrzewska, Krystyna, Lavery, Richard, Orozco, Modesto, "Unraveling the sequence-dependent polymorphic behavior of d(CpG) steps in B-DNA.", Nucleic Acids Res, 42, 18, 11304-20, 2014
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- » Yolanda Guillén, Núria Rius, Alejandra Delprat, Anna Williford, Francesc Muiyas, Marta Puig, Sònia Casillas, Miquel Ràmia, Raquel Egea, Barbara Negre, Gisela Mir, Jordi Camps, Valentí Moncunill, Francisco J. Ruiz-Ruano, Josefa Cabrero, Leonardo G. de Lima, Guilherme B. Dias, Jeronimo C. Ruiz, Aurélie Kapusta, Jordi Garcia-Mas, Marta Gut, Ivo G. Gut, David Torrents, Juan P. Camacho, Gustavo C.S. Kuhn, Cédric Feschotte, Andrew G. Clark, Esther Betrán, Antonio Barbadilla, and Alfredo Ruiz, "Genomics of ecological adaptation in cactophilic *Drosophila*", *Genome Biology Evolution*, 7, 1, 349-66, 2014

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- » Lecina, Daniel, Takahashi, Ryoji, Guallar, Victor, "Binding free energy and ligand orientation calculations using Monte Carlo method with Markov State analysis", *Entropy in Biomolecular Systems Workshop*. Vienna, Austria , 2014
- » Moal, I.H, Fernandez-Recio, J., "EVALUATING SCORING FUNCTIONS FOR PROTEIN-PROTEIN DOCKING", *3DSIG: STRUCTURAL BIOINFORMATICS AND COMPUTATIONAL BIOPHYSICS*, Boston (US), 2014
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- » Pallara, C., Rueda, M., Fernández-Recio, J., "Conformational selection mechanism in protein-protein association: insights from docking", *II Jornada de Bioinformàtica i Biologia Computacional*, 2014

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- » Adam Hospital, "High Throughput Computational Studies of Macromolecular Structure Flexibility", Supervised by: Josep Ll. Gelpi and Modesto Orozco, 2014

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- » A.J. Bates, D.J. Doorly, R. Cetto, H. Calmet, A.M. Gambaruto, N.S. Tolley, G. Houzeaux, R.C. Schroter, "Dynamics of Airflow in a Short Inhalation", *J. R. Soc. Interface*, 12, 42005, 2014
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- » Felix Rubio, Mauricio Hanzich, Albert Farrès, Josep de la Puente, José Ma. Cela, "Finite-Difference Staggered Grids in GPUs for Anisotropic Elastic Wave Propagation Simulation", *Computers and Geosciences*, 2014
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- » Xavier Rubio-Campillo, Francesc Xavier Hernández Cardona, María Yubero Gómez, "The Spatiotemporal Model of an 18th-Century City Siege", *Social Science Computer Review*, 2014
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- » F. Magoulès, F.X. Roux, G. Houzeaux, "Cálculo científico paralelo", 2014
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- » Cristina Montañola-Sales, Xavier Rubio-Campillo, Josep Casanovas-García, José Ma. Cela, A. Kaplan-Marcusán, "Large-Scale Social Simulation, Dealing with Complexity Challenges in High Performance Environments", *Interdisciplinary Applications of Agent-Based Social Simulation and Modeling*, 106-123, 2014
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- » D. Mira, M. Zavala, M. Avila, Herbert Owen, J.C. Cajas, G. Houzeaux, M. Vázquez, "Heat transfer effects on a fully premixed methane impinging flame", 10th International ERCOFTAC. Symposium on Engineering Turbulence Modelling and Measurements, Marbella (Spain), 2014
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- » D. Zebbar, G. Houzeaux, K. Mostefa, S. Kherris, "La mise en évidence de l'oscillation radiale du segment de piston d'un moteur à combustion interne", CMVA-ACVM-CIRI 2014, Montréal (Canada), 2014
- » Felix Rubio, Mauricio Hanzich, Josep de la Puente, Natalia Gutierrez, "Lossy Data Compression with DCT Transforms", EAGE Workshop on High Performance Computing for Upstream, 7th-10th September, Crete, Greece, HPC30, 2014
- » Fonseca-i-Casas, Pau, Fonseca i Casas, Pau, Codina-Sancho, Esteve, Codina Sancho, Esteve, Montero-Mercadé, Lidia, Montero Mercadé, Lidia, Linares, M.Paz, Cristina Montaña-Sales, Montaña-Sales, C., Montaña-Sales, C., Tolk, A., Diallo, S. D., Ryzhov, I. O., Yilmaz, L., Buckley, S., Miller, J. A., "Formal and operational validation of a bus stop public transport network micro simulation", Proceeding of the 2014 Winter Simulation Conference WSC'14, Savannah (GA) 7-10 December 2014, Piscataway, NJ, USA, 604-615, 2014
- » Guasch, Toni, Figueras, Jaume, Fonseca-i-Casas, Pau, Cristina Montaña-Sales, Montaña-Sales, C., Josep Casanovas-García, "Simulation analysis of a dynamic ridesharing model", Proceeding of the 2014 Winter Simulation Conference WSC'14, Savannah (GA) 7-10 December 2014, Piscataway, NJ, USA, 1965-1976, 2014
- » H. Calmet, A. Gambaruto, G. Houzeaux, A. Bates, "Challenge of visualising large airway flows and particle transport", The 5th International Conference on

Computational Methods (ICCM2014), Cambridge (UK), 2014

- » J. Cajas, G. Houzeaux, M. Zavala, M. Vázquez, B. Uekermann, B. Gatzhammer, M. Mehl, Y. Fournier, C. Moulinec, "Multi-Physics Multi-Code Coupling On Supercomputers", 1st International Workshop on Software Solutions for ICME, Aachen (Germany), 2014
- » J. Remesal, A. Díaz-Guilera, B. Rondelli, Xavier Rubio-Campillo, A. Aguilera, G. Rull, "The EPNet Project. Production and distribution of food during the Roman Empire: Economics and Political Dynamics", Information Technologies for Epigraphy and Cultural Heritage: Proceedings of the First EAGLE International Conference, 455-464, 2014
- » Jean Kormann, Juan Esteban Rodriguez, Natalia Gutierrez, Josep de la Puente, Mauricio Hanzich, José Ma. Cela, "Retrieving Elastic Parameters from Short Offset Geometry Acquisition", 76th EAGE Conference & Exhibition, Expanded Abstract, Th-E106-05, 2014
- » Josep de la Puente, Mauricio Hanzich, Natalia Gutierrez, Juan Esteban Rodriguez, Jean Kormann, "HPC Solutions for Geophysical Exploration Problems: Efficiency, Reliability and Maintenance for Real-Life Applications", Platform of Advanced Scientific Computing (PASC 2014) 1st Conference, Zürich, Switzerland, 2014
- » Linares, M.Paz, Carmona, Carlos, Barcelo, Jaume, Cristina Montaña-Sales, Montaña-Sales, C., "Validation of a new multiclass mesoscopic simulator based on individual vehicles for dynamic network loading", Proceeding of the 2014 Winter Simulation Conference WSC'14, Savannah (GA) 7-10 December 2014, Piscataway, NJ, USA, 2060-2071, 2014
- » M. Vázquez, G. Houzeaux, F. Rubio, C. Simarro, "Alya multiphysics simulations on Intel's Xeon Phi accelerators", Communications in Computer and Information Science, 485, 248-254, 2014
- » Martinez-Ruiz, A., Cristina Montaña-Sales, "A Review on Strategies to Factor Matrices and Parallelize Algorithms", 2014
- » Mauricio Hanzich, "Roofline-based Optimization of Elastic Wave Propagation on Xeon Processors for Large-scale Execution", 2014
- » Mauricio Hanzich, Jean Kormann, Juan Esteban Rodriguez, Josep de la Puente, José Ma. Cela, "Developing Full Waveform Inversion Using HPC Frameworks: BSIT", EAGE Workshop on High Performance Computing for Upstream, HPC29, 2014
- » Mauricio Hanzich, Juan Esteban Rodriguez, Natalia Gutierrez, José Ma. Cela, "BSIT: A FLEXIBLE PLATFORM FOR DEVELOPMENT OF EFFICIENT SIMULATION SOFTWARE", IACM - ECCOMAS, Barcelona, Barcelona, Spain, 2014
- » Miguel Ferrer, Josep de la Puente, José E. Castillo, "3D Viscoelastic Anisotropic Seismic Modelling with High-Order Mimetic Finite Differences", International Conference on Spectral and High Order Methods (ICOSAHOM). June 23rd-27th, Salt Lake City, USA, 2014
- » N. Ashton, D. Mira, C. Moulinec, A. Revell, Herbert Owen, M. Vázquez, G. Houzeaux, "Application of RANS and hybrid RANS-LES models to a high-lift aircraft wing and fuselage", ERCOFTAC XXI Fluid Mechanics Conference, Krakow (Poland), 2014
- » Raúl de la Cruz, Mauricio Araya-Polo, "Modeling Stencil Code Optimizations", Performance Optimization for Stencils and Meshes Workshop, SIAM Conference on Parallel Processing for Scientific Computing, 2014
- » Raúl de la Cruz, Mauricio Araya-Polo, "Modeling Stencil Computations on Modern HPC Architectures", 5th International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS14) held as part of SC14, 2014
- » Raúl de la Cruz, Mauricio Hanzich, José Ma. Cela, "Stencils Computations: from Academy to Industry", Parallel Processing Conference, Portland, Oregon, USA, 2014
- » S. Gövert, D. Mira, M. Vázquez, G. Houzeaux, J.B.W. Kok, "Turbulent combustion modeling of a confined premixed methane/air jet flame using tabulated

chemistry for {RANS} and {LES}", 12th International Conference on Combustion and Energy Utilisation, Lancaster (UK), 2014

- » Uceda-Sosa, Rosario, Cormenzana, Berta, Marrero, Monica, Rueda, Salvador, Marinescu, Maria-Cristina, Fabregas, Ferran, "An Ontology for Urban Ecology. SUM+Ecology", 28th-AAAI Conference Workshop on Semantic Cities, QuZbec, Canada, 2014
- » Vladimir Puzyrev, "Modeling multiple source locations using block Krylov methods", 22 EM Induction Workshop, Weimar, Germany, 2014
- » Vladimir Puzyrev, Pilar Queral, Juanjo Ledo, Eloi Vilamajó, Alex Marcuello, Josep de la Puente, José Ma. Cela, "CSEM monitoring of a CO2 reservoir imaged by MT", 76th EAGE Conference & Exhibition - Workshops, 2014
- » Wittek, Peter, Lim, IkSoo, Xavier Rubio-Campillo, Atmanspacher, Harald, Haven, Emmanuel, Kitto, Kirsty, Raine, Derek, "Quantum Probabilistic Description of Dealing with Risk and Ambiguity in Foraging Decisions", Quantum Interaction: Lecture Notes in Computer Science, 296-307, 2014
- » Xavier Rubio-Campillo, "Pandora: A Versatile Agent-Based Modelling Platform for Social Simulation", Proceedings of SIMUL 2014, The Sixth International Conference on Advances in System Simulation, 29-34, 2014

National Conferences

- » D. Zebbar, G. Houzeaux, S. Kherris, K. Mostefa, "Définition de l'épaisseur du microfilm de lubrification dans la jonction segment-chemise d'un moteur à combustion interne", International Conference of Modeling and Simulation 2014, Blida (Algeria), 2014
- » Josep de la Puente, "Advanced Algorithms for the Modelling and Inversion of 3D Seismic and Electromagnetic Waves: An HPC Approach", M2OPIII 2014 – Third International Workshop on Multiphysics, Multiscale and Optimization Problems. May 22nd-23rd. Bilbao, Spain, 2014
- » Lin, Lin, Georg Huhs, Garcia, Alberto, Yang, Chao, "SIESTA-PEXSI: Massively parallel method for efficient and accurate ab initio materials simulation", Bulletin of the American Physical Society, 59, 2014

PhD Theses

- » Beatriz Eguzkitza, "HERMESH : a geometrical domain composition method in computational mechanics", Supervised by: Guillaume Houzeaux, 2014
- » Chiara Scaini, "Modelling strategies for volcanic ash dispersal and management of impacts on civil aviation", Supervised by: Arnau Folch, 2014
- » Ruth Arís Sánchez, "Electromechanical Large Scale Computational Models of the Ventricular Myocardium", Supervised by: Mariano Vazquez, 2014

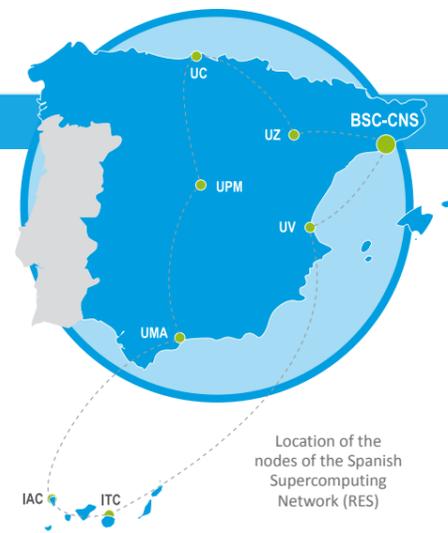
Education and Training 2014 Publications

Journals

- » Alexandrov, N, "Measuring business value of learning technology implementation in higher education setting", Procedia Computer Science - 2014 International Conference on Computational Science, 29, 1846-1858, 2014
- » Maria Ribera Sancho, "BSC Methodology and Best Practices in Professional Training and Teaching at PG Level for the HPC Ecosystem", SC14 Workshop on Best Practices for HPC Training, 2014
- » Montse González, "HPC Resources & Training in the BSC-CNS, the RES and PRACE", HPC Advisory Council Spain Conference, 2014
- » Montse González, "HPC Resources & Training in the BSC-CNS, the RES and PRACE", Ibergrid, 2014
- » Nia Alexandrov, "Bridging the HPC Talent Gap with Computational Science Research Methods", ICCS, 2014

- » Raul Ramirez-Velarde, Raul Perez-Cazares, Nia Alexandrov, Jose Jesus Garcia-Rueda, "Education 2.0: Student generated learning materials through collaborative work", Procedia Computer Science - 2014 International Conference on Computational Science, 29, 1835-1845, 2014

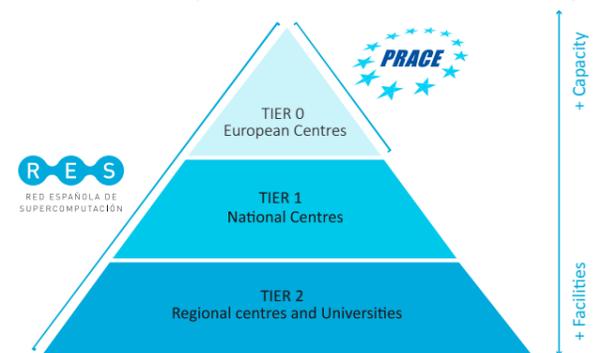




A total of 237 activities were run on RES nodes during 2014. This brings to more than 2.380 the number of different projects awarded computing time on the RES network since its establishment in 2006. The year also saw increased participation in RES scientific and dissemination events, as well as training seminars that aim to broaden user groups amongst all scientific fields, ensuring that the HPC resources of the RES are fully utilized to support scientific progress throughout the country.

ESFRI's vision of the European HPC service and how RES and PRACE fit within it

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



The RES as a national and local-level HPC service provider is intended to provide tier-1 and tier-2 level infrastructure. The upgraded MareNostrum3, a PRACE Europe-wide infrastructure, will provide tier-0 service to Europe and also to the RES, while the other RES nodes will provide tier-1 or 2 service according to their capabilities.

RES history, main goals, resources and members

The Spanish government created the Spanish Supercomputing Network (Red Española de Supercomputación) in July 2006 in response to the need of the Spanish scientific community for intensive calculation resources, with supercomputing infrastructure and services considered to be an indispensable asset

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

Access protocol and allocations in the RES

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

The Expert Panels

- Astronomy, Space and Earth Sciences
 - Life and Health Sciences
 - Mathematics, Physics and Engineering
 - Chemistry and Materials Science and Technology
- Each panel is composed of a coordinator, an assistant, and eight reviewers.

Access Committee Core Team

- Francisco Herrada, MINECO.
- Julio Bravo, ANEP.
- Alfonso Tarancón, BIFI-Universidad de Zaragoza.
- Jordi Torres, BSC-CNS.

RES Processing Power in TFLOPS/s in December 2014



The allocation of access to the supercomputing facilities is based on efficacy, efficiency and transparency criteria. First, formal and technical reviews are produced for each project. Then the evaluation process is mediated by a double filter system, with potential projects first being evaluated by the ANEP (National Agency of Evaluation and Prospective) if they have not been previously evaluated by other relevant national or international institutions, followed by a review by the RES Access Committee (Core Team and four Scientific Expert Panels formed by prestigious scientists external to BSC-CNS and defined according to the classification established by the Spanish Foundation of Science and Technology (FECYT)).

More than 117 million hours were awarded by the Access Committee in the 3 calls for applications that took place during 2014. In addition to internal research activities of the RES nodes, more than 110 external research projects made use of the RES system in 2014. It is important to note that many scientific projects often request several periods of access during the year (each access lasts 4 months) in order to perform different work activities. As specified in the Access Protocol, each request is treated separately and must pass the evaluation procedure of the Access Committee. Consequently, the number of activities reported by the RES is higher than the number of projects registered for the year.

Access requests and usage of RES resources

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

The chart below shows the evolution of requested, awarded and consumed TFLOP since the RES was founded in 2006. It

clearly shows that demand is consistently higher than the resources offered, and that all capacity upgrades are quickly absorbed, as can be clearly seen during the first and second MareNostrum upgrades in 2008 and 2013.

CURES, the RES Users Committee

CURES Members

- Miguel Ángel Aloy, UV
- Javier Junquera, UC
- Fernando Martín García, UAM
- Rubén Pérez, UAM
- Antoni Planas, URL
- Marcel Swart, IQCC-UdG
- Daniel Stich, UGR
- Carme Rovira, PCB-UB (Chair)

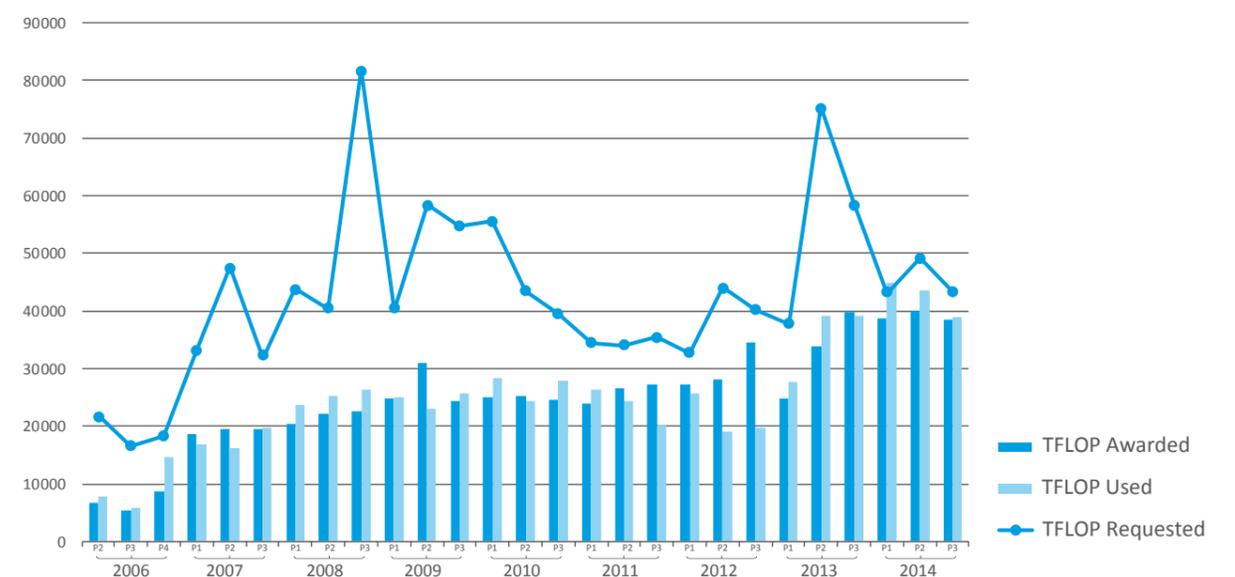
CURES was established in 2010 to provide advice and feedback to RES management on the current state and future delivery of the resources and services provided by the RES network. CURES aims to promote the effective use of the facilities by sharing information on experiences in

using the different systems, suggesting new research and technology directions in scientific computing and, above all, voicing user concerns.

To this end CURES undertakes various communication activities, such as holding regular meetings, establishing shared databases, and posting information. CURES also assists with the Survey on RES User Satisfaction, which gathers data and guides improvements in services.

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

Evolution of requested, awarded and consumed RES resources



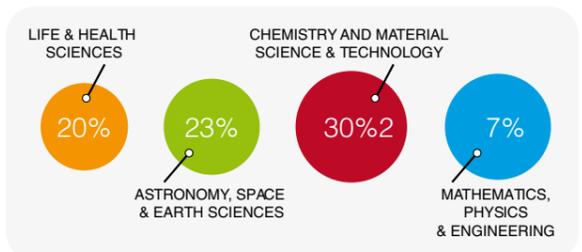


Geographical precedence of the RES users during 2014

Broad Impact on Scientific Research

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

The different research activities carried out on RES supercomputers during 2014 were led by prominent researchers from institutions all over Spain, Europe and overseas, and covered a huge range of scientific fields, whose results were disseminated in seminars and conferences all over the world, in prestigious peer-reviewed journals, and also to broader audiences via the BSC-CNS website and social networks.



Percentage of RES resources used by Scientific Area in 2014

8th RES User Conference

The 8th RES Users Conference took place on the 23rd September 2014 in Santander, Spain. The goal of the meeting was to promote available resources and services, to explain procedures for requesting time and reviewing of proposals, to disseminate the results obtained using the RES, and to offer a discussion forum among users, the CURES, and RES coordinators.



Four different sessions were held: Resources and services offered by the RES and PRACE; The challenge of moving from Tier-1 to Tier-0 supercomputers; Computational technology, Cosmology and Materials; and Quantum Mechanics and Technological development. Planned to coincide with the Users Conference, the 3rd Annual HPC Advisory Council Spain Conference was held the next day, co-organised by BSC-CNS and the HPC Advisory Council, a network of experts from some of the leading global HPC companies. Further information at <http://www.bsc.es/res-and-hpcac-2014>.

RES User Trainings

The fifth edition of the Programming and Tuning Massively Parallel Systems summer school (PUMPS) was held in Barcelona and co-organised by PRACE and RES. It was aimed at enriching the skills of researchers, graduate students, and teachers with cutting-edge technique and hands-on experience in developing applications for many-core processors with massively parallel computing resources like GPU accelerators in addition to PUMPS, the RES also cooperated with the organisation and dissemination of all the BSC-CNS PATC Trainings during 2014.

The program and related information available at <http://bcw.ac.upc.edu/PUMPS2014>

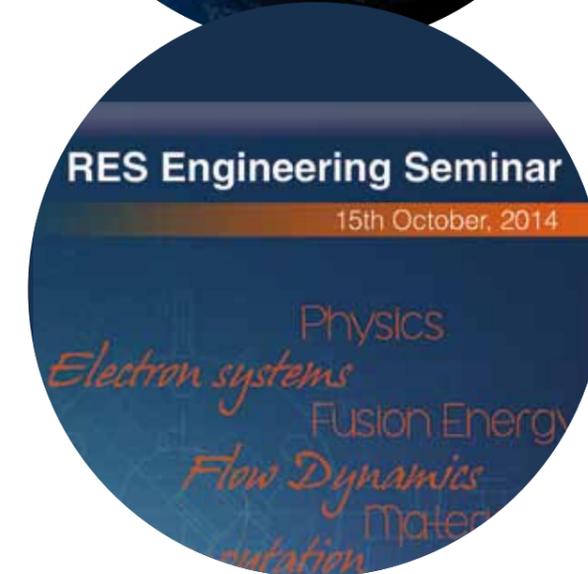
Scientific seminars



Attendees to the Earth Sciences seminar

Earth Sciences. This seminar was organised with the co-operation of the Earth Sciences Department at BSC-CNS. The objective of this seminar was to show researchers computational applications and problems in the study of Earth Sciences, specifically analysing the usage of supercomputing in Climate, Weather, and Seismic areas. Renowned scientists and researchers shared their findings from projects and studies. See <http://www.bsc.es/res-earth-sciences-2014>

Engineering. This seminar was organised with the co-operation of the CASE Department, to provide a common forum for Mathematics, Physics, and Engineering researchers who usually access RES resources, with special focus on analysing the usage of supercomputing in the areas of Fusion Energy, Study of Turbulence, Materials, Eigensolvers, and others. Renowned scientists and researchers shared their findings from projects and studies as well as their successes and problems regarding the usage of HPC services. See <http://www.bsc.es/engineering-seminar-2014>



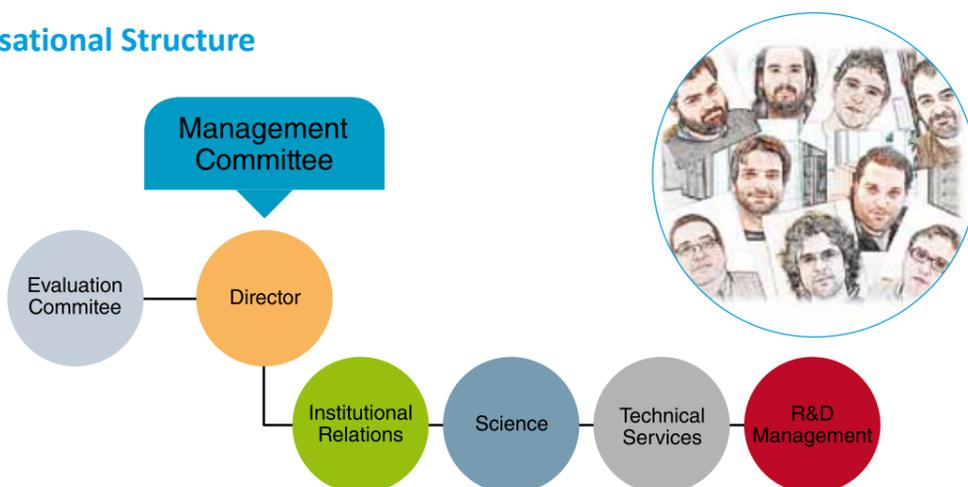
Earth Sciences Seminar & RES Engineering Seminar posters



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

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

Organisational Structure



Technical and Scientific Highlights 2014

Key Publications 2014

Articles

- *Analysis of SnS₂ hyperdoped with V proposed as efficient absorber material*, Yohanna Seminovski, Pablo Palacios y Perla Wahnón.
- *Ab initio molecular dynamics: Relationship between structural phases and the sound velocity in dense hydrogen*, Carlo L. Guerrero, Santiago Cuesta-Lopez y José M. Perlado.
- *Distributed Estimation of Distribution Algorithms for continuous optimization: How does the exchanged information influence their behavior?*, S. Muelas, A. Mendiburu, A. LaTorre y J. Peña.
- *Effect of the computational domain on direct simulations of turbulent channels up to Re⁺=4200*, Adrián Lozano-Durán y Javier Jiménez.
- *Fast ignition driven by quasi-monoenergetic ions: Optimal ion type and reduction of the ignition energies with an ion beam array*, J.J. Honrubia, J.C. Fernandez, B.M. Hegelich, M. Murakami y C.D. Enríquez.
- *Hybrid Quantum Magnetism in Circuit QED: From Spin-Photon Waves to Many-Body Spectroscopy*, Andreas Kurcz, Alejandro Bermudez y

Juan José García-Ripoll.

- *Maturation of Rhizobium leguminosarum Hydrogenase in the Presence of Oxygen Requires the Interaction of the Chaperone HspC and the Scaffolding Protein HupK*, Marta Albareda, Luis F. Pacios, Hamid Manyani, Luis Rey, Belén Brito, Juan Imperial, Tomás Ruiz-Argüeso y José M. Palacios.
- *Molecular Dynamics of Major Allergens from Alternaria*, Birch Pollen and Peach, María Garrido-Arandia, Cristina Gómez-Casado, Araceli Díaz-Perales y Luis F. Pacios.
- *Quantum metropolitan optical network based on wavelength division multiplexing*, A. Ciurana, J. Martínez-Mateo, M. Peev, A. Poppe, N. Walenta, H. Zbinden y V. Martín.
- *Self-consistent relativistic band structure of the CH₃NH₃PbI₃ perovskite*, E. Menéndez-Proupin, P. Palacios, P. Wahnón y J.C. Conesa.
- *Time-resolved evolution of coherent structures in turbulent channels: characterization of eddies and cascades*, Adrián Lozano-Durán y Javier Jiménez.
- *Twinning of Polymer Crystals Suppressed by Entropy*, N. C. Karayianis, K. Foteinopoulou y M. Laso.
- *V-substituted In₂S₃: an intermediate band material with photocatalytic in the whole visible light range*, R. Lucena, J.C. Conesa, I. Aguilera, P. Palacios y P. Wahnón.

Phd Thesis

- *Theoretical Study of Thermodynamic and Optoelectronic Properties of New Intermediate Band Photovoltaic Materials*, Yohanna Seminovski Pérez. *Proceedings*

Proceedings

- *New Generation of Materials for More Efficient Solar Energy Use: Quantum Modelling and Experimental Realizations*, P. Wahnón, P. Palacios, I. Aguilera, Y. Seminovski, R. Lucena y J.C. Conesa.

Conference

- *Designer-driven 3D Buildings Generated Using Variable Neighbourhood Search*, J.M. Peña, J. Viedma, S. Muelas, A. LaTorre y L. Peña.
- *Packing of athermal polymers in the bulk and under confinement*, P. Ramos, K. Foteinopoulou, N. C. Karayianis y M. Laso.

Technical Report

- *Hydrodynamic and acoustic results of the AQUO propeller.*, Leo M. González.

Misc

- *Monte Carlo simulations of athermal polymers under confinement*, P. Ramos.

Key Projects 2014

- *Implementation of new exchange correlation functionals and molecular dynamics calculations in Octopus*, Joseba Alberdi.
- *Sulfur Dioxide Capture by Ionic Liquids from a molecular point of view: A Density Functional Theory Study*, Santiago Aparicio.
- *Study of bulk and nanoconfined liquid water from ab initio simulations*, Emilio Artacho.
- *Evaluación de métricas de similitud aplicadas a sistemas de recomendación*, Jesús Bobadilla Sancho.
- *Ketonic decarboxylation over metal oxides: MgO and ZrO₂*, Mercedes Boronat.
- *Understanding the dynamics of water-silicate interactions at the nanoscale*, Stefan Bromley.
- *Investigating the protomeric space of Hairpin DNA by CPMD simulations*, Paolo Carloni.
- *Simulación de agua subenfriada*, Jose Antonio Cobos Marquez.
- *Parameter Control of Genetic Algorithms*, Juan Antonio Fernández del Pozo de Salamanca.
- *Catalysis modelling: gold nanoparticles supported on yttrium modified anatase as efficient WGS and CO oxidation catalysts*, Javier Fernández Sanz.
- *Complex flow calculations oriented to Biofluid and Liquid Crystalline Flows*, Katerina Foteinopoulou.
- *QUITEMAD: QUINFOG*, Juan José García Ripoll.
- *Cálculo de inestabilidades de flujos aerodinámicos*, Leo González.

- *Mining Software Repositories*, Israel Herraiz Tabernero.
- *Ignición rápida de blancos fusión inercial: desde la aceleración de electrones hasta la ignición del combustible*, José Javier Honrubia Checa.
- *Electronic structure of semiconductors by means of quasiparticle calculations: relevance to photocatalysis*, Francesc Illas.
- *Simulación del comportamiento en solución de proteínas implicadas en el ensamblaje de la hidrogenasa*, Juan Imperial Ródenas.
- *Aplicación de supercomputación distribuida al análisis de secuencias genómicas y a la modelización enzimática*, Juan Imperial Ródenas.
- *Caracterización del microbioma de la caña de azúcar*, Juan Imperial Ródenas.
- *Aplicación de la física estadística a la mecánica de medios granulares*, Rafael Jimenez.
- *Modelling of Synthetic and Biological Micromolecules Through a Hierarchical Multiscale Approach*, Nikos Karayianis.
- *Determination of the Stress-optical coefficient and plateau modulus from atomistic simulations of polyethylene melts*, Vicente Lorenzo.
- *Multiscale dynamics of turbulent flows*, Adrián Lozano Durán.
- *QUITEMAD: Cryptography, Computation and Simulation*, Miguel Ángel Martín-Delgado Alcántara.
- *Constraints on inflationary models of the universe based on CMB data*, Enrique Martínez González.
- *Formation energies of point defects in cadmium telluride*, Eduardo Menéndez.
- *Effect of defects on the two-photon photoemission (2PP) resonance for methanol and water on TiO₂(110)*, Annapaola Migani.
- *Heart visualization and supervised classification*, María Montoya.
- *Advanced high-performance vehicle routing & scheduling through emerging parallel architectures ADITI*, Santiago Muelas Pascual.
- *Theoretical Characterization of the optimized geometry and energy levels in an hybrid nanostructure*, Pablo Palacios Clemente.
- *Blue Brain Project*, José María Peña Sánchez.
- *Optimization Algorithms*, José María Peña Sánchez.
- *Simulación de estructuras con dinámica molecular cuántica*, José Manuel Perlado Martín.
- *PNOF5-PT2: A new benchmark tool in computational chemistry*, Mario Piris.
- *Binding of glycosylated surfactants to concanavalin A*, Antoni Planas.
- *Evidence of Conformational Selection in a Glycosyltransferase Structure*, Antoni Planas.
- *Método Montecarlo en resolución de problemas competitivos*, Alfonso Rodríguez-Paton.
- *Octopus GS and TD scaling testing in new architectures*, Angel Rubio.
- *Sistema de predicción de la calidad del aire de tercera generación*, Roberto San José García.
- *Development of a numerical multiphase flow tool for applications to petroleum Industry*, Eusebio Valero Sánchez.
- *Validación de herramientas Xflow en configuraciones de High-Lift*, Eusebio Valero Sánchez.
- *Diseño, Síntesis y Caracterización de Materiales Fotovoltaicos Avanzados de Alta Eficiencia*, Perla Wahnón Benarroch.
- *Design and Characterization of Advanced Photovoltaic Materials with High Efficiency*, Perla Wahnón Benarroch.
- *Electronic and optical properties of two-dimensional materials. Graphene and transition metal dichalcogenides*, Ludger Wirtz.



Financed by the Ministry of Economy and Competitiveness (MINECO), LaPalma supercomputer is one of the eight nodes belonging to the RES. It is located in the "Centro de Astrofísica de La Palma (CALP)", in Breña Baja.

The installation of LaPalma in 2007 was a strategic step with the objective to boost the observation activities in the Observatorio del Roque de Los Muchachos - above all through the incorporation of the Gran Telescopio CANARIAS (GTC) - and therefore reinforce the telecommunication development on the island.

At the end of 2012 LaPalma doubled the number of cores but kept the number of blades (256). With 1024 PowerPC cores, the maximum processing capacity increased from 4.5 TFLOP/s to 9 TFLOP/s. The power consumption however increased only by 20%. LaPalma, installed in a controlled environment room of 32 square metres, has two terabytes of principal memory in addition to its 38.5 TB of hard-disc data storage.

Organisational Structure

The Time Assignment Commission manages 50 percent of the CPU time of LaPalma for local users (the rest of the time is assigned via the RES). Its members come from different divisions of the Instituto de Astrofísica de Canarias (IAC).

For administration and management of the supercomputer node, the IAC makes available its IT support team and additionally has employed one engineer dedicated full-time to fulfil these functions.



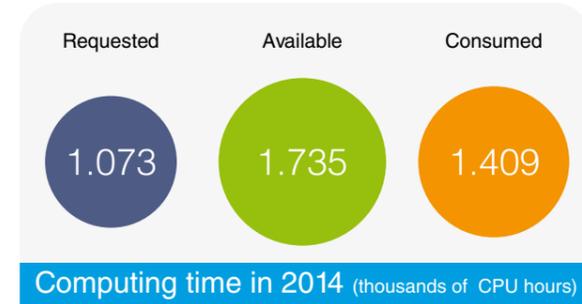
LaPalma team (left to right): (back) Carlos Martín, Justo Luna, Ubay Dorta, Antonio Dorta, Víctor Plasencia (front) Antonio Jiménez, Antonio Díaz.

The LaPalma Supercomputer Systems & Support Team:

Antonio Jiménez Mancebo (PhD), Head of the I.T. Common Services (SIC); Carlos Martín Galán (Senior Engineer), Technician Responsible of SIC; Antonio Díaz Chinae (Senior Engineer), System Administrator; Justo Luna López (Engineer), System Administrator; Ubay Dorta Guerra (Engineer), System Administrator and UserSupport; Antonio Dorta Lorenzo (PhD), User Support; Víctor Plasencia Darias (Operator), User Support.

Technical and Scientific Highlights 2014

The research groups, belonging to several subject areas of the IAC, consumed 1.4 million CPU hours of LaPalma in 2014. That amount represents 81% of time available for local users.



Key Publications 2014

Journals

- Sanromá, E.; Pallé, E.; Parenteau, M. N.; Kiang, N. Y.; Gutiérrez-Navarro, A. M.; López, R.; Montañés-Rodríguez, P., *Characterizing the Purple Earth: Modeling the Globally Integrated Spectral Variability of the Archean Earth*, The Astrophysical Journal, V780, A52 (2014).
- Socas-Navarro, H.; de la Cruz Rodríguez, J.; Asensio Ramos, A.; Trujillo Bueno, J.; Ruiz Cobo, B., *An open source, massively parallel code for non-LTE synthesis and inversion of spectral lines and Zeeman-induced Stokes profiles*, Astronomy & Astrophysics (2014).
- Socas-Navarro, H., *The solar oxygen abundance from an empirical three-dimensional model*, Astronomy & Astrophysics (2014).
- Yelles Chaouche, L.; Moreno-Insertis, F.; Bonet, J. A., *The power spectrum of solar convection flows from high-resolution observations and 3D simulations*, Astronomy & Astrophysics (2014).

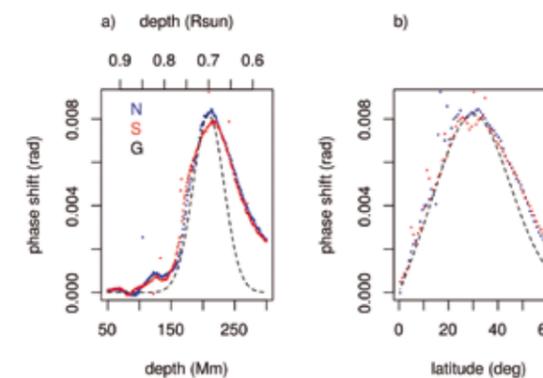
Thesis

- Sanromá Ramos, E., *The Earth through time as a template for the characterization of inhabitable exoplanets*, 2014 (thesis advisor E. Pallé).

Key Projects 2014

Seismic Holography of the Tachocline along the Solar Cycle (P.I.: Manuel Díaz Alfaro)

The aim of this project is the study of the tachocline and the deep part of the convection zone in the Sun along the solar cycle, using techniques of seismic holography. The tachocline is a thin layer located between the radiative interior and the convective envelope of the Sun, where the solar dynamo is believed to be generated, creating the magnetic cycle of solar activity. The technique, using observations of the velocity field in the solar surface and a model of the solar interior, reconstructs the travel of acoustic waves from the solar interior towards the solar surface. In this way, we can create seismic maps of perturbations with respect to the model of the solar interior at different depths. This study was performed for a range of different depths, including the tachocline, with simulated data and with observations taken by the GONG (Global Oscillation Network Group) between 2002 and 2014 along the solar cycle.



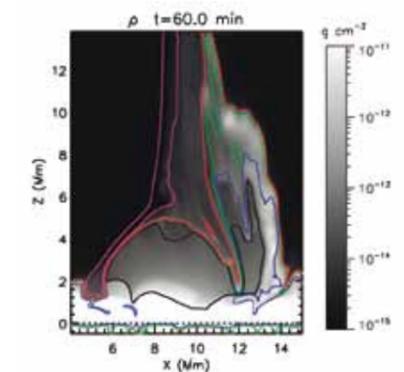
Relative phase shift with respect to depth and latitude between two datasets simulating the whole Sun, where 2D Gaussian-shaped sound-speed perturbations have been introduced centered at 0.7 Rsun and 30° in both hemispheres, with central peak values of the sound-speed perturbations of 0.70% and 0.65% in the Northern hemisphere (blue) and 0.50% and 0.55% in the Southern hemisphere (red). The Northern difference has been reversed to be expressed in positive values. A model Gaussian with the perturbation parameters is shown in black for comparison.

The dynamics and magnetism of the solar atmosphere (P.I.: Fernando Moreno Insertis)

We study different physical processes that take place in the solar atmosphere (corona, chromosphere, photosphere) or in the convection cells in the topmost few Megameters of the solar interior.

The basic method used is the numerical modelling and experimentation using the Bifrost radiation-MHD code, which can be run in massively parallel computers over hundreds of CPUs using Message Passing Algorithms.

The code contains LTE radiation transfer, scattering, optically thin radiation cooling and thermal conduction. The processes studied in 2014 centered around the emission of a cool jet with temperatures around 10.000 degrees as a by-product of the collision of emerging and ambient-coronal magnetized regions. The complicated dynamical, thermodynamical and electromagnetic phenomena involved in this process were studied in detail.





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 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. 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. and offers 96TB of storage disk.

Organisational Structure



M^a Belén Esteban Sánchez (System Administrator and User Support)

The technical staff of Atlante comprises a computing engineer from ITC (María Belén Esteban Sánchez), who is responsible for system management and user support, and a group manager (José Manuel Pérez Pérez). A local Access Committee allocates the 80% of local CPU time amongst users from the Government of Canary Islands, private companies and R&D groups, while the remaining processing time is provided to the RES network.

Technical and Scientific Highlights 2014

In 2014 Atlante's local access granted 7 local projects corresponding to Canary Islands companies and researchers. They ran 1.2M hours of CPU time, related to the following projects and publications:

Key Publications 2014

Journals

- Imaculada Menéndez, Emma Pérez-Chacón, José Mangas, Esperanza Tauler, Johann P Engelbrecht, Edward Derbyshire, Luis Cana, Ignacio Alonso. *Dust deposits on La Graciosa Island (Canary Islands, Spain): texture, mineralogy and transport*. Elsevier Catena 2014, 117, 133-144.
- C. Vericat, M. E. Vela, G. Corthey, E. Pensa, E. Cortés, M. H. Fonticelli, F. Ibañez, G. E. Benitez, P. Carro and R. C. Salvarezza. *Self-assembled monolayers of thiolates on metals: a review article on sulfur-metal chemistry and surface structures*. Royal Society of Chemistry Adv., 2014, 4, 27730.

- P. Carro, X. Torrelles and R. C. Salvarezza. *A novel model for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ alkanethiolate-Au(111) phase based on alkanethiolate-Au adatom complexes*. Phys.Chem.Chem.Phys., 2014, 16, 19017.

Key Projects 2014

Analysis of a wide range of Measure-Correlate-Predict (MCP) methods used to estimate long-term wind characteristics at a target site

So-called Measure-Correlate-Predict (MCP) methods have been extensively proposed in renewable energy related literature to estimate the wind resources that represent the long-term conditions at a target site where a short-term wind data measurement campaign has been held. The main differences between the various MCP methods lie fundamentally in the type of relationship established between the wind data (speed and direction) recorded at the target site and the wind data recorded simultaneously at one or various nearby weather stations which serve as reference stations and for which long-term data series are also available.

This project analyses and compares a wide range of MCP methods that have been proposed in the context of wind energy analysis, a number of which have been implemented in wind energy industry software applications. This analysis includes the initial methods first proposed in the 1940s which generally attempted only to estimate the long-term mean annual wind speed from a single reference station, and extends up to the most recent methods proposed in the present century based on automatic learning techniques which use several reference stations. It is intended that, the extensive collection of MCP methods which is brought together and analysed in this project, ranging from the simplest and easiest-to-use models to the most complicated computational ones which require specific user experience, comprises an extremely useful catalogue when it comes to choosing the best predictor method.

Sensitivity of Korea South wind energy to turbine characteristics

Using output from a high-resolution meteorological simulation (WRF model), we evaluate the sensitivity of Korea South wind energy generation to variations in key characteristics of current wind turbines. These characteristics include hub height, rotor diameter and rated power, and depend on turbine make and model. They shape the turbine's power curve and thus have large implications for the energy generation capacity of wind farms. In the case of the sensitivity to rotor diameter, the change in energy output per unit change in rotor diameter at any location is directly proportional to the weighted average wind speed between the cut-in speed and the rated speed.

The sensitivity to rated power variations is likewise captured by the percent of the wind speed distribution between the turbines rated and cut-out speeds. Finally, the sensitivity to hub height is proportional to lower atmospheric wind shear. Our study underscores the need for joint analysis of regional climate, turbine engineering and economic modelling to optimize wind energy production.

Improving short-term wind energy prediction with wind farm data using the NCAR WRF RTFDAA models

The number of wind farms and the demand for accurate forecasting techniques increases. Harmattan Solutions uses WRF model since a couple of years to produce, among other applications, operational three-day forecasts. Since 2012, a wind farm parameterisation scheme has been added to the WRF model (Fitch et al, 2012). The WRF model allows for the possibility of parameterising the effects that the wind turbines exert over the atmospheric evolution.

The parameterisation represents the turbines as an elevated sink of momentum and a source of turbulent kinetic energy following Blahak et al. (2010). However, it uses the thrust coefficient instead of the factor loss to represent the influence of the wind turbines (Fitch et al. 2012). Harmattan solutions started an evaluation study to assess the forecasting quality of this scheme. The simulations are performed with the Weather Research and Forecasting mesoscale model configured at a high horizontal resolution of 333 m.

The scheme has been slightly adapted such that it reads power curve data from a file instead of using a parameterised power curve. Since version 3.4 WRF incorporates a parameterisation to improve the effects produced by topography over the surface winds (Jimenez and Dudhia, 2012, 2013). The parameterisation allows for the speed up of the flow over mountains and hills and to represent the drag exerted by the unresolved topography over plains and valleys.

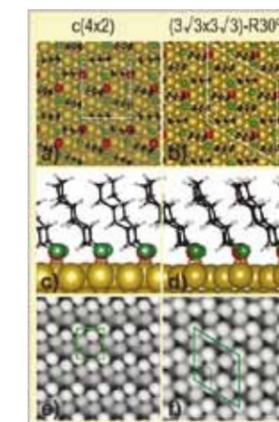
Valuation of travel time savings and reductions in risk of road accidents: application to the evaluation of transport projects

The objective of this Project is to determine the value of travel time savings as well as the willingness to pay for reducing the risk of accidents in order to use these figures in the social evaluation of transport projects.

In this study, the team analysed both passengers and freight transport, and will make a thorough analysis of all the methodological issues that should be followed in transportation demand studies and project evaluation.

The project illustrates theoretical results with several empirical applications that could be used by the Spanish Ministry of Transport as reference case studies.

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



Optimised hexanethiolate surface structures on Au(111)

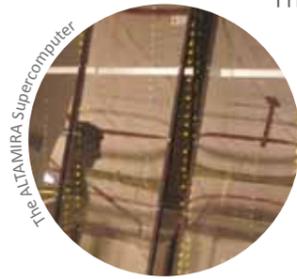
Metallic nanoparticles (NPs) appear as promising materials to be used in biomedicine, as efficient catalysts and electrocatalysts, and as active elements in electronic and sensing devices.

The most common strategy to protect these NPs is by using thiolate self-assembled monolayers (SAMs), a strategy that has proved useful to control the physical and chemical properties of extended solid surfaces. However, the knowledge of structure and

chemistry of thiol-metal interfaces yet remain elusive, although it is crucial for understanding how NPs interact with molecules, biomolecules and living cells, and also for a better design of NP-based devices. This work strives to show the complexity of the thiol-metal NP interface. If the size of the metallic core is large the NP interface properties approach those of SAMs on planar surfaces.

Atmospheric numerical prediction

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



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

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

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

The ALTAMIRA node was upgraded in June 2012 with the installation of a new system at IFCA datacenter room and became fully operational in October 2012. The current systems in the ALTAMIRA node is composed of 158 IBM-iDataPlex servers interconnected with Mellanox InfiniBand fabric. Also, ALTAMIRA has a small GPU based cluster, with 5 IBM servers, each one with 2 GPU cards, and a cluster with IBM POWER7 blades, with capacity for up to 700 processes to execute intensive CPU applications.

Organisational Structure

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



Miguel Angel Nuñez and Luis Cabellos.



Technical and Scientific Highlights 2014

In 2014 the Altamira node executed applications corresponding to local users at the University of Cantabria with about five million hours of CPU.

Key Publications 2014

Journals

- CMS Collaboration. Measurement of the t t-bar production cross section in the dilepton channel in pp collisions at $\sqrt{s} = 8$ TeV. *Journal of High Energy Physics*.
- Planck Collaboration. III. LFI systematic uncertainties, XII. Diffuse component separation, XIX. The integrated Sachs-Wolfe effect, XXIII. Isotropy and statistics of the CMB, XXIV. Constraints on primordial non-Gaussianity. *Planck 2013 results*.
- Fernández-Cobos, R.; Vielva, P.; Pietrobon, D.; Balbi, A.; Martínez-González, E.; Barreiro, R. B. Searching for a dipole modulation in the large-scale structure of the Universe. *Monthly Notices of the Royal Astronomical Society*.
- Benedicto Crespo-Facorro; Carlos Prieto; Jesus Sainz. Schizophrenia Gene Expression Profile Reverted to Normal Levels by Antipsychotics. *International Journal of Neuropsychopharmacology*.
- Crespo-Facorro B; Prieto C, Sainz J. Schizophrenia Gene Expression Profile Reverted to Normal Levels by Antipsychotics. *International Journal of Neuropsychopharmacology*.
- Elza C. de Bruin et al. Spatial and temporal diversity in genomic instability processes defines lung cancer evolution. *Science Magazine*.
- Jon Infante; Carlos Prieto; María Sierra; Pascual Sánchez-Juan; Isabel González-Aramburu; Coro Sánchez-Quintana; José Berciano; Onofre Combarros; Jesús Sainz. Identification of candidate genes for Parkinson's disease through blood transcriptome analysis in LRRK2-G2019S carriers, idiopathic cases, and controls. *Neurobiology of Aging*.
- David Osca; Iker Irisarri; Christiane Todt; Cristina Grande; Rafael Zardoya. The complete mitochondrial genome of *Scutopus ventrolineatus* (Mollusca: Chaetodermomorpha) supports the Aculifera hypothesis. *BMC Evolutionary Biology*.
- David Osca; José Templado; Rafael Zardoya. The mitochondrial genome of *Ifremeria nautili* and the phylogenetic position of the enigmatic deep-sea *Abyssochrysoidea* (Mollusca: Gastropoda). *Gene*.
- Y. F. Nie; Y. Zhu; C. -H. Lee; L. F. Kourkoutis; J. A. Mundy; Javier Junquera; Ph. Ghosez; D. J. Baek; S. Sung; X. X. Xi; K. M. Shen; D. A. Muller; D. G. Schlom. Atomically precise interfaces from non-stoichiometric deposition. *Nature Communications*.
- Pablo Fuentes; José Luis Bosque; Ramón Bevide; Mateo Valero; Cyriel Minkenberg. Characterizing the Communication Demands of the Graph500 Benchmark on a Commodity Cluster. *2014 International Symposium on Big Data Computing*.

Key Projects 2014

Computation from the Instituto de Biomedicina y Biotecnología de Cantabria

Ignacio Varela leads the computing work in Instituto de Biomedicina y Biotecnología de Cantabria. The IBBTEC is a strategic centre for the development of biomedical science in Cantabria. It was created in April 2007 as a joint Centre between CSIC (Spanish National Research Council), University of Cantabria and Government of Cantabria. The main mission of this Institute is to carry out a high level research as well as the transfer of technology in order to stimulate the productive sectors related to health and biotechnology. With the help of Altamira supercomputer IBBTEC has been conducting studies on lung cancer, Parkinson's disease, and others.

Constraints on inflationary models of the universe based on CMB

Enrique Martinez leads the Cosmic Microwave Background Radiation (CMB) research group at IFCA. CMB represents an essential tool for the research in Modern Cosmology. There are a large number of ground-based, balloon-borne and satellite experiments both current and planned. The existence of the CMB is a proof of the primordial explosion widely known as Big-Bang. The anisotropies of the black body radiation temperature measured in different directions of the sky provide valuable information about the primordial epochs of the universe and its evolution. The standard inflation theory, developed in the 1980's and nowadays widely accepted, predicts that these anisotropies follow very closely a Gaussian distribution. The detection of non-Gaussian deviations in the CMB would have far-reaching consequences for our understanding of the universe.

RNA-seq analysis service

Rafael Zardoya and Etienne Kornobis lead the development of a Genomic service that uses Altamira. High throughput sequencing (HTS) methods are drastically changing the face of modern Biology studies. RNA-seq refers to the use of such methods to characterise the RNA content of a biological sample. Currently, the analysis of the data produced by these new methods require both high computing resources and Bioinformatic know-how. Consequently, they are developing TRUFA, a free webserver designed for fast and user-friendly RNA-seq analysis by using the Altamira cluster and reducing the amount of Bioinformatic knowledge necessary.



Picasso is a RES node located in the Bio-Innovation Building of the University of Málaga (UMA) at the Technological Park of Andalusia (PTA), close to the city of Málaga. It is managed by the SCBI (Supercomputing and Bioinformatics Centre) of the UMA, which runs several integrated computational infrastructures supporting research activities within the University and in the Andalusian region.

These include a 7 node cluster of 80 cores and 2TB RAM computers, 32 nodes with 16 cores, 41 nodes with 24 cores and 16 nodes with 2 GPUs each, totalling 63 TFLOP/s. All these resources share computer room, cooling, power and fire extinguishing systems.

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

Organisational Structure

The SCBI draws on 15 years of experience of the Computational Laboratory of the University of Málaga in running production supercomputers to support scientific research in several fields. It also incorporates a multidisciplinary research infrastructure, the Bioinformatics Platform of Andalusia, whose mission is to provide computational resources and commercial software licenses, and to transfer knowledge and experience on bioinformatics research to the scientific community in Andalusia.



SCBI team at Málaga (left to right):
Rafael Larrosa, Darío Guerrero

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 UMA whose main research areas are analysis, design, and evaluation of high performance architectures, from the application level to the lower hardware levels.

Technical and Scientific Highlights 2014

In 2014 new computer resources were made available to users, with more cores, more disk space and a wider selection of systems. Four different systems are offered, from a cluster of big memory computers with 2TB of RAM each, to a cluster of computers with GPUs, all under the control of the same queue manager, thereby enabling users to select the one which best matches their research needs.

Biocomputation was one of the main areas that used most of the node's resources, taking special advantage of the big-

mem cluster for the assembly of genomes, and using the rest of the system for other processes. Quantum mechanics, protein folding and custom simulations, where users write their own code, were also heavy users of the system, as can be seen in the publications list.

Key Publications 2014

Articles

- *3GPP QoS Based Scheduling Framework for LTE*. Pablo Ameigeiras, Jorge Navarro-Ortiz, Juan M. López-Soler et al. 2014 - International Journal of Communications Systems.
- *A combined MD/QM and experimental exploration of conformational richness in branched oligothiophenes*. Jonas Sjöqvist, Rafael Carlos González-Cano, Juan T. López Navarrete et al. 2014 - Physical Chemistry Chemical Physics.
- *A Histogram Transform for Probability Density Function Estimation*. Ezequiel López-Rubio. 2014 - IEEE Transactions on Pattern Analysis and Machine Intelligence.
- *A Performance/Cost Evaluation for a GPU-Based Drug Discovery Application on Volunteer Computing*. Ginés D. Guerrero, Baldomero Imbernon, Horacio Pérez-Sánchez et al. 2014 - BioMed Research International.
- *Accelerating GWAS Epistatic Interaction Analysis Methods*. Upton A, Orue P, Trelles O. 2014 - Proc. XII Symp. Bioinformatics.
- *Alkoxy-Functionalized Thienyl-Vinylene Polymers for Field-Effect Transistors and All-Polymer Solar Cells*. Hui Huang, Nanjia Zhou, Rocio Ponce Ortiz et al. 2014 - Advanced Functional Materials.
- *An adaptive system for compressed video deblocking*. Ezequiel López-Rubio, Rafael Marcos Luque-Baena. 2014 - Signal Processing.

- *An Efficient Solvent Accessible Surface Area calculation applied in Ab Initio Protein Structure Prediction*. D. Bonetti, H. Pérez-Sánchez, A. Delbem. 2014 - IWBBIO 2014.
- *Antiaromatic Bisindeno-[n]thienoacenes With Small Singlet Biradical Characters: Syntheses, Structures and Chain Length Dependent Physical Properties*. Xueliang Shi, Paula Mayorga Burrezo, Sangsu Lee et al. 2014 - Chemical Science.
- *Application of parallel blind docking with BINDSURF for the study of platinum derived compounds as anticancer drugs*. J. P. Cerón-Carrasco, J. Cerezo, J. Zúñiga et al. 2014 - IWBBIO 2014.
- *Bregman Divergences for Growing Hierarchical Self-Organizing Networks*. Ezequiel López-Rubio, Esteban José Palomo and Enrique Domínguez. 2014 - International Journal Of Neural Systems.
- *Chameleon-like behaviour of cyclo[n]paraphenylenes in complexes with C70: on their impressive electronic and structural adaptability as probed by Raman spectroscopy*. Miriam Peña Álvarez, Paula Mayorga Burrezo, Takahiro Iwamoto et al. 2014 - Faraday Discussions.

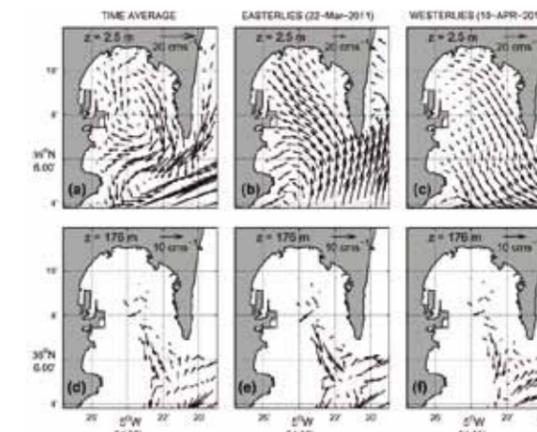
Seminars and conferences

- *Cold response in Olive tree; A RNAseq Study*. Leyva-Pérez M.O., Valverde A., Jiménez-Ruiz J. et al. 2014 - Congress: 5th Workshop of Cost Action.
- *La respuesta a estrés por frío en el olivo (Olea europea L.) se produce mediante cambios transitorios de la expresión génica a la vez que por cambios adaptativos estables durante la persistencia del estrés*. María de la O Leyva-Pérez, Antonio Valverde, Jaime Jiménez-Ruiz et al. 2014 - Congress: XXXIX Congreso de la Sociedad Española de Genética.
- *Un gen marcador de la infección por Verticillium dahliae del olivo cultivado (Olea europaea L.)*. Leyva M.O., Schilirò E., Jiménez-Ruiz J. et al. 2014 - Congress - XII Reunión De Biología Molecular de Plantas.
- *Parallel Computation of Non-Bonded Interactions in Drug Discovery: Nvidia GPUs vs. Intel Xeon Phi*, J. Fang, A. Lucia Varbanescu, B. Imbernon, J. M. Cecilia, H. Pérez-Sánchez, (2014), International Work-Conference on Bioinformatics and Biomedical Engineering, IWBBIO 2014, 579-588.

Key Projects 2014

Physical oceanography research

The physical oceanography research group of the University of Malaga conducted a simulation of the circulation and renew times of the water in the Bay of Algeciras. The evolution of possible oil spills, taking into account currents and meteorological forces, is studied, with the objective of optimising interventions in case disaster strikes. The Bay is a place of singular complexity. The clash between Atlantic and Mediterranean water flows that develop in the adjacent Strait of Gibraltar, and its study is of particular interest to the scientific oceanographic community.



Experimental and numerical characterisations of harbour oscillations in the port of Málaga were also done. The harbour is characterised by abnormal oscillations of the sea level. Its trigger seems to be the resonance between high-frequency oscillations of the sea level induced by the atmospheric fronts and the harbour structure. With this research the effect of future expansions can be studied and design optimised in order to avoid such problems.

An adaptive system for compressed video deblocking

The icai research group of the University of Málaga developed a video deblocking system which is based on the properties of the DCT. Many state of the art methods for video compression rely on the Discrete Cosine Transform (DCT) and the quantization of its coefficients. Hence it is suitable for MPEG-2 compressed videos, since the MPEG-2 standard belongs to this class of compression formats. The system carries out an online analysis of the video in order to adapt its operation to the characteristics of the incoming video frames. Experiments with benchmark real videos are shown, which demonstrate the performance of our proposal both in quantitative and qualitative terms.

HVAC simulation

The fluid mechanics group of the University of Málaga inside the general research of flows, jets, vortices, etc. analysed the work of a HVAC diffuser, developing a Micro/Macro Level Approach (MMLA) method to model a conventional diffuser. This procedure reduces the number of points in order to solve the airflow in a room. This can be seen as a numerical box method, and it provides a number of variables at the inlet of the room (outlet of the diffuser) which are difficult to obtain experimentally, e.g. turbulent properties. Flow visualizations were carried out to determine the shape of the plume. These qualitative experimental data are also compared with numerical temperature fields for sufficiently high Reynolds numbers and give accurate results. In addition, we report the throw and drop of the diffuser for different flow rates. Finally, the pressure drop of the terminal device was obtained experimentally, and it is also shown that numerical results can predict it accurately. A discussion of two different methods to compute the pressure drop is given, showing the differences in relation to the airflow characteristics near the outlet of the diffuser.



The RES node located at the University of Valencia was inaugurated in January 2008. The supercomputer's name Tirant refers to the main character in the "Tirant lo Blanc" novel written by the Catalan author Joanot Martorell in 1490. The node is installed in a specially designed data centre and is managed by technicians of the Servei d'Informàtica de la Universitat de València (SIUV).

The SIUV has broad experience in managing supercomputers and has been key to the university's efforts in the field of scientific computing since 1978. The SIUV also hosts the RedIris PoP of the Valencian region, the network infrastructure of the university, the central database, the university web page, e-mail services, application services and other computer services.

In December 2012, Tirant was upgraded as a consequence of the installation of MareNostrum3, by virtue of the agreement between RES nodes. Tirant now has 2048 processors and 4TB of distributed memory.

Organisational Structure



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

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

Technical and Scientific Highlights 2014

In 2014, Tirant offered more than 7,7 million CPU hours, of which 4,8 million (~62%) hours were used by the scientific community of Valencia, including researchers at the host University. The rest was consumed by RES users.

Key Publications 2014

Journals

- Aranda, J., Zinoviev, K., Roca, M., and Tuñón, I. *Dynamics and Reactivity in Thermus Aquaticus N6-Adenine Methyltransferase*, Journal of the American Chemical Society 136, 16227-16239 (2014)

- Zinoviev, K., and Tuñón, I. *Exploring Chemical Reactivity of Complex Systems with Path-Based Coordinates: Role of the Distance Metric*, Journal of Computational Chemistry 35, 1672-1681 (2014)
- Luk, L. Y. P., Ruiz-Pernía, J. J., Dawson, W. M., Loveridge, E. J., Tuñón, I., Moliner, V., and Allemann, R. K. *Protein Isotope Effects in Dihydrofolate Reductase from Geobacillus Stearothermophilus Show Entropic-Enthalpic Compensatory Effects on the Rate Constant*, Journal of the American Chemical Society 136, 17317-17323 (2014)
- M. Boronat, A. Leyva-Pérez, A. Corma. *Theoretical and Experimental Insights into the Origin of the Catalytic Activity of Subnanometric Gold Clusters: Attempts to Predict Reactivity with Clusters and Nanoparticles of Gold*. Accounts of Chemical Research 47, 834 – 844 (2014)
- M. Boronat, T. López-Ausens, A. Corma. *Making C-C bonds with gold catalysts: a theoretical study of the influence of gold particle size on the dissociation of the C-X bond in aryl halides*. Journal of Physical Chemistry C 118, 9018 – 9029 (2014)
- M. Boronat, S. Laursen, A. Leyva-Perez, J. Oliver-Meseguer, D. Combita, A. Corma. *Partially oxidized gold nanoparticles: A catalytic base-free system for the aerobic homocoupling of alkynes*. Journal of Catalysis 315, 6 – 14 (2014)
- M. Boronat, A. Pulido, P. Concepción, A. Corma. *Propene Epoxidation with O₂ or H₂/O₂ Mixtures over Silver Catalysts: Theoretical Insights into the Role of Particle Size*. Phys. Chem. Chem. Phys. 16, 26600 – 26612 (2014)

Contributed talks and posters 2014

- Oral contribution at 15th International Conference on Theoretical Aspects of Catalysis ICTAC 15, London. *Theoretical investigation of the exceptional oxidation activity of gold clusters of low atomicity*. M. Boronat, P. Concepción, A. Corma.
- **Conference:** *Simulation of atomization process in diesel*. F.J. Salvador, D.Jaramillo-Ciscar, J.-V. Romero and M. D. Rosello, Modelling engineering and human behaviour, September 2014, ISBN 978-84-606-5746-0.

Key Projects 2014

Development of novel treatments for myotonic dystrophy: in vivo drug discovery

Myotonic dystrophy type 1 (DM1) is caused by the expansion of noncoding CTG repeats in the DMPK gene. Mutant transcripts form CUG hairpins that sequester RNA-binding factors into nuclear foci, including MBNL1 protein, which regulate alternative splicing and gene expression. A previous study in our lab proved that D-amino acid hexapeptides can bind to CUG hairpins and improve the phenotype of a DM1 Drosophila melanogaster model, but the activity of these peptides was weak. Using the Tirant supercomputer we developed a computational model of the interaction between the hexapeptides and the CUG RNA and are using this structural information to develop peptides with stronger affinity for CUG repeat expansions.

Thermal conductivity of GaN nanowires

In this work the group led by Heruy Mengistu investigates the thermal conductivity of GaN nanowires with wurtzite structure by using Green-Kubo approach. The molecular dynamics calculations are performed by using LAMMPS code. Calculations show that the thermal conductivity of GaN nanowires decreases with decrease of diameter from 2.6 to 0.781 nm. It was also observed that for all the diameters considered, the thermal conductivity becomes less affected by higher temperatures values. This shows that the contribution of the surface scattering to the conductivity of the wires is dominant but decreases with temperature.

Acid base reactivity of zirconia polymorphs

ZrO₂ has high thermal and chemical stability, as well as structural versatility. It has weak acid and basic centres, and therefore shows interesting acid-base bifunctional catalytic properties. This project, led by Mercedes Boronat, theoretically investigated the acid-base catalytic properties of the most stable facets of monoclinic and tetragonal ZrO₂ polymorphs, and their influence on selected acid-base catalysed reactions: ketonic decarboxylation, Knoevenagel and Claisen-Schmid condensations, and Meerwein-Ponndorf-Verley reduction.

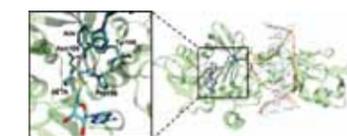
Monte Carlo study of the SU(2) Higgs Model

This project, led by Pilar Hernandez, aims to study the existence of a scaling window in the four-dimensional gauged non-linear sigma model, which at low energy could describe the Higgs-gauge sector of the Standard Model. In JHEP 1311 (2013) 213 the group found strong indications for the existence of such a scaling window up to the TeV scale. However the results for the observables used for this scaling study had rather large statistical errors, and a large share of the CPU time allocated on TIRANT in 2014 was devoted to reduce those. Also, the group studied the effective tree-level vector-bosons coupling at finer lattice resolutions and confirmed that such coupling is a fac-

tor 2 – 3 larger than in the Standard Model. Finally the group optimized the setup for the search of excited states and non Standard-Model states, which would represent striking signatures of the model and could be searched at LHC.

Molecular simulations of enzymatic reactions

The research group led by Ignacio Tuñón focuses on the simulation of enzymatic reactions using hybrid techniques, combining mechano quantum description (QM) of the active site while using molecular mechanics (MM) for the rest of the system (protein and solvent). We use these hybrid QM/MM methods to simulate reaction mechanisms in complex biomolecular systems, testing them against accurate experimental data and reproducing subtle effects such as the change in the mass of some protein atoms. One of the latest applications of our QM/MM methodology was carried out for the study of the reaction mechanism catalysed by the N6-DNA-Methyltransferase, an enzyme involved in the epigenetic methylation process of DNA in bacteria. The most feasible reaction mechanism in terms of free energy barriers was characterized.



Structure of the N6-DNA-Methyltransferase M.TaqI enzyme in complex with a decamer of DNA used in our simulations, (PDB ID: 1G38). An inset of the active site is shown

Simulations of relativistic flows in active galaxies and binary stars

During 2014, this group led by Manel Perucho published results of simulations performed during previous years at Tirant and Mare Nostrum. Results were published on long-term jet evolution and their influence on the intergalactic medium and on mass-load of jets by stellar winds. In addition, the group continued the study of wind/wind interaction in a binary system formed by a non-accreting pulsar and a massive star. The aim was to study the locations of high-energy emission produced by the interaction of the dilute, relativistic pulsar wind, with the slow, dense and inhomogeneous wind from a massive star. The objective is to achieve a quasi-steady-state scenario and perturb it with typical stellar wind inhomogeneities.

Simulation of atomization process in diesel

In 2014, the group led by Francisco Javier Salvador continued the study on the internal flow and cavitation phenomenon on Diesel injectors. The study focused on geometrical influences of nozzle parameters and on the differences between turbulence models to properly simulate diesel behaviour in the injector. The study focused on an incompressible monophasic solver. It showed similar values in terms of mass flow error, around 2% for all the turbulence models studied except for the standard k-epsilon that showed an average error of 6%. This study was also extended to a non-simplified solver, considering the compressibility of the liquid under a non-cavitating geometry.



The Institute for Biocomputation and Physics of Complex Systems of the University of Zaragoza (BIFI-UNIZAR) is a research organisation 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: HPC, grid computing, cloud computing, GPUs, dedicated computers (FPGAs) and volunteer computing.

CAESARAUGUSTA II (locally also known as "Memento") at the University of Zaragoza, is a founding node of the Spanish Supercomputing Network (RES). The supercomputer, located at BIFI's premises in the Río Ebro Campus of the University, is managed by the High Performance Computing group of the Institute. It is equipped with 3072 computing cores, 12TB of RAM memory, 72TB of raw storage and Infiniband QDR interconnection network (40Gb/s), offering an overall raw performance (Rpeak) of 25,8 TFLOPS (Rmax is 20 TFLOPS). The portion of CAESARAUGUSTA II shared through the RES during 2014 was equal to 768 cores; 512 for RES users and 256 for local users.

This second version of Caesaraugusta superseded the former Caesaraugusta (2007-2013), PowerPC-based, hosted in the Faculty of Science of the University of Zaragoza.

Organisational Structure



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

CAESARAUGUSTA is maintained by technical staff of the Computing Area at BIFI, namely the HPC group. 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 periodically (each four months, coinciding with RES schedule) allocates the CPU time reserved for local projects (the portion equivalent to 256 cores mentioned above) among applicant activities. This time is assigned by the Committee after evaluating the applications received. During 2014, the members of the local Access Committee were: Prof. Pablo Ibáñez Marín, Prof. Luis Rández García, and Prof. Alfonso Tarancón Lafita

Technical and Scientific Highlights 2014

In 2014 CAESARAUGUSTA's local Access Committee granted a total of 20 local projects, consuming 1.878.000 hours of CPU time. These activities have produced numerous scientific results and publications.

Key Publications 2014

Journals

- Structure and magnetism of Tm atoms and monolayers on W(110); Corneliu Nistor, Aitor Mugarza, Sebastian Stepanow, and Pietro Gambardella, Kurt Kummer, José Luis Díez-Ferrer, David Coffey, César de la Fuente, Miguel Ciria, and Jose I. Arnaudus; *PHYSICAL REVIEW B* 90, 064423 (2014), DOI: 10.1103/PhysRevB.90.064423
- Roca-Lopez, D.; Tejero, T.; Merino, P. DFT Investigation of the Mechanism of E/Z Isomerization of Nitrones. *J. Org. Chem.* 2014, 79, 8358-8365.
- Roca-López, D.; Tejero, T.; Caramella, P.; Merino, P., [2n2π + 2n2π] Cycloadditions: An alternative to forbidden [4π + 4π] processes. The Case of Nitrones Dimerizations. *Org. Biomol. Chem.* 2014, 12, 517-525.
- Roca-López, D.; Marqués-López, E.; Alcaine, A.; Merino, P.; Herrera, R. P., Friedel-Crafts alkylation mechanism using aminoindanol derived thiourea catalyst. *Org. Biomol. Chem.* 2014, 12, 4503-4510.
- Merino, P.; Tejero, T.; Díez Martínez, A., Theoretical Elucidation of the Mechanism of the Cycloaddition between Nitronyl Ylides and Electron-deficient Alkenes. *J. Org. Chem.* 2014, 79, 2189-2202.
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- Nguyen, D. H.; Greger, I.; Perez-Torrente, J. J.; Jiménez, M. V.; Modrego, F. J.; Lahoz, F. J.; Oro, L. A. *Organometallics* 2013, 32, 6903-6917. ONO Dianionic Pincer-Type Ligand Precursors for the Synthesis of σ,π-Cyclooctenyl Iridium(III) Complexes: Formation Mechanism and Coordination Chemistry DOI:10.1021/om400767d

- Jiménez, M. V.; Bartolomé, M. I.; Perez-Torrente, J. J.; Gómez, D.; Modrego, F. J.; Oro, L. A. *ChemCatChem* 2013, 5, 263-276. Mechanistic Studies on the Catalytic Oxidative Amination of Alkenes by Rhodium(I) Complexes with Hemilabile Phosphines DOI:10.1002/cctc.201200510
- Baya, M.; Belío, U.; Martín, A. Synthesis, Characterization, And Computational Study of Complexes Containing Pt···H Hydrogen Bonding Interactions *Inorg. Chem.* 2014, 53, 189-200.
- García-Monforte, M. A.; Baya, M.; Betoré, M. P.; Martín, A.; Menjón, B. Mononuclear anionic AO2X3 compounds with non-VSEPR structure *Dalton Trans.* 2014, 43, 7615-7621.
- Sabater, S.; Baya, M.; Mata, J. A. Highly Active Cp*Ir Catalyst at Low Temperatures Bearing an N-Heterocyclic Carbene Ligand and a Chelated Primary Benzylamine in Transfer Hydrogenation *Organometallics* 2014, 33, 6830-6839.

Key Projects 2014

Theoretical study of chemical and enzymatic reactions

Led by Pedro Merino (UNIZAR). Investigations on several reaction mechanism regarding organic reactions including nucleophilic additions, cycloadditions and rearrangements were carried out. Particular attention was focused on the mechanism of enzymatic reactions, e.g. transglycosylation reactions and protein-glycosylation reactions and small systems including organocatalytic reactions resembling enzymatic processes. The study in detail of the model reactions is crucial for understanding the mechanism of action of the enzymes and it can serve as the basis for the design of specific therapeutic agents acting as inhibitors and/or modulators of the target proteins.

Detailed long-term weather predictions for the construction of a Typical Meteorological Year for Spain

Led by Norberto Fueyo Díaz (UNIZAR). The project involves performing highly detailed Numerical Weather Predictions (NWP) simulations for Spain for the construction of a high-resolution Typical Meteorological Year, TMY. The overarching aim is the re-evaluation of the potential and cost of renewable energies in Spain, using the calculated TMY. It is part of the wider project ENE2011-27264: Rigorous quantification of energy scenarios for Spain, funded by the Spanish Ministry for Science and Innovation.

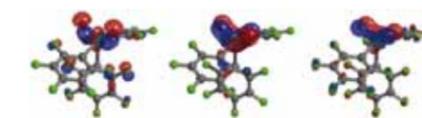


The figure shows the average wind speed at 80 meters in Spain (calculated with a spatial resolution of 2.5 km and a time resolution of 1 h.)

A TMY of Spain with a spatial resolution of 2.5 km and a time resolution of 1 h will be available free in the web page of the Fluid Numerical Group (gfn.unizar.es) of the University of Zaragoza in order to help develop research activities by other groups.

Modellization of Chemical Processes of Theoretical and Practical Importance

Led by Miguel Baya García (ISQCH). Our scientific interests are centred in the study of



Molecular Orbitals describing the pi-bonding of the molybdenyl unit in complex [MoO2(C6F5)3]

chemical reactions involving organometallics. For example, we described and characterized hydrogen-bonding interactions in platinum (II) square-planar systems, both in the solid state and in solution. We also prepared and studied a rare mononuclear molybdenum (IV) dioxo complex, which shows an unusual structure that can be described as an edge-capped tetrahedron. Furthermore we designed novel Iridium (III) catalysts active in transfer hydrogenation reactions, which showed to induce moderate enantiomeric excesses in the reduction of prochiral ketones.

Computational Modelling of Homogeneous Catalytic Reactions

Led by Francisco Javier Modrego Pérez (ISQCH). The project was developed along the research line "Catalysis and catalytic processes" within the ISQCH. The computational chemistry methodology allowed for a detailed analysis of the reaction mechanisms and the homogeneous catalysis processes as a whole, obtaining results which are not amenable to experimental studies alone. The use of the supercomputing facilities at CAESARAUGUSTA enabled us to use realistic models of the molecules and processes avoiding simplifications which are not always advisable.

First-principles calculations of the spin coupling between lanthanide adatoms and iron islands

Led by Cesar de la Fuente. By using non-collinear spin polarized (SP) DFT-based first-principles calculations, we performed a study of the electronic properties of Tm and Lu adatoms over an Fe monolayer (ML) on (110) W. The agreement with the spin-polarized scanning tunneling microscopy (SP-STM) experimental results was very good. All first principle calculations were done on CAESARAUGUSTA.

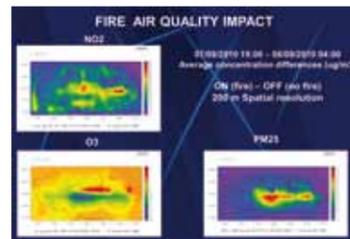
Structure and magnetism of Tm atoms and monolayers on W(110)

Led by Cesar de la Fuente. We investigated the growth and magnetic properties of Tm atoms and monolayers deposited on a W(110) surface using scanning tunnelling microscopy and x-ray magnetic circular and linear dichroism. The equilibrium structure of Tm monolayer films is found and calculated by first principle calculations. The triangular structure of the Tm lattice suggests the presence of significant magnetic frustration in this system, which may lead to either a non-collinear staggered spin structure or intrinsic disorder.

Fuel moisture content models to forest fire behaviour forecast, Roberto San José, UPM Computer Science School

Abstract

A new information system for wildland fire forecast is being developed based on WRF-Fire. The goal is to simulate real wildland fires in Spain and use the information to plan and respond to fires. A new fuel moisture content model was developed. The new module allows each time step to calculate the fuel moisture content of dead fuels (1hr, 10hr, and 100hr) and live fuels. The system has capabilities to assimilate data from measurement networks and/or satellite data. The system should be evaluated and applied with collected data from real wildland fires. The objective is to show that the designed system really has the ability to simulate wildland fires. The task is part of the research project PROMETEO "Technologies for the comprehensive fighting of forest fires and for the conservation of our forests".



Results

The new Fuel Moisture Content (FMC) model was validated with wildland fire model WRF-Fire. The results, from the fire behavior model runs with FMC input values calculated by the new developed model, were compared with real wildfires in Spain. The final spatial resolution of 20m requires supercomputing facilities in order to conclude the calculation within a reasonable timeframe. Results show that the system can produce realistic simulations of fire behavior using the geographical information available of the fire in a real case scenario. Simulations to analyse the impact on air pollution concentration of a fire were also implemented using the WRF/Chem model and the Fire model implemented into WRF in on-line mode. The amount of the chemical species created is determined from the amount of fuel burned, simulated by the fire model.

Publications

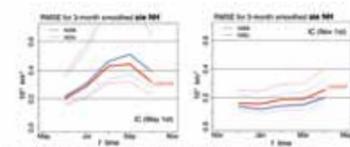
- Roberto San José, et. al. A CUSTOMIZED FMC MODEL FOR WILDLAND FIRE SIMULATIONS USING WRF-FIRE MODEL OVER SPAIN. Fresenius Environmental Bulletin Volume 23, No 11. 2014
- Roberto San José, et. al. ANALYSIS OF FIRE BEHAVIOUR SIMULATIONS OVER SPAIN WITH WRF-FIRE. Int. J. Environment and Pollution, Vol. 55, Nos. 1/2/3/4, 2014

Ocean tuning in high-resolution climate prediction experiments, Francisco J. Doblas-Reyes, Institut Català de Ciències del Clima

Abstract

The objective of this project is to find a set of values for the namelist parameters in the enhanced-resolution ocean-component of EC-Earth. Finding the best combination of model input parameters requires a series of runs to adequately handle the imbrication of the ocean source-code.

The outcome of this work will contribute to the progress of EC-Earth by reaching a configuration able to translate the increase in ocean resolu-



Root Mean Square Error of Sea Ice extent in 1000 sources, in real and 1000 (changed) values of sea ice, in March for May start date (M5) and November start date (N5). The blue lines show the confidence interval at 95% of the Root Mean Square Error.

tion into more accurate coupled outputs, also setting a benchmark for subsequent coupled high-resolution-ocean studies.

Results

Based on suggestions from various partners of the EC-Earth consortium, it was decided to focus this study more specifically on two parameters of the NEMO namelist: rn_ebb the input of kinetic energy from wind stress at the surface (rn_ebb) and the parametrization of the sea ice albedo. The EC-Earth 3 forecast system has a strong cold bias in the sea surface temperatures (SSTs) of Northern hemisphere in summer. This bias has been suggested to be a limiting factor for the predictability of the Northern Atlantic Oscillation among other phenomena. The main finding of the study is that the reduction of the rn_ebb parameter were shown to be an important factor for SSTs in the summer hemisphere, as a decreased value of this parameter tends to warm the SST in the Northern hemisphere in summer and thus reduce the bias in this region. This result is very encouraging, showing that an appropriate tuning can lead to an important reduction of systematic biases, and thus it has been implemented at the different resolution of EC-Earth.

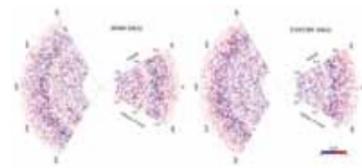
Publications

- A paper based on these experiments is in preparation and will be submitted before summer of 2015.

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

Abstract

The Marenstrum Numerical Cosmology Project (<http://astro.ft.uam.es/marenstrum>) is an international collaboration with the aim of using the exceptional capabilities of the new Marenstrum-III supercomputer to carry out grand challenge cosmological simulations of the formation of galaxies, groups and clusters of galaxies and the large scale structures in the universe. The scientific objective is to understand the physical processes that were involved in the formation and evolution of these objects from initial conditions that are compatible with the early epochs of the Universe derived from the observations of the



Cosmic Microwave Background radiation. The project uses state-of-the-art numerical codes for our simulations, based on different techniques, SPH, VPH and AMR. All of them are fully MPI + OpenMP parallelized.

Results

Work undertaken during 2014 focused on two main lines of research:

- 1) Simulations of Clusters of Galaxies (MUSIC project) - a continua-

tion of the work started in 2012 with the generation of the largest database of simulated galaxy clusters called MUSIC. During 2014 the database was complemented with a new set of runs that include the effects of black hole physics and AGN feedbacks, in collaboration with Trieste Observatory. The full database can be accessed from <http://music.ft.uam.es>.

- 2) Large Volume Simulations for galaxy surveys - the results on the clustering of halos and dark matter from the analysis of the new Multidark Simulations (<http://www.multidark.org>) that were run in Supermuc thanks to a PRACE grant, were used to calibrate a set of new codes developed by the Group with collaborators in Potsdam, Beijing, Bolonia and Marseille to generate massive mock catalogues for lensing and galaxy surveys.

Publications

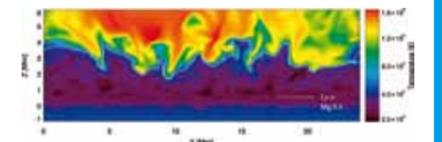
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- Dark matter in the Local Universe, Gustavo Yepes, et. al., New Astronomy Reviews 1 58 (2014).
- Hydrodynamical simulations of coupled and uncoupled quintessence models - II. Galaxy clusters, Edoardo Carlesi, et. al., Monthly Notices of the Royal Astronomical Society 2958 439 (2014).
- Hydrodynamical simulations of coupled and uncoupled quintessence models - I. Halo properties and the cosmic web Edoardo Carlesi, et. al., Monthly Notices of the Royal Astronomical Society 2943 439 (2014).
- Modelling baryon acoustic oscillations with perturbation theory and stochastic halo biasing, Francisco-Shu Kitaura, et. al., Monthly Notices of the Royal Astronomical Society L21 439 (2014).
- The MUSIC of galaxy clusters - II. X-ray global properties and scaling relations, Biffi, V., et. al., Monthly Notices of the Royal Astronomical Society 588 439 (2014).
- EZmocks: extending the Zel'dovich approximation to generate mock galaxy catalogues with accurate clustering statistics, Chia-Hsun Chuang, et. al., ArXiv e-prints arXiv:1409.1124 (2014).
- The Imprint of Reionization on the Star Formation Histories of Dwarf Galaxies, Alejandro Benitez-Llambay, et. al., ArXiv e-prints arXiv:1405.5540 (2014).

Three Dimensional Simulations Of The Generation And Transfer Of Polarized Radiation In The Solar Outer Atmosphere, Javier Trujillo Bueno, Instituto de Astrofísica de Canarias (IAC)

Abstract

Deciphering and understanding the magnetic activity of the outer solar atmosphere requires measuring and modelling the polarization

produced by anisotropic radiation pumping and the Hanle and Zeeman effects in strong spectral lines.



The interpretation of the observations requires solving a complex non-equilibrium radiative transfer problem, because the plasma of the solar atmosphere is highly inhomogeneous and dynamic. This implies the need to solve the problem of the generation of polarized radiation in realistic 3D models of the solar atmosphere. To this end, the Group developed the radiative transfer code PORTA. With PORTA and the MareNostrum supercomputer the Group is investigating the magnetic sensitivity of chromospheric and transition region lines, whose polarization will be measured by novel telescopes such as CLASP and SOLAR-C.

Results

To study the physics of the chromosphere-corona transition region and above (i.e. the place where the coronal heating takes place, the solar wind is driven and the near-Earth space weather generated) it is necessary to develop and apply plasma diagnostic techniques based on the polarization produced by scattering processes and the Hanle and Zeeman effects in strong spectral lines. To this end, the Group solved the multilevel problem of the generation and transfer of polarized radiation, considering realistic 3D models of the solar atmosphere resulting from magneto-hydrodynamic simulations. Detailed numerical simulations were carried out of the linear polarization signals produced in the core of the following resonance lines: hydrogen Lyman-alpha, Mg II k and Ca II K, which originate in the upper solar chromosphere. Of particular importance was investigating the magnetic sensitivity of the scattering polarization in such spectral lines, and to develop strategies for determining the magnetization of the solar chromosphere. For more information see: <http://www.iac.es/proyecto/magnetism/>

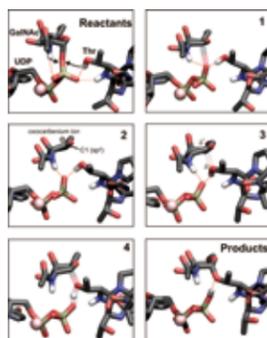
Publications

- Stepan, J., 'PORTA: A Massively Parallel Code for 3D Non-LTE Polarized Radiative Transfer', Invited Review in the international conference "Solar Polarization 7", ASP Conf. Series, Vol. 489, 243, (2014).
- Trujillo Bueno, J., 'Polarized Radiation Diagnostics for Probing the Magnetism of the Outer Solar Atmosphere', Invited Review in the international conference "Solar Polarization 7", ASP Conf. Series, Vol. 489, 137, (2014).
- Trujillo Bueno, J., 'Polarized Radiation Diagnostics for Exploring the Magnetic Activity of the Chromosphere, Transition Region and Coronai', Invited Review in 40th COSPAR Scientific Assembly. 2-10 Aug 2014, Moscow, Russia.
- Stepan, J., & Trujillo Bueno, J., 'Three-dimensional Radiative Transfer Simulations of Scattering Polarization and the Hanle Effect in Magneto-hydrodynamical Chromospheric Models', Invited Review in the IAU Symposium 305. 1-5 Dec 2014, Punta Leona (Costa Rica).
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- Stepan, J., et. al., 'Three-dimensional Radiative Transfer Simulations of the Scattering Polarization of the Hydrogen Ly-alpha line in a Magneto-hydrodynamical Model of the Chromosphere-Corona Transition Region', The Astrophysical Journal, (2014).

Elucidating the catalytic mechanism of retaining glycosyltransferases, Carme Rovira, Parc Científic de Barcelona (Universitat de Barcelona)

Abstract

Glycosyltransferases are the enzymes responsible for the formation of the glycosidic bond, one of the most important chemical reactions in nature. However, their mechanism of action is very controversial. A very unusual mechanism with little chemical precedence ("front-face") has been proposed. Yet the lack of mechanistic insight prohibits elucidation of whether this mechanism is feasible in the enzyme environment. The project aims to elucidate whether the front-face mechanism is feasible for some glycosyltransferases.



Results

By means of ab initio metadynamics dynamics techniques the project demonstrated that the "front-face" type mechanism is feasible for some glycosyltransferase enzymes, in particular, for those not displaying a carboxylate group near the active site, such as trehalose-6-phosphate synthase and polypeptide GalNAc-transferase 2. In these cases, the front-face reaction takes place thanks to the formation of a positively-charged species (a carbocation) with an extremely short half-life that moves quickly from the donor to the acceptor.

Glycosyltransferases are responsible for the structure of many carbohydrates and, therefore, the knowledge of their mechanism of action will help to modify their function, thereby improving the synthesis of known carbohydrates and new structures. It will also contribute to the design of inhibitors for those GTs that are involved in infectious diseases.

The large amount of multiple-processor calculations necessary to obtain the free energy landscape of the reaction process makes this process unfeasible without high-performance computing resources.

Publications

- E. Lira-Navarrete, J. Iglesias-Fernández, W. F. Zandberg, I. Compañón, Y. Kong, F. Corzana, B. M. Pinto, H. Clausen, J. M. Peregrina, D. Vocadlo, C. Rovira, R. Hurtado-Guerrero. 'Combined structural snapshots and metadynamics reveal a substrate-guided front-face reaction for polypeptide GalNAc-transferase T2j. *Angew. Chem. Int. Ed.* 2014, 126, 8345-8349.

Microbial Oceanomics using Next-Generation Sequencing (454/Illumina), Ramiro Logares, ICM-CSIC

Abstract

Microbes are vital for the functioning of the biosphere. Still, the extent of their diversity and their spatiotemporal structuring patterns are barely known. Similarly, not much is known about their ecological interactions. During the last five years, powerful high throughput molecular tools became available, allowing deeper insights into microbial diversity, distributions and evolution. For example, today one can investigate the order of magnitude of microbial diversity and possibly determine whether there is a 'rare biosphere'. Furthermore, one can start asking whether microbes have biogeographies or are randomly distributed over different spatiotemporal scales. The data gathered by research in these latter areas will be vital for understanding how the Earth's ecosystems work.



Results

MareNostrum was used to analyse large amounts of genetic data from marine organisms as well as to run models that help to understand how the ocean functions. Given the dimensions of the global ocean, such knowledge is vital to increase our understanding of the biosphere and the effects of climate change.

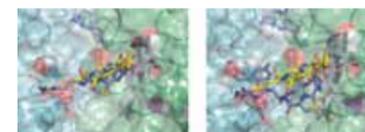
Publications

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Novel compounds against angiogenesis: Design of selective inhibitors against alpha v/beta 3 integrins, Fco. Javier Luque Garriga, Faculty of Pharmacy, University of Barcelona

Abstract

Polythiazole amino acids clasp linear peptides to generate cyclic derivatives, and the resulting species are not mere stapled peptides but bear a complex heterocyclic moiety unfolding its intrinsic set of interactions. This strategy was followed to improve the pharmacological properties of a series of cyclic RGD-containing peptides acting as potential inhibitors of integrins, and hence with a promising role in regulating angiogenesis. Compared to cilengitide, the novel stapled peptides exhibit improved integrin selectivity against alpha_v/beta_3 and remarkable antiangiogenic in vivo activity. The molecular basis of the binding to alpha_v/beta_3 and the selectivity relative to alpha_v/beta_5 will be examined in this project.



Results

Using a modular strategy for the preparation of a new (poly)thiazole-containing cyclic peptide, compound 2 was found to exhibit considerably increased integrin selectivity toward avb3 compared to the parent cilengitide. This is of particular relevance, since avb3 integrin is highly expressed in several tumor tissues, whereas avb5 is commonly found in healthy cells. While compound 2 superposes well with the structure of cilengitide upon binding to avb3, a significant relocation of the cyclopeptide backbone is observed upon binding to avb5, an effect that can be attributed to the electrostatic influence exerted by Asp279. In fact, binding of compound 2 to avb3 was predicted to be more favorable than to avb5, which agrees qualitatively with the 70-fold increase in selectivity determined experimentally for compound 2. These results open up new avenues for the design of and synthetic access to new analogues with enhanced integrin selectivity, a key issue for the development of therapeutic antiangiogenic agents.

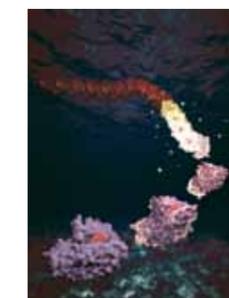
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Study of the nucleotide conformational switch in bacterial cell division proteins by all-atom simulations, Pablo Chacón, IQFR (CSIC)

Abstract

FtsZ and TubZ are crucial cytoskeleton proteins. Both proteins assemble forming filaments whose dynamics is modulated by the binding and GTP hydrolysis. Only very recently the assembled states of a straight FtsZ and two-stranded helical TubZ filaments have been solved at atomic detail. Using this novel information, the goal is to perform all-atom simulations of long filaments bound to GTP or GDP to investigate the induced conformational changes. In particular, to shed light on the molecular mechanism of activation of the assembly and correlate the findings with their eukaryotic homolog, tubulin. Ultimately, understanding the relationship between the assembly molecular mechanism and the binding of modulators may help the rational design of new antibiotics.



Results

Large scale FtsZ filament dynamics studies were performed and interpreted in the context of the assembly cycle of this essential cell division protein. In contrast with all previous studies based on the inactive (not functional) closed-cleft FtsZ conformation studies, the simulations disclose different filament curvatures supported by nucleotide-regulated interfacial dynamics. Moreover, for the first time the relaxation from the active polymer conformation to the inactive closed-cleft conformation of FtsZ monomers was monitored. In agreement with experimental data, these groundbreaking results unravel the natural mechanism of the FtsZ assembly switch. Integrating this assembly switch and the nucleotide-dependent interfacial filament stability, the work offers a detailed molecular interpretation of the assembly-disassembly FtsZ cycle and its inhibition. These results were recently published and a related drug-design paper has been submitted.

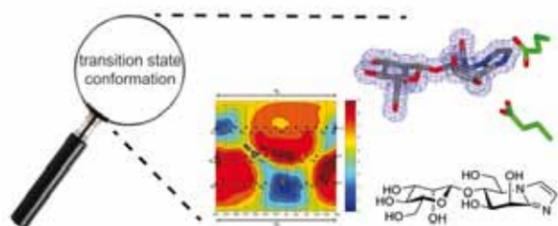
Publications

- Ramirez-Aportela E., López-Blanco J.R., Andreu J.M., and Chacón P. (2014). Understanding Nucleotide-Regulated FtsZ Filament Dynamics and the Monomer Assembly Switch with Large-Scale Atomistic Simulations. *Biophys J.* 107 (9):2164-2176
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Conformational free energy landscapes of carbohydrates, Carme Rovira, Universitat de Barcelona

Abstract

Carbohydrate-active enzymes are the focus of enormous interest due to the critically important roles that complex glycans play in health and disease, as well as the rekindled interest in enzymatic biomass conversion. The project uses state-of-the-art ab initio molecular dynamics (enhanced sampling) methods to analyse the conformational free energy landscapes of isolated monosaccharides and substrates of carbohydrate-active enzymes to predict catalytically-competent conformations that can be used to guide inhibitor design.



Results

The results obtained show that the conformational free energy landscape of isolated sugars (e.g. beta-glucose, or beta-xylose) inform on the type of transition state of glycosylation reactions. In addition, it was demonstrated that the conformational free energy landscape of glycosidase inhibitors can be used to assess transition state mimicry (i.e. how much the inhibitor resembles the transition state of the enzymatic reaction). This opens the door to develop new molecules with the desired energy landscape that can be used as a potent inhibitors to treat diseases related to glycosidase malfunction.

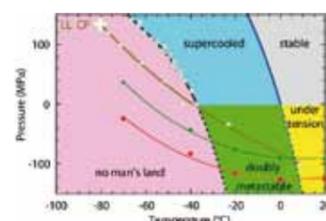
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Existence of the liquid-liquid critical point in supercooled water, Jose Luis Fernandez Abascal, Universidad Complutense de Madrid

Abstract

Water anomalies still defy explanation. One problem of fundamental importance is the study of the putative liquid-liquid critical point which attempts to explain many of the water anomalies. The project also aims to contribute to understanding the behaviour of supercooled liquid water, a fundamental question of great scientific interest. Describing the liquid-liquid critical point with molecular dynamics simulations of a reliable water model would explain the origin of the anomalous behaviour of supercooled water.



Results

In the supercooled liquid, many quantities show a large increase. The question is whether these quantities diverge or go through a maximum. The answer, key to our understanding of water anomalies, has remained elusive in experiments because crystallization always occurred before any extremum is reached.

The project collaborated with an experimental team in order to analyse their measurements of the sound velocity of water in a scarcely explored region of the phase diagram, where water is both supercooled and at negative pressure (i.e., doubly metastable). Several anomalies were found (maxima in the adiabatic compressibility) reminiscent of the behaviour of supercritical fluids. To support this interpretation, large scale simulations were performed with the TIP4P/2005 model with good agreement, suggesting the existence of a line of maxima in compressibility.

The simulations required significant computer time only possible because of the computing power of Minotauro.

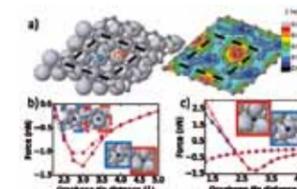
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First principles simulations of Scanning Probe Microscopies experiments on graphene heterostructures and metal oxides, Rubén Pérez, Universidad Autónoma de Madrid

Abstract

This project combines first-principles calculations with state-of-the-art SPM experiments in order to provide the basis for (1) the understanding of the role of the defects the catalytic properties of metal oxides, (2) the study of the interaction of graphene with other 2D related materials and with molecules, and (3) the SPM-assisted manipulation of organic molecules on inorganic surfaces. The simulation of these systems share common problems: the requirement of an accurate description of the electronic configuration and the need for large cells to minimize the density of defects. Therefore, these studies can only be accomplished with computational resources provided by the supercomputers as those integrated in the RES.



Results

The response of graphene (G) to the AFM was studied: On G on Pt it was shown that the AFM operated in dynamic mode is able to disclose the subtle differences between different C atoms of the Moiré pattern, this differences originate from different stiffness instead of differences in heights or electronic properties. The DFT simulations showed that atomic vacancies on G do not directly increase the layer strength as shown in recent experiments but, due to the vacancy reconstruction, they do locally stretch the G which can modify the thermal fluctuations of the layer controlled by the out of plane modes. Large molecular dynamic simulations based on classical potentials are currently being performed to quantify the effect of this induced strain field on the mechanical properties of graphene.

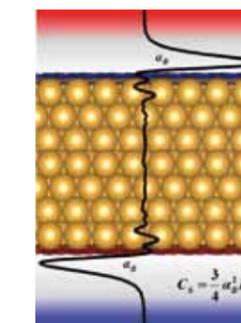
Publications

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Theoretical Modeling of Aquous Phase Reforming: 1st period, Nuria López, ICIQ

Abstract

Aqueous Phase Reforming (APR) is a process of high industrial interest to produce biomass-derived alcohols. In 2010, the world's first biogasoline employing this technique was presented in a demonstration plant in Madison, WI by Virent Energy Systems, Inc. In the reaction sugar feedstocks are directly converted into gasoline. This project aims to employ Density Functional Theory in the framework of a slab model to study the reactivity of alcohols on selected surfaces of metals and oxides. The project will analyse the reactivity, role of water and the effect of water dynamics on the activity and selectivity of the process. In parallel the role of oxides as potentially interesting supports and/or catalysts will be considered.



Results

APR includes reforming to generate hydrogen, dehydrogenation of alcohols/hydrogenation of carbonyls, deoxygenation reactions, hydrogenolysis and cyclization. In all these parts of the process the water-metal interface is the key that controls activity. The computational resources at BSC-RES enabled, for the first time, the generation of complete knowledge of the most relevant ingredients that are required in order to fully take into account the complexity of the water-metal interface. With this purpose massive computational simulations based on Born-Oppenheimer Molecular Dynamics were carried out for different water configurations. The simulations showed that it is possible to define a suitable water-metal model where all the reactivity taking place in the APR can be explicitly addressed for a wide variety of metals. The results pave the way for the complete understanding and adequate tuning of new formulations of this important catalytic system.

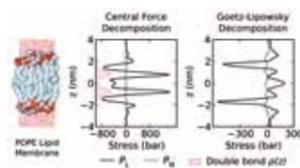
Publications

- "A first principles comparison of methanol decomposition and reverse reactions on metal surfaces" R. Garcia-Muelas, Q. Li, N. Lopez, *ACS Catal.* (submitted)
- "Costless Derivation of Dispersion Coefficients for Metal Surfaces" N. Al-mora-Barrios, G. Carchini, P. Blonski, and N. López, *J. Chem. Theor. Comp.* 10, 5002 (2014)
- "Free energy assessment of water structures and their dissociation on Ru(0001)" G. Revilla-Lopez, P. Blonski, and N. Lopez, submitted
- "Homolytic Products from Heterolytic Paths in H₂ Dissociation on Metal Oxides: The example of CeO₂" M. Garcia-Melchor and N. Lopez, *J. Phys. Chem. C* 118, 10921 (2014)
- "Unique Reaction Path in Heterogeneous Catalysis: The Concerted Semi-Hydrogenation of Propyne to Propene on CeO₂" M. Garcia-Melchor, L. Bellarosa, and N. López *ACS Catal.* 4, 4015 (2014)

Bridging the scales in biomolecular mechanics: membranes and coiled-coils, Marino Arroyo Balaguer, UPC

Abstract

The effective behaviour of biomolecular systems often results from phenomena at multiple spatial and temporal scales. As a result, it is very difficult to understand them from purely molecular simulations. There is a pressing need to understand how to correctly upscale molecular models to rationalize these systems from a continuum viewpoint. Here we investigate the molecular-to-continuum relation in two model systems: (1) biomembranes and (2) filamentous coiled-coil proteins. The mechanical state of biomembranes is of singular biological importance due to the different stresses and deformations they must bear for the proper function of the cell. Coiled-coils are the main component of intermediate filaments, one of the three major filaments of the cell cytoskeleton.



Results

It has long been recognized that the mapping from the statistical mechanics of molecular systems to a continuum stress field is not unique and depends, for instance, on the method employed to decompose interatomic forces into pairwise terms. Although appreciated by theoreticians, the practical consequences have been largely overlooked. We investigate the significance of this non-uniqueness and provide a canonical definition of the stress for biomolecular systems. We perform MD simulations of biomembranes and coiled-coils with the GROMACS 4.5.5 package and compute the microscopic stress with a customized version of GROMACS 4.5.5 (publicly available at <http://www.lacan.upc.edu/LocalStressFromMD>). Strikingly, we find that a widely used definition of the microscopic stress leads to stresses that are inconsistent with standard continuum mechanics and therefore do not have a clear mechanical interpretation. In contrast, we propose a canonical force decomposition that results in physically meaningful fields by construction.

Publications

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- Vanegas, J. M. et al. "Force Transduction and Lipid Binding in MscL: A Continuum-Molecular Approach." *PLOS one*, 9(12) e113947, 2014.

Diffusion Monte Carlo simulation of quantum gases and solids, Grigory E. Astrakharchik, Departament de Física i Enginyeria Nuclear, Universitat Politècnica de Catalunya

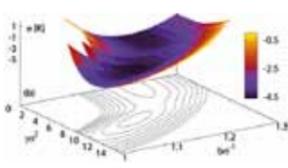
Abstract

Quantum Monte Carlo methods are used to simulate properties of matter at zero temperature. The energy calculated in variational Monte Carlo method provides an

upper bound to the ground-state energy. By minimizing the energy with respect to variational parameters an explicit analytic expression is obtained which closely approximates the many-body wave function. This provides an insight to the physics of ultracold matter. Diffusion Monte Carlo method is used to find the exact ground-state energy.

The quantum systems studied are: helium 4 (liquid and hcp solid), helium 3 in 1D, dipolar bilayer, a mixture of 1D Bose gases in traps.

Ground-state energy is calculated and is used to locate quantum phase transitions at zero temperature. The correlations and coherence is investigated by calculating the correlation functions.



Results

- 1) The variational method was used with a simple yet exchange-symmetric and fully explicit wave function. The explicit form of the wave function allows various contributions to be considered to the phase transition. It was found that the employed wave function is an excellent candidate for describing both a first-order quantum phase transition and the ground state of a Bose solid.
- 2) The Luttinger liquid theory is found to describe the long-range properties of the correlation function. The density dependence of the Luttinger parameter is reported. Identified regimes include an "ideal Fermi gas", a "Bose-gas", a "super-Tonks-Girardeau".
- 3) It was found that by decreasing the interlayer distance for fixed value of the strength of the dipolar interaction, the dipolar bilayer system undergoes a quantum phase transition from a single-particle to a pair superfluid. The single-particle superfluid is characterized by a finite value of both the atomic condensate and the super-counterfluid density.
- 4) The complete phase diagram for one-dimensional binary mixtures of bosonic ultracold atomic gases in a harmonic trap was presented.

Publications

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First-principles modelling of radiation-resistant materials: interfaces between immiscible and incoherent transition metals, César González Pascual, University of Oviedo

Abstract

The project aims to perform a comprehensive study of different aspects of He atoms behaviour at the interfaces of immiscible incoherent transition metallic systems (Cu/Nb or Cu/W). Assessment of the energetics, stability and mobility of the impurity atoms at the interfaces and close

internal layers is envisaged. The possible differences between fcc and bcc metals on both sides of the interface shall be specifically evaluated. The systematic approach proposed will contribute to understanding the diffusion and solubility of He atoms inside the pure metallic matrices. This materials-by-design modelling effort can be regarded as a pioneering attempt to tailor the stability and self-healing properties of nanoscale interfaces and their potential uses as radiation-resistant systems for fusion reactor technologies.



Results

Density Functional Theory (DFT) calculations were performed of the complex semi-coherent Cu/Nb interface. In a first stage, it was found that the vacancies and He atoms are more comfortable at the interface than in the metallic Cu and Nb bulks. Both defects have to cross a lower energy barrier to reach the interface when they are close to it. Once a vacancy or a He atom has emerged at the interface, it prefers to stay in the so-called misfit dislocation intersections (MDI), where the Nb atoms fall precisely or nearly over the Cu atoms at the interface. This result can be explained in terms of geometrical effects. The He atoms are accommodated in the vacancies at the interface, better than at the pure interface or in a vacancy in the metallic bulk. Finally, both defects have to cross a relatively high energy barrier in their motion along the interface. These results suggest that the He atoms and vacancies will try to reach the interface and be stabilized there.

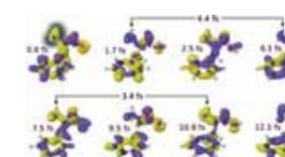
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- C. Gonzalez et al. "Migration mechanisms of helium in copper and tungsten", *Journal of Material Science*, 49, 8127-8139, August 2014.
- C. Gonzalez, et al. "Point defects stability in a semicoherent metallic interface"(submitted).

XUV/X-ray laser pulses for ultrafast electronic control in molecules,Name: Fernando Martin, UAM

Abstract

Ultrafast electronic and nuclear dynamics of molecules can be investigated by using ultrashort (atto- and femtosecond) laser pulses. A full theoretical description of the dynamics of molecules subject to ultrashort laser pulses remains a challenge due to the computational difficulty to include all electronic and vibrational degrees of freedom. Our group has developed time-dependent ab initio treatments that overcome this difficulty. The project aims to perform: i) a systematic study on the influence of laser parameters on autoionization processes, ii) attosecond pump-probe numerical



experiments on molecules, and iii) a study on single and double ionization of molecules induced by strong fields as well as by single and trains of ultrashort laser pulses.

Results

A theoretical study was performed of the interaction of small molecules with ultrashort laser pulses, using parallel codes, MPI and PET-Sc, as well as the computational support available at Mare Nostrum. Main studies: - In H2: UV coherent control of molecular dynamics by (XUV+IR)-pump-IR-probe dynamics. Ultrafast (1-fs-scale) electron and nuclear dynamics with XUV-pump-XUV-probe pulses. Electron streaking, focusing on autoionization. Circular dichroism. UV-pump-UV-probe schemes to create a molecular interferometer. - The first study of ultrafast electron dynamics on an aminoacid, phenylalanine, initiated by single attosecond pulses. - Photoionization of molecular fluorine from inner and valence shells. - Vibrationally resolved photionization cross sections of CF4. In addition: - A hybrid Gaussian-B-spline basis was developed for studying the electronic continuum in photoionization. - A resolvent-operator method was used to study correlated kinetic energy spectra in the H2+ molecule.

Publications

- A. Palacios, et al. "XUV lasers for ultrafast electronic control in H2." *Ultrafast phenomena in molecular sciences*. Springer Series in Chemical Physics, Vol. 107, pp 25-48 (2014).
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- F. Catoire, et al. "The molecular Resolvent Operator Method: electronic and nuclear dynamics in strong-field ionization". *Physical Review A* 89 023415 (2014).
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- A. Palacios, et al. "Electron streaking and dissociation in laser-assisted photoionization of molecular hydrogen". *Journal of Physics B* 47 124013 (2014).
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- D. Ayuso, et al. "Dissociative and non-dissociative photoionization of molecular fluorine from inner and valence shells". *Journal of Electron Spectroscopy and Related Phenomena* 195 320 (2014).
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- F. Calegari, et al. "Ultrafast Electron Dynamics in a Biomolecule Initiated by Attosecond Pulses". *Science* 346 336 (2014).
- J. F. Pérez-Torres, et al. "Circular dichroism in molecular frame photoelectron angular distributions in the dissociative photoionization of H2 and D2 molecules". *Physical Review A* 90 043417 (2014).

Astronomy, Space & Earth Sciences 2014 Projects

- » **3D geoelectrical characterization of geological reservoirs** - Leader Name: Pilar Queral, Leader Institution: Universitat de Barcelona- Dept. Geodinàmica i Geofísica
- » **Coalescence of Black Hole Binary systems** - Leader Name: Sascha Husa, Leader Institution: Universitat de les Illes Balears
- » **Constraints on inflationary models of the universe based on CMB data** - Leader Name: Enrique Martinez Gonzalez, Leader Institution: Instituto de Física de Cantabria
- » **Development And Consolidation Of Geo-Spatial Sustainability Services For Adaptation Of Environmental And Climate Change Urban Impacts (Decumanus)** - Leader Name: Roberto San Jose, Leader Institution: UPM Computer Science School
- » **European framework for online integrated air quality and meteorology modeling** - Leader Name: Roberto San Jose, Leader Institution: UPM Computer Science School
- » **From the Galactic Fountain to Single Stars** - Leader Name: Paolo Padoan, Leader Institution: ICREA and ICC - UB
- » **Fuel moisture content models to forest fire behaviour forecast** - Leader Name: Roberto San Jose, Leader Institution: UPM Computer Science School
- » **Gaia: Data Processing and Simulation of Telemetry Stream** - Leader Name: Jordi Torra i Roca, Leader Institution: Universitat de Barcelona (UB), Departament d'Astronomia i Meteorologia
- » **Gaia: Simulation of Telemetry Stream** - Leader Name: Jordi Torra i Roca, Leader Institution: Universitat de Barcelona (UB), Departament d'Astronomia i Meteorologia
- » **Impact of ocean resolution and initialisation in climate seasonal predictions** - Leader Name: Francisco J. Doblas-Reyes, Leader Institution: Institut Català de Ciències del Clima
- » **Impact Of Solar Forcing On Future Climate Change Using A Chemistry Climate Model – Continuation** - Leader Name: Natalia Calvo Fernández, Leader Institution: Universidad Complutense de Madrid
- » **Ocean tuning in high-resolution climate prediction experiments** - Leader Name: Francisco J. Doblas-Reyes, Leader Institution: Institut Català de Ciències del Clima
- » **Simulations of dynamics of partially ionized solar atmosphere** - Leader Name: Elena Khomenko, Leader Institution: Instituto de Astrofísica de Canarias
- » **Tectonic/surface processes modeling of the Neogene Mesopotamian basin evolution** - Leader Name: Charlotte Fillon, Leader Institution: Instituto Jaime Almera-CSIC
- » **The Marenstrum Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe** - Leader Name: Gustavo Yepes, Leader Institution: Universidad Autonoma de Madrid
- » **The MICE project -1. Mapping the high-redshift universe** - Leader Name: Pablo Fosalba, Leader Institution: ICE (IEEC-CSIC)
- » **The MICE project -2. Volume and mass resolution effects on small-scale dark matter clustering** - Leader Name: Pablo Fosalba, Leader Institution: ICE (IEEC-CSIC)
- » **Three Dimensional Simulations Of The Generation And Transfer Of Polarized Radiation In The Solar Outer Atmosphere** - Leader Name: Javier Trujillo Bueno, Leader Institution: Instituto de Astrofísica de Canarias (IAC)

Biology and Life Sciences 2014 Projects

- » **Allosteric regulation of the SHIP2 phosphatase by its C2 domain.** - Leader Name: Daniel Lietha, Leader Institution: Spanish National Cancer Research Center (CNIO)
- » **Binding of novel activators to AMPK and theoretical study of the activation mechanism** - Leader Name: Fco. Javier Luque Garriga, Leader Institution: Faculty of Pharmacy, University of Barcelona
- » **Collective variables from Structural Alphabets for protein model refinement** - Leader Name: Arianna Fornili, Leader Institution: Kings College London
- » **Development of novel treatments for myotonic dystrophy: in vivo drug discovery** - Leader Name: Jordi Teixidó, Leader Institution: Institut Químic de Sarrià (IQS, URL)
- » **Effect of the S31N mutation on the inhibition of the M2 proton channel of influenza virus** - Leader Name: Fco. Javier Luque Garriga, Leader Institution: Faculty of Pharmacy, University of Barcelona
- » **Elucidating the catalytic mechanism of retaining glycosyltransferases** - Leader Name: Carme Rovira, Leader Institution: Universitat de Barcelona
- » **Evidence of Conformational Selection in a Glycosyltransferase Structure?** - Leader Name: Antoni Planas, Leader Institution: Laboratory of Biochemistry. IQS - Universitat Ramon Llull
- » **Exploration of the unusual biophysics of Intrinsically Disordered Proteins using Monte Carlo simulations** - Leader Name: Ramon Crehuet Simon, Leader Institution: Institute of Advanced Chemistry of Catalonia (IQAC/CSIC)
- » **Exploring the Small Molecule Binding effects in protein folding equilibrium** - Leader Name: Ramon Crehuet Simon, Leader Institution: Institute of Advanced Chemistry of Catalonia (IQAC/CSIC)
- » **Improvement of the affinity of a membrane receptor ligand** - Leader Name: Ernest Giralt Lledó, Leader Institution: Institute for Research in Biomedicine (IRB)
- » **In silico evolution of the gap gene network: how to turn one fly into another** - Leader Name: Johannes Jaeger, Leader Institution: EMBL/CRG Research Unit in Systems Biology
- » **ligand binding and unbinding to the M2 proton channel** - Leader Name: Fco. Javier Luque Garriga, Leader Institution: Faculty of Pharmacy, University of Barcelona
- » **Microbial Oceanomics using Next-Generation Sequencing (454/Illumina)** - Leader Name: Ramiro Logares-Haurie, Leader Institution: Instituto de Ciencias del Mar, CMIMA, CSIC
- » **Modulation of immune receptors function as a novel therapeutic strategy for acute CNS damage** - Leader Name: Jordi Villà-Freixa, Leader Institution: Polytechnic School, University of Vic - Central University of Catalonia
- » **Molecular Dynamics Of Gpcrs In Lipid Rafts Of Cns Diseases** - Leader Name: Jana Selent, Leader Institution: Pompeu Fabra University
- » **New strategies in GPCR drug discovery** - Leader Name: Leonardo Pardo, Leader Institution: Universitat Autònoma Barcelona
- » **Novel compounds against angiogenesis: Design of selective inhibitors against α_v/β_3 integrins** - Leader Name: Fco. Javier Luque Garriga, Leader Institution: Faculty of Pharmacy, University of Barcelona
- » **Redesign of enzymes in silico. Testing the BindScan algorithm.** - Leader Name: Xevi Biarnés, Leader Institution: Institut Químic de Sarrià
- » **Reverse-engineering embryo segmentation patterning in flies: from Clogmia to Megaselia** - Leader Name: Johannes Jaeger, Leader Institution: EMBL/CRG Research Unit in Systems Biology

- » **Structural modeling of an RNA stem-loop that regulates the alternative splicing of SMN2: a new therapeutic target in Spinal Muscular Atrophy** - Leader Name: Leonardo Scapozza, Leader Institution: University of Geneva
- » **Study of Phe allosteric site of phenylalanine hydroxylase by molecular dynamics** - Leader Name: Prof. Adriana Zagari, Leader Institution: University of Naples Federico II
- » **Study of the fluctuations of neurotoxic proteins** - Leader Name: Mariano Carrión-Vázquez, Leader Institution: Instituto Cajal - CSIC
- » **Study of the nucleotide conformational switch in bacterial cell division proteins by all-atom simulations** - Leader Name: Pablo Chacon, Leader Institution: IQFR(CSIC)
- » **Study of the role of EGFR activating mutations in the development of drug resistance in non-small cell lung cancer treatment** - Leader Name: Jordi Teixidó, Leader Institution: Institut Químic de Sarrià (IQS, URL)
- » **The mechanics of unfolding in coiled-coils** - Leader Name: Marino Arroyo Balaguer, Leader Institution: upc
- » **Transmembrane Ion Transport through alpha, gamma-Peptide Nanotubes** - Leader Name: Rebeca García Fandiño, Leader Institution: Universidad de Santiago de Compostela

Chemistry and Material Sciences 2014 Projects

- » **Ab initio molecular dynamics of organic ion-radical pairing in solution** - Leader Name: Juan José Novoa Vide, Leader Institution: University of Barcelona
- » **Ab initio molecular dynamics of photovoltaic organic self-assembled monolayers adsorbed on metal surfaces** - Leader Name: Sergio Diaz Tendero, Leader Institution: UAM
- » **Ab-initio calculations of thermoelectric properties in nanostructures: silicene, germanene, Si/Ge heterostructure, and two-dimensional transition-metal-dichalcogenides** - Leader Name: Angel Rubio, Leader Institution: Universidad País Vasco/CSIC/FHI
- » **Accessing multiscale properties of biological systems (DNA, proteins) via large-scale atomistic molecular dynamics.** - Leader Name: Rubén Pérez, Leader Institution: Universidad Autónoma de Madrid
- » **Accuracy of Density Functional Theory Techniques in Prediction of Boron Nitride Gas-Adsorbent Materials** - Leader Name: Claudio Cazorla, Leader Institution: Institute of Materials Science of Barcelona (ICMAB-CSIC)
- » **Adsorption of Atomic Hydrogen on Defective Non-Stoichiometric Surfaces of Cosmic Dust** - Leader Name: Albert Rimola, Leader Institution: UAB
- » **Adsorption of proteins on defective surfaces with large-scale molecular dynamics simulations** - Leader Name: Rubén Pérez, Leader Institution: Universidad Autónoma de Madrid
- » **Alkane oxidation over CeO2 nanoparticles: role of defects** - Leader Name: Avelino Corma Canós, Leader Institution: Instituto de Tecnología Química UPV-CSIC
- » **Bingel-Hirsch additions on Endohedral Metallofullerenes. How are they affected by the metallic cluster, the strain energy and the solvent effects?** - Leader Name: Miquel Solà, Leader Institution: universitat de Girona
- » **Calculating delta-G of Associative and Dissociative Organometallic Reaction Steps: The case of Pd-Catalysts in Cross-Coupling** - Leader Name: Gregori Ujaque, Leader Institution: UAB
- » **Characterization of Cu active centers in Cu-zeolite catalysts for the selective reduction of NOx** - Leader Name: Mercedes Boronat, Leader Institution: Instituto de Tecnología Química UPV-CSIC
- » **Charge transfer and self-assembly of molecules on modified metal surfaces**

- Leader Name: Manuel Alcamí, Leader Institution: UAM
- » **Competition between phonons and electron-hole pair excitations in ab-initio molecular dynamics simulations of gas/surface reactivity** - Leader Name: Maite Alducin Ochoa, Leader Institution: Centro de Física de Materiales, centro mixto CSIC-UPV/EHU
- » **Computational exploration of fullerene and endohedral metallofullerenes charge transfer properties for organic photovoltaic devices** - Leader Name: Miquel Solà, Leader Institution: universitat de Girona
- » **Conformational free energy landscapes of carbohydrates** - Leader Name: Carme Rovira, Leader Institution: Universitat de Barcelona
- » **Effect of defects on the two-photon photoemission (2PP) resonance for methanol and water on TiO2(110)** - Leader Name: Annapaola Migani, Leader Institution: CSIC-ICN2
- » **Electronic structure of semiconductors by means of quasiparticle calculations: relevance to photocatalysis** - Leader Name: Francesc Illas, Leader Institution: Universitat de Barcelona
- » **Existence of the liquid-liquid critical point in supercooled water** - Leader Name: Jose Luis Fernandez Abascal, Leader Institution: Universidad Complutense de Madrid
- » **First principles simulations of Scanning Probe Microscopies experiments on graphene heterostructures and metal oxides** - Leader Name: Rubén Pérez, Leader Institution: Universidad Autónoma de Madrid
- » **First-principles design of gold catalysts for C-C bond forming reactions: optimizing particle size and morphology for dissociation of C-X bonds with X = Cl, Br, I.** - Leader Name: Mercedes Boronat, Leader Institution: Instituto de Tecnología Química UPV-CSIC
- » **First-principles investigation of intrinsic screening mechanisms in ferroelectric thin film** - Leader Name: Emilio Artacho, Leader Institution: CIC nanoGUNE Consolider and University of Cambridge
- » **First-principles simulations of metal oxide surface chemistry and defects aided by scanning probe microscopies** - Leader Name: Rubén Pérez, Leader Institution: Universidad Autónoma de Madrid
- » **Formation energies of point defects in cadmium telluride** - Leader Name: Eduardo Menendez Proupin, Leader Institution: Universidad Politécnica de Madrid
- » **Fragmentation and reaction dynamics of charged and excited molecules in gas phase** - Leader Name: Manuel Alcamí, Leader Institution: UAM
- » **Ice crystallization** - Leader Name: Carlos Vega, Leader Institution: Universidad Complutense de Madrid, Dep. Química Física
- » **Improving the Performance of the IO and Density Fragment procedures on OCTOPUS code.** - Leader Name: Joaquim Jornet Somoza, Leader Institution: Universitat de Barcelona
- » **Large-scale radiation damage cascades from first principles** - Leader Name: Emilio Artacho, Leader Institution: CIC nanoGUNE Consolider and University of Cambridge
- » **Mechanical properties of biological systems as measured by atomic force microscopy** - Leader Name: Rubén Pérez, Leader Institution: Universidad Autónoma de Madrid
- » **MEMOIR: Multiferric and magnetoElectric Metal Organic frameworks** - Leader Name: Alessandro Stroppa, Leader Institution: CNR-SPIN
- » **Molecular-level understanding of CeO2 as catalyst for partial alkyne hydrogenation** - Leader Name: Maria Veronica Ganduglia-Pirovano, Leader Institution: Instituto de Catalis y Petroleoquímica, CSIC
- » **New Frontiers on Scanning Probe Microscopies: charge density distribution, subsurface resolution and atomic manipulation with the force and the electric current studied by First Principles simulations.** - Leader Name: Pablo Pou Bell, Leader Institution: Universidad Autónoma de Madrid

- » **New local multipole implementation and visualization for Octopus code** - Leader Name: Joseba Alberdi-Rodríguez, Leader Institution: Euskal Herriko Unibertsitatea UPV/EHU
- » **Oxidative addition at Pd centers by explicit solvent ab initio molecular dynamics** - Leader Name: Agustí Lledós, Leader Institution: UAB
- » **Oxygen induced step-doubling transition of the vicinal Pt(997) surface.** - Leader Name: Annapaola Migani, Leader Institution: CSIC-ICN2
- » **Performance of Time Dependent Density Functional Theory in the strong field photoionisation of noble gas atoms** - Leader Name: Angel Rubio, Leader Institution: Universidad Pais Vasco/CSIC/FHI
- » **Rationalization of the different reactivity of CeO2 crystallographic facets from first principles calculations** - Leader Name: Avelino Corma Canós, Leader Institution: Instituto de Tecnología Química UPV-CSIC
- » **Reveling insulator-to-metal transition in Mott materials with delocalization measures** - Leader Name: Ángel Martín Pendás, Leader Institution:
- » **Role of surface defects on the formation of the 2-dimensional electron gas at polar interfaces** - Leader Name: Emilio Artacho, Leader Institution: CIC nanoGUNE Consolider and University of Cambridge
- » **Role of triplet excitons in the photocatalysis of water and methanol on rutile TiO2(110).** - Leader Name: Annapaola Migani, Leader Institution: CSIC-ICN2
- » **Simulation of nanoparticles of pristine and Co-doped ZnO** - Leader Name: Victor Manuel García Suarez, Leader Institution: Universidad de Oviedo
- » **Structure, stability and spectroscopic properties of charged PAH (Polycyclic Aromatic Hydrocarbons) and PAH clusters** - Leader Name: Manuel Alcamí, Leader Institution: UAM
- » **Study of 2-dimensional nanoconfined water from ab initio simulations** - Leader Name: Emilio Artacho, Leader Institution: CIC nanoGUNE Consolider and University of Cambridge
- » **Theoretical Modeling of Aqueous Phase Reforming: 1st period** - Leader Name: Nuria Lopez, Leader Institution: ICIQ
- » **Towards more realistic modelling of industrially important Pd/CeO2 and Pt/CeO2 catalysts** - Leader Name: Konstantin Neyman, Leader Institution: Uni Barcelona
- » **Towards realistic models of stoichiometric and doped TiO2 nanoparticles relevant to photocatalysis: Atomic and electronic structure from Density Functional Theory and Quasiparticle GW calculations** - Leader Name: Francesc Illas, Leader Institution: Universitat de Barcelona
- » **Understanding monofunctional active sites for the water-gas shift reaction on model Ni/ceria catalysts** - Leader Name: María Verónica Ganduglia-Pirovano, Leader Institution: Instituto de Catalis y Petroleoquímica, CSIC
- » **Understanding Polytypism in Group IV Nanowires from an Ab initio perspective** - Leader Name: Michele Amato, Leader Institution: Université Paris-Sud
- » **Understanding the nature of the driving force of the phase transitions in switchable phenalenyl-base molecular materials** - Leader Name: Juan Jose Novoa Vide, Leader Institution: University of Barcelona

Physics and Engineering 2014 Projects

- » **3D Elastic Full Waveform Inversion: Toward Reflection Based Inversion** - Leader Name: Jean Kormann, Leader Institution: BSC-CNS
- » **Activation and conversion of CO2 through novel catalysts based on Au and Cu nanoparticles supported on molybdenum carbides** - Leader Name: Francesc Illas, Leader Institution: Universitat de Barcelona
- » **Approximating the Ground State of a Many-Particle Quantum System with Semi-Definite Relaxations** - Leader Name: Peter Wittek, Leader Institution: University of Boras
- » **Bridging the scales in biomolecular mechanics: membranes and coiled-coils** - Leader Name: Marino Arroyo Balaguer, Leader Institution: upc
- » **Development of the GPGPU generation of DNS codes.** - Leader Name: Javier JIMENEZ Sendin, Leader Institution: School of Aeronautics, Universidad Politecnica Madrid
- » **Diffusion Monte Carlo simulation of quantum gases and solids.** - Leader Name: Grigory E. Astrakharchik, Leader Institution: Departament de Física i Enginyeria Nuclear, Universitat Politècnica de Catalunya
- » **Direct Numerical Simulation of stabilised jet flames.** - Leader Name: Assensi Oliva, Leader Institution: Universitat Politècnica de Catalunya
- » **Direct numerical simulations of Taylor-Couette flow for the Princeton experimental setup.** - Leader Name: Francisco Marques Truyol, Leader Institution: UPC
- » **Disconnected contributions for the nucleon form factors from GPUs** - Leader Name: Alexandrou, Leader Institution: University of cyprus
- » **Electrostatic microinstabilities and zonal flows in stellarator plasmas.** - Leader Name: Edilberto Sánchez, Leader Institution: Laboratorio Nacional de Fusion-CIEMAT
- » **First-principles modelling of radiation-resistant materials: interfaces between immiscible and incoherent transition metals** - Leader Name: César González Pascual, Leader Institution: University of Oviedo
- » **High performance adaptive finite element methods for turbulent flow and fluid-structure interaction with applications in biomechanics, aerodynamics and aeroacoustics** - Leader Name: Johan Jansson, Leader Institution: Basque Center for Applied Mathematics (BCAM)
- » **High Performance Computing of the flow past a spinning cylinder. Application to flow control.** - Leader Name: Assensi Oliva, Leader Institution: Universitat Politècnica de Catalunya
- » **Implementation of new exchange correlation functionals and molecular dynamics calculations in Octopus** - Leader Name: Joseba Alberdi-Rodríguez, Leader Institution: Euskal Herriko Unibertsitatea UPV/EHU
- » **Improving the scalability of balancing substructuring domain decomposition methods for computational fusion** - Leader Name: Santiago Badia, Leader Institution: UPC & CIMNE
- » **Massively parallel Smoothed Particle Hydrodynamics scheme using GPU clusters.** - Leader Name: Ramon Gómez Gesteira, Leader Institution: Universidade de Vigo
- » **Mixing features of swirling flows in combustors** - Leader Name: Teresa Parra, Leader Institution: University of Valladolid
- » **Multi-physics coupled simulations: interaction of turbulence with radiation. Application to direct numerical simulation of turbulent Rayleigh-Bénard convection in a radiatively participating medium.** - Leader Name: Assensi Oliva, Leader Institution: Universitat Politècnica de Catalunya
- » **Optimal Control of Molecular Spectra in 1D Model Systems and 3D Molecular Systems** - Leader Name: Jessica Walkenhorst, Leader Institution: Universidad del Pais Vasco UPV/EHU

- » **Phase field modeling of biomembrane dynamics and crack propagation** - Leader Name: Marino Arroyo Balaguer, Leader Institution: upc
- » **Random Field Ising Model in four spatial dimensions and beyond** - Leader Name: Victor Martin Mayor, Leader Institution: Universidad Complutense de Madrid
- » **Self assembly in active suspensions** - Leader Name: Ignacio Pagonabarraga, Leader Institution: University of Barcelona
- » **Time-resolved evolution of vorticity and momentum cascades in statistically stationary homogeneous shear turbulence** - Leader Name: Javier JIMENEZ Sendin, Leader Institution: School of Aeronautics, Universidad Politecnica Madrid
- » **Time-resolved evolution of vorticity and momentum cascades in statistically stationary homogeneous shear turbulence** - Leader Name: Javier JIMENEZ Sendin, Leader Institution: School of Aeronautics, Universidad Politecnica Madrid
- » **Turbulent flow through a square duct: direct numerical simulation and advanced turbulence modeling** - Leader Name: Assensi Oliva, Leader Institution: Universitat Politècnica de Catalunya
- » **XUV/X-ray laser pulses for ultrafast electronic control in molecules** - Leader Name: Fernando Martin, Leader Institution: UAM

