



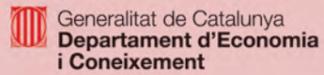
Barcelona Supercomputing Center ~ Red Española de Supercomputación

Jordi Girona, 31
Torre Girona Building
08034 Barcelona (Spain)
www.bsc.es

2013 Annual Report



BSC-CNS Patrons



BSC-CNS gratefully acknowledges the support of:



2013 Annual Report



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The 2013 Combined Annual Report of the Barcelona Supercomputing Center - Centro Nacional de Supercomputación (BSC-CNS) and the Spanish Supercomputing Network (RES) summarises the various support and research activities for the year and provides a short description of the two organisations.

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» 2013 Review



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

It is pleasing to report that 2013 was another year of growth and development for BSC-CNS, with the successful installation of a new world-class supercomputer, dramatically visible progress on the new building which will be the future headquarters of BSC-CNS, and excellent scientific results from all research departments, with increased project activity and industry collaborations across the board.

BSC-CNS has established its **international profile as a leader in both HPC research** and interaction with leading industry, as also evidenced by its ever-increasing capacity to attract international talent from around the world for both fundamental and applied research activities. During 2013, some 464 people performed research or provided support at the centre. Over 43% of staff are of foreign nationality, with over 48 countries represented including: Albania, Algeria, Argentina, Austria, Belgium, Bosnia, Brazil, Bulgaria, Canada, Colombia, Cuba, Chile, China, Denmark, Ecuador, Ethiopia, Finland, France, Germany, Greece, Holland, Hungary, India, Iran, Ireland, Italy, Japan, Lithuania, Mexico, Montenegro, Pakistan, Peru, Poland, Portugal, Romania, Russia, Serbia, Slovakia, Slovenia, Switzerland, Syria, Thailand, Turkey, Ukraine, United Kingdom, USA, Venezuela and Spain.

Mission

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



World Map of Countries of Origin

The work carried out by the scientists at BSC-CNS resulted in **over 146 journals, books and book chapter publications**, and some 150 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.

In 2013, **BSC-CNS participated in ninety-three projects**, with a total BSC-CNS grant of over 28 million euros. Fifty-one projects were funded by the extremely competitive Framework Seven Programme of the European Commission (FP7). Eight of these FP7 projects were led by BSC-CNS, in which the Centre coordinated a total of sixty partners based throughout Europe and Latin America. Two of these were projects for the international coordination of nationally funded research, and one was funded by the Artemis Joint Technology Initiative. Fourteen projects were funded by Spanish National or Catalan funds. Of the twenty-seven other projects, seventeen were research activities funded by private companies, five were funded by Spanish and international public bodies, including the UN, and three were funded by the European Space Agency (ESA). The centre also managed 59 personnel grants funded by ICREA, the Marie Curie programme, la Caixa, and CONACYT, among many others.

MareNostrum III, the main supercomputer at BSC-CNS, **was brought into full operation with 33,600 cores** on 2nd January 2013, following a shutdown for upgrade in the last part of 2012. A further upgrade was implemented in June (without requiring shutdown), giving a final configuration of 48,128 Intel Sandy Bridge cores and a total computing capability of 1,1 PFlops. 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.

A total of **268 activities were run on RES nodes** during 2013. This brings to more than 2.150 the number of different projects awarded time on the RES network since its establishment in 2006. Comple-

Broad Access

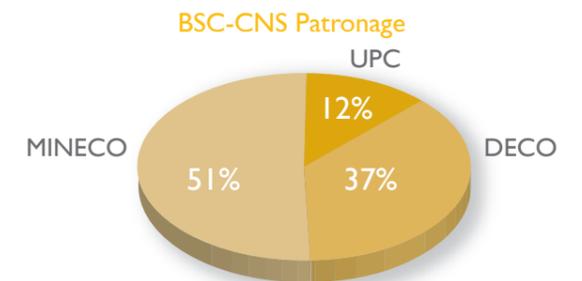
The powerful resources of the MareNostrum III Supercomputer and the RES nodes are accessed by a broad spectrum of Spanish and international scientists. 70% of MareNostrum III computing time is allocated to the international community via PRACE, while 24% is allocated to Spanish users by the Access Committee, composed of prestigious Spanish scientists external to BSC-CNS. The final 6% of computing time is reserved for BSC-CNS scientists and commercial projects to enable Spanish companies to maintain international competitiveness.

ting the series of RES node upgrades commenced in 2012, during 2013 MareNostrum increased its capacity to 1,1 PFLOP/s and Picasso achieved 63 TFLOP/s, thereby tripling the global computing capacity of the supercomputers participating in the RES network. Despite this dramatic increase in computing capacity, demand continues to exceed supply by a significant factor, with increasing numbers of scientists from increasingly diverse fields requesting access.

The **income of BSC-CNS in 2013 was €24 M**, of which 14 M corresponded to ordinary budget and strategic investments funded by the patrons of BSC-CNS, the Spanish and Catalan Governments (down from €21.5 M in the previous year, which was exceptionally high due to the MareNostrum upgrade); and €10.1M from competitive projects (up from €9.1 M in the previous year), one quarter of which was derived from projects with private companies.

Patrons of BSC-CNS

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



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 and NVIDIA), as well as major multinationals from other sectors, such as Repsol and Iberdrola. A total of 17 collaborative projects with industry were active in 2013, in addition to 15 national competitive R&D projects and 4 training projects. Of particular note, 2013 saw a significant increase in the number of European and international competitive R&D projects, up from 47 in 2012 to 61 in 2013.

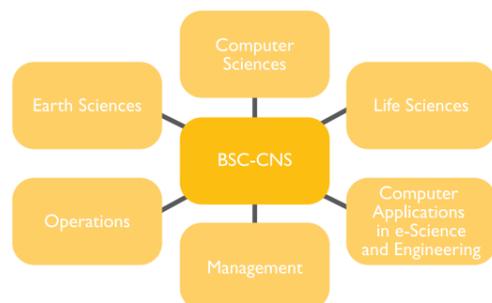
BSC-CNS is extremely proud to be one of the first centres in Spain awarded the Severo Ochoa distinction. The BSC-CNS Severo Ochoa program, which aims to design supercomputing hardware, software and applications targeted at solving significant social challenges in health and climate change, completed its second year in 2013, with a comprehensive progress report submitted to the Spanish Ministry of Economy and Innovation. All research lines are advancing well, and the recruitment, training and mobility actions facilitated by the grant have made a notable difference to BSC-CNS capabilities in fostering excellence and international talent attraction.



Support and Research

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

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



The 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.

BSC-CNS's commitment to PRACE and to **providing a distributed supercomputing infrastructure** for the best European researchers is perhaps the greatest demonstration of our international vocation. PRACE, together with the HPC Technology Platform, which designs the roadmap for HPC technology, as well as the future centres of excellence for HPC applications, will form the basis of the HPC ecosystem in Europe. BSC-CNS is well positioned in all of them.



The new BSC-CNS building advanced well during 2013, benefiting from the significant financial support from Repsol Foundation. The entire structure above ground was raised, including the roof and the

covered bridge that connects the main building with the Chapel that hosts MareNostrum III. This building will eventually house all BSC-CNS staff who are currently spread out amongst various sites in the UPC campus.

BSC-CNS is, and aims to continue being, a globally recognised centre of excellence in HPC related disciplines and this will mean even more international participation than ever. This is why BSC-CNS is already preparing more than 50 proposals for the Horizon 2020 Programme. It also means that BSC-CNS looks beyond Europe and tries to participate with excellent partners from all around the world, participating in the global Open MP consortium, being an active member of the worldwide Big Data and Extreme-scale Computing initiative, and collaborating closely with the best international IT companies including IBM, Intel, Microsoft, NVIDIA from the US and Samsung from Korea.

BSC-CNS is cooperating intensely with Latin America in various initiatives, and future opportunities are also being explored with China, Japan, Israel and Qatar. The Centre is well aware that the greatest challenges of today can only be tackled through international cooperation.

The **Computer Science Department** was extremely active across the full breadth of HPC fields and it continues to influence the future of computer architecture and systems through intensive collaborations with industry leaders, including Intel, NVIDIA, Microsoft, IBM, Samsung, Xilinx, and Qualcomm, amongst others. The Department also took prominent roles in key international and national HPC initiatives, with partners such as the European Space Agency (ESA), and the G8-ECS (Enabling Climate Simulations at Extreme Scale).

Particularly pleasing in 2013 was the further development of large-scale projects that require internal integration and collaboration between the various research groups within the Department, 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.

Earth Sciences continues to play an important role in global climate endeavours, hosting the Northern Africa-Middle East-Europe (NA-ME-E) Node of the SDS-WAS Regional Center, to deliver timely and quality sand and dust storm forecasts, and also hosting the first WMO CBS Regional Specialized Meteorological Center (RSMC-ASDF) which will build and maintain a web portal to provide forecast products, related information, verification results and services on the Internet. It also continues to develop and grow the number of regions in Spain covered by the Caliope air quality forecast system, as well as numerous other models relating to chemical transport, aerosols, mineral dust, and air quality, and their integration at mesoscale and with wave and other models.

During 2013 the **Life Sciences Department** participated in both national and international projects, of which highlights included PELE, an Advanced ERC grant to provide a fast and accurate tool for obtaining atomic detailed mechanisms of protein-ligand induced fit, International Cancer Genome Consortium for chronic lymphocytic leukaemia, and Trans-national Infrastructure for Plant Genomic Science to develop a trans-national infrastructure for plant genomic science. The Department is highly integrated with research groups at the IRB Barcelona, with the Joint Program continuing to function well and produce excellent results. Last year it also organised the "In silico Humans" scientific meeting, co-sponsored by PRACE, EESI and B-DEBATE, to debate the current state and future of human simulation.

The **CASE Department** expanded even further the range of applications to which its codes are applied, taking part in a dozen international and European projects and some half a dozen projects with industry. These include highly complex biomechanical simulations, such as airflows in the human respiratory system and the region around the face, and a complete electromechanical simulation of the heart. Industrial applications include fluid dynamics to improve yacht designs and wind farm placement, chemical reaction simulations to improve chemical reactors, and geophysical simulations to better map subsea oilfields. Social applications include simulating ancient societies to better understand human social behaviour, and improving the designs of interactive museums. The department is also working on Smart Cities, integrating urban data to capture the structures and processes that occur in urban environments; doing simulations and exploiting the publicly available data from social networks, so as to being able to alert to the presence of events, behaviour patterns, or emerging trends whose knowledge can improve the decision making processes.

The **Operations Department** of BSC-CNS not only successfully installs and operates some of Europe's most powerful supercomputers, but it also takes leading roles in key international platforms and projects that are defining the future of European HPC infrastructure, including PRACE, EESI2, EUDAT and RDA-Europe, amongst others, as well as overseeing the Spanish Supercomputing Network (RES), providing technical support and training to all seven nodes.

In summary, 2013 was a year that saw **BSC-CNS continue to thrive and grow**, managing both operational aspects, including the construction and installation of world-class HPC facilities and research activities, participating in an ever-increasing array of European and international projects, and further extending already deep collaborations with industry. Challenges remain, including the need to more actively engage local industry and entrepreneurial opportunities, and to maintain global competitiveness in the difficult climate of the ongoing economic crisis. However, with the truly outstanding efforts of BSC-CNS staff, students, and collaborators, and the continued strong support of its patrons, MINECO, DECO and UPC, and other key funding and support agencies such as the European Commission, Repsol, ICREA and the European Research Council, the future is bright. The Directors wish to extend their heartfelt gratitude to all BSC-CNS staff and friends, without whom none of these accomplishments would be possible.

Mateo Valero, Director

Francesc Subirada, Associate Director

Directors' Office



The Directors' Office is a new staff organization that comprises 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 program, the co-ordinators for European relations and Latin American relations, the Education and Training team, and the coordinator of Media Relations and Protocol.

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.

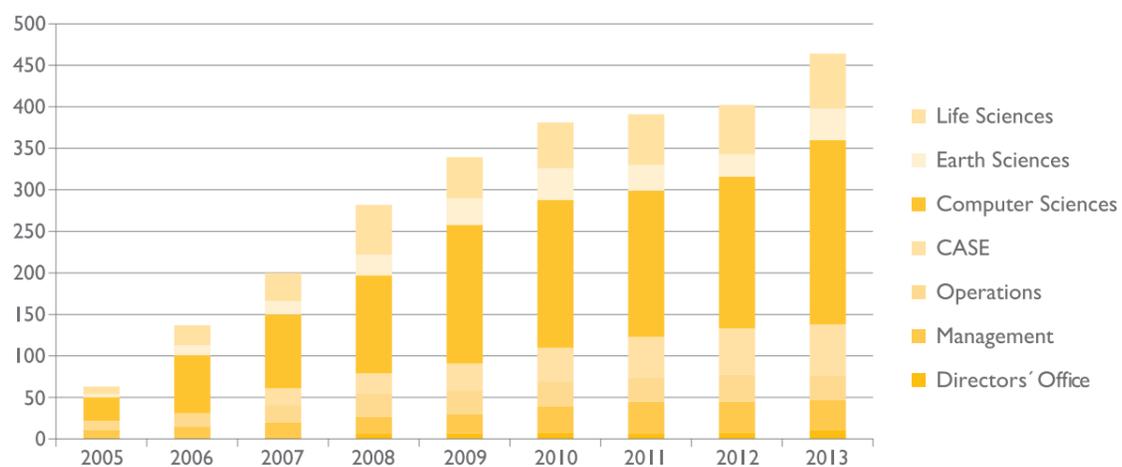
As at 31st December 2013, the core staff of BSC-CNS included 104 permanent positions, 158 dedicated to specific projects and 65 scholarship students. These numbers were significantly augmented by additional staff who participated in BSC-CNS via a number of programs.

Total personnel who worked at BSC-CNS throughout the year increased from 402 during 2012 to 464 during 2013, mainly through new temporary and shared staff, resident students, and collaborating and visiting researchers.

Shared Staff and Human Resource Programs

In addition to its own staff, BSC-CNS hosts shared staff from other public institutions such as the Universitat Politècnica de Catalunya • BarcelonaTech (UPC), the Institute for Research in Biomedicine (IRB) and the Consejo Superior de Investigaciones Científicas (CSIC). In 2013, BSC-CNS also welcomed high level scientific personnel from special human resources public programs such as the Ramón y Cajal Program, the ICREA Program and other personnel training research programs sponsored by various Spanish Ministries.

Annual BSC-CNS Staff and Collaborators



The BSC-CNS Fellowship Program

The BSC-CNS Fellowship program invites applicants from relevant scientific disciplines to participate in several European research projects and collaborations with international industry such as IBM and Microsoft. These fellowships are offered for periods of one year, renewable for the duration of the project. During 2013, BSC-CNS hosted 115 student researchers associated to 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 five ICREA professors during 2013.



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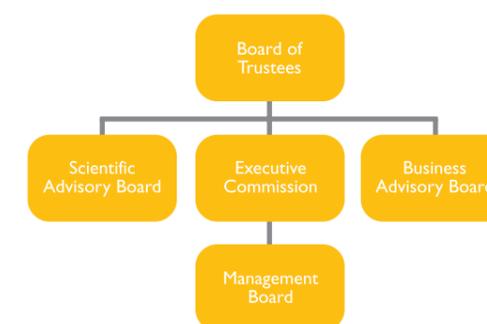
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Prof. Leonard Barrie, Vice-President of Research, The Cyprus Institute (Cyl)

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.



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Management Board Vice-Chairman

Francesc Subirada, Associate Director

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Eduard Ayguadé, Computer Sciences Associate Director

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Sergi Girona, Operations Director

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Joaquín Serrano, Ministerio de Ciencia e Innovación

Eduard Ayguadé, Barcelona Supercomputing Center-Centro Nacional de Supercomputación

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

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 Associate Researcher: Alejandro Pajuelo
 Associate Researcher: Emery Berger
 Associate Researcher: Kamil Kedzierski

Associate Researcher: Miquel Moretó
 HPC Visitor: Sascha Uhrig
 Visitor: Suzana Milutinovic

Performance Tools

Performance Tools Group Manager: Judit Giménez
 Senior Researcher: José Carlos Sancho
 Junior Developer: Eloy Martínez
 Junior Developer: Pedro Antonio González
 Postdoctoral Researcher: Claudia Andreina Rosas
 Postdoctoral Researcher: Vladimir Subotic
 Junior Researcher: Francesc Xavier Pegenaute
 Junior Researcher: Germán Llort
 Junior Researcher: Harald Servat
 Junior Researcher: Juan González
 Doctoral Student: Arturo San Emeterio
 Doctoral Student: Sergi Sisó
 HPC Visitor: Oleg Tsemaylo

Programming Models

Parallel Programming Models Group Manager: **Xavier Martorell**
 Senior Developer: Julián David Morillo
 Senior Researcher: Isaac Juan Rudomín
 Senior Researcher: Vicenç Beltran
 Junior Developer: Jorge Bellón
 Junior Developer: Marçal Solà
 Junior Developer: Víctor López
 Junior Researcher: Javier Teruel
 Junior Researcher: Roger Ferrer
 Doctoral Student: Ahimed Yazdanpanah Ahmadabadi
 Doctoral Student: Alejandro Fernández
 Doctoral Student: Antonio Filgueras
 Doctoral Student: Benjamin Hernández
 Doctoral Student: Diego Caballero
 Doctoral Student: Ettore Speziale
 Doctoral Student: Guray Ozen
 Doctoral Student: Jaume Pujantell
 Doctoral Student: Javier Bueno
 Doctoral Student: Lluc Álvarez
 Doctoral Student: Lluís Vilanova
 Doctoral Student: Michail Alvanos
 Doctoral Student: Rajiv Nishtala
 Doctoral Student: Sara Royuela
 Doctoral Student: Tassadaq Hussain
 Doctoral Student: Zeus Gómez
 Trainee Developer: Florentino Sainz
 Trainee Developer: Guillermo Miranda
 Trainee Developer: Sergi Mateo
 Associate Researcher: Gladys Utrera
 Associate Researcher: Juan José Costa
 Associate Researcher: Julita Corbalán
 Associate Researcher: Marc González
 Associate Researcher: Marisa Gil
 Associate Researcher: Montse Farreras
 HPC Visitor: Alessandro Cilaro
 HPC Visitor: Fisnik Kraja

BSC-CNS Staff and Collaborators during 2013

Visitor: Cyril Fournier
Visitor: Evan Alexander Johnson

Storage Systems

Storage Systems Group Manager: **Antonio Cortés**
Senior Researcher: Anna Queralt
Senior Researcher: Ramón Nou
Junior Researcher: Ernest Artiaga
Junior Researcher: Jonathan Martí
Junior Researcher: Paul Hermann
Doctoral Student: Alberto Miranda
Trainee Developer: Daniel Gasull
Visitor: Andrés Pardo
Visitor: Isak Nuhic

Unconventional Computer Architecture and Networks

ICREA Prof. and Unconventional Computer Architecture and Networks Group Manager: **Mario Nemirovsky**
Doctoral Student: Damián Roca
Visitor: Francesco Ciaccia

Earth Sciences Department

Earth Sciences Director: **Jose María Baldasano Recio**
Research Support Coordinator Technician: Kim Serradell
Research Support Technician: Albert Soret
Research Support Technician: David Carrió
Research Support Technician: Francesc Martínez
Research Support Technician: Miguel Castrillo
Visitor: Baris Ozdemir
Visitor: Ebru Celik
Visitor: Karahman Oguz
Visitor: Matías Méndez

Air Quality

Air Quality Group Manager: **Santiago Gassó**
Senior Researcher: Gustavo Arévalo
Postdoctoral Researcher: María Teresa Pay
Postdoctoral Researcher: Valentina Sicardi
Research Support Technician: Marc Guevara
Doctoral Student: Marina Ealo Alonso
Doctoral Student: Víctor Manuel Valverde
Visitor: Robert Banks

Atmospheric Modelling

Atmospheric Modelling Group Manager: **Oriol Jorba**
Senior Researcher: Georgios Markomanolis
Postdoctoral Researcher: Enza Di Tomaso
Doctoral Student: Alba Badía
Doctoral Student: Ángel Rincón
Doctoral Student: Michele Spada
Doctoral Student: Vincenzo Obiso
Visitor: Nick Shutgens
Visitor: Rocio Baro

Climate Change

Trainee Student: Lola Guerreiro

Associate Researcher: Maria Gonçalves
Visitor: Vicente Pastor

Meteorological Modelling

Meteorological Modelling Group Manager: **Oriol Jorba**

Mineral Dust

Postdoctoral Researcher: Sara Basart
Research Support Technician: Francesco Benincasa
Doctoral Student: Lluís Vendrell
Associate Researcher: Carlos Pérez
Associate Researcher: Enric Terradellas
HPC Visitor: Anna Pederzoli
HPC Visitor: Eduard Chemyakin
Visitor: Carla Gama

Life Sciences Department

Life Sciences Director: **Modesto Orozco**

Computational Genomics

ICREA Prof. and Computational Genomics Group Manager: **David Torrents**
Postdoctoral Researcher: Josep Maria
Postdoctoral Researcher: Lisa Olivia Andrieux
Research Support Technician: Ana Milovanovic
Research Support Technician: Friman Sánchez
Research Support Technician: Marco Paulo Seco
Doctoral Student: Laura Martínez
Doctoral Student: Leyden Fernández
Doctoral Student: Mercè Planas
Doctoral Student: Santiago González
Doctoral Student: Sílvia Bonás
Associate Researcher: Ana Rojas

Electronic and Atomic Protein Modelling

ICREA Prof. and Electronic and Atomic Protein Modelling Group Manager: **Victor Guallar**
Senior Researcher: Armin Madadkar Sobhani
Postdoctoral Researcher: Maria De Fatima Assunção
Postdoctoral Researcher: Martin Ivanov Kotev
Postdoctoral Researcher: Ryoji Takahashi
Postdoctoral Researcher: Suwipa Saen Oon
Research Support Technician: Daniel Lecina
Research Support Technician: Manuel Augusto Rivero
Research Support Technician: Pedro Riera
Research Support Technician: Xavier Oro
Doctoral Student: Emanuele Monza
Doctoral Student: Israel Cabeza De Vaca
Doctoral Student: Óscar Alejandro Esquivel
Doctoral Student: Sandra Acebes
Doctoral Student: Seyed Ali Hoseini
Doctoral Student: Víctor Gil
Visitor: Alba Rincón
Visitor: Ignacio Viciano
Visitor: James Valdés
Visitor: Marc Noguera

INB-Computational Node 2

INB - Computational Group Manager: **Josep Gelpí**
Research Support Technician: Anna Mantsoki
Research Support Technician: Dmitry Reptchevski
Research Support Technician: Laia Codó Tarraubella
Research Support Technician: Montserrat Puiggròs
Research Support Technician: Pau Andrio
Research Support Technician: Romina Royo
Research Support Technician: Stamatina Fragkogian
Research Support Technician: Valenti Moncunill

Molecular Modelling and Bioinformatics

Senior Researcher: Josep Ramón Goñi
Senior Researcher: Manuel Rueda
Postdoctoral Researcher: Robert Soliva
Research Support Technician: Carles Fenollosa
Research Support Technician: Jorge Cortés
Research Support Technician: Núria Villegas
Doctoral Student: Diana Camila Buitrago
Doctoral Student: Ricard Illa
Visitor: Ardita Shkurti
Visitor: Lucía Díaz
Visitor: Yabebal Ayalew

Protein Interactions and Docking

Protein Interactions and Docking Group Manager: **Juan Fernández**
Postdoctoral Researcher: Iain Moal
Postdoctoral Researcher: Santiago Esteban
Doctoral Student: Brian Jiménez
Doctoral Student: Chiara Pallara
Doctoral Student: Didier Barradas
Doctoral Student: Laura Pérez Cano
Doctoral Student: Miguel Romero
Associate Researcher: Solene Grosdidier
Visitor: Mark Agostino
Visitor: Massimo Simoniello
Visitor: Mireia Rosell
Visitor: Triki Dhoha

Computer Applications in Science & Engineering Department

Computer Applications in Science and Engineering Director: **José María Cela**
Senior Developer: Albert Farrés
Senior Developer: George Huhs
Senior Developer: Mónica Marrero
Senior Developer: Rogeli Grima
ICREA Prof. and Senior Researcher: Mervi Johanna
Senior Researcher: José De La Puente
Senior Researcher: Mauricio Hanzich
Senior Researcher: Volodymyr Puzyrov
CASE Director Assistant: Beatriz López
Junior Developer: Hadrien Calmet
Junior Developer: Luis Beltran
Junior Developer: Natalia Gutiérrez
Postdoctoral Researcher: Angel Coppola

Postdoctoral Researcher: Jean Antoine Kormann
Postdoctoral Researcher: Maria Cristina Marinescu
Postdoctoral Researcher: Xavier Rubio
Junior Researcher: Félix Rubio
Junior Researcher: Xavier Sáez
Associate Researcher: Carles Serrat
HPC Visitor: Alister Bates
HPC Visitor: Etienne Boileau

Environmental Simulations

Environmental Simulations Group Manager: **Arnau Folch**
Postdoctoral Researcher: Matías Óscar Ávila
Junior Researcher: Alejandro Martí
Junior Researcher: Raúl De La Cruz
Doctoral Student: Chiara Scaini
Visitor: Soledad Osoro

High Performance Computational Mechanics

High Performance Computational Mechanics Group Manager: **Mariano Vázquez**
Senior Developer: Antoni Artigues
Postdoctoral Researcher: Alberto Gambaruto
Postdoctoral Researcher: Daniel Mira
Postdoctoral Researcher: Fernando Martín Cucchiatti
Postdoctoral Researcher: Jazmín Aguado
Junior researcher: Miguel Zavala
Visualisation Technician: Guillermo Marín
Doctoral Student: Alexis Torrano
Doctoral Student: Edgar Olivares
Doctoral Student: Juan Carlos Cajas
Doctoral Student: Margarida Moragues
Doctoral Student: Ruth Aris
HPC Visitor: Esteban Ferrer
HPC Visitor: Peter Wittek
Visitor: Alice Elisabeth Rosam

Physical and Numerical Modelling

Physical and Numerical Modelling Group Manager: **Guillaume Houzeaux**
Junior Developer: Genís Aguilar
Junior Developer: Juan Esteban Rodríguez
Junior Developer: Miguel Ferrer
Junior Developer: Mohammad Jowkar
Postdoctoral Researcher: Eva Casoni
Junior Researcher: Tano Varadinov Ognyanov
Doctoral Student: Augusto Samaniego
Doctoral Student: Beatriz Eguzkitza
Doctoral Student: Jelena Koldan
Doctoral Student: Óscar Francisco Peredo
Doctoral Student: Vincent Boyer
HPC Visitor: Benjamín Uekermann
Visitor: Djallel Zebbar
Visitor: Romain Aubry
Visitor: Ruslan Gabbasov

Smarter City Initiative

Associate Researcher: Jorge García

BSC-CNS Staff and Collaborators during 2013

Operations Department

Operations Director: **Sergi Girona**
 Operations Director Assistant: Núria Saavedra
 Facility Management Consultant Operations: Ramón Pallisa
 RES Technical Support: Montserrat González

Facility Management

Facility Management Group Manager: **Ahmet Emin Senata**
 Maintenance Technician: Albert Riera
 Maintenance Technician: Miguel Armenta

System Administration

Systems Group Manager: **Javier Bartolomé**
 Helpdesk Technician: Antonio Espinar
 Helpdesk Technician: Ferran Sellés
 Helpdesk Technician: Pedro Gómez
 Network Technician: Albert Benet
 Performance Technician: Alejandro Lucero
 Performance Technician: Carles Fenoy
 System Administration: Anibal Moreno
 System Administration: David Ocaña
 System Administration: Gabriele Carteni
 System Administration: Jordi Valls
 System Administration: Sergi Moré
 Visitor: Alejandro Flores
 Visitor: Daniel Ortiz

User Support

Support Applications Consultant: Christian Simarro
 Support Applications Consultant: Jorge Rodríguez
 Support Applications Consultant: Pablo Ródenas
 User Support Group Manager: David Vicente
 Visualisation Technician: Carlos Tripiàna
 Web Graphical Designer: Jasmina Tomic
 Web Graphical Designer: Laura Bermúdez
 Webmaster: Silvina Rusinek
 First Level Support: Miguel Bernabeu

Management Department

Management Director: **Ernest Quingles**

Business Administration

Administration, Finances and Human Resources Group
 Manager: **Mercè Calvet**
 Information System Developer: Toni Matas

Administration and Purchasing

General Assistant: Laura Gutiérrez
 General Assistant: Núria Sirvent
 Purchasing Officer: Cristina Vargas
 Purchasing Officer: Neus Jiménez
 Administration Trainee Student: Aurora Rodríguez

Finance and Accounting

Accounting Manager: **M^a Cristina Calonge**
 Support Accounting Technician Alba Delclòs
 Support Accounting Technician: Irene Belda
 Support Accounting Technician: Judit Soldevila
 Technical Support for Economic Management Project: Laia Traveset
 Technical Support for Economic Management Project: Laura Viñas

Human Resources

HR Technician: Anna Martín
 HR Technician: Lara Cejudo
 HR Trainee Student: Carla Santamaría

Education and Training

HPC Professional Training: Evguenia Stoilova Alexandrova

Project Management and Communication

Project Management Office & Communication Group Manager:

Eugene Griffiths

Projects and Technology Transfer

Prace Project Manager: **Carlos David Mérida**
 Project Manager: Francesca Arcara
 Project Manager: Gina Michelle Alioto
 Project Manager: Guadalupe Moreno
 Project Manager: Javier Salazar
 Project Manager: Marta Rosselló
 Project Manager: Oriol Pineda
 Project Manager: Pilar Callau
 Business Analyst: Marcin Ostasz
 Visitor: Diego Rudomín

Communication

Communications Officer: Cristina Jiménez
 Communications Officer: María José Barroso
 Communications Officer: Núria Masdó
 Communications Officer: Sara Ibáñez
 Dissemination Project Officer: Nagham Salman
 Marketing Officer: Renata Giménez
 Marenostrium Visits Manager: Oriol Riu

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

» **Activities** • There is a long standing tradition of BSC-CNS leadership at national and European levels providing excellent training and professional skills development for researchers and industry. BSC-CNS has also been closely involved with postgraduate studies in the broad area of HPC ecosystems and application areas through its collaborations with local universities, UPC and UB.

Training Courses • As the PRACE Advanced Training Centre (PATC), BSC-CNS delivered 10 courses in the 2012-2013 academic year and designed a further 2 new courses based on the PRACE curriculum, which will be delivered in the 2013-2014 academic year. By organising the training events at a postgraduate level of comprehension, and marketing them across diverse communities, BSC-CNS has 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 have been very highly rated by the attendees, placing BSC-CNS in a leading position among the other centres in Europe. BSC-CNS has a long history of leadership in developing Latin American (LA) HPC capacity through various projects and initiatives. In 2013, under several projects and using the PATC curricula, BSC-CNS lecturers and researchers delivered eight courses in several countries across the continent – Peru, Brazil, Colombia and Mexico. Since 2011 some 986 trainees have participated in BSC-CNS led courses in Latin America.

Fostering Collaboration with Universities • The relationship with UPC, and in particular with the Barcelona School of Informatics, was further developed through the extensive PATC program offered to students at Master and PhD levels, and particularly to those enrolled in the MIRI MSc course who can take them as credited seminars. BSC-CNS was closely involved in the design and delivery of the HPC Stream of the MIRI Master program, and from the Autumn of 2013 is offering MSc Scholarships under the BSC-CNS Severo Ochoa project. The first four students holding the scholarship started their studies in the HPC stream in September 2013.

Summer Schools • PUMPS Summer School, which held its fourth edition in 2013, is 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. It is organised and delivered by the specialists from the CUDA Center of Excellence awarded by NVIDIA to BSC-CNS in association with UPC. “Distributed Multi-scale Computing” - the second MAPPER seasonal school co-organised by BSC-CNS was another opportunity to gather young scientists from EU countries in a pre- ICCS 2013 conference event with the objective to train the participants to use MAPPER tools, services, and methodologies developed for distributed multi-scale computing in various application areas. The school addressed e-scientists from all disciplines.

The Severo Ochoa Research Seminar which started in the spring of 2013 is organised by the Education and Training Team to provide state-of-the-art information through a series of lectures given by researchers on current projects. It is also used as a platform for visiting researchers to introduce their work. Its aim is to encourage cross-disciplinary collaboration. These series run in parallel with the departmental subject specific seminars and attract audiences from across the BSC-CNS departments and PhD programs, and are run with an open-doors policy, inviting participation of interested researchers from RES and UPC.

» **Involvement in Key Projects** • In 2013 the team was engaged in: PRACE 2IP and 3IP project with WP4 Training and PATC OMB; Severo Ochoa project with the Training and Mobility Work Package; ESSI project, RISC (A Network for Supporting the Coordination of Supercomputing Research Between Europe and Latin America), EU Brazil OpenBio project.

Conferences, Presentations and Papers

- ▶ In January 2013 the book : “Technological Advances in Interactive Collaborative Learning”, edited by Nia Alexandrov, Raul Ramirez, and Vassil Alexandrov, was published by Taylor and Francis (ISBN-9781466502086).
- ▶ The Education and Training team was involved in the organization of the International Conference on Computational Science in Barcelona in June 2013.
- ▶ Nia Alexandrov gave the talk “Measuring Business Value of Learning Technology Implementation in Higher Education Setting” at the Workshop on Teaching Computational Science (WTCS) 2013 at the ICCS 2013, Barcelona.
- ▶ Nia Alexandrov gave the talk “The Significance of Stochastic Methods as Part of Postgraduate Research Skills Teaching” at the Ninth IMACS Seminar on Monte Carlo Methods, Annecy, France in July 2013.
- ▶ Vassil Alexandrov presented the keynote talk “Technological Advances in Interactive Collaborative Learning” at the International Conference on Interactive Collaborative Learning, 25-27 September 2013, Kazan, Russia.
- ▶ Jesús Labarta, Eduard Ayguadé, Álex Ramírez, and Rosa M. Badia delivered a tutorial with practical training session on “Asynchronous Hybrid and Heterogeneous Parallel Programming with MPI/OmpSs and its Impact in Energy Efficient Architectures for Exascale Systems” at the SC13, 16 - 22 November, Denver, USA.

The financial accounts for 2013 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 2013 was composed of ordinary income derived from contributions by its patrons, as well as project income derived from competitive funding sources and agreements reached with private organisations. This income was then employed to cover expenses, including costs of operations and fulfilment of all financial obligations.

» Income

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

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

Other Income includes strategic investments, overheads and capital transfers.

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

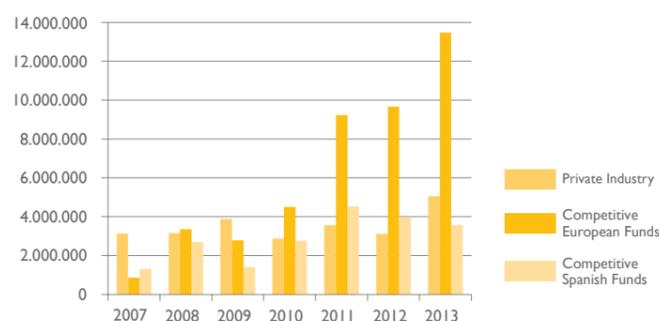
Overheads are incomes derived from ordinary projects, which according to the norms of BSC-CNS are charged 10% to cover overhead expenses.

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

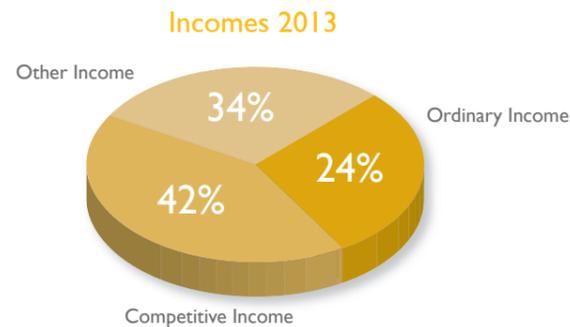
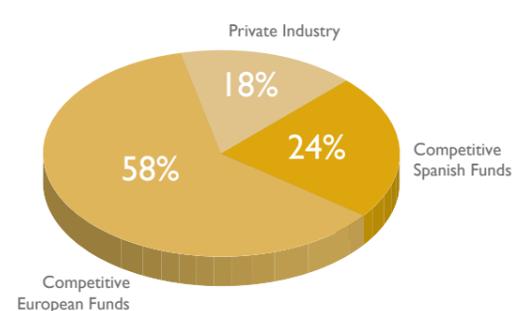
» Breakdown of Competitive Income

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

Competitive Income Evolution



Competitive Funding 2013



INCOMES 2013	AMOUNT €
Ordinary Income	5.694.144,33
Ministerio de Economía y Competitividad	4.288.320,00
Generalitat de Catalunya	1.405.824,33
Competitive Income	10.082.032,15
Ministerio de Economía y Competitividad	1.724.168,49
Generalitat de Catalunya	169.516,69
European Commission	5.698.858,74
Private Companies	2.489.488,23
Other Income	8.250.502,77
Applied Previous Reserves	6.368.657,10
Strategic Investment	290.924,00
Overheads/Capital transfers	1.590.921,67
TOTAL INCOME	24.026.679,25

» Expenses

EXPENSES	AMOUNT €		
	Ordinary Budget	Projects Budget	Total
Personnel	4.341.437	6.691.966	11.033.403
Investments	5.940.511	437.277	6.377.788
Current Expenses	3.286.959	3.328.530	6.615.489
TOTAL EXPENSES	13.568.906	10.457.773	24.026.679

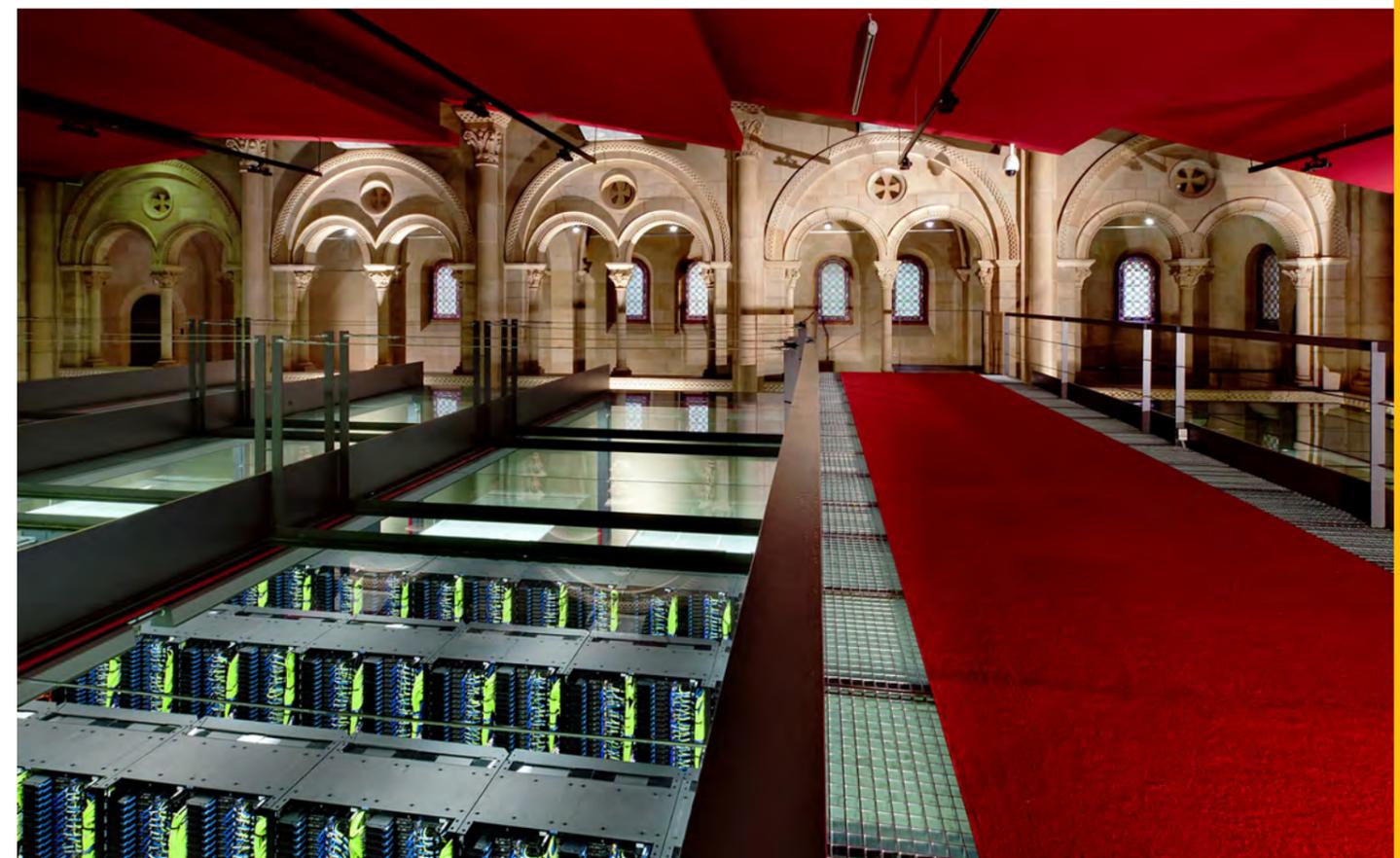
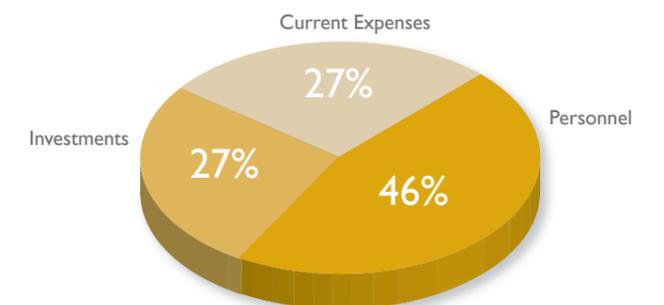
Personnel refers to salaries and associated charges directly related to the employment of staff contracted by BSC-CNS. It does not include salaries and associated charges of visitors or other collaborators who continued to be paid via their originating institution.

Investments include 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.

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 10 public tender contracts were signed during the year.

Expenses 2013



» BSC-CNS - Center of Excellence Severo Ochoa



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

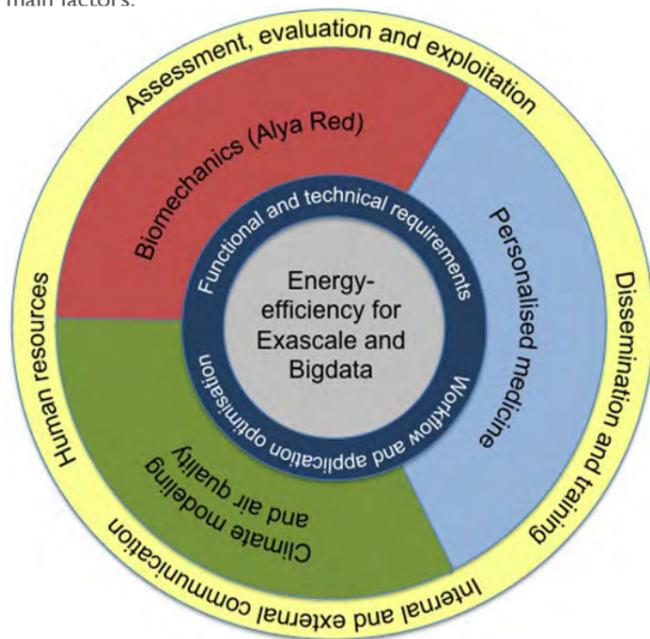
BSC-CNS received the “Severo Ochoa Centres of Excellence” support and accreditation in the 2011 call, a programme of the Secretary of State for Research, Development and Innovation of the Ministry of Economy and Competitiveness that aims to promote excellence in scientific research in Spain. The award confirmed BSC-CNS’s reputation as one of the world’s leading centres applying and doing research on supercomputing technologies. The program commenced in January 2012 with an ambitious research program: 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 program also plans to consolidate best practices in support services, based on the recognition that efficient management of human resources, training and communication are key elements for promoting outstanding results in research.

» The BSC-CNS Severo Ochoa Project

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



The image on the left summarizes the BSC-CNS Severo Ochoa program, which is made up of four main scientific sub-projects: the proposal and development of novel models in three application domains which rotate around novel components in the hardware and software stacks to achieve the Exascale and Big Data. In the following paragraphs the three applications and achievements during 2013 are described.

► **Personalised medicine** (Life Sciences Department): In the Severo Ochoa project the combination of genomics, proteomics and transcriptomics analysis with computer simulation is explored to create models capable of predicting certain diseases or the effects of drugs on patients before a pathology starts. During 2013 the following aspects were addressed: 1) Cancer genomics: collection of genomes from Leukaemia patients, the participation in the International Pan-Cancer consortium and the development of a new

strategy to predict cancer somatic mutations; 2) Genetic markers: participation and leading of important studies for Asthma, Diabetes type 2 and autoimmune diseases; the portability of GWAS tools to COMPSs and the design new predictive strategies were completed. 3) Personalised drug discovery: a Chemoinformatics server and the PELE web server for the study of personalised drug-targets (for example HIV-1) were completed; collaborations with CASE and Computer Sciences departments in order to improve the usability of tools and to deal with the large amount of data produced. 4) Protein networks: new tools for protein-protein interaction study were produced and their use to predict the effects of genetic mutants in protein networks was studied.

- **Multi-scale air quality climate modelling** (Earth Sciences Department): In the Severo Ochoa project a high-resolution modelling system for short- and long-term applications is being developed, 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. During 2013, the system was improved with the implementation of a secondary aerosol module (in collaboration with the University of California Irvine) and the coupling of data assimilation capabilities using the technique of Local Ensemble Transform Kalman Filter (in collaboration with the University of Oxford). In collaboration with the Computer Sciences Department, the computational performance of the model was studied with Extrae and Paraver tools, figuring out which functions are degrading performance and identifying a generic issue with the I/O. Additionally, the use of COMPSs has sped-up the pre-process of the system and further implementations are envisaged.
- **Computational biomechanics-Alya Red** (Computer Applications in Science and Engineering Department): In the Severo Ochoa program a new Cardiac Computational Model (CCM) is going to be developed, through the implementation and validation of various advanced physiological models. During 2013 the CCM was improved with new cell models which enable the use of Alya to simulate anti-arrhythmia drug tests. Additionally, other aspects of the cardiovascular system, such as the rupture risk in cerebral aneurysms, were studied.
- **Novel components in the hardware and software stacks to achieve the Exascale and Big Data** (Computer Sciences Department). During 2013 the Computer Sciences Department focussed on implementing first prototypes of novel technologies to facilitate the implementation of the applications including:
 - 1) the adaptation of the BSC-CNS’s programming models COMPSs/OmpSs for the data demands of workflow applications and energy-efficiency of the target architectures;
 - 2) design of methodologies and technologies to support data organisation in key/value non-relational databases;
 - 3) proposal of Self-Contained Objects (SCO), 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 architectures.

The four scientific sub-projects benefit from the support provided by three additional support sub-projects: a clear Human Resources policy, efficient management and well-structured communications and training activities. During the first year of the program, BSC-CNS designed an Education and Training Strategy, including the BSC-CNS PRACE Advanced Training Centre and the Severo Ochoa mobility programme which will include financial help for incoming and outgoing short stays.

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

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



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



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



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

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

During 2013, more than 400 IT and senior executives from over 250 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 20 sectorial visits were organised. Some of the industrial sectors covered were: aeronautics, automotive, telecommunications, robotics, pharma, logistics, textile, and governmental IT related organisations.

The existing collaborative R&D program agreements that BSC-CNS has with Repsol, Microsoft, Intel, IBM and Nvidia were extremely active, with significant progress and successful results obtained in multiple projects. During 2013 a new program agreement was signed with Samsung, as well as other specific projects with different companies. All of them are described in the following list;

» IBM-BSC Research Collaboration



During 2013, the collaboration with IBM focused on four main directions: 1) Workload management of data analytics workloads composed of a set of MapReduce jobs running on top of a NoSQL back-end and transactional workloads producing data to be dumped to the NoSQL back-end; 2) High performance architectures for Big Data with particular attention to the IBM BlueGene Active Storage (BGAS) architecture and the Parallel In-Memory Database (PIMD) as the key/value store; 3) Power modeling for the IBM POWER7 processor; and 4) Software-driven resource allocation and adaptive data prefetching techniques in PowerPC processors. A new 3-year collaboration framework was defined during 2013 with the aim of starting new joint research agreements during 2014.

» 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 2013 the collaboration mainly focussed on fault tolerance transparently managed by highly scalable parallel run-time systems (OmpSs) and on performance analysis and prediction for HPC code targeting these future exascale systems. In addition, the research on transparent support for heterogeneity in the OmpSs programming model, dynamic load balancing (DLB) in hybrid MPI/OmpSs applications and tools to predict the potential parallelism in sequential applications (Tareador) has continued during 2013.

» Microsoft-BSC Research Centre



The BSC-Microsoft Research Centre (BSCMSRC) continued research activities on transactional memory (TM), including efficient compiler and runtime support for new best-effort hardware transactional memory implementations such as Intel Haswell, the Atomic Dataflow Model combining TM and dataflow including formal verification of the model, and TM support for reliability. During 2013 the Center started a new line of research aiming to study the performance characteristics of MapReduce deployments, to provide deep understanding of what software and hardware parameters affect the throughput of Hadoop-based workloads and how they can be tuned properly, and TLB characterization of big data workloads. Finally, the Center continued exploring the suitability of low-power vector processors for mobile and data intensive workloads, including the design of their Instruction Set Architecture (ISA), including low-power vector ALU design, and new vector architectures with configurable interconnect.

» 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 BSC's broad-based research success in leveraging the NVIDIA CUDA technology and GPU computing. As part of the CCoE training, during 2013 several courses were offered in graduate and master programs at UPC, as part of the PRACE Advanced Training Center (PATC), the Spanish Supercomputing Network (RES) and the Red Iberoamericana de Supercomputación (RISC) activities. Besides them, a well renowned success has been the Programming and Tuning Massively Parallel Systems (PUMPS) Summer School held in Barcelona since 2010. During 2013 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) Leveraging CUDA for productive programming using OmpSs; 3) Optimization of applications in different domains in conjunction with the CASE, Life and Earth sciences departments; 4) Facial recognition and security video surveillance with the UPC start-up company HERTA Security; 5) The development of software infrastructures to ease the development on multi-GPU systems, and mechanisms and policies for scheduling multiprogrammed workloads.

» SAMSUNG Collaboration



The collaboration agreement between BSC and Samsung started during 2013 in the context of memory technologies for HPC systems. On one side, the collaboration focusses on analyzing how production HPC applications exercise the current DRAM memory system and evaluating the frequency and locality of memory errors in exiting DDR3 technologies. On the other side, the collaboration pursues the proposal of new architectures and management algorithms to exploit the upcoming non-volatile STT-MRAM memory technologies in HPC systems.

» Fundación Botín



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

» Repsol-BSC Research Center



The Center is undertaking various research projects to develop advanced technologies applicable to the exploration of hydrocarbons and other areas of interest to Repsol, such as modelling of subterranean and subsea reserves, fluid flows, etc. The establishment of the Center is the result of many years of successful collaboration between BSC-CNS and Repsol, a highlight of which was the now commercialised Kaleidoscope project which developed algorithms that enable Repsol to process subterranean seismic images up to 15 times faster than its competitors, and was voted one of the five most innovative projects in the global energy sector. During 2012, the Repsol-BSC Research Center was involved in the following research topics:

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

» Iberdrola-BSC Research Collaboration



BSC-CNS and Iberdrola Renovables are collaborating to design mathematical models to improve the design of Iberdrola's wind farms. Led by the CASE Department, the project tackles the extremely challenging simulations of wind farms. The main objective is to significantly increase the efficiency and power of wind farms by developing numerical techniques to optimise placement of wind turbines.

» Xilinx-BSC Research Collaboration



During 2013 the joint collaboration with Xilinx focussed on the development of FPGA support in the OmpSs programming model (both Mercurium and Nanos++). Currently the infrastructure generates both the ARM binary and the FPGA bitstreams necessary to run the application in systems with multiple FPGA accelerators. An improved task management mechanism that allows fast task dispatching when several independent tasks are executed has been implemented in the Nanos++ runtime. Several Zynq boards and licenses of state-of-the-art Xilinx tools have been donated through the Xilinx University Program to the BSC-CNS.

» European Space Agency



In 2013 the collaboration with the European Space Agency (ESA) has been structured around two projects: 1) 'Architectural solutions for the timing predictability of next-generation multi-core processors', with the objective of enabling the Worst Case Execution Time analysis of time-critical space applications in a multi-core execution environment (such as the New Generation Multi-Core Processor NGMP); and 2) 'Multicore OS Benchmark', with the objective of evaluating the time-predictability behavior of multicore processor and task scheduling.

» Other Industry and Institutional Collaborations

In addition to the major collaborations detailed above, BSC-CNS has signed a new contract with the company Anaxomics Biotech S.L. with the objective of transferring technology related to the design and optimisation of industrial enzymes. Also, a new contract has been signed with the company Cetemmsa to work on the simulation of the printing process of bio-inks to reduce time and costs of real experiments. Beyond its relationships with private industry, BSC-CNS works with public agencies on a range of applied projects. During 2013, BSC-CNS collaborated with over 100 private companies both within Spain and internationally, either in direct R&D collaborations or via European or nationally sponsored project consortia.

1.7 PRACE: Supercomputing Infrastructure for Europe



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;

- ▶ **WMO SDS-WAS:** to coordinate together with AEMET a Regional Center in Barcelona for Northern Africa, Middle East and Europe in Barcelona. Also the WMO Barcelona Dust Forecast Center was approved by the Executive Council of WMO in May 2013.



- ▶ **AEMET (The State Meteorological Agency):** to implement, disseminate and validate the operational prediction of the North African dust transport in the Iberian Peninsula as well as to perform modelling, detection, follow-up and characterisation studies of atmospheric material.



- ▶ **Environment and Water Agency of Andalusia:** to provide the Andalusia Government with an operational air quality forecasting and assessment service, which will allow the simulations of photochemical and particulate matter pollution with high spatial and temporal resolution for Andalusia: 1 km² and 1 hour.



- ▶ **International Research Institute for Climate and Society:** to enable cooperative efforts between the IRI and BSC-CNS in areas connecting climate, atmospheric aerosols and health.



- ▶ **National Oceanic and Atmospheric Administration - National Centers for Environmental Predictions and Environmental Modeling Center:** to develop a new chemical weather prediction system and chemical transport model intended to be a powerful tool for research and to provide experimental efficient global and regional chemical weather forecast.



- ▶ **Spanish Ministry of the Environment:** to develop and implement an operational high-resolution air quality forecasting system for Spain, providing end-users with an air quality forecasting and assessment service for Spain and Europe with higher detail for some hot spot areas.



- ▶ **Government of the Canary Islands:** to develop an information system for air quality forecast and surveillance of the Canary Islands.



PRACE - Partnership for Advanced Computing in Europe

» Background

The Partnership for Advanced Computing in Europe (PRACE) is a pan-European Research Infrastructure for High Performance Computing (HPC) and forms the top level of the European HPC ecosystem. The infrastructure consists of several tier-0 supercomputers (including one at BSC-CNS) distributed across 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, European scientists and technologists in the 25 member countries are being provided with world-class supercomputers with capabilities comparable to those available in the USA and Japan. These leadership class systems will help the continent's scientists and engineers to remain internationally competitive. During 2013, the 5th Call for Project Access served as the test-platform for an entirely new form of access to Europe's top-level systems: PRACE Multi-Year Access. A limited group of 7 outstanding projects from academia and industry were awarded more than 175 million core hours for the first year of their research program, while an additional 175 million core hours were reserved for their second year.

» BSC-CNS and PRACE



BSC-CNS played a key role in the creation of the PRACE Research Infrastructure at all levels, with Sergi Girona serving as Chairman of the Board of Directors, significant technical contributions, and leadership of the organisational design. This included the selection of the best legal form, design of the governance structure, funding and usage models, and the peer review process, resulting in the PRACE statutes and initial agreement which were signed in May 2010. 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. 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. For the second year in a row, in 2013, BSC-CNS PATC courses were rated 8 or above (out of 10) in overall performance by course participants, placing BSC-CNS amongst the best performing PATC centres. Three EC funded projects supporting the Implementation of the PRACE Research Infrastructure were running in parallel during 2013, all with a significant level of involvement of BSC-CNS. Within the 1st Implementation Project, BSC-CNS worked on the application scaling for capability science projects on the Intel MIC architecture available on MareNostrum, amongst other tasks. 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 the research on best practice for HPC system commissioning and novel programming techniques. Finally, within the 3rd Implementation Project, BSC-CNS continued many of the PRACE IIP activities including research on organisational aspects and the development of an impact assessment framework.

» Spanish participation in PRACE • Spanish scientists were very successful in participating in important research projects that won computing time on the various PRACE nodes. Some of the projects are:

- ▶ Time-resolved evolution of vorticity and momentum cascades in statistically stationary homogeneous shear turbulence, Prof. Javier Jimenez Sendin (UPM), 20 million hours on JUQUEEN
- ▶ Longitudinal and Transverse Electronic Transport in Atomically Doped Graphene from First Principles, Prof. Stephan Roche (ICN2), 22 million hours on CURIE
- ▶ Molecular crowding effect on protein landscape, Prof. Modesto Orozco (IRB), 33 million hours on MareNostrum
- ▶ LATTQCDNf3 - Chiral properties of Lattice QCD with three dynamical quark flavours, with the participation of IFIC (CSIC) and UAM, 70 million hours on FERMI
- ▶ ContQCD - The continuum limit of QCD with up, down and strange quarks, with the participation of IFIC (CSIC), 40 million hours on SuperMUC
- ▶ HiResClim: High Resolution Ensemble Climate Modeling, Prof. Francisco Doblas-Reyes (IC3), 50 Million hours on MareNostrum
- ▶ The optical absorption spectra of a real Light Harvesting Complex from first-principles: the spinach case, Prof. Angel Rubio (ETSF), 21 million hours on MareNostrum

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

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



Artist's impression of the New BSC-CNS Building



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

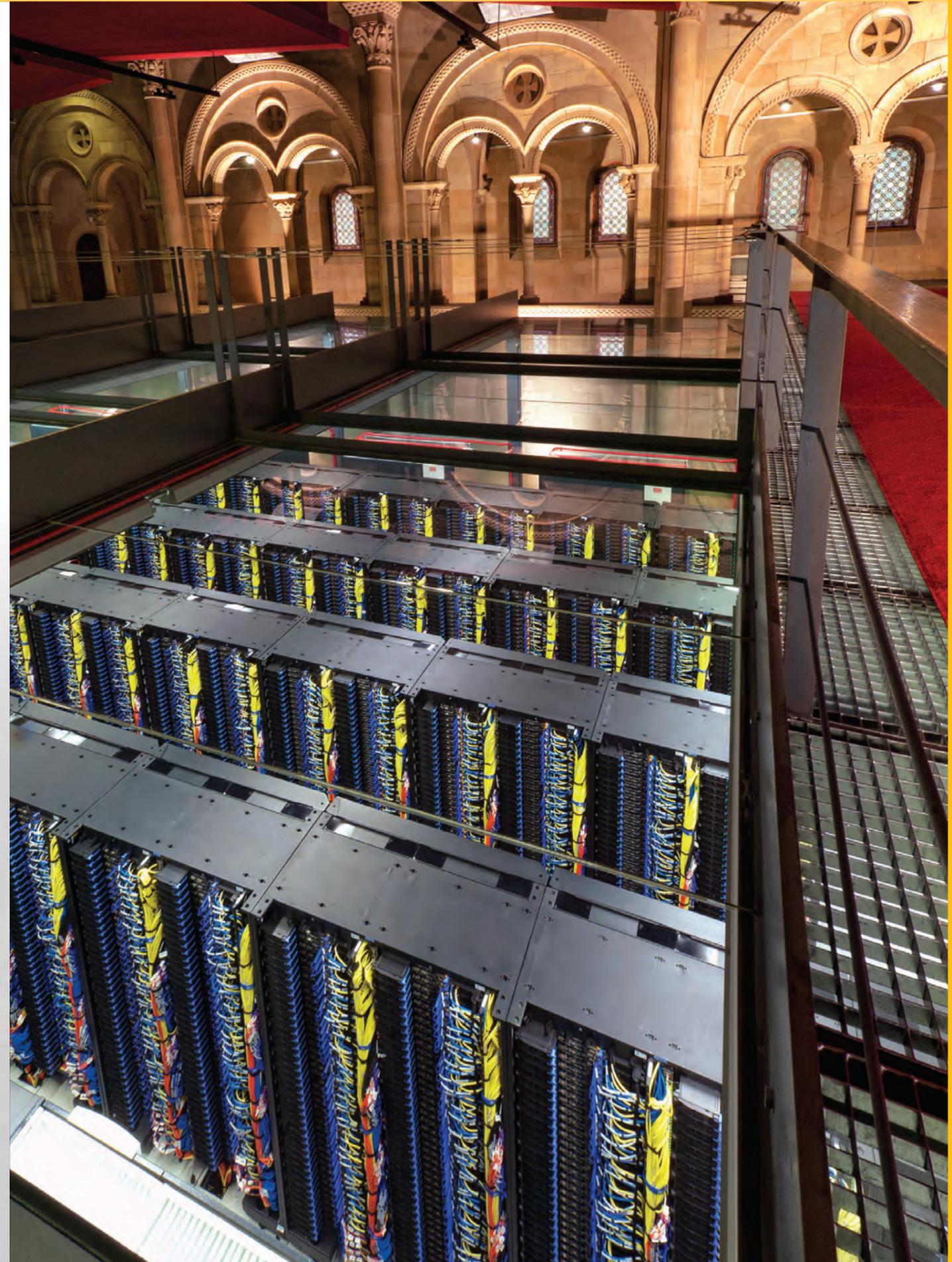
Following the granting of the tender for Phase 2 of the building construction to the company Dragados S.A. in December 2012, construction of this phase began in May 2013, and was completed in December 2013.

In this phase, the entire structure above ground was raised, including the roof and the covered bridge that, resembling a hanging tunnel, connects the main building with the Chapel that hosts MareNostrum III.

Additional minor works such as covering the car park level with concrete were also performed.

A new tender for the next stage, to finish the building's facade and the primary closings of the underground levels, will be launched in early 2014 such as water recycling, automatic illumination to maximise use of natural light, and natural cooling to achieve a B-level energy efficiency rating.

Images showing construction of Phase 2 of the New BSC-CNS Building



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



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

» Overview

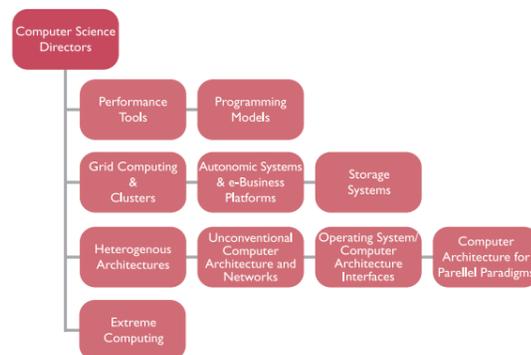
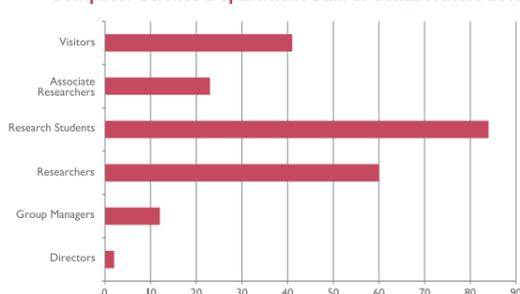
The Computer Sciences Department, led by Jesús Labarta and Eduard Ayguadé, is structured in 10 research groups. Although each group has its own specialised lines of research, the teams often come together to collaborate on projects that require vertical integration, such as the Exascale EU projects Mont-Blanc/Mont-Blanc2 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.

» Unique Strength

The combination of broad coverage of all facets of computer systems design and programming, along with in-depth expertise in each area, are somewhat unique amongst supercomputing centres. This unique strength of the Computer Sciences Department has attracted leading computing companies to invest during 2013 in collaborative systems design R&D projects.

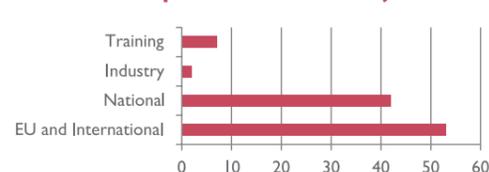
» Organisational Structure

Computer Science Department Staff & Collaborators 2013



During 2013, some 153 staff and students, and a further 69 associated or visiting researchers, worked within the Department, organised in 10 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), 2 focused on improving productivity when programming and optimising parallel applications on large scale parallel systems (Programming Models and Performance Tools), 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).

Computer Sciences Projects 2013



» Key Projects and Networks

During 2013, the Computer Sciences Department participated in the following:

EU projects:

- ▶ 30 FP7 projects: ASCETIC, AXLE, COMPOSE, DEEP, DEEP-ER, EnCORE, EUBrazil CloudConnect, EUBrazil OpenBio, EuroServer, HOPSA-EU, Human Brain Project HBP, IOLanes, Lightness, Mont-Blanc, Mont-Blanc2, OPTIMIS, ParaDIME, parMERASA, PROARTIS, PROXIMA, P-Socrates, Re-NewIT, RETHINK Big, RoMoL ERC, ScalaLife, SECURED, TERAFLUX, TEXT, TransPLANT and ARTEMIS VeTeSS;

- ▶ RoMoL (Riding on Moore's Law) ERC grant;
- ▶ The Second Implementation Phase in the PRACE EU FP7 project FTI and energy-efficient prototype;
- ▶ 2 networks of excellence: HiPEAC-3 and RISC;
- ▶ The European Technology Platform for HPC (ETP4HPC), contributing to the draft of the European Strategic Research Agenda towards Exascale computing;

Collaborations with IT companies:

- ▶ Intel Corporation with a multi-year agreement Intel-BSC Exascale Lab, on topics related to auto-tuning, resilience, analysis of applications and performance prediction tools;
- ▶ NVIDIA through the CUDA Center Of Excellence (CCoE), in association with the Universitat Politècnica de Catalunya (UPC-BarcelonaTECH); the centre was one of the 4 finalists in the 2013 CCoE awards;
- ▶ 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 SoW: "Scalable Data Centric Computing", "Middleware and Virtualization Management" and "Power management" with IBM Research Watson and "PGAS programming models" with IBM Toronto;
- ▶ 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;
- ▶ The G8-ECS (Enabling Climate Simulations at Extreme Scale) international collaboration initiative;
- ▶ ORNL (USA) on the Extreme-scale Simulator (xSim) toolkit.

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;
- ▶ The Spanish Consolider program "Supercomputing and eScience", coordinating the Basic Research in Supercomputing workpackage;

» Scientific Output • For additional information, please see the Detailed Report of Research Activities 2013.

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 Symposium on Microarchitecture (MICRO), Annual Design Automation Conference (DAC), International Conference on Computer Design (ICCD), International Conference on Supercomputing (ICS), International Conference on High Performance Computing, Networking, Storage and Analysis (Supercomputing (SC), Symposium on Applied Computing (SAC), International Parallel & Distributed Processing Symposium (IPDPS), Design, Automation, and Test in Europe (DATE) conference, International Conference on Computing Frontiers (CF), IEEE International Conference on High Performance Computing (HiPC), Great Lakes Symposium on VLSI and International Conference on Field Programmable Logic and Applications (FPLA).

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

Communication & Dissemination 2013	
Publishing	
Journal Articles	35
Book Chapters	3
Conference Presentations	
International	61
National	3
Workshops	
Workshops	18
Education	
Theses Read	7

» Research Groups Heterogeneous Architectures



Led by Álex Ramirez, this Group aims to design and evaluate the next generation of HPC systems capable of achieving the 50 GFlops/Watt energy efficiency required by future Exaflop supercomputers. The Group believes that energy-efficient 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 2013, the Group performed a series of performance and energy efficiency evaluations on a series

of small-scale prototypes (as PRACE prototypes) and contributed to the design and bring-up of the large-scale Mont-Blanc prototype, in the framework of the EU FP7 Mont-Blanc project. The group also participated in the FP7 EuroServer project, evaluating the use of energy-efficient technologies from the mobile market for BigData processing, and started a new collaboration with Samsung, evaluating the memory behaviour of HPC production applications and the frequency and locality of memory errors. Finally, the Group continues to develop architecture innovations to further increase the energy efficiency of next-generation HPC systems.

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 represents the core of the BSC-Microsoft Research Centre (www.bscmsrc.eu) which focuses its research on lowering the programmability wall raised by multicore architectures; research areas include low-power vector processors, transactional memory, programming language runtimes and synchronisation. During 2013, the group continued its work in two FP7 projects (ParaDIME and AXLE) and also on reliability as part of the Intel-BSC Laboratory and the G8 Enabling Climate Simulation at Extreme Scale project. During 2013 two new FP7 projects started: ICT-Energy FET coordination action and RETHINK Big to construct the roadmap of hardware and networking technologies for Big Data processing and analysis.



Operating System / Computer Architecture Interface

In the last year the CAOS Group has centred its activities on embedded real-time and high-performance systems. In the area of real-time systems the group successfully completed the EU FP7 PROARTIS project, started a follow up EU FP7 project, PROXIMA, both led by the CAOS group, and continued his participation in the EU FP7 parMERSA and ARTEMIS VeTeSS projects, as well as the collaboration with the European Space Agency. In the area of high-performance systems, the group continued its work on energy and CPU accounting and on ultra-low power operation. Finally, in 2013 a new research activity started to converge real-time and high performance, in collaboration with the Programming Models group, under the scope of the EU FP7 P-SOCRATES project.



Unconventional Computer Architecture and Networks

Led by Mario Nemirovsky, the Group is conducting research on massive multithreaded architectures focused on big data, latency sensitive and network processing architectures (e.g. IoT, cloud and data centres). In this direction, the Group is developing the concept of FOG, a highly distributed computing and storage platform at the network from the core to the edge. In addition, as new materials became available, in special grapheme, new architectures driven by the use of these materials need to be researched. In order to support their design, the group is developing a new kind of architecture simulators based on queuing models, allowing much faster simulations with an excellent accuracy. During 2013, the Group concentrated on studying these systems and defining new architectures to address these challenges.



Programming Models

Led by Xavier Martorell, the Group explores new programming models and their efficient implementation for current and future architectures, 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 2013, the Group improved the support for GPU, the MIC, FPGA and clusters in OmpSs, interoperability with MPI with DLB (Dynamic Load Balancing), designed a new platform to support the proposal of DSL (Domain Specific Languages) targeting OmpSs and CUDA, continued the work on power modelling for multicore architectures and code transformations for processors with local memories. During 2013, the Group also continued the participation in the EU FP7 EnCORE (finalized), Mont-Blanc, DEEP and TERAFLUX projects as well as in the HiPEAC-3 network of excellence and the research collaboration with Intel, IBM and Xilinx Research Labs in Dublin. Finally, the Group also started the participation in the new Mont-Blanc-II and DEEP-ER projects, complementary to the work being done in Mont-Blanc and DEEP, respectively, and the Human Brain Project.

Performance Tools

Led by Judit Giménez, this Group is working on the design of tools to instrument, analyse and predict the behaviour of parallel applications on parallel systems. The main goal of the Group is to provide technology to understand the issues that determine the actual perfor-



mance of a parallel application or that contribute to the application bottlenecks. This knowledge is extremely important both in novel homogeneous and heterogeneous multi-core architectures as well as in highly scalable cluster systems. During 2013, the activities of the Group focused on improving the tools infrastructures and their integration, evolving the Group research lines targeting performance analytics and models, participating in EU FP7 projects (HOPSA, ScalaLife, Mont-Blanc, DEEP and PRACE) and the joint Intel-BSC Exascale Laboratory, and disseminating our work through publications and training activities. Finally, new projects started by the end of 2013, including the extensions of the EU Exascale projects (Mont-Blanc2 and DEEP-ER), and a collaboration with IBM to support in Extrae the new OpenMP instrumentation interface.

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 2013 focussed on further development of the COMPSs programming model in order to enable the inclusion of web-services as elements of the applications, on extensions to enable the deployment of the applications themselves as web-services, the development of a graphical IDE to help application developers and the interoperability of the runtime back-end with different Cloud middle wares. The Group has also worked on the integration of COMPSs with the self-contained objects layer in development by the Storage Group (as part of the Severo Ochoa program) and the extension of new language bindings (Python and C/C++). Finally, the Group has continued its participation in several EU FP7 projects (OPTIMIS, ScalaLife, transPLANT, EU-Brazil OpenBIO and HBP) and started new projects (ASCETIC, EuroServer and EUBrazil CloudConnect), all of them related with extensions of COMPSs and porting of applications.



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.

Storage Systems

Led by Toni Cortés, this Group explores appropriate solutions to the scalability of parallel storage systems in large installations (in which very large volumes of data need to be generated and accessed), new file-system approaches to increase their performance and/or usability (file system virtualisation), and new approaches to store and manage Big Data. In 2013, the Group focussed on increasing the performance and adaptability of parallel file systems, applying the Group's virtualised file system to cloud environments, and on developing a new storage abstraction based on self-contained objects. During 2013 the research activities of the Group have been supported by the Severo Ochoa program, the IOLanes and HBP EU projects, and SCALUS Marie Curie Initial Training Network.



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, scalable mathematical and Monte Carlo methods and algorithms. In particular, scalable Monte Carlo and hybrid algorithms are developed for linear algebra, optimization, 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 2013 the Group completed the participation and leadership in the EU Brazil OpenBio and RISC EU projects.



José María Baldasano, Director of the Earth Sciences Department



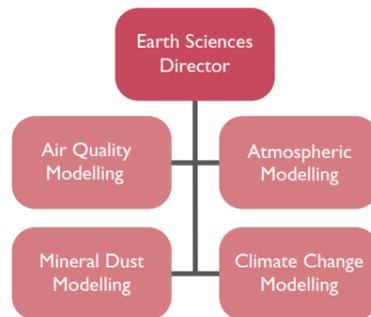
The Earth Sciences Department of BSC-CNS has the aim of modelling and understanding the behaviour of the Earth System, focusing its research activities on atmospheric processes and climate change modelling.

» Overview

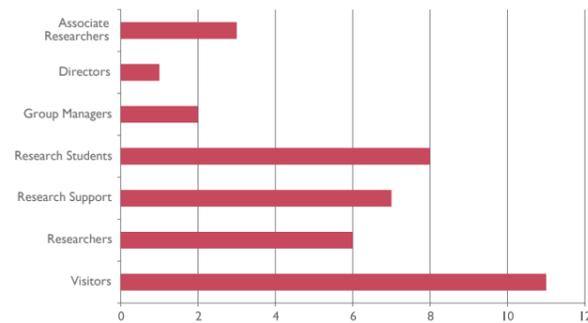
The high performance capabilities of MareNostrum enable the Earth Sciences Department to increase the spatial and temporal resolution of earth systems, in order to improve knowledge of dynamic patterns of air pollutants in complex terrains and interactions and feedbacks of physico-chemical processes occurring in the atmosphere. Also possible are analyses with high-resolution global circulation models and downscaling to regional models. This coupling of global and regional climate models will contribute to a detailed description of the impacts of climate change. The main topics of research are: high-resolution air quality and atmospheric modelling; global and regional mineral dust modelling; global and regional climate modelling.

» Organisational Structure

The Department is structured in four Groups that represent the main topics of Earth Sciences research: air quality modelling, mineral dust modelling, atmospheric modelling and global and regional climate modelling. These Groups are inter-related and work in a cooperative form. They are led by a senior scientist and composed of a researcher, post-doctoral fellows and doctoral students. The technical support staff is shared by all the research Groups. During 2013 some 34 staff, collaborators and visitors worked with the Department.



Earth Sciences Department Staff & Collaborators 2013



Earth Sciences Projects 2013



» Key Projects

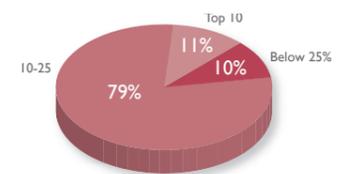
- ▶ Initiated IS-ENES2 project Infrastructure for the European Network for Earth System modelling - Phase 2 is an FP7 Integrating Activity in the Capacities Programme;
- ▶ Continued the APPRAISAL project. Air Pollution Policies for Assessment of Integrated Strategies At regional and Local scales is an FP7 Environment project;
- ▶ Concluded the FIELD_AC project. Fluxes, Interactions and Environment at the Land-Ocean Boundary. Downscaling, Assimilation and Coupling is an FP7 Space Programme project;
- ▶ Continued the participation in European consortium for the development of EC-Earth: European Earth System model based on ECMWF modelling systems. Currently, the EC-Earth consortium consists of 22 academic institutions and meteorological services from 10 countries in Europe (FP7-Project);
- ▶ Continued the MACC-II (Monitoring Atmospheric Composition and Climate) FP7-project in collaboration with AEMET, to establish the core global and regional atmospheric environmental services to be delivered as a component of Europe's GMES initiative;
- ▶ Led the Earth Science work package in the SyeC Consolidator Program coordinated by the BSC-CNS and funded by MICINN;

- ▶ Continued the CICYT project: Coupling of a fully online multi-component aerosol module within the atmospheric global-regional NMMB model funded by MICINN;
- ▶ Participated in the CICYT project: Currents, waves and wind: Improving Risk Assessment through Assimilation in Numerical models of the Coastal Environment (COVARIANCE) funded by MICINN, in collaboration with LIM/UPC, CSIC and Servei Meteorològic de Catalunya;
- ▶ Continued the extension of the CALIOPE project to the Autonomous Community of Andalusia, funded by the Junta de Andalucía;
- ▶ Concluded the extension of the CALIOPE project to the Autonomous Community of Canarias, funded by the Canarias Government;
- ▶ Generation of climate projections for the 21st century in Catalonia, supported by the "Servei Meteorològic de Catalunya" of the Territory and Sustainability Department of Catalonia Government;
- ▶ Participated in the COST Action ES1004. European framework for online integrated air quality and meteorology modelling (EuMetChem) - is focusing on a new generation of online integrated Atmospheric Chemical Transport (ACT) and Meteorology (Numerical Weather Prediction and Climate) modelling with two-way interactions between different atmospheric processes including chemistry (both gases and aerosols), clouds, radiation, boundary layer, emissions, meteorology and climate;
- ▶ Participated in the COST Action ES1002. European framework for Weather Intelligence for Renewable Energies (WIRE), to enhance the methodologies of forecasting wind and solar power production in the time domain of a few minutes up to several days ahead;
- ▶ Participated in the European Network for Earth System Modelling (ENES);
- ▶ Participated in the European Aerosol Research Lidar Network: EARLINET. The dataset generated is used to validate and improve models that predict the future state of the atmosphere and its dependence on different scenarios;
- ▶ Participated in AERONET (AErosol RObotic NETwork), an optical ground based aerosol monitoring network and data archive supported by NASA's Earth Observing System and expanded by federation with many non-NASA institutions;
- ▶ Hosted the Northern Africa-Middle East-Europe (NA-ME-E) Node of the SDS-WAS Regional Center. The SDS-WAS mission is to enhance the ability of countries to deliver timely and quality sand and dust storm forecasts, observations, information and knowledge is supported by the WMO;
- ▶ Hosted the first CBS Regional Specialized Meteorological Center with activity specialisation on Atmospheric Sand and Dust Forecast (RSMC-ASDF). This centre is requested to 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;
- ▶ Collaborated with The National Centers for Environmental Prediction (NOAA/NCEP/EMC) within the framework of a Memorandum of Understanding (MoU). Under this MoU it is intended that both institutions will continue collaborating for NMMB/BSC-CTM development, international joint project proposals and researcher mobility;
- ▶ Collaborated with the The Trustees of Columbia University in the City of New York for the International Research Institute for Climate and Society (IRI) within the framework of an MoU. Under this MoU it is intended that both institutions will continue collaborating for areas connecting climate, atmospheric aerosols and health, as well as sharing of dust model data;
- ▶ Organised the "3rd Training course on WMO SDS-WAS products", in collaboration with the WMO and EUMETSAT;
- ▶ Actively contributed as a member of the Spanish network RETEMCA (Red Temática de Modelización de la Contaminación Atmosférica).

» Scientific Output

For additional information, please see the Detailed Report of Research Activities 2013 for the Earth Sciences Department, available in the online version of this report.

Distribution of 2013 Published Articles by JCR-IF rank journal in subject area



The diffusion 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 2013, 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. The number of ISI-JCR publications in 2013 increased compared to 2012 (from 12 in 2012 to 15 in 2013). The JCR publications in 2013 had an average quality of 3,2 (Average JCR Science Edition Impact Factor). The ISI-JCR publications of the ES department are mostly ranked in the first quartile of their subject category (90 percent).

Communication & Dissemination 2013

Publishing	
Journal Articles	20
Book Chapters	2
Conference Presentations	
International	35
National	5
Workshops	
Workshops	11
Education	
Theses Read	1

» Research Groups
Air Quality

The Air Quality Group focuses its research on understanding the physico-chemical processes in the atmosphere that contribute to a decrease of air quality, and analyses the interactions between air pollutants and atmospheric processes, with the aim of obtaining a precise estimation of the air quality through high-resolution mode-



Figure 1 - Screen views of CALIOPE App

lling, especially the relation between emissions, atmospheric transport, chemistry and deposition. For that purpose, an air quality modelling system with high spatial and temporal resolution (1 km – 4 km and 1 hour) is under development, implementation and validation under supercomputing infrastructures. It will consist of a set of models that will take into account emissions of anthropogenic and natural pollutants, meteorology and chemistry.

In 2013 the activities of the Group were mainly related to maintaining and improving the daily operational air quality forecast of the CALIOPE system, developed in the framework of the CALIOPE project, funded by the Spanish Ministry of the Environment and Rural and Marine Affairs. CALIOPE encompasses an operational high resolution air quality forecasting system, namely WRF-ARW/HERMESEMEP/CMAQ/BSC-DREAM8b, being applied to Europe as a mother domain: 12 km x 12 km, 1 h as well as to Spain as the nested domain: 4 km x 4 km, 1 h, and with higher detail for some hot spot areas (<http://www.bsc.es/caliope>). Such high resolution of the modelling system is made possible by its implementation on the MareNostrum supercomputer hosted by BSC-CNS.

During 2013, the following improvements in the CALIOPE system were done: HERMESv2 (emission inventory), WRFv3.5 (meteorological model), CMAQv5.0.1 (photochemical transport model) and the boundary conditions (NCARG MOZART-4/GEOS-5 (6h)). Other significant developments were the increase of horizontal resolution for Andalusia domain to 1km x 1km, the expansion of Catalonia domain (before Barcelona domain) and the incorporation of Madrid domain, both with 1km x 1km.

The CALIOPE website was also updated, especially with the implementation of a user-friendly maps visor. The number of measurement and evaluation points over Spain was increased, from 344 to 443. An app (web application) for mobiles and tablets devices was developed with the hourly main results of the CALIOPE forecast for Iberian Peninsula and Canaries Islands (Fig. 1).

Technology transfer activities were also undertaken with some institutions, especially Junta de Andalucía.

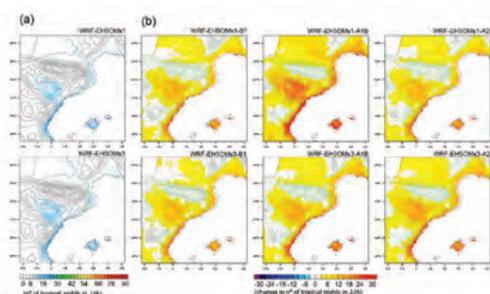


Figure 2 - Climatological mean from the WRF-EH5OMs1 and s3 simulations for 1971-2000 (a) and projected changes for 2021-2050 as derived from WRF-EH5OMs1 and s3 according to B1, A1B and A2 scenarios for the tropical nights (TR) in JJA (b) in the North Western Mediterranean Basin.

observational databases available for the 20th century as a reference. Climate indices to characterise the amplitude, persistence and frequency of extreme temperature and precipitation events were derived and analysed both geographically and temporarily.

In parallel, the group continued its activities of dynamic downscaling over the Western Mediterranean region, in collaboration with the Servei Meteorològic de Catalunya.

Within this project, present time climate conditions were obtained by means of the Regional Climate Model WRF-ARW, forced by the ERA40 reanalysis, for the 1971-2000 period. Future projections covered the 2001-2050 period and the A2, A1B and B1 emissions scenarios defined in the SRES report of the IPCC. 2013 activities included the preparation of two scientific articles related to the temperature and precipitation analysis. The first included the analysis of the effect of the resolution on climate projections in areas with complex topography and a high climatic variability. The second analysed the capabilities of the regional modelling system to assess temperature and precipitation extreme climate events. Additionally, some preliminary assessments of the impact of climate change on socio-economical variables in Catalonia were developed.

First efforts focused on the evaluation of the model capabilities to reproduce the wind field, considering both climatological means and extremes. This assessment constitutes a first step for the derivation of possible wind changes in future climate scenarios, which could affect wind power generation and preferred locations for wind farms. Additionally, an initial estimation of changes in energy needs for maintaining comfort conditions in buildings below climate change scenarios was performed.

The group continued its involvement in the second phase project of the distributed e-infrastructure of models, model data and metadata of the European Network for Earth System Modelling (ENES). This network gathers together the European modelling community working on understanding and predicting climate variability and change. Performance analyses of different model components of the EC-Earth Earth System Model are conducted in the framework of the IS-ENES2 project. Also, within this framework, BSC-CNS was selected as a host for the second IS-ENES Summer School on Earth System Models, which will be held in Barcelona in the summer of 2014.

Atmospheric Modelling

The research group continued the developments of the modelling system NMMB/BSC-Chemical Transport Model (NMMB/BSC-CTM) in 2013. Currently, the system provides aerosol forecasts at global scale and high-resolution dust forecast over a European domain. The group has participated in the international initiative of online model intercomparison AQMEII-Phase2. Regional simulations have been conducted following the requirements of the intercomparison initiative and evaluated with

several observational datasets (Figure 3). The multicomponent global aerosol module is under development and the secondary aerosol module was evaluated in collaboration with the NASA Goddard Institute for Space Studies and the University of California Irvine. During 2013, the meteorological driver of the NMMB/BSC-Chemical Transport model was upgraded, and now includes the capability to run simultaneous nest domains.

In the framework of the Severo-Ochoa project, the Group continued collaboration with the Computer Sciences Department to improve and extend the computing

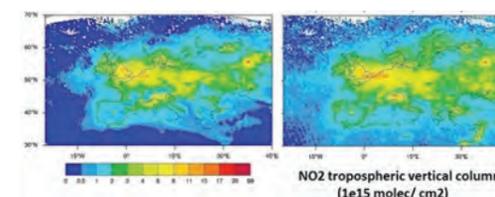


Figure 3 - Comparison of NMMB/BSC-CTM modelled (left panel) NO2 vertical tropospheric columns with OMI satellite data (middle panel) for autumn 2010.

performance of the NMMB/BSC-CTM system, to prepare it for future exascale architectures. Under this framework, the modelling system is using the parallel paradigms developed by the Computer Sciences Department (COMPSs, ompSs) to extend the range of applicability to very high-resolutions at global scale. In parallel, an aerosol data assimilation system was coupled with the NMMB/BSC-CTM in collaboration with the University of Oxford. The technique used was the Local Ensemble Transform Kalman Filter. It is a development of the ensemble Kalman Filter particularly suited to high-performance computing applications. It requires running multiple predictions using different initial conditions (i.e. an ensemble). Ideally, the amount of ensemble spread should be related to the uncertainty of the forecast.

Mineral Dust Modelling

The Mineral Dust Group provides daily operational forecasts of mineral dust for North Africa, Middle East, Europe and East Asia based on the updated version of BSC-DREAM8b version 2.

The model is participating in the Sand and Dust Storm Warning and Assessment and Advisory System (SDS-WAS) Regional Centre for Northern Africa, Middle East and Europe. Also BSC-DREAM8b is offline coupled in an air quality forecasting system CALIOPE, and therefore CALIOPE is the unique operational forecasting air quality system over Europe including the contribution of Saharan dust on an hourly basis.

In 2013 the group continued with the development of the NMMB/BSC-Dust model. This model is on-line coupled to the new generation unified atmospheric model NMMB of the National Centers for Environmental Prediction (NCEP). NMMB/BSC-Dust includes a physically-based dust emission scheme taking into account the effects of saltation and sandblasting, soil moisture and viscous diffusion close to the ground.

The new modelling system is intended to be a powerful tool for research and to provide efficient global and regional chemical weather forecasts at sub-synoptic and mesoscale resolutions on MareNostrum in the framework of the NMMB/BSC-CTM project. In this period, the NMMB/BSC-Dust model is in operational status and provides operational dust forecast over North Africa- Middle East-Europe and global regions. The dust forecast are daily published and evaluated (against ground-based and satellite observations) in the website of the model (<http://www.bsc.es/projects/earthscience/NMMB-BSC-DUST/>). Moreover, the NMMB/BSC-Dust website includes a new operational product: the vertical cross section and profile dust concentration interface which includes vertical dust concentrations for all EARLINET sites (Figure 4).

Furthermore, the NMMB/BSC-Dust model is participating in the International Cooperative on Aerosol Prediction (ICAP) model intercomparison initiative (<http://www.nrlmry.navy.mil/aerosol/icap.I087.php>) as well as in SDS WAS Regional Centre for Northern Africa, Middle East and Europe.

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

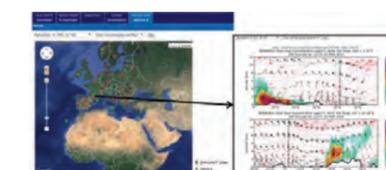


Figure 4 - New vertical dust forecast product of the NMMB/BSC-Dust website for 2th March 2014 at 12UTC for the regional (left panel) and global (right panel) domains.

SDS-WAS WMO Regional center

Activities in the framework of World Meteorological Organization (WMO) Sand and Dust Storm Warning and Assessment and Advisory System (SDS-WAS) Regional Centre for Northern Africa, Middle East and Europe (NA-ME-E), hosted by AEMET and the BSC-CNS, were also undertaken.

The web portal of the NA-ME-E Regional Center (<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. At present, 7 operational dust forecast systems (BSC-DREAM8b, DREAM8-NMME-MACC, MACC, NMMB/BSC-Dust, MetUM, GEOS-5 and NGAC) are included in the daily activities of NA-ME-E Regional Center.

During 2013, in addition to AERONET observations, the dust forecast evaluation includes MODIS aerosol product (Figure 5). In 2013, the Regional Center organised and coordinated the "3rd Training course on WMO SDS-WAS products" held in Muscat in December 2013 and participated in one training course, the 'Workshop on Meteorology, Sand and Dust Storm (SDS), Combating Desertification and Erosion' held in Istanbul, Turkey, 28-31 October 2013.

The experience acquired during the management in coordination with Spanish Weather Agency (AEMET) of the WMO SDS-WAS NA-ME-E Regional Center have been contributed to the creation of the first World Meteorological Organization (WMO) Regional Meteorological Center specialised in Atmospheric Sand and Dust Forecast.

The Barcelona Dust Forecast Center (BDFC) will significantly contribute to the creation of specialised products for the end-users.

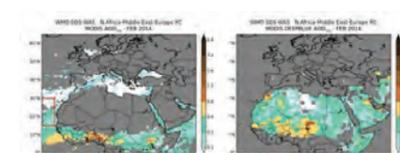


Figure 5 - MODIS satellite aerosol products for February 2014 used in the model evaluation of the WMO Regional Centre for Northern Africa, Middle East and Europe. Extracted from: <http://sds-was.aemet.es/>



Modesto Orozco, Director of the Life Sciences Department

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

» Overview

The Department benefits greatly from its unique situation in a major supercomputer centre, and also exists within a large and active environment of research in experimental biology. Its research line is tightly integrated in a collaborative effort with the Institute for Research in Biomedicine (IRB) 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), commencing in 2014.



The Department has 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 2013 include publications in leading journals with interdisciplinary impact such as Nature Genetics, Nature Nanotechnology, Nature Methods, GUT, JACS Genome Biology or PNAS; the organization of "in Silico Human Simulation" co-sponsored by PRACE, EESI and B-DEBATE; advances made within the International PanCancer consortium, the meeting of Life Sciences work group from the European Exascale Software Initiative and the publication of advances in auto-immune diseases and diabetes type II.

» Joint IRB-BSC Program on Computational Biology

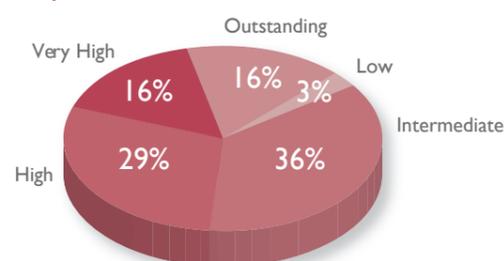


INSTITUTE FOR RESEARCH IN BIOMEDICINE

The Computational Biology Program was created as a joint venture between BSC-CNS and IRB 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 Barcelona, and from the Life Science Department of BSC-CNS. In 2013 researchers from CRG incorporated to the program. During the lifetime of the Program the scientists will enjoy access to computational resources from BSC-CNS (including MareNostrum) and services and facilities at the IRB Barcelona and CRG.

The Program, which in 2013 involved some 105 people, pursues excellence in research in bioinformatics and computational biology. Its research lines range from atomistic studies on bio-macromolecules to the analysis of high-order cell regulatory mechanisms, sequence analysis, gene regulation and expression, systems biology, network medicine and drug design. The Program published almost 70 journal papers during the year, 10 of them with an outstanding impact factor. Also of note, three principal investigators of the Program are currently holding an ERC grant.

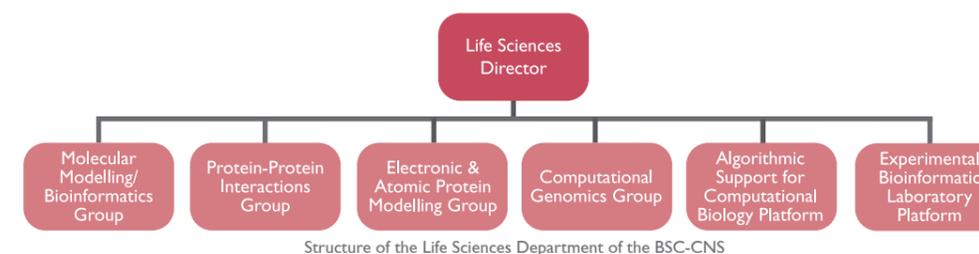
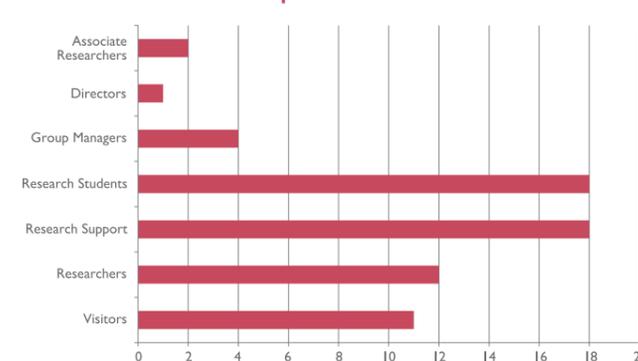
ISI Impact Factor of Articles published in 2013



» Organisational Structure

The structure of the Department and the technology platforms enables coverage of the entire field of computational biology, from atomistic detail to holistic views of the entire ecosystem. The Groups integrate different independent researchers, led by senior scientists who work in different aspects of computational biology. The Department is composed of 4 research groups and 2 research platforms: BSC-CNS research groups Electronic and Atomic Protein Modelling (EAPM), Protein Interactions and Docking (PID) and Computational Genomics (CG), the Molecular Modelling and Bioinformatics (MMB) and the Experimental Bioinformatics Laboratory (EBL), jointly run by BSC-CNS and IRB, the Computational Node (CN) of the National Institute of Bioinformatics, jointly run by BSC-CNS and INB.

Life Sciences Department Staff & Collaborators 2013



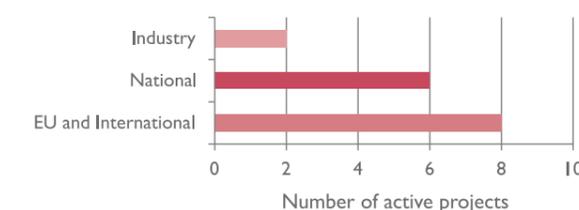
» EU & National Projects

Highlights among 2013 projects include:

- ▶ **PELE** - a la carte drug design tools. ERC Advanced Grant. The project aims to provide, to the large community of scientists working in molecular target therapies, a fast and accurate tool capable of obtaining an atomic detailed mechanism of the protein-ligand induced fit, of its recognition process and of the ligand migration. In 2013, the project published the web-server simulation of PELE.
- ▶ **ICGC** - International Cancer Genome Consortium. The Life Sciences department participates in the Spanish consortium for chronic lymphocytic leukemia, supporting the Genome and Exome analysis. In 2013, consortium activities towards a PanCancer initiative were launched.

- ▶ **TransPLANT** - Trans-national Infrastructure for Plant Genomic Science. Funded by FP7. The project address the challenges of large and complex genomes of plants to develop a trans-national infrastructure for plant genomic science. During 2013, the work focused on the development of a more efficient analysis framework.

Life Sciences Projects 2013



» Scientific Output

The Life Sciences Department defines a unique environment that combines very active groups working in computational biology with top supercomputing and experimental resources.

The research efforts can be classified into four main areas:

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

Organised Events:

In 2013 the Department's dissemination activities included the organisation of the "In silico Humans", one of the B-Debate series of meetings (www.bdebate.org). The meeting brought together a small number of scientific leaders and policy makers in both private and public institutions to debate on the current state and future of human simulation. Scientific topics covered simulations (from atomistic to whole organism level), and also parallel topics such as the evolution of computers, the impact of this research in pharma and biotech companies, and the actions that are planned from public and private research institutions to fuel this new kind of research.

Communication & Dissemination 2013	
Publishing	
Journal Articles	45
Conference Presentations	
International	11
Education	
Theses Read	2

» Research Groups



Molecular Modelling and Bioinformatics (MMB) Group

The Group's long term objective is to understand the behaviour of living organisms by means of theoretical models, whose roots are anchored in the basic principles of physics and chemistry. With this general aim the Group works with different methodolo-

gies, 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 set of techniques: classical and quantum simulations.

Protein Interaction and Docking (PID) Group

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



Computational Genomics (CG) Group

The aim of the Computational Genomics Group is to investigate different processes of the biology of genomes and to contribute to the understanding of how the sequence and the structure of these macromolecules determine their basic functions. The Group's research lines 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 invests time in developing tools for the analysis of the cancer genome in the context of the Cancer Genome Project to identify somatic mutations, with particular interest in those affecting regulatory regions. Finally, the Computational Genomics Group devotes collaborative efforts within high impact projects related to the assembly and the primary analysis of genomes and metagenomes.



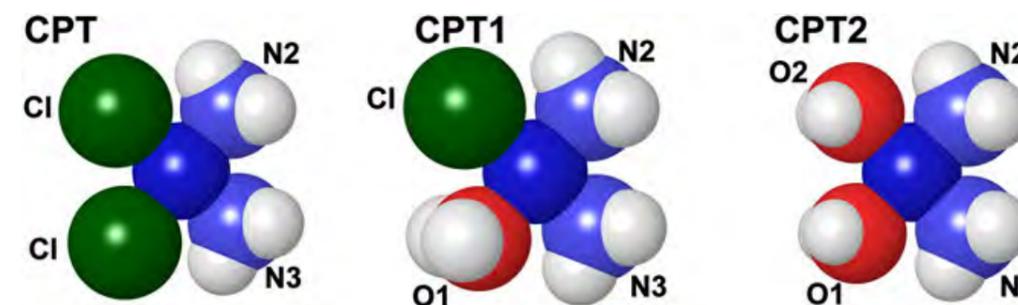
INB-BSC-CNS

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

biological databases, both generic and related to supported projects, and to develop web services and applications covering a broad range of analysis software.

Experimental Bioinformatics Laboratory (EBL) Platform

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





José María Cela, Director of the CASE Department

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

» Overview

The applications developed by the CASE department are truly 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, 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, High Energy Physics (plasma core and edge transport, plasma wall interaction), Biomechanics (Cardiovascular and Respiratory systems), Geophysics and Atmospheric flows. Recently, CASE has also opened a new line in large scale social simulation and smart cities.

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

- ▶ **Alya:** HPCM system. Fluid mechanics, Solid mechanics, Electric propagation, Combustion, etc.
- ▶ **FAIL3D:** Volcanos ash transport. Used in production in South American Volcanic Ash Advisory Centres (VAAC)
- ▶ **BSIT (Barcelona Seismic Imaging Tools):** Acoustic/Elastic waves, Forward Modelling, RTM, FWI. Promoted by Repsol.
- ▶ **SIESTA:** Ab-initio molecular dynamics. CASE is a co-developer of this code.
- ▶ **Pandora:** An HPC Agent-Based Modelling framework for social simulation.
- ▶ **Waris:** Atmospheric Flows, Structured Meshes, running on accelerators.

» Organisational Structure

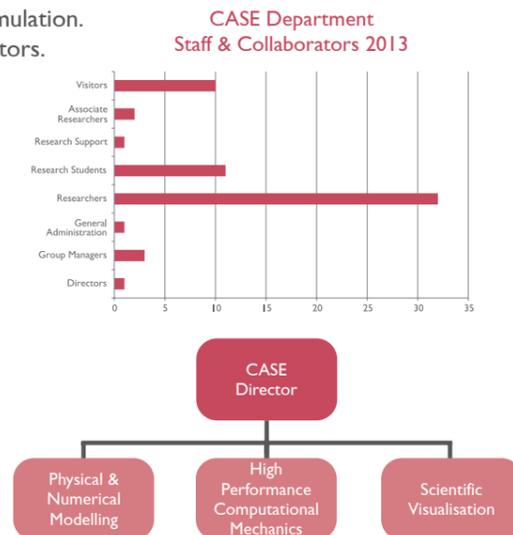
The CASE Department is led by José María Cela. The research lines fall naturally in three main Groups: Physical & Numerical Modelling (PNM), High Performance Computational Mechanics (HPCM) and Scientific Visualisation. Each Group consists of around 25 people, comprising several senior scientists, post and pre-doctoral students and visiting scientists. PNM research lines are horizontal and HPCM lines are vertical, in the sense that the PNM Group is in charge of developing the core components which are then assembled and modified as required by the HPCM Group into applications, tailor-made to meet specific project needs. Due to the multidisciplinary character of CASE research activities, both groups are involved in all projects.

» Key Projects • In 2013, the CASE Department carried out work under the scope of the following projects:

EU funded projects:

- ▶ **PRACE 2IP-3IP:** Partnership for Advanced Computing in Europe.
- ▶ **ETSF:** Generating a software infrastructure for support of the spectroscopy community.
- ▶ **C2CA:** Recycling of Concrete to Cement and Aggregates. The Department models combustion, compressible flows, radiation and solid N-body impact.

- ▶ **COPA-GT:** A Marie Curie training project for Turbines operation in Aerospace and energy production plants with research in compressible flows, combustion, aeroelasticity and optimisation algorithms.
- ▶ **NEMO:** A Marie Curie training project for the next generation of European volcanologists.



- ▶ **INNFACTO2011:** Wind model based on the open source CFD code OpenFoam and applied supercomputing techniques.
- ▶ **Scalable Parallel Simulation for Policy Analysis.** This project aims to create high-performance computing tools useful in the analysis of migration processes.
- ▶ **MontBlanc:** The Department ports to the MontBlanc Architecture the EUTERPE code.

Enterprise funded projects:

- ▶ **Repsol-BSC research centre:** RTM, elastic forward modelling, full wave-form inversion, controlled source electromagnetic method.
- ▶ **OptiReact:** optimization of chemical reactors using response surface method and adjoint method based on a reactor modelling with Alya.
- ▶ **Resvolver phase I:** expert system for simplifying the user interface of multiphysics massively parallel simulations.
- ▶ **Iberdrola:** Optimisation of wind farms both on-shore and off-shore (in Alya code).
- ▶ **Confidential Partner:** Race yacht design (in Alya code).
- ▶ **Simulplay, with La Caixa:** Simulation videogames for technosocial learning. This project is funded by the RecerCaixa program, and its main aim is to develop new tools for communicating to society how scientists use simulation to explore human behaviour.

Nationally funded projects:

- ▶ **Coordination of Supercomputación y e-Ciencia (CONSOLIDER):** to develop a set of scientific Grand Challenges for Petaflop supercomputers and design the architecture of these machines.
- ▶ **Simulpast (CONSOLIDER).** Simulating the past to understand human behaviour: to develop an innovative and interdisciplinary methodological framework to model and simulate ancient societies and their relationship with environmental transformations.
- ▶ **ATMOST (Plan Nacional):** to model ashes and contaminant dispersion in the atmosphere.
- ▶ **MIVAL3D (GenCat):** to simulate the cardiac mytral valve.
- ▶ **S4E (Plan Nacional):** Supercomputing for Energy. Three specific topics are considered: hydrocarbon exploration, wind energy and marine energy.

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

- ▶ **Airflow in the Human Respiratory System:** with the Aeronautics and Bioengineering Depts. at Imperial College London. A simulation of the complete human respiratory system, including the air surrounding the face, and particle transport simulation in order to catch the deposition patterns according to the particle types (density, diameter). Supported by HPC-Europa.

» Scientific Output

For additional information, please see the *Detailed Report of Research Activities 2013 for the CASE Department*, available in the online version of this report.

Except for work that is private and confidential and can not be published, research results of the CASE Department were presented in congresses and conference lectures as well as a number of scientific publications, including: International Journal for Numerical Methods in Biomedical Engineering, Journal of Volcanology and Geothermal Research, International Journal of Modeling and Optimization, and others.

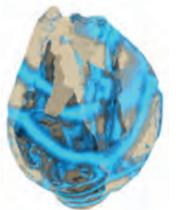
» Research Groups • CASE department consists of three formal groups: Physical and Numerical Modelling and High Performance Computational Mechanics and Environmental Simulations. However, due to the industrial impact of the Kaleidoscope project and the work carried out by its associated team, the Seismic Imaging "group" deserves a separate and detailed description. Due to the increasing activities in the field of scientific visualisation, a visualisation team was formally created as well.



- ▶ **Airflow in large and small airways:** with the Aeronautics and Bioengineering Depts. at Imperial College London and Jackson State University.
- ▶ **Computational Cardiac Mechanics:** Coupled electromechanical simulation of the heart, including the mytral valve. Collaboration with UAB, Htal. St. Pau, Htal. Clinic, Htal. Bellvitge, T-Systems, PULSO, UPC, Univ. Lleida, IMDEA Materiales and the University of Cape Town.
- ▶ **Skeletal muscles:** with Univ. of Illinois, USA.
- ▶ **Material Science:** with Laurence Berkeley National Lab, USA, IC-MAB-CSIC, ICN2, Humboldt-Universität zu Berlin, and Université catholique de Louvain.

Other collaborations:

- ▶ **Solid Mechanics:** with Oxford University (UK) and IMDEA in the development of a HP solid mechanics module, including X-FEM for fracture simulations.
- ▶ **Turbulence:** Application of turbulence models to high Reynolds number flows: with EDF (France), Univ. Manchester (UK), Science & Technology Facilities Council, Daresbury (UK).
- ▶ **Participation in "Adaptation of historical spaces to teaching museums via reactive applications with multiplatform, mobile telephony and tactile surface contents"** from DIDPATRI (UB).
- ▶ **Collaboration with IPHES** to develop a dynamic population simulator for hominid groups based on agents on a supercomputing infrastructure.
- ▶ **Participation in "Arqueología y memoria de la aviación republicana (1938-1939)"** to apply new research methodologies to the understanding of the role of aviation during the Spanish Civil War.
- ▶ **Euterpe code:** Collaboration with Max Planck IPP and CIEMAT to port the EUTERPE code to new hardware platforms.



Propagation of the electric impulse in the heart

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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.

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

Among these developments are: 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; and Speed up tests were carried out on the main European supercomputers on up to 22528 CPUs: Lindgren - Cray XE6 - Sweden, Jugene - Blue Gene/P - Germany and Curie - BullX - France.

Computational Social Sciences • Since 2009, the Group has worked on the design of applications specially designed for use in social sciences and policy analysis areas. **The Group is developing a new simulator capable of executing Agent-Based Models of human societies in a HPC environment, in order to explore:** Emergence of behavioural patterns in human societies, understood as complex systems; Interaction between societies and their relationship with environment and landscape; Impact of change in human groups and population dynamics (both ancient and present); Design of artificial societies as models to understand human behaviour; and Methodological and theoretical foundations of social simulation.

High Performance Computational Mechanics (HPCM)

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

The activities of the HPCM Group are driven by direct interaction with users and industry.

Usually the core problem requires modelling of physical processes which then must be solved by intensive numerical calculation.

Some of the applications developed by the HPCM Group during 2013 include:

- ▶ A large-strain solid mechanics simulation for anisotropic cardiac tissue. Collaboration with Hosp. Sant PAU, Univ. Autònoma de Barcelona.
- ▶ DES simulation of car aerodynamics. Collaboration with Univ. Hiroshima.
- ▶ High accuracy racing yacht hydrodynamics. Confidential contract.
- ▶ Simulation and optimisation of a plastics recycling setup. W2Plastics project.
- ▶ Airflow simulations of the human large airways during normal breathing cycles. HPCEuropa2 project, collaboration with Imperial College (UK).
- ▶ An elastic 3D Full Wave-form Inversion Code. Repsol contract.
- ▶ Wind farm simulation using RANS models. Iberdrola contract.
- ▶ Dynamic atmospheric mesoscale simulation.
- ▶ Ash transport: el Hierro (Spain), Puyehue (Patagonia), Eyjafjallajökull (Iceland).

Environmental simulations

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; and 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 consi-



dering 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; and Tailored modelling postprocess using GoogleEarth to facilitate visualization and standard data interchange.

REPSOL-BSC Research Center

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

The research focuses on the use of elastic and electromagnetic wave modelling and inversion to develop new imaging algorithms, and in the practical implementation of those algorithms on different computer architectures. In recent years state-of-the-art seismic imaging tools were developed (Kaleidoscope project) and received international recognition and awards. These tools used acoustic wave equations, requiring computers of 100 TFlops peak performance, however, improved solutions require the use of elastic waves, multiplying computational needs 50-fold. The capability of working with elastic waves, furthermore, opens the possibility of a real full waveform inversion procedure, potentially the most accurate tool for inverting the reservoir's properties to date. As a consequence, elastic wave modelling will lead us to retrieve even more accurate models of the Earth's subsurface. In addition, the group aims to investigate the inversion of electromagnetic waves to obtain images of the subsurface's resistivity, which is directly associated with the different reservoir's fluid contents (water, hydrocarbons). Finally, a joint elastic and electromagnetic inversion could further constrain the properties of the hydrocarbon reservoirs beyond the capabilities of seismic or electromagnetic methods alone.

The research is focused on solving 4 grand challenges in hydrocarbon exploration: use elastic wave equation for modelling large onshore exploration surveys; Develop a full waveform inversion algorithm based on elastic waves; Develop a geophysical inversion method for electromagnetic waves; and Couple the elastic and the electromagnetic inversion procedures to obtain a novel reservoir characterisation tool.



Scientific Visualisation

The Scientific Visualisation Team 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; and publication of results from a scientist to other experts in the field. For this purpose, the team is composed of scientists and visual communication and interaction experts, aimed to enhance the quality of the visualisations produced at the BSC while maintaining their scientific value.

The team works on and develops visual protocols to transmit quantitative information in the most efficient manner.

The images and videos result of this process are typically included in papers and presentations, used to create films that non-experts can understand and enjoy, or to help scientists explore and extract information from their data more efficiently.

Achievements and work during 2013:

Data exploration: Development of a pipeline for post-processing large scale simulation data. This process of data conversion is a necessary step to treat simulation results in terms of image. These tools are used in most of our production, in particular for the creation of outreach videos. One of the biggest challenges faced by modern visualisation is Big Data treatment: how to display and allow the exploration of very large data sets, in this case produced by simulations.

To address this problem, a parallel data visualisation system was developed, tested, and implemented. In this setup, simulation data distributed across a cluster (using Hadoop) is coupled to Paraview, where user exploration is translated to queries using Hive and Impala that return results in an interactive manner. In this manner, researchers can continue to use tools they are familiar with, but connected to potentially huge sets of results.

Science outreach

- ▶ The video "Alya Red: A Computational Heart" (<http://youtu.be/tKD2hff27rM>) produced by the Team, was awarded in February 2013, First Place winner of the 2012 International Science and Engineering Visualization Challenge by The National Science Foundation and the Journal Science.
- ▶ Within the frame of the European CONSOLIDER project SyEC, the Team produced the shortfilm documentary "Supercomputers" (<http://youtu.be/b5bQdTL0wAg>).

Through high-end render visualisations and interviews the film explains the impact of high performance computing on science, technology, and society.

For data publication

- ▶ Short videos and static images for scientists of the Red Española de Supercomputación.
- ▶ A technical video describing the features of software developed at BSC-CNS.
- ▶ A technical video showcasing simulation results calculated with software developed at BSC-CNS.
- ▶ Various images for papers 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. Further core objectives are to manage upgrades to the MareNostrum and other RES nodes; facilitate access to RES facilities, including online electronic applications, remote access, and porting of code; manage the environmental aspect of the BSC-CNS installations; manage the technical aspects of integration of the MareNostrum in the DEISA and European HPC network grids; and ensure that RES staff receive appropriate training and skills development in order to be able to professionally carry out their duties in an environment of constant technological change and advancement.

» Overview

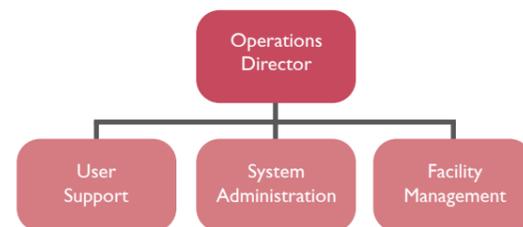
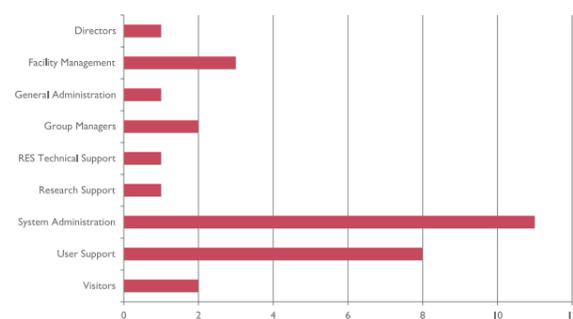
The Operations Department, led by Sergi Girona, ensures the continuous daily functioning of the RES supercomputers and remote access by users both within Spain and internationally. In addition to all the routine maintenance and operations tasks, the Department staff are also heavily involved in planning and designing new systems and support facilities. Furthermore, the entire Department participates in European projects such as PRACE, EESI-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 BSC team requires a continue remodeling of premises to accommodate the new employees, and to facilitate the development of their research. Until the BSC headquarters building is ready to be used, maintenance and extension of current computer rooms, office space and meeting rooms requires an intensive effort.

» Organisational Structure

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

Operations Department Staff & Collaborators 2013



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

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

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

» Key Projects

The Operations Department was involved in the following projects during 2013:

► **RES (Red Española de Supercomputación):** The Spanish Supercomputing Network offers coordinated HPC services to the Spanish scientific community. The Operations Department is responsible for the coordination of the network, including all support and administration services.

► **PRACE IIP:** In the PRACE First Implementation Phase, the Operations Department is involved in WP6, WP7 and WP8, and coordinates the participation of the BSC-CNS in the project.

► **PRACE 2IP:** In the PRACE Second Implementation Phase, the Operations Department is involved in WP2, WP7 and WP10, and coordinates the participation of the BSC-CNS in the project.

► **PRACE 3IP:** In the PRACE Third Implementation Phase, the Operations Department is involved in WP2, WP7, WP10 and WP12, and coordinates the participation of the 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 that 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 to support 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.



Active Archive

During the first half of 2013 the Operations department worked to put in production the Active Archive storage system. The Active Archive is a 4.1 Petabytes long-term storage based on GPFS technology for scientific data; this data can come from the rest of BSC HPC facilities or produced/consumed from other sources through Internet. This facility is permitting BSC-CNS to be a data-centric computing infrastructure to any Scientific Community.

The Active Archive also has a private cloud that permits to provide different data services for any that may need it. During 2013 projects from different areas are using this new storage and their associated cloud infrastructure, such as EUDAT, RES, EGA, PanCancer, etc.

Upgrade of connectivity to Internet

In addition to the Active Archive installation, during 2013 the connectivity to Internet of BSC-CNS was upgraded from a dedicated 1Gbit (Gigabit) link to a dedicated 10Gbit link. This upgrade will permit BSC-CNS to harness the demand on data transfer and data services to the rest of centres and researchers around the globe, with transfer rates that can reach a Gigabyte per second.

Phi Cluster

During July of 2013, a rack of cluster of heterogeneous nodes was installed and integrated within the actual MareNostrum3 cluster. This cluster is composed of:

- 42 compute nodes with the same characteristics that the rest of MareNostrum3
- Fat nodes in terms of memory having 64GB per node (4GB/core)
- 2x Xeon Phi 5110P
- 2 Infiniband FDR10 interfaces

This cluster will permit researchers to adapt tools and programming models developed at BSC-CNS to this technology, having in mind the exascale paradigm that will come in the next years.

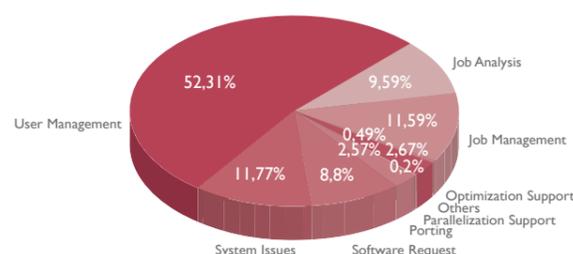
» User Support

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.

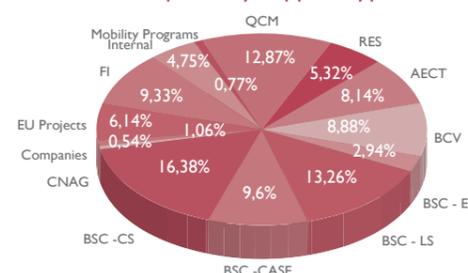
Some 7382 support requests were received in 2013 as presented in the figures below, split by support request area and by topic.



Requests by support area



Requests by support type



Highlighted Projects

► Support to new MN3 and the first PRACE TIER-0 users

During 2013 BSC put in production the new MareNostrum3 machine. It was a grand challenge in terms of installation, but also in terms of tuning applications and supporting the new users. The User Support group coordinated the installation of all the software stack required for the new system. It was split in 4 levels of porting.

- The compilers, so they change from IBM compilers for PowerPC to INTEL compilers for x86 architecture,
- MPI implementation. The system currently supports 3 implementations of MPI: the IBM implementation (POE), the INTEL implementation (IMPI) and the OpenMPI implementation
- Mathematical libraries. The new system supports the INTEL MKL mathematical libraries, which substitute the IBM ESSL libraries that were used previously in the MN2 environment.
- Batch system. The system was moved from a SLURM/MOAB system to a LSF. It implied the modification of all the scripts for the users, as well as new examples and new documentation.

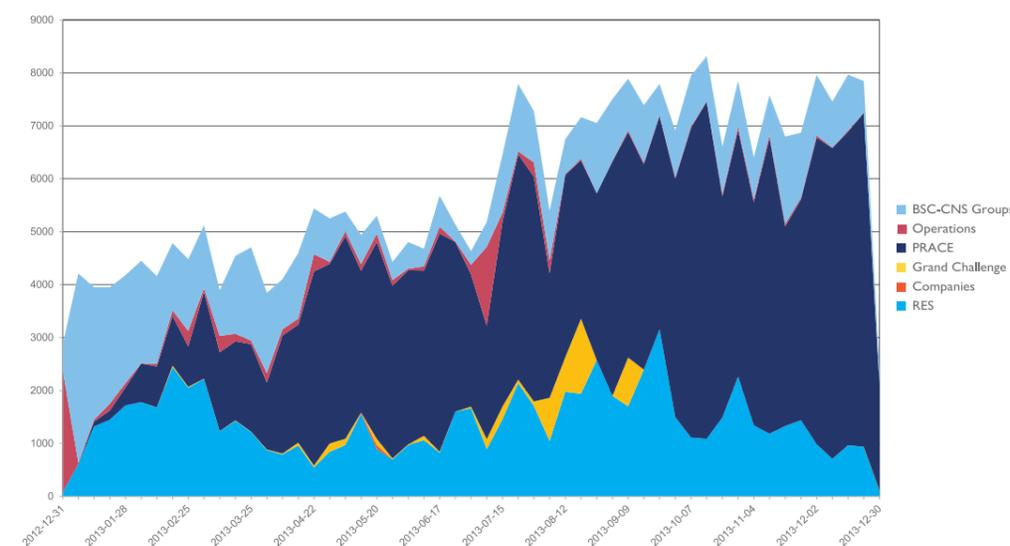
In less than 6 months the support team has installed more than 150 applications with its bunch of versions.

MareNostrum Performance 2013

MareNostrum was in full production from 2nd January 2013. The system was installed in two phases: the first phase, with 33600 cores, from January until June, and the second phase, which is the final configuration for the MN3 machine for a total of 48128 cores. Using these numbers for the year 2013, the observed system utilisation was approximately 86.68%. In addition to BSC-CNS internal groups, more than 260 external groups accessed the MareNostrum system during the year.

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

MareNostrum Weekly Performance 2013 (in 1000's hours)



» Facility Management

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

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

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



Finished MareNostrum 3 facility upgrade

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

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

BMS (Building Management System)

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

Highlight features include:

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



Chill Water Exchanger



Ernest Quingles, Management Department Director

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

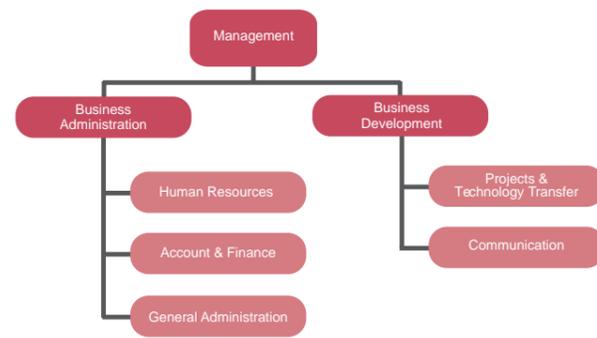
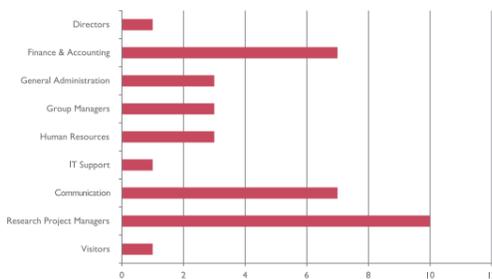
» Overview

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

» Organisational Structure

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

Management Department Staff & Collaborators 2013



» Finance and Business Administration

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

Finance & Accounting

The Finance & Accounting Group is responsible for financial resources management of all BSC-CNS activities (expenses, budgets, audits, bank relations, suppliers, receiving payments and control budget deviations). With support from the Administration Group they manage and safeguard the patrimony of BSC-CNS according to existing financial legislation and accountancy norms. The Group also prepares financial reports for project audits in coordination with the Project Office and principal researchers.

Due to the economic environment and public funding delays, the Group was forced to increase the role of the controller and work on the automation of certain data analysis and exploitation processes. A semiannual follow-up of financial indicators was also introduced. In 2013 the Group continued working on a SAP BI Tool with a system upgrade for better reporting capabilities and also developed new finance queries.



Human Resources

The Human Resources Group is responsible for managing selection processes, hiring and training, job descriptions, labour relations and collective bargaining, planning careers and internal promotions, and preventing work-related accidents. In 2013, the Group continued work on a professional development system for all BSC-CNS staff. To measure motivation and retention of talent, a new web tool was implemented to manage the BSC-CNS Staff Professional Development Plan. The tool facilitated the annual staff evaluation, monitoring of the Plan's development, and keeping it aligned with annual goals of the department as well as of the entire Centre.

During 2013, BSC-CNS committed to implement and apply the principles of the code of conduct to work towards an award of excellence in Human Resources and management policies, with the aim of promoting transparency, accessibility and equity in the recruitment and promotion of researchers.

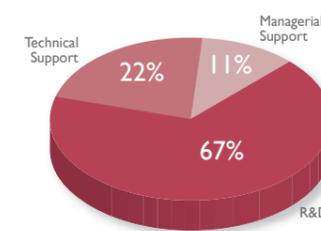
To this end, BSC-CNS became a member of the HR Strategy Group promoted by the European Commission. An initial gap analysis was conducted in preparation for the first meeting of the working group, highlighting some issues to analyse and develop:

- ▶ Improvements related to equal opportunity and promoting female scientific careers;
- ▶ Actions to integrate disabled people at the Centre;
- ▶ A survey of values and action principles promoting internal collaboration among all BSC-CNS staff;
- ▶ Training development actions to acquire new skills and competencies focused on teamwork, interdepartmental relationships and communication.

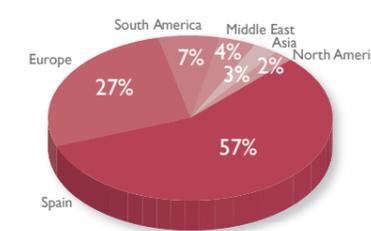
BSC-CNS continues to attract researchers from all over the world and currently 43% of its researchers are from abroad (from a total of 48 countries). The International Postdoctoral Programme at BSC-CNS currently hosts around 58 postdocs supported by internal and competitive funding from highly prestigious institutions and by the Postdoctoral Fellowship Programme, co-funded by the European Commission and the Spanish government. In 2013, 26 external fellowships and postdoctoral contracts were awarded to BSC-CNS postdocs.

In 2013, the 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 five candidates selected in the "la Caixa" call started their PhD thesis in September, after a highly competitive selection process involving significantly number of candidates (145 candidates from over 26 countries).

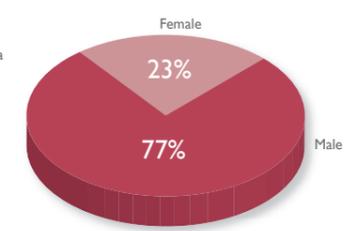
2013 Personnel by Function



2013 Personnel by Region of Origin



2013 Personnel by Gender



General Administration

The General Administration Group is responsible for activities such as the 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 office 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 2013, the Group strengthened the administrative support structure in order to meet growing internal needs for support of both senior staff and new projects, and also to increase efficiency. To this end, some new reception and secretarial services were established for individual departments.

During the year, BSC-CNS invited 10 public calls in order to accept 6 supply tenders, 3 services tenders and 1 works tender.

A total of 76 administration contracts were signed during the year. Activities of the purchasing unit increased significantly, and the works tender was held to start the 2nd phase construction of the new BSC-CNS building and to finalise the new supercomputer installation. For both actions, BSC-CNS will receive grants from the European Regional Development Fund (FEDER).



» Project Management

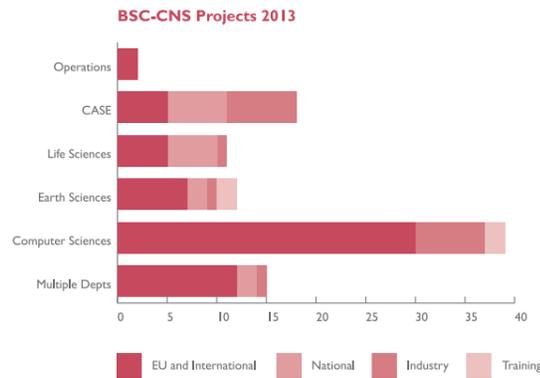
Project Management Office

The BSC-CNS Project Management Office (PMO) is staffed by seven experienced project managers, who work closely with the centre's Principal Investigators. PMO is responsible for detecting and communicating research funding opportunities; coordinating and contributing to project proposals; managing contract negotiations and managing all legal, financial and administrative aspects of contracts and projects. This includes both publicly funded projects 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 following and anticipating developments in relevant funding programmes and helping the centre to adapt to changing requirements. The aim is to increase BSC-CNS's capacity to leverage competitive funding and professionally manage results-oriented research. In 2013 the focus was on preparing for the new Horizon 2020 research funding programme of the European Commission.

In 2013, BSC-CNS participated in ninety-three projects (excluding personnel grants), with a total BSC grant of over twenty-eight million euros. Fifty-one projects were funded by the extremely competitive Framework Seven Programme of the European Commission (FP7). Eight of these FP7 projects were led by BSC-CNS, in which the centre coordinated a total of sixty partners based throughout Europe and Latin America. Two were COST-funded projects for the international coordination of nationally funded research and one was funded by the Artemis Joint Technology Initiative. Fourteen projects were funded by Spanish National or Catalan funds. Of the twenty-seven other projects, seventeen were research activities funded by private companies, five were funded by Spanish and international public bodies, including the UN, and three were funded by the European Space Agency (ESA).

In addition to managing active projects, in 2013, the Project Management Office assisted BSC-CNS researchers in submitting one-hundred and fourteen new project proposals to help ensure continued funding for BSC-CNS research activities, including proposals for forty-two personnel grants.



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. Highlights of 2013 included the publication of the ETP4HPC Strategic Research Agenda which identified specific research areas which need to be advanced up to 2020 in order to develop European HPC technologies.

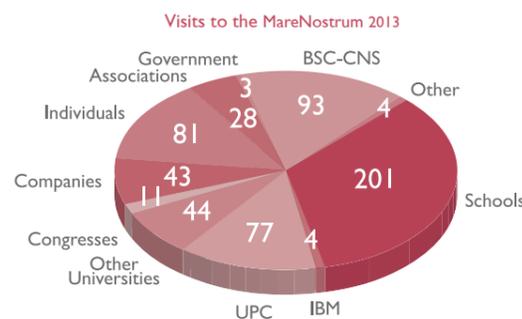


» Communication Area

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 2013, BSC-CNS received a total of 8644 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, our technology and our research lines. Most visits are tailored depending on the target audience and often incorporate videos and a visit to the BSC's collection of "antique" supercomputers.



BSC-CNS in the Media

BSC-CNS was mentioned 428 times in national and international newspapers and magazines in 2013. Most coverage was received in the print media, with online press in second place, followed by TV, radio and news agencies. In total, BSC-CNS sent out 17 press releases in Spanish, Catalan and English, all posted on the Press section of the BSC-CNS website. All identified press impacts were also included on the web.

Web and Social Media

In 2013, the Communications team made a major effort to strengthen BSC-CNS's web presence and social media networks. The website had more than 1,000,000 visits. More than 60 articles were published on the corporate website and 800 posts were made, mainly on Facebook and Twitter. During this period, the number of Facebook fans increased by 100% and the number of Twitter followers, by 80%. The Youtube Channel has 200 subscribers and about 100,000 views.

Internal Communication

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

Events, Seminars and Workshops

In 2013, BSC-CNS hosted and organised the following events: Consolider Final Conference, 27-28 May; ICCS, June 5-7; PUMPS Summer School, July 8-12; B-Debate: In silico human simulation, 18-20 September; Open Days 2013, 19-20 September; EUDAT conference, October 28-30; 2nd IUGG-WMO workshop on Ash dispersal forecast and civil aviation, 18-20 November; PRACE Summer of HPC Award Ceremony, 2nd December.

Participation in international supercomputing conferences

The Communications team prepared the BSC-CNS presence at the exhibitions of the International Supercomputing conference 2013 and at the SuperComputing13 and coordinated logistics resulting in the presence of BSC-CNS researchers in both prestigious conferences. Furthermore, BSC-CNS participated also at the exhibition of the SEG International Exposition and 83rd Annual Meeting, 22-27 September 2013.

Dissemination of European and National Projects

The Communications team also carried out BSC-CNS dissemination tasks for 20 European and National projects. PRACE, Mont-Blanc, EUDAT and Consolider were the projects with most dissemination time assigned to BSC-CNS in 2013.



» Computer Sciences 2013 Publications

Journals

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- » Greg Katsaros, Josep Subirats, Oriol Fitó, Jordi Guitart, Pierre Gilet, Daniel Esping, "A service framework for energy-aware monitoring and VM management in Clouds", *Future Generation Computer Systems*, Vol. 29 (8), 2077–2091, 2013
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- » Jordá Polo, Yolanda Becerra, David Carrera, Malgorzata Steinder, Ian Whalley, Jordi Torres, Eduard Ayguadé, "Deadline-based MapReduce Workload Management", *IEEE Transactions on Network and Service Management*, 10, 231–244, 2013
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- » Vassil Alexandrov, "Scalable Algorithms", Scalable Algorithms, 2013

Books

- » Alexandrov, Nia, Ramírez Velarde, Raúl, Vassil Alexandrov, "Technological Advances in Interactive Collaborative Learning", *book*, New York, 2013
- » Mario Nemirovsky, Dean Tullsen, Dean Tullsen, "Multithreading Architectures", Morgan & Claypool publishers, 2013
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- » Adrià Armejach, Anurag Negi, Adrián Cristal, Osman Unsal, Per Stenström, Tim Harris, "HARP: Adaptive Abort Recurrence Prediction for Hardware Transactional Memory", *IEEE Conference on High Performance Computing (HiPC 2013)*, Bengaluru, India, 2013
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- » Antonio Filgueras, Eduard Gil, Carlos Álvarez, Daniel Jiménez, Xavier Martorell, Jan Langer, Juanjo Noguera, "Heterogeneous tasking on SMP/FPGA SoCs: the case of OmpSs and the Zynq", *21st IFIP/IEEE International Conference on Very Large Scale Integration (VLSI-SoC)*, Istanbul, Turkey, 290–291, 2013
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- » Daniele Lezzi, Francesc Lordan, Roger Rafanell, Rosa M. Badia, "Execution of scientific workflows on federated multi-cloud infrastructures", *Euro-Par 2013*, Aachen, Germany, 2013
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 - » Milos Panic, Germán Rodríguez, Eduard Quiñones, Jaume Abella, Francisco J. Cazorla, "On-Chip Ring Network Designs for Hard-Real Time Systems", 21st International Conference on Real-Time Networks and Systems, Sophia Antipolis, France, 23–32, 2013
 - » Milovan Duric, Óscar Palomar, Aaron Smith, "ReCompAc: Reconfigurable Compute Accelerator", International Conference on Reconfigurable Computing and FPGAs 2013, 2013
 - » Mladen Slijepcevic, Leonidas Kosmidis, Jaume Abella, Eduard Quiñones, Francisco J. Cazorla, "DTM: Degraded Test Mode for Fault-Aware Probabilistic Timing Analysis", 25th Euromicro Conference on Real-Time Systems (ECRTS'13), Paris, France, 2013
 - » Myron King, Asif Khan, Abhinav Agarwal, Oriol Arcas, Arvind, "Generating Infrastructure for FPGA-Accelerated Applications", 23rd International Conference on Field Programmable Logic and Applications, Porto, Portugal, 1–6, 2013
 - » Nikola Rajovic, Alejandro Rico, James Vipond, Isaac Gelado, Nikola Puzovic, Álex Ramirez, "Experiences With Mobile Processors for Energy Efficient HPC", ACM/IEEE Design, Automation, and Test in Europe (DATE), Grenoble, France, 464–468, 2013
 - » Nikola Rajovic, Paul Carpenter, Isaac Gelado, Nikola Puzovic, Álex Ramirez, Mateo Valero, "Supercomputing with commodity CPUs: are mobile SoCs ready for HPC?", SC13: International Conference for High Performance Computing, Networking, Storage and Analysis, Denver, United States, 40–40, 2013
 - » Paul Lensing, Toni Cortés, Andre Brinkmann, "Direct Lookup and Hash-Based Metadata Placement for Local File Systems", 6th International System and Storage Conference (Systor 2013), 2013
 - » Rahul Gayatri, Rosa M. Badia, Eduard Ayguadé, "Loop Level Speculation in a Task Based Programming Model", IEEE Conference on High Performance Computing (HiPC 2013), Bengaluru, India, 1–10, 2013
 - » Saravanan Karthikeyan, Paul Carpenter, Álex Ramirez, "Power/Performance evaluation of Energy Efficient Ethernet (EEE) for High Performance Computing", IEEE International Symposium on Performance Analysis of Systems and Software (ISPASS-2013), Austin, United States, 2013
 - » Saša Tomić, Ege Akpınar, Adrián Cristal, Osman S. Ünsal, Mateo Valero, "EcoTM: Conflict-Aware Economical Unbounded Hardware Transactional Memory", International Conference on Computational Science, ICCS 2013, www.sciencedirect.com, 2013
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 - » Subotic, V., José Carlos Sancho, Labarta, J., Valero, M., "Identifying Critical Code Sections in Dataflow Programming Models", Parallel, Distributed and Network-Based Processing (PDP), 2013 21st Euromicro International Conference on, Belfast, Ireland, 29-37, 2013
 - » Sylvain Girbal, Miquel Moretó, Arnaud Grasset, Jaume Abella, Eduard Quiñones, Francisco J. Cazorla, Sami Yehia, "On the Convergence of Mainstream and Mission Critical Markets", 50th Annual Design Automation Conference (DAC), Austin (Texas), United States, 1–10, 2013
 - » Theo Ungerer, Christian Bradatsch, Mike Gerdes, Florian Kluge, Ralf Jahr, Michele, Jörg, Joao Fernandes, Pavel Zaykov, Petrov Zlatko, Bert Boddeker, Sebastian Kehr, Hans Regler, Andreas Hugel, Christine Rochange, Haluk Ozaktas, Hugues Cassé, Bonenfant Armelle, Pascal Sainrat, Nick Lay, Ian Broster, David George, Milos Panic, Eduard Quiñones, Francisco J. Cazorla, Jaume Abella, Sascha Uhrig, Mathias Rohde, Arthur Pyka, "parMERASA Multi-Core Execution of Parallelized Hard Real-Time Applications Supporting Analysability", Euromicro Conference on Digital System Design, DSD 2013, Santander, Spain, 363–370, 2013
 - » Thomas Grass, "Task Sampling: Computer Architecture Simulation in the Many-Core Era", 22nd international conference on Parallel Architectures and Compilation Techniques, Edinburgh, United Kingdom, 405–406, 2013
 - » Toni Cortés, Anna Queral, "Enabling flexible and efficient data sharing without losing control", CloudScape V. Cloud for savings, Cloud for quality, 2013
 - » Ugljesa Milic, Isaac Gelado, Nikola Puzovic, Álex Ramirez, Milo Tomasevic, "Parallelizing general histogram application for CUDA architectures", 2013 International Conference on Embedded Computer Systems: Architectures, Modeling, and Simulation (SAMOS XIII), Samos, Greece, 11–18, 2013
 - » Vasileios Karakostas, Saša Tomić, Osman Unsal, Mario Nemirovsky, Adrián Cristal, "Improving the Energy Efficiency of Hardware-Assisted Watchpoint Systems", 50th Annual Design Automation Conference (DAC), Austin (Texas), United States, 2013
 - » Vassil Alexandrov, Janko Strassburg, "Hybrid Scalable Monte Carlo Methods for Approximate Matrix Inversion", Hybrid Scalable Monte Carlo Methods for Approximate Matrix Inversion" submitted to 9th IMACS Seminar on Monte Carlo Methods 2013", 2013
 - » Vesna Smiljkovic, Martin Nowack, Nebojša Miletić, Tim Harris, Osman Unsal, Adrián Cristal, Mateo Valero, "TM-dietlib: A TM-aware Real-world System Library", The 27th IEEE International Parallel and Distributed Processing Symposium (IPDPS 2013), Boston, United States, 2013
 - » Zoe Stephenson, Jaume Abella, Tullio Vardanega, "Supporting Industrial Use of Probabilistic Timing Analysis with Explicit Argumentation", 11th IEEE International Conference on Industrial Informatics (INDIN), Bochum, Germany, 734–740, 2013
- ## National Conferences
- » Emanuele Naboni, Yi Zhang, Alessandro Maccarini, Elian Hirsch, Daniele Lezzi, "Extending the use of parametric simulation in practice through a cloud based online service", 1st IBPSA-Italy Conference: BSA2013 Building Simulation Applications Conference, Bolzano, Italy, 105–112, 2013
 - » Jorge Ejarque, Anthony Sulistio, Francesc Lordan, Pierre Gilet, Raül Sirvent, Rosa M. Badia, "Service Construction Tools for Easy Cloud Deployment", 7th Iberian Grid Infrastructure Conference, Madrid, Spain, 119–132, 2013
 - » Pablo Pessolani, Toni Cortés, Silvio Gonnet, Fernando Tinetti, "Un mecanismo de IPC de microkernel embebido en el kernel de Linux", Workshop de Investigadores en Ciencias de la Computación, Parana Entre Ríos, Argentina, 2013
- ## Workshops
- » Adrián Cristal, Osman Unsal, Gulay Yalcin, Christof Fetzer, Jons-Tobias Wamhoff, Pascal Felber, Derin Harmanci, Anita Sobe, "Leveraging Transactional Memory for Energy-efficient Computing below Safe Operation Margins", 8th ACM SIGPLAN Workshop on Transactional Computing (TRANSACT 2013), Texas, United States, 2013
 - » Antonio Filgueras, Eduard Gil, Carlos Álvarez, Jiménez-González, Daniel, Xavier Martorell, Jan Langer, Juanjo Noguera, "Heterogeneous tasking on SMP/FPGA SoCs: the case of OmpSs and the Zynq", workshop @VLSI-SOC: WIA (Special Session 2): Are processors the NAND gates of the future?", 2013
 - » Cecilia González, Ishikawa, Haruku, Hayashi, Akihiro, Daniel Jiménez, Carlos Álvarez, Kimura, Keiji, Kasahara, Hironori, "Automatic Design Exploration Framework for Multicores with Reconfigurable Accelerators", WRC 2013 : 7th HiPEAC Workshop on Reconfigurable Computing, Berlin, Germany, 1–10, 2013
 - » Diego Caballero, Alejandro Duran, Xavier Martorell, "An OpenMP Barrier Using SIMD Instructions for Intel Xeon Phi(TM) Coprocessor", 9th International Workshop on OpenMP (IWOMP), Canberra, Australia, 99–113, 2013
 - » Fahimeh Yazdanpanah Ahmadbadi, Daniel Jiménez, Carlos Álvarez, Yoav Etsion, Rosa M. Badia, "FPGA-Based Prototype of the Task Superscalar Architecture", WRC 2013 : 7th HiPEAC Workshop on Reconfigurable Computing, Berlin, Germany, 1–10, 2013
 - » Francisco J. Cazorla, Tullio Vardanega, Eduard Quiñones, Jaume Abella, "Upper-bounding Program Execution Time with Extreme Value Theory.", 13th International Workshop on Worst-Case Execution Time Analysis, Paris, France, 61–70, 2013
 - » Fulvio Riso, Mario Nemirovsky, Antonio Manzanini, "Some Controversial Opinions on Software-Defined Data Plane Services", IEEE Software Defined Networks for Future Networks and Services 2013, Italy, 2013
 - » Jokanovic, Ana, Jokanovic, A., Prisacari, Bogdan, Prisacari, B., Rodríguez, German, Rodríguez, G., Minkenber, Cyriel, Minkenber, C., "Randomizing Task Placement Does Not Randomize Traffic (Enough)", Proceedings of the 2013 Interconnection Network Architecture: On-Chip, Multi-Chip, New York, NY, USA, France, 9–12, 2013
 - » Jonathan Martí, Dani Gasull, Anna Queral, Toni Cortés, "Towards DaaS 2.0: Enriching Data Models", Services 2013 - 3rd International Workshop on Formal Methods in Services and Cloud Computing, 2013
 - » Josep Lluís Berral, Ricard Gavaldà, Jordi Torres, "Power-aware Multi-DataCenter Management using Machine Learning", 2nd International Workshop on Power-aware Algorithms, Systems, and Architectures, Pittsburgh, United States, 858–867, 2013
 - » Juan González, Judit Gimenez, Jesús Labarta, "Performance Analytics: understanding parallel applications using cluster and sequence analysis", 5th International Workshop on Parallel Tools for High Performance Computing, Germany, 2013
 - » Martin Tilleenius, Elisabeth Larsson, Rosa M. Badia, Xavier Martorell, "Resource-aware task scheduling.", 4th Workshop on Parallel Programming and Run-Time Management Techniques for Many-core Architectures (PARMA), Berlin, Germany, 6–11, 2013
 - » Rafael Amaral, Rosa M. Badia, Ignacio Blanquer, Leonardo Candela, Donatella Castelli, Renato De Giovanni, William Alexander Gray, Daniele Lezzi, Pasquale Pagano, Vanderlei Perez-Canhos, Roger Rafanell, Vinod Rebello, Erik Torres, "EU-Brazil Open Data and Cloud Computing e-Infrastructure for Biodiversity", 5th International Workshop on Science Gateways, Zurich, Switzerland, 2013
 - » Ramon Nou, Jacobo Giral, Toni Cortés, "DYON: Managing a New Scheduling Class to Improve System Performance in Multicore Systems", 1st Workshop on Runtime and Operating Systems for the Many-core Era (ROME 2013) - Best paper award, 2013
 - » Sylvain Girbal, Miquel Moretó, Arnaud Grasset, Jaume Abella, Eduard Quiñones, Francisco J. Cazorla, Sami Yehia, "The Next Convergence: High-performance and Mission-critical Markets", Workshop on High-performance and Real-time Embedded Systems (HiRES), Berlin, Germany, 1–11, 2013
 - » Tanasic, Ivan, Lluís Vilanova, Marc Jorda, Javier Cabezas, Isaac Gelado, Nacho Navarro, Wen-mei W. Hwu, "Comparison Based Sorting for Systems with Multiple GPUs", GPGPU-6 - Six Workshop on General Purpose Processing Using GPUs, Houston, TX, United States, 2013
 - » Vesna Smiljkovic, S. Stipić, Osman Unsal, Adrián Cristal, Mateo Valero, "Transaction Coalescing - Lowering Transactional Overheads by Merging Transactions", Sixth Workshop on Programmability Issues for Heterogeneous Multicores (MULTIPROG-2013), Berlin, Germany, 2013

- » Xavier Teruel, Michael Klemm, Kelvin Li, Xavier Martorell, Stephen Olivier, Christian Terboven, "A Proposal for Task-Generating Loops in OpenMP", 9th International Workshop on OpenMP (IWOMP), Canberra, Australia, 1–14, 2013

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- » Aidan Fries, "The use of Java in large scientific applications in HPC environments", 2013
- » Alejandro Rico, "Raising the Level of Abstraction: Simulation of Large Chip Multiprocessors Running Multithreaded Applications", 2013
- » Enric Tejedor, "Programming and Parallelising Applications for Distributed Infrastructures", 2013
- » Juan González, "Application of clustering analysis and sequence analysis on the performance analysis of parallel applications", 2013
- » Michail Alvanos, "Optimization Techniques for Fine-grained Communication in PGAS Environments", 2013
- » Petar Radojkovic, "Improving the Effective use of Multithreaded Architectures: Implications on Compilation, Thread Assignment, and Timing Analysis", 2013
- » Vladimir Subotic, "Evaluating techniques for parallelization tuning in MPI, OpenMP and MPI/OpenMPs", 2013

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Journals

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- » C. Cuvelier, P. Thunis, D. Karam, M. Schaap, C. Hendriks, R. Kranenburg, H. Fager-

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International Conferences

- » A. Rincón, O. Jorba, L. Delle Monache, Baldasano, J. M., "Solar Irradiance Forecast System Based On Post-Processing Techniques Applied On WRF-ARW Meteorological Simulations In Spain", *ICEM 2013: 2nd International Conference Energy&Meteorology*, 26-28 June, 2013. Toulouse, France, 2013
- » A. Badia, O. Jorba, R. Nuterman, Baklanov, A., Baldasano, J. M., "Model inter-comparison study between NMMB/BSC-CTM and Enviro-HIRLAM on-line systems contributing to the AQMEII-Phase2 initiative", *33rd International Technical Meeting on Air Pollution Modelling and its Application*, 26-30 August, 2013, Miami, Florida USA, 2013
- » A.P. Fernandes, J. Ferreira, Miranda, A.I., Baldasano, J. M., O. Tchepel, "Análise de episódios de poeiras utilizando a modelação da qualidade do ar e dados de satélite", *10ª CNA-12ª CNEA: 10ª Conferência Nacional do Ambiente- 12º Congresso Nacional de Engenharia do Ambiente*, 6-8 November, 2013. Aveiro, Portugal, 2013
- » Baklanov, A., Heinke, K., Suppan, P., Baldasano, J. M., Brunner, D., Gauss, M., Maurizi, A., Moussiopoulos, N., Seigneur, C., Kong, X., O. Jorba, Joffre, S., "Online integrated meteorology-chemistry models: needs and benefits for Numerical Weather Prediction, Air Quality and Climate communities (European experience)", *33rd International Technical Meeting on Air Pollution Modelling and its Application*, 26-30 August, 2013, Miami, Florida (USA), 2013
- » Baldasano, J. M., "Air Quality Forecasting Systems: Needs of Computational Resources and Database", *International Computing for the Atmospheric Sciences Symposium 2013*, 8-12 September, 2013. Annecy (France), 2013
- » Baldasano, J. M., "AQFS: Sistemas de Pronóstico de la Calidad del Aire. Funciones y Requerimientos", *Seminario de Reducción de Gases de Efecto Invernadero*, 13 November, 2013. Toluca (México), 2013
- » Baldasano, J. M., "Dust prediction models", *3rd Training Course on WMO SDS-WAS products (satellite and ground observation and modelling of atmospheric dust)*, 10 November, 2013. Muscat (Oman), 2013
- » Baldasano, J. M., "Mineral dust forecast models", *Summer of School 2013. ITaRS (Initial Training for atmospheric Remote Sensing)*, 23 September-4 October, 2013. Bucharest (Romania), 2013
- » Baldasano, J. M., "Mineral dust modelling from meso to global scales", *RIC-TA2013 1st Iberian Meeting on Aerosol Science and Technology*, 1-3 July, 2013. Évora, Portugal, 2013
- » Baldasano, J. M., "Modelización numérica de la tormenta tropical DELTA" sobre las Islas Canarias. Importancia de la alta resolución", *XIX Congreso de la División de Dinámica De Fluidos*, 13-15 November, 2013. Jiutepec, Morelos (México), 2013
- » Baldasano, J. M., "Sistemas de pronóstico de la calidad del aire: funciones básicas y requerimientos", *Jornada Luso-Española de Calidad del Aire*, 31 Octubre, 2013. Madrid, Spain, 2013
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- » O. Jorba, A. Badia, Michele Spada, C. Perez, Sara Basart, Baldasano, J. M., Z. Janjic, D. Dabdub, "Multiscale Air Quality Modelling with the NMMB/BSC Chemical Transport model", XIX Jornades Eduard Fontseré (JEF) 2013, 22-24 November, 2013. Barcelona. Spain, 2013
- » O. Jorba, C. Perez, A. Badia, Michele Spada, Z. Janjic, Baldasano, J. M., D. Dabdub, "The NMMB/BSC Chemical Transport model air quality results from global to regional scales", 4th International Meeting on Meteorology and Climatology of the Mediterranean (4th IMMCM), February 27 - March 1, 2013. Banyuls (Roussillon), France, 2013
- » Papadimas, C., A. Gkikas, Hatzianastassiou, N., Matsoukas, C, S. Kazadzis, Sara Basart, Baldasano, J. M., Vardavas, I., "Dust radiative effect over Europe, Mediterranean, Sahara and Middle East from a radiative transfer model using BSC-DREAM8b aerosol optical data", European Geosciences Union (EGU) General Assembly 2013. Geophysical Research Abstracts, 07-12 April, 2013. Viena, Austria, 15, 2013
- » Pay, M.T., Gustavo Arévalo, Baldasano, J. M., "Evaluating the impact of increasing horizontal resolution on Air quality modelling systems over big metropolitan areas in Spain", 12th Annual CMAS Conference, 28-30 October, 2013. Chapel Hill, NC (USA), 2013
- » R. E. Mamouri, A. Nisantzi, D.G. Hadjimitsis, A. Ansmann, A. Schwarz, Sara Basart, Baldasano, J. M., "Complex Vertical Layering and Mixing of Aerosol over the Eastern Mediterranean: Active and passive remote sensing at the Cyprus University of Technology", First International Conference on Remote Sensing and Geoinformation of Environment RSCy 2013, 8-10 April 2013. Paphos, Cyprus, 2013
- » Sara Basart, Baldasano, J. M., O. Jorba, C. Pérez, "Desert dust modelling and forecasting in the Barcelona Supercomputing Center (BSC): developments and activities", XIX Jornades Eduard Fontseré (JEF) 2013, 22-24 November, 2013. Barcelona. Spain, 2013
- » Sara Basart, E. Terradellas, Huneus, N., Baldasano, J. M., Morcrette, J.J., J. Mulcahy, G. Pejanovic, da Silva, A., Lu, S., Benincasa, F., "Intercomparison and evaluation of dust prediction models", 4th International Meeting on Meteorology and Climatology of the Mediterranean (4th IMMCM), February 27 - March 1, 2013. Banyuls (Roussillon), France, 2013
- » Sara Basart, M. Sicard, Baldasano, J. M., Lane, D., Adolfo Comerón, "Optical characteristics of biomass burning and desert dust over the Western Mediterranean during summer: a case study", European Geosciences Union (EGU) General Assembly 2013. Geophysical Research Abstracts, 07-12 April, 2013. Viena, Austria, 15, EGU2013-8223, 2013
- » Sara Basart, Oriol Jorba, E. Terradellas, Benincasa, F., Baldasano, J. M., "Desert dust modelling and forecasting in the BSC: Activities and developments", ICAP 5th working group meeting: Recent Progress in Aerosol Observability for Global Modeling, 5-8 November, 2013. Tsukuba, Japan, 2013
- » Wichink Kruit, R., D. Simpson, R. Stern, B. Bessagnet, M. Engardt, C. Geels, Baldasano, J. M., Pay, M.T., K. Cuvelier, D. Hauglustaine, C.H. Flechard, M. Schaap, "ÉCLAIRE Model Comparison for Atmospheric Nitrogen Components over Europe", ACCENT-Plus Symposium 2013, 17-20 September, 2013. Urbino, Italy, 2013

National Conferences

- » Baldasano, J. M., "CALIOPE-AQFS como instrumento de planificación. Análisis de casos", 25-26 Junio, 2013. Santander, Spain, 2013
- » Baldasano, J. M., "Projecte ESCAT: Escenaris Climàtics amb Alta Resolució per

- a Catalunya: 2000-2050", Ecotendències: Canvi climàtic. Hi som a temps, de mitigar el canvi climàtic?, COSMOCAIXA, 27 November, 2013. Barcelona (Spain), 2013
- » Baldasano, J. M., "Qualitat de l'Aire i Salut", 5ª Jornades d'Anàlisi i Debat sobre les Ciències Ambientals DIÀLEGS AMBIENTALS'13 MOBILITAT I SALUT, ACCA, 3 Octubre, 2013. Barcelona (España), 2013
- » Baldasano, J. M., E. Terradellas, E. Cuevas, "Sistema d'avaluació i Avis de Tempestes de Pols i Sorra de L'OMM (WMO SDS-WAS)", XIX Jornades de Meteorologia Eduard Fontseré, 22-24 November, 2013. Barcelona. Spain, 105-118, 2013
- » Baldasano, J. M., Santiago Gassó, "Presentació projecte APPRAISAL. Model per avaluació de mesures", Jornada Plans de millora de la qualitat de l'aire. Mesures i experiències, 31 Octubre, 2013. Barcelona, Spain, 2013

Workshops

- » A. Mortier, P. Goloub, T. Podvin, D. Tanré, C. Deroo, A. Diallo, Th. Diallo, E. Cuevas, Sara Basart, Baldasano, J. M., "Variability of aerosol properties and radiative forcing over M'Bour (Senegal) as revealed by a 6 year coincident sunphotometer and LIDAR dataset", 7th International Workshop on Sand/Duststorms and Associated Dustfall. ESA/ESRIN, 02-04 December, 2013. Frascati (Rome), Italy, 2013
- » Baldasano, J. M., "Air Quality Modelling. Evaluation and post-processing techniques", ITaRS (Initial Training for atmospheric Remote Sensing) Start-up workshop, 13-15 February, 2013. Athens, Greece, 2013
- » Baldasano, J. M., "Climate Change and its relation with ecosystems in the Central America & Caribbean context", EUCARINET/ENLACE Europe, Central America&Caribbean: Climate Change and Biodiversity Dialogue Workshop, 22-23 April, 2013. Ciudad de Panamá (Panamá), 2013
- » Baldasano, J. M., "HPC in Environmental Issues", H2020: Challenges and opportunities for HPC, RISC Workshop, 25 November, 2013. México D.F. (México), 2013
- » Baldasano, J. M., Pay, M.T., Gustavo Arévalo, Santiago Gassó, "Evaluation of Chemical Initial and Boundary on Ozone Concentrations in the Spanish CALIOPE AQFS", 5th International Workshop on Air Quality Forecasting Research (IWAQFR), October 8-9, 2013. Santiago, Chile, 2013
- » Baldasano, J. M., Sara Basart, "Mineral dust modelling from meso to global scales", Workshop CV Dust Atmospheric Aerosols in Cape Verde Region, 11 January, 2012. Aveiro, Portugal, 2013
- » E. Terradellas, Sara Basart, Baldasano, J. M., Morcrette, J.J., G. Pejanovic, Oriol Jorba, M.E. Brooks, da Silva, A., Lu, S., Benincasa, F., "SDS-WAS: Evaluation of Dust Forecast Models", 7th International Workshop on Sand/Duststorms and Associated Dustfall. ESA/ESRIN, 02-04 December, 2013. Frascati (Rome), Italy, 2013
- » O.T.chepele, C. Gama, J. Ferreira, J. Cardoso, Sara Basart, Baldasano, J. M., C. Borrego, C. Pio, "Mineral dust modelling in Cape Verde", Workshop CV Dust Atmospheric Aerosols in Cape Verde Region, 11 January, 2012. Aveiro, Portugal, 2013
- » Sara Basart, C. Gama, O. Jorba, Michele Spada, C. Perez, Baldasano, J. M., "Desert dust and sea-salt evaluation of the NMMB/BSC-CTM model for Capo Verde (North Africa) salt evaluation of the NMMB/BSC-CTM model for Capo Verde (North Africa)", 7th International Workshop on Sand/Duststorms and Associated Dustfall. ESA/ESRIN, 02-04 December, 2013. Frascati (Rome), Italy, 2013
- » Sara Basart, F. Dulac, Baldasano, J. M., P. Nabat, M. Mallet, L. Roblou, F. Solmon, B. Laurent, J. Vincent, L. Menut, El Amraoui, B. Sic, J.-P. Chaboureaud, J.-F. Léon, Vogel, B., J.-B. Renard, F. Ravetta, J. Pelon, C. Di Biagio, P. Formenti, I. Chiapello, J.-L. Roujean, X. Ceamanos, D. Carrer, M. Sicard, H. Delbarre, J.-L. Attié, "Dust Model Intercomparison for Summer 2012 in the Western Mediterranean and comparison to the Pre-ChArMEx/TRAQA Campaign Observations", 7th International Workshop on Sand/Duststorms and Associated Dustfall. ESA/ES-

RIN, 02-04 December, 2013. Frascati (Rome), Italy, 2013

- » W.A. Sessions, A. Benedetti, P. Lynch, J.J.S. Reid, Baldasano, J. M., Sara Basart, P.R. Colarco, da Silva, A., O. Jorba, Lu, S., Morcrette, J.J., M. Razinger, Michele Spada, T.T. Sekiyama, T.Y. Tanaka, "International Cooperative for Aerosol Prediction Multi-Model Ensemble (ICAP-MME)", 7th International Workshop on Sand/Duststorms and Associated Dustfall. ESA/ESRIN, 02-04 December, 2013. Frascati (Rome), Italy, 2013

Theses

- » A Rincón, "Sistema de pronóstico de radiación solar a corto plazo a partir de un modelo meteorológico y técnicas de post-proceso para España", 2013

Life Sciences 2013 Publications

Journals

- » Agius, Rudi, Torchala, Mieczyslaw, Moal, Iain H, J. Fernández-Recio, Bates, Paul A, "Characterizing changes in the rate of protein-protein dissociation upon interface mutation using hotspot energy and organization.", *PLoS computational biology*, 9, 9, e1003216, 2013
- » Agustí Emperador, Solernou, Albert, Pedro Sfriso, Carles Pons, José Luis Gelpi, J. Fernández-Recio, Modesto Orozco, "Efficient relaxation of protein-protein interfaces by discrete molecular dynamics simulations", *Journal of Chemical Theory and Computation*, 9, 2, 1222-1229, 2013
- » Aviñó, Anna, Portella, Guillem, Ferreira, Ruben, Gargallo, Raimundo, Mazzini, Stefania, Gabelica, Valérie, Modesto Orozco, Eritja, Ramon, "Specific loop modifications of the thrombin-binding aptamer trigger the formation of parallel structures.", *The FEBS journal*, 2013
- » Candotti, Michela, Alberto Pérez, Ferrer-Costa, Carles, Manuel Rueda, Tim Meyer, Gelpi, Josep Lluís, Modesto Orozco, "Exploring early stages of the chemical unfolding of proteins at the proteome scale", *PLoS computational biology*, 9, 12, e1003393, 2013
- » Candotti, Michela, Esteban-Martín, Santiago, Salvatella, Xavier, Modesto Orozco, "Toward an atomistic description of the urea-denatured state of proteins", *Proceedings of the National Academy of Sciences of the United States of America*, 110, 15, 5933-8, 2013
- » Chen, Yang, Tascón, Igor, Neunuebel, M Ramona, Pallara, Chiara, Brady, Jacqueline, Kinch, Lisa N, J. Fernández-Recio, Rojas, Adriana L, Machner, Matthias P, Hierro, Aitor, "Structural basis for Rab1 de-AMPylation by the Legionella pneumophila effector SidD", *PLoS pathogens*, 9, 5, e1003382, 2013
- » D'Abbramo, Marco, Castellazzi, Chiara Lara, Modesto Orozco, Amadei, Andrea, "On the nature of DNA hyperchromic effect", *The journal of physical chemistry. B*, 117, 29, 8697-704, 2013
- » T. Dršata, A. Pérez, M. Orozco, A. V. Morozov, J. Sponer, F. Lankaš, "Structure, Stiffness and Substates of the Dickerson-Drew Dodecamer", *Journal of chemical theory and computation*, 9, 1, 707-721, 2013
- » Durán, Elisa, Djebali, Sarah, Santi González, Flores, Óscar, Mercader, Josep Maria, Guigó, Roderic, David Torrents, Soler-López, Montserrat, Modesto Orozco, "Unravelling the hidden DNA structural/physical code provides novel insights on promoter location", *Nucleic acids research*, 41, 15, 7220-30, 2013
- » Gil, Victor A, Guallar, Victor, "pyRMSD: a Python package for efficient pairwise RMSD matrix calculation and handling", *Bioinformatics (Oxford, England)*, 29, 18, 2363-4, 2013
- » Gracia, Eduard, Farré, Daniel, Cortés, Antoni, Ferrer-Costa, Carles, Modesto Orozco, Mallol, Josefa, Lluís, Carme, Canela, Enric I, McCormick, Peter J, Franco, Rafael, Fanelli, Francesca, Casadó, Vicent, "The catalytic site structural gate of adenosine deaminase allosterically modulates ligand binding to adenosine receptors", *FASEB journal: official publication of the Federation of American*

Societies for Experimental Biology, 27, 3, 1048-61, 2013

- » Hospital, A, Gelpi, J.L., "High-throughput molecular dynamics simulations: toward a dynamic view of macromolecular structure", *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 2013
- » Hospital, Adam, Faustino, Ignacio, Collepardo-Guevara, Rosana, González, Carlos, Gelpi, Josep Lluís, Modesto Orozco, "NAFlex: a web server for the study of nucleic acid flexibility", *Nucleic acids research*, 41, Web Server issue, W47-55, 2013
- » Hosseini, Ali, Espona-Fiedler, Margarita, Soto-Cerrato, Vanessa, Quesada, Roberto, Pérez-Tomás, Ricardo, Guallar, Victor, "Molecular Interactions of Prodigins with the BH3 Domain of Anti-Apoptotic Bcl-2 Family Members.", *PLoS one*, 8, 2, e57562, 2013
- » Islam, Barira, Sgobba, Miriam, Loughton, Charlie, Modesto Orozco, Sponer, Jiri, Neidle, Stephen, Haider, Shozeb, "Conformational dynamics of the human propeller telomeric DNA quadruplex on a microsecond time scale.", *Nucleic acids research*, 41, 4, 2723-35, 2013
- » Jiménez-García, Brian, Carles Pons, J. Fernández-Recio, "pyDockWEB: a web server for rigid-body protein-protein docking using electrostatics and desolvation scoring.", *Bioinformatics (Oxford, England)*, 29, 13, 1698-9, 2013
- » Julià, Antonio, Domènech, Eugeni, Ricart, Elena, Tortosa, Raül, García-Sánchez, Valle, Gisbert, Javier Pérez, Nos Mateu, Pilar, Gutiérrez, Ana, Gomollón, Fernando, Mendoza, Juan Luis, García-Planella, Esther, Barreiro-de Acosta, Manuel, Muñoz, Fernando, Vera, Maribel, Saro, Cristina, Esteve, Maria, Andreu, Montserrat, Alonso, Arnald, López-Lasanta, María, Codó, Laia, Gelpi, Josep Lluís, García-Montero, Andres C, Bertranpetit, Jaume, Absher, Devin, Panés, Julián, Marsal, Sara, "A genome-wide association study on a southern European population identifies a new Crohn's disease susceptibility locus at RBX1-EP300", *Gut*, 2013
- » Julià, Antonio, Domènech, Eugeni, Ricart, Elena, Tortosa, Raül, García-Sánchez, Valle, Gisbert, Javier Pérez, Nos Mateu, Pilar, Gutiérrez, Ana, Gomollón, Fernando, Mendoza, Juan Luis, García-Planella, Esther, Barreiro-de Acosta, Manuel, Muñoz, Fernando, Vera, Maribel, Saro, Cristina, Esteve, Maria, Andreu, Montserrat, Alonso, Arnald, López-Lasanta, María, Codó, Laia, Josep L Gelpi, García-Montero, Andrés, Bertranpetit, Jaume, Absher, Devin, Panés, Julián, Marsal, Sara, "A genome-wide association study on a southern European population identifies a new Crohn's disease susceptibility locus at RBX1-EP300", *Gut*, 2013
- » Lucas, M Fátima, Guallar, Victor, "Single vs. multiple ligand pathways in globins: A computational view.", *Biochimica et biophysica acta*, 2013
- » Lucas, M Fátima, Guallar, Victor, "Single vs. multiple ligand pathways in globins: A computational view", *Biochimica et biophysica acta*, 2013
- » Madadkar-Sobhani, Armin, Guallar, Victor, "PELE web server: atomistic study of biomolecular systems at your fingertips", *Nucleic acids research*, 41, Web Server issue, W322-8, 2013
- » Manuel Rueda, Modesto Orozco, Totrov, Maxim, Abagyan, Ruben, "BioSuper: a web tool for the superimposition of biomolecules and assemblies with rotational symmetry", *BMC structural biology*, 13, 32, 2013
- » Martín-Pintado, Nerea, Deleavey, Glen F, Portella, Guillem, Campos-Olivas, Ramón, Modesto Orozco, Damha, Masad J, González, Carlos, "Backbone FCH-O Hydrogen Bonds in 2'-F-Substituted Nucleic Acids", *Angewandte Chemie (International ed. in English)*, 2013
- » Michal Jamroz, Modesto Orozco, Andrzej Kolinski, Sebastian Kmiecik, "Consistent View of Protein Fluctuations from All-Atom Molecular Dynamics and Coarse-Grained Dynamics with Knowledge-Based Force-Field", 2013
- » Miki, Yuta, Pogni, Rebecca, Acebes, Sandra, Lucas, Fátima, Fernández-Fueyo, Elena, Baratto, Maria Camilla, Fernández, María I, de Los Ríos, Vivian, Ruiz-Dueñas, Francisco J, Sinicropi, Adalgisa, Basosi, Riccardo, Hammel, Kenneth E, Guallar, Victor, Martínez, Angel T, "Formation of a tyrosine adduct involved in lignin degradation by Trametesopsis cervina lignin peroxidase: a novel peroxidase acti-

- vation mechanism.", *The Biochemical journal*, 452, 3, 575-84, 2013
- » Moal, Iain H, Moretti, Rocco, Baker, David, J Fernández-Recio, "Scoring functions for protein-protein interactions.", *Current opinion in structural biology*, 23, 6, 862-7, 2013
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 - » Modesto Orozco, "The dynamic view of proteins: comment on Comparing proteins to their internal dynamics: exploring structure-function relationships beyond static structural alignments". *Physics of life reviews*, 10, 1, 29-30; discussion 39-40, 2013
 - » Moretti, Rocco, Fleishman, Sarel J, Agius, Rudi, Torchala, Mieczyslaw, Bates, Paul A, Kastritis, Panagiotis L, Rodrigues, João P G L M, Trellet, Mikael, Bonvin, Alexandre M J J, Cui, Meng, Rومان, Marianne, Gillis, Dimitri, Dehouck, Yves, Moal, Iain, Romero-Durana, Miguel, Perez-Cano, Laura, Pallara, Chiara, Jimenez, Brian, J Fernández-Recio, Flores, Samuel, Pacella, Michael, Praneeth Kilambi, Krishna, Gray, Jeffrey J, Popov, Petr, Grudin, Sergei, Esquivel-Rodriguez, Juan, Kihara, Daisuke, Zhao, Nan, Korkein, Dmitry, Zhu, Xiaolei, Demerdash, Omar N A, Mitchell, Julie C, Kanamori, Eiji, Tsuchiya, Yuko, Nakamura, Haruki, Lee, Hasup, Park, Hahnbeom, Seok, Chaok, Sarmiento, Jamaica, Liang, Shide, Teraguchi, Shusuke, Standley, Daron M, Shimoyama, Hiromitsu, Terashi, Genki, Takeda-Shitaka, Mayuko, Iwadate, Mitsuo, Umeyama, Hideaki, Beglov, Dmitri, Hall, David R, Kozakov, Dima, Vajda, Sandor, Pierce, Brian G, Hwang, Howook, Vreven, Thom, Weng, Zhiping, Huang, Yangyu, Li, Haotian, Yang, Xiufeng, Ji, Xiaofeng, Liu, Shiyong, Xiao, Yi, Zacharias, Martin, Qin, Sanbo, Zhou, Huan-Xiang, Huang, Sheng-You, Zou, Xiaoqin, Velankar, Sameer, Janin, Joël, Wodak, Shoshana J, Baker, David, "Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions.", *Proteins*, 81, 11, 1980-7, 2013
 - » Naganathan, Athi N, Modesto Orozco, "The conformational landscape of an intrinsically disordered DNA-binding domain of a transcription regulator.", *The journal of physical chemistry. B*, 117, 44, 13842-50, 2013
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 - » Pedro Sfriso, Hospital, Adam, Emperador, Agustí, Modesto Orozco, "Exploration of conformational transition pathways from coarse-grained simulations.", *Bioinformatics (Oxford, England)*, 29, 16, 1980-6, 2013
 - » Pérez-Cano, Laura, Eliahoo, Elad, Lasker, Keren, Wolfson, Haim J, Glaser, Fabian, Manor, Haim, Bernadó, Pau, J Fernández-Recio, "Conformational transitions in human translin enable nucleic acid binding", *Nucleic acids research*, 41, 21, 9956-66, 2013
 - » Portella, Guillem, Battistini, Federica, Modesto Orozco, "Understanding the connection between epigenetic DNA methylation and nucleosome positioning from computer simulations", *PLoS computational biology*, 9, 11, e1003354, 2013
 - » Raimondi, Francesco, Felling, Angelo, Portella, Guillem, Modesto Orozco, Fanelli, Francesca, "Light on the structural communication in Ras GTPases", *Journal of biomolecular structure & dynamics*, 31, 2, 142-57, 2013
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 - » Rao, Satish, Raj, Saurabh, Cossins, Benjamin, Marro, Monica, Guallar, Victor, Petrov, Dmitri, "Direct observation of single DNA structural alterations at low forces with surface-enhanced Raman scattering.", *Biophysical journal*, 104, 1, 156-62, 2013
 - » Saen-oon, Suwipa, Lucas, Maria Fatima, Guallar, Victor, "Electron transfer in pro-

- teins: theory, applications and future perspectives.", *Physical chemistry chemical physics : PCCP*, 15, 37, 15271-85, 2013
- » Sciabola, Simone, Cao, Qing, Modesto Orozco, Faustino, Ignacio, Stanton, Robert V, "Improved nucleic acid descriptors for siRNA efficacy prediction.", *Nucleic acids research*, 41, 3, 1383-94, 2013
 - » Spyralis, Francesca, Lucas, Fátima, Bidon-Chanal, Axel, Viappiani, Cristiano, Guallar, Victor, Luque, F Javier, "Comparative analysis of inner cavities and ligand migration in non-symbiotic AHb1 and AHb2.", *Biochimica et biophysica acta*, 2013
 - » Terrazas, Montserrat, Alagia, Adele, Faustino, Ignacio, Modesto Orozco, Eritja, Ramon, "Functionalization of the 3'-ends of DNA and RNA strands with N-ethyl-N-coupled nucleosides: a promising approach to avoid 3'-exonuclease-catalyzed hydrolysis of therapeutic oligonucleotides", *Chembiochem: a European journal of chemical biology*, 14, 4, 510-20, 2013
 - » Tim Meyer, Gabelica, Valérie, Helmut Grubmüller, Modesto Orozco, "Proteins in the gas phase", 2013
 - » Torchala, Mieczyslaw, Moal, Iain H, Chaleil, Raphael A G, J Fernández-Recio, Bates, Paul A, "SwarmDock: a server for flexible protein-protein docking", *Bioinformatics (Oxford, England)*, 2013
 - » Valdés, James J, Schwarz, Alexandra, Cabeza de Vaca, Israel, Calvo, Eric, Pedra, Joao H F, Guallar, Victor, Kotsyfakis, Michalis, "Tryptogalinin is a tick Kunitz serine protease inhibitor with a unique intrinsic disorder", *PLoS one*, 8, 5, e62562, 2013
 - » Wallrapp, Frank H, Voityuk, Alexander A, Guallar, Victor, "In-silico assessment of protein-protein electron transfer: a case study: cytochrome c peroxidase-cytochrome c.", *PLoS computational biology*, 9, 3, e1002990, 2013

International Conferences

- » Modesto Orozco, "DNA simulation in the postgenomic era". Plenary lecture. Department of Pharmacy, North Carolina State University", North Carolina, US, 2013
- » Modesto Orozco, "Expanding the frontiers of molecular dynamics simulations of DNA". CECAM Conference. University of Vienna", Vienna, Austria, 2013
- » Modesto Orozco, "Exploring protein flexibility". Plenary Lecture. Cambridge University", Cambridge, UK, 2013
- » Modesto Orozco, "In Silico Biology" Ciclo de Conferencias Montpellier", Zaragoza, Spain, 2013
- » Modesto Orozco, "Multilevel simulation of DNA". Invited lecture. American Chemical Society Meeting, New Orleans, US, 2013
- » Modesto Orozco, "New challenges in the representation of protein dynamics". Plenary Lecture. Institute of Nanosciences", Lucca, Italy, 2013
- » Modesto Orozco, "The molecular basis of the transport cycle of APC antiporters". Invited Talk. PRACE Scientific Conference", Leipzig, Germany, 2013
- » Modesto Orozco, "When mass spectroscopy and molecular simulations meet". Invited Talk. CECAM Meeting. Frontiers of Computational Biomolecular Spectroscopy and Mass Spectrometry", Jülich, Germany, 2013
- » Modesto Orozco, "When physics and biology meet. The 2013 Nobel Award of Chemistry". Sant Albert Plenary Lecture. Physical Engineering Sant Albert Plenary Lecture", Barcelona, Spain, 2013
- » Modesto Orozco, "Data deluge in genomics". Roche-Instituto Principe Felipe meeting on "Sequencing in the clinical practices", Valencia, Spain, 2013
- » Modesto Orozco, "DNA from the electron to the chromatin VIII", Biogune Anniversary Distinguished Lecture", Bilbao, Spain, 2013

Theses

- » Ignacio Faustino Pló, "Estudio teórico de formas inusuales y modificadas de los ácidos nucleicos", 2013
- » Pérez Cano, Laura, "Structural prediction and characterization of protein-RNA interactions", 2013

» Computer Applications in Science & Engineering (CASE) 2013 Publications

Journals

- » A Costa, Arnau Folch, G Macedonio, "Density-driven transport in the umbrella region of volcanic clouds: Implications for tephra dispersion models", *Geophysical Research Letters*, 40, 41760, 2013
- » A. Arbona, Antoni Artigues, C. Bona-Casas, J. Massó, B. Miñano, A. Rigo, M. Trias, C. Bona, "Simflowny: A general-purpose platform for the management of physical models and simulation problems", *Computer Physics Communications*, 184, 10, 2321-2331, 2013
- » B. Eguzkitza, Guillaume Houzeaux, H. Calmet, Mariano Vázquez, B. Soni, S. Alibadi, A. Bates, D. Doorly, "A Gluing Method for Non-Matching Meshes", *Computers and Fluids*, 2013
- » Bonasia, Rosanna, Scaini, Chiara, Capra, Lucia, Nathenson, Manuel, Araña Salinas, Lilia, Siebe, Claus, Arnau Folch, "Long-range hazard assessment of volcanic ash dispersal for a Plinian eruptive scenario at Popocatepet volcano (Mexico): implications for civil aviation safety", *Bulletin of Volcanology*, 76, 789, 2013
- » A. Cresti, T. Louvet, F. Ortmann, D. Van Tuan, P. Lenarczyk, G. Huhs, S. Roche, "Impact of Vacancies on Diffusive and Pseudodiffusive Electronic Transport in Graphene", *Crystals*, 3, 289-305, 2013
- » Daniel Mira, Xi Jiang, "Large-eddy simulations of unsteady hydrogen annular flames", *Computers & Fluids*, 80, 429 - 440, 2013
- » Daniel Mira, Xi Jiang, "Numerical investigations of a hydrogen impinging flame with different finite-rate chemical kinetic mechanisms", *Fuel*, 109, 285-296, 2013
- » Daniel Mira, Xi Jiang, Charles Moulinec, D.R. Emerson, "Numerical investigation of the effects of fuel variability on the dynamics of syngas impinging jet flames", *Fuel*, 103, 646-662, 2013
- » Daniel Mira, Xi Jiang, Charles Moulinec, David R. Emerson, "Numerical simulations of turbulent jet flames with non-premixed combustion of hydrogen-enriched fuels", *Computers & Fluids*, 88, 688 - 701, 2013
- » E. Collini, M.S. Osoro, Arnau Folch, J. Viramonte, Villarosa, G., Salmuni, G., "Volcanic ash forecast during the June 2011 Cordón-Caulle eruption", *Natural hazards*, 66, 389-412, 2013
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- » Felix Rubio, Albert Farrès, Mauricio Hanzich, Josep de la Puente, Miguel Ferrer, "Optimizing Isotropic and Fully-anisotropic Elastic Modelling on Multi-GPU Platforms", 75th EAGE Conference & Exhibition, Tu-P10-13, 2013
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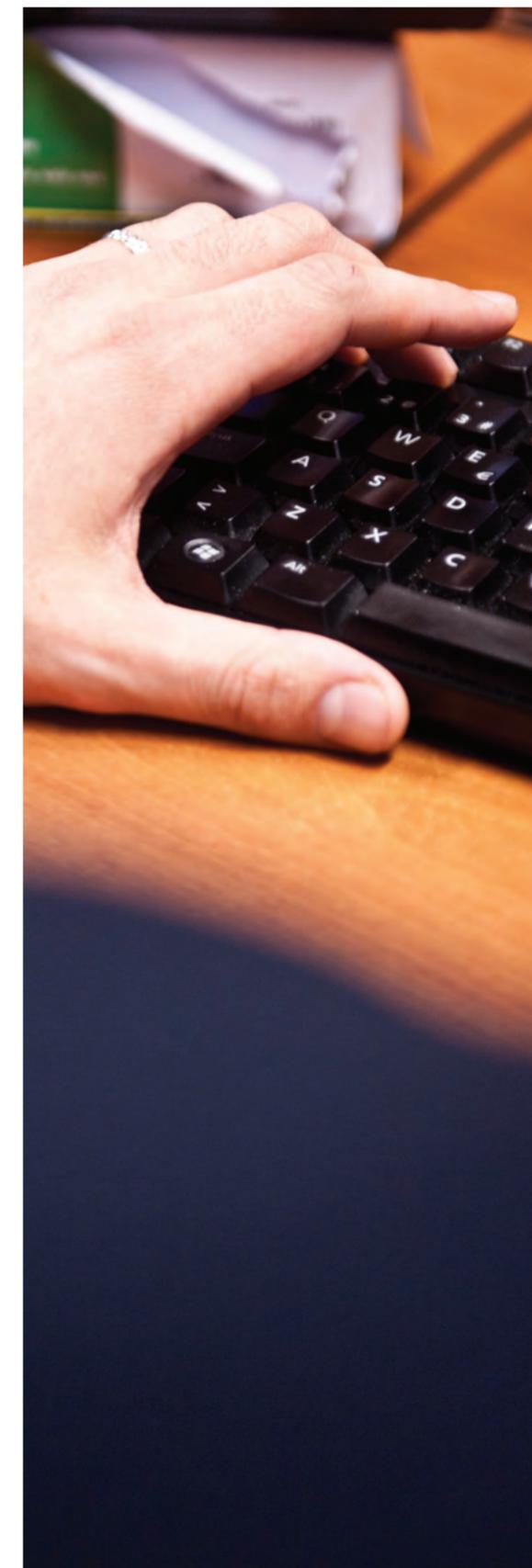
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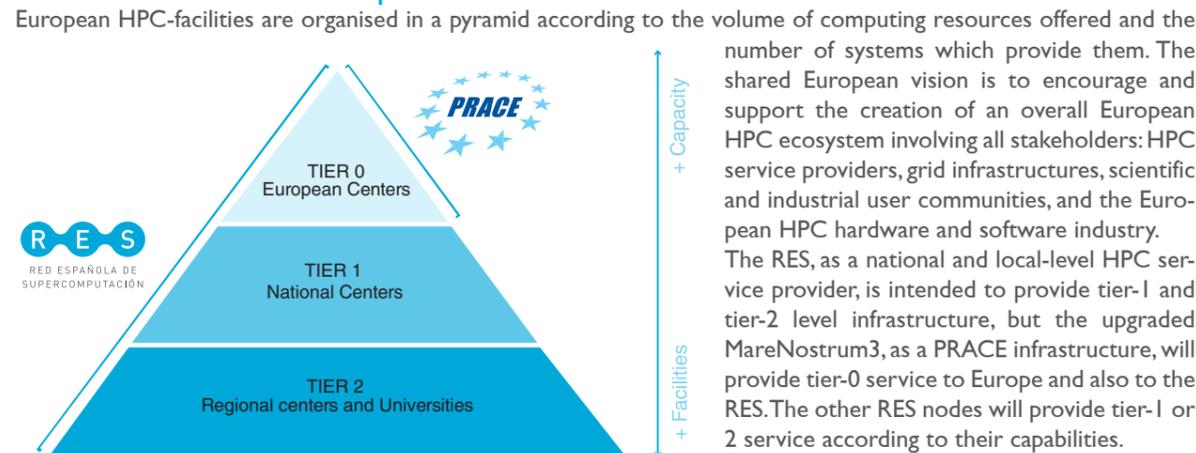


Two RES nodes were significantly upgraded in 2013: MareNostrum increased its capacity reaching 1,1 PFLOP/s and Picasso achieved 63 TFLOP/s, thereby tripling the global computing capacity of the supercomputers participating in the RES network. In spite of these increased resources, the long-term trend of increasing user demand meant that demand still exceeded available capacity by 47%. A total of 268 activities were run on RES nodes during 2013. This brings to more than 2.150 the number of different projects awarded 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 the user groups amongst all scientific fields, ensuring that the HPC resources of the RES are fully utilised to support scientific progress throughout the country.



Location of the nodes of the Spanish Supercomputing Network (RES)

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



» 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.

RES Processing Power in TFLOPs/s in December 2013



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 user support.

A major upgrade which commenced in 2012 was completed in 2013, with 7 of the 9 supercomputers included in the RES alliance upgraded during this period. Of particular note, the new MareNostrum offers eleven times the processing capability of the former machine. Such major upgrades require significant long term planning and coordination amongst all RES nodes, support teams and equipment suppliers, demonstrating the commitment of the Spanish government and the RES network to provide top-class HPC services to the Spanish scientific community, hence ensuring the competitiveness of Spanish science.

» 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, and are evaluated by a single Access Committee.

The allocation of access to the supercomputing facilities is based on criteria of efficacy, efficiency and transparency. First a formal and technical review 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. This is composed of a Core Team and four Scientific Expert Panels formed by prestigious scientists external to BSC-CNS and defined according to the classification established by the Spanish Foundation of Science and Technology (FECYT).

The Expert Panels

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

The Access Committee Core Team in 2013

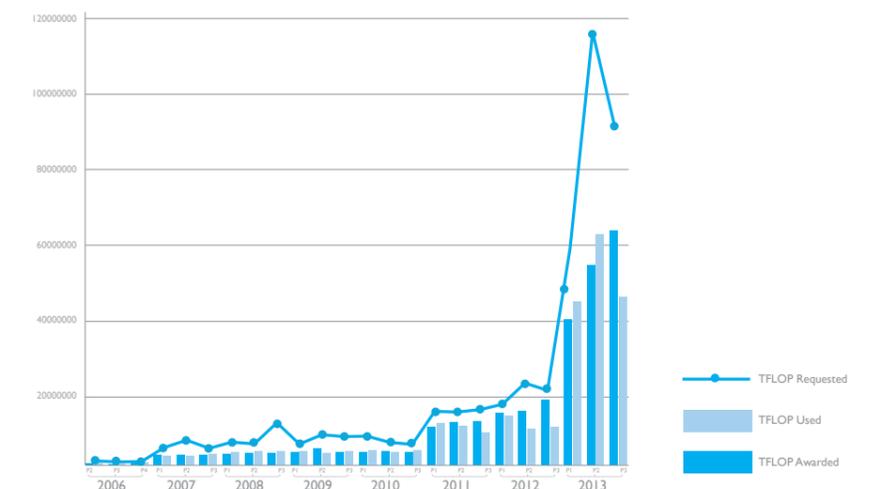
- ▶ Joaquin Serrano, MINECO
- ▶ Julio Bravo, ANEP
- ▶ Alfonso Tarancón, BIFI-Universidad de Zaragoza
- ▶ Eduard Ayguadé, BSC-CNS

More than 98 million hours were awarded by the Access Committee in the 3 calls for applications that took place during 2013. In addition to internal research activities of the RES nodes, more than 100 external research projects made use of the RES system in 2013. It is important to note that many scientific projects often request several periods of access during the year (each access lasts 4 months) in order to perform different work activities. As specified in the Access Protocol, each request is treated separately and must pass the evaluation procedure of the Access Committee. Consequently, the number of activities reported for the RES is 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 the users, preparing their software for loading and running, and ensuring access to results data and also statistics on the performance of the code, so as to facilitate future code improvements.

The graph shows the evolution of requested, assigned and used TFLOP since the founding of the RES. It clearly shows how demand has always remained higher than the resources offered, and how any upgrades in capacity are quickly absorbed, as can be clearly seen in the first and second upgrades of MareNostrum that took place in 2008 and 2013. The used TFLOP bar in the last period of 2013 is lower because the usage ends in February 2013 and therefore the data is incomplete.



» CURES, the RES Users Committee

The 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.

The CURES members in 2013

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

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

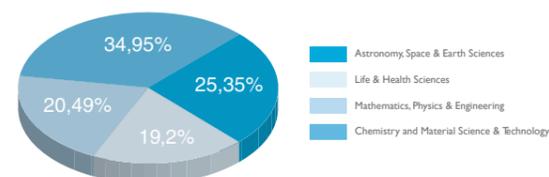
» Broad Impact on Scientific Research

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



Geographical precedence of the RES users during 2013

The different research activities carried out on RES supercomputers during 2013 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 2013

» 7th RES User Conference



Poster of the 7th RES User Conference

The 7th RES Users Conference took place in Barcelona on 13th September 2013. The aim of the meeting was to promote the available resources and services, explain procedures for requesting time and reviewing of proposals, disseminate the results obtained using the RES, and to offer a discussion forum between users, the CURES and RES coordinators.

Five different sessions were held: Resources and services offered by the RES and PRACE, The challenge of moving from Tier-I to Tier-0 supercomputers, Service to research for technological development, Service to fundamental research, and Visualization as a tool for research. Planned to coincide with the Users Conference, the 2nd Annual HPC Advisory Council Spain Conference was held on the previous day, co-organised by BSC-CNS and the HPC Advisory Council, a network of experts from some of the leading global HPC companies.

More information is available at <http://www.bsc.es/marenostrum-support-services/hpc-education-and-training/res-trainings-seminars/res-users-meetings>

» RES User Trainings

Access to supercomputing services in BSC-CNS, RES and PRACE • Two meetings were organised in the first quarter of 2013 in Madrid (co-organised with CSIC) and Barcelona, to inform the national scientific community of the new resources available following the upgrade of several RES supercomputers. The characteristics of PRACE were explained to facilitate Spanish scientists applying to the PRACE 6th and 7th Regular Call.

Details on Access to supercomputing services in BSC-CNS, RES and PRACE + Specific training for RES users in the IAC • User meeting and training sessions were held in Tenerife at the request of scientists at IAC. Training was provided on how to submit serial jobs to the LaPalma node, and information was provided on the resources available at RES and PRACE, and on how to apply to the PRACE 7th Regular Call.

Access to supercomputing services in UMA, BSC, RES and PRACE • A similar event was held in Málaga in order to let the researchers know the characteristics and services offered by the new Picasso and the other RES supercomputers, as well as the mechanism to request access to PRACE and promote the application to the PRACE 7th Regular Call.

Access to supercomputing services in BIFI-UZ, BSC, RES and PRACE • The user meeting was held in Zaragoza to report on the HPC services offered by BIFI-UZ via the supercomputers Terminus, Memento and Caesarugusta or the possibility of hosting clusters of research teams. Moreover, the computing services through Grid and Cloud computing were explained because the BIFI-UZ cooperates in several projects as NGI and Ibergrid, EGI-InSPIRE, SCI-BUS, CloudSME, AraGrid and Cloud OpenStack. Also details were provided regarding the Ibercivis Foundation, a private non-profit organization created in 2011 and whose main objective is to promote the distributed computing effort using the resources provided by citizens. Finally, information about the RES supercomputers was supplied, as well as the mechanism to request access to PRACE and promote the application to the PRACE 7th Regular Call.

PUMPS Summer School • The fourth edition of the Programming and Tuning Massively Parallel Systems summer school (PUMPS) was held in Barcelona and coorganised 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.

Scientific seminars • Scientific Supercomputing in Euskadi 2013 • This was the first RES conference celebrated in Euskadi and was organized with support and cooperation of i2Basque, a program of the Department of Education, Linguist and Cultural Policy of the Basque Government, that provides academic and research institutions of communications services, High Performance Computing, video and multimedia content and online repositories. The conference was broadcasted to 4 different locations to maximize its diffusion and attendance. It was aimed to inform the scientific community of the Basque Country about the supercomputing resources and services that provide the BSC-CNS, the RES, PRACE, i2Basque and the EHU (Euskal Herriko Unibertsitatea). Furthermore, relevant projects developed by Basque researchers, such as the Biosoft Project, were presented. Besides, two projects with access to RES and PRACE, respectively, were presented, to let the researchers share its experience with the attendees and promote the usage of the available resources.



Poster of the Access to supercomputing services in BSC, RES and PRACE meetings

» Overview



Magerit Supercomputer

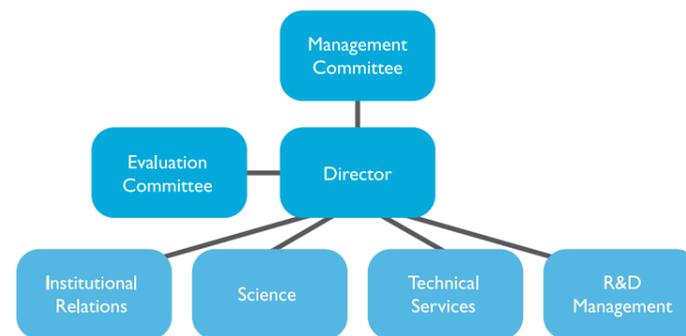
CeSViMa (Supercomputing and Visualization Centre of Madrid, in Spanish "Centro de Supercomputación y Visualización de Madrid") is located in the Excellent IT and Technology Transfer Montegancedo Campus, one of the sites of the Technical University of Madrid Science & Technology Park. CeSViMa, which is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

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

» Organisational Structure



CeSViMa Team as of January 2013



» Technical and Scientific Highlights 2013

Key Publications 2013

Articles

- A methodology to compare Dimensionality Reduction algorithms in terms of information loss, Gracia, A. and González, S. and Robles, V. and Menasalvas, E.
- Analysis of a rate-adaptive reconciliation protocol and the effect of leakage on the secret key rate, Elkouss, David and Martínez-Mateo, Jesús and Martín, Vicente
- BaP (PAH) air quality modelling exercise over Zaragoza (Spain) using an adapted version of WRF-CMAQ model, Roberto San José AND Juan Luis Pérez AND María Soledad Callén AND José Manuel López AND Ana Mastral
- Effect of van der Waals interaction on the properties of SnS₂ layered semiconductors, Y. Seminóvski, P. Palacios, P. Wahnón
- Evolution of a long-lived FLOSS project, Jesús González-Barahona, Gregorio Robles, Israel Herraiz, Felipe Ortega
- Improving collaborative filtering based recommender systems using Pareto dominance, Ortega, F., Sánchez, J. L., Bobadilla, J., Gutiérrez, A.
- Incorporating group recommendations to recommender systems: Alternatives and performance, Ortega, F., Bobadilla, J., Hernando, A., Gutiérrez, A.
- Incorporating reliability measurements into the predictions of a recommender system, Hernando, A., Bobadilla, J., Ortega, F., Tejedor, J.
- Key Reconciliation for High Performance Quantum Key Distribution, Martínez-Mateo, Jesús and Elkouss, David and Martín, Vicente
- Learning mixtures of polynomials of multidimensional probability densities from data using B-spline interpolation, López-Cruz, P. L. and Bielza, C. and Larrañaga, P.
- Nonequilibrium and nonperturbative dynamics of ultrastrong coupling in open lines, Peropadre, B. and Zueco, D. and Porras, D. and García-Ripoll, J.
- Obtaining an Intermediate Band Photovoltaic Material through the Bi insertion in CdTe, Y. Seminóvski, P. Palacios, P. Wahnón

- Parameter control of genetic algorithms by learning and simulation of Bayesian networks— A case study for the optimal ordering of tables, Bielza C., Fernández del Pozo JA, Larrañaga P.
- Recommender systems survey, Bobadilla J., Hernando, A., Ortega, F., Gutiérrez, A.
- Reduction of the fast electron angular dispersion by means of varying-resistivity structured targets, A. Debayle, L. Gremillet, J. J. Honrubia and E. d'Humieres
- Simple model for chain packing and crystallization of soft colloidal polymers, R. S. Hoy and N. C. Karayiannis
- Statistical mechanics as guidance for particle-based computational methods, I. G. Tejada and R. Jimenez
- Toward a self-consistent model of the interaction between an ultra-intense, normally incident laser pulse with an overdense plasma, A. Debayle, J. Sanz, L. Gremillet, and K. Mima
- Trees for explaining recommendations made through collaborative filtering, Hernando, A., Bobadilla, J., Ortega, F., Gutiérrez, A.

Phd Thesis

- Contributions to Bayesian network learning with applications to neuroscience, López-Cruz, P. L.

Proceedings

- Bulk modulus for solid molecular tritium: ab initio approximation, Carlo Guerrieri AND Jose M. Perlado
- Sample size vs. bias in defect prediction, Foyzur Rahman, Daryl Posnett, Israel Herraiz, Premkumar Devanbu

Conference

- Sample size vs bias in defect prediction, Foyzur Rahman and Daryl Posnett and Israel Herraiz and Premkumar Devanbu

Key Projects 2013

- Implementation of new exchange correlation functionals and molecular dynamics calculations in Octopus, Joseba Alberdi
- Properties of epitaxial graphene on Ru(0001), Manuel Alcamí Peretejo
- 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
- Super resolution studies, Pablo Benitez Giménez
- 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, José Antonio Cobos Márquez
- Parameter Control of Genetic Algorithms, Juan Antonio Fernández del Pozo de Salamanca
- Catalysis modeling: 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
- MEDVIR: 3D visual interface applied to gene profile analysis, Santiago González Tortosa
- Paralelización de algoritmos de optimización aplicados a la segmentación de imágenes multispectrales, Consuelo Gonzalo Martín
- Mining Software Repositories, Israel Herraiz Tabernero
- Electron acceleration in relativistic laser-plasma interactions, José Javier Honrubia Checa
- Electronic structure of semiconductors by means of quasiparticle calculations: relevance to photocatalysis, Francesc Illas
- Caracterización del microbioma de la caña de azúcar, Juan Imperial Ródenas
- Aplicación de supercomputación distribuida al análisis de secuencias genómicas y a la modelización enzimática, Juan Imperial Ródenas
- Simulación del comportamiento en solución de proteínas implicadas en el ensamblaje de la hidrogenasa, Juan Imperial Ródenas
- Aplicación de la física estadística a la mecánica de medios granulares, Rafael Jimenez
- Modeling of Synthetic and Biological Micromolecules Through a Hierarchical Multiscale Approach, Nikos Karayiannis
- 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: GICC-UPM, Vicente Martín Ayuso
- 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
- Role of triplet excitons in the photocatalysis of water and methanol on rutile 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
- Numerical study of disordered localized electronic systems using energy minimization, Matteo Palassini
- Optimization Algorithms, José María Peña Sánchez
- Blue Brain Project, José María Peña Sánchez
- Heuristic Optimization Tuning, José María Peña Sánchez
- Primer Extractor Browser Plugin, David Perez del Rey
- QUITEMAD: MIC, David Pérez García
- Carbon nanostructures and hydrogen production and storage by first-principles calculations and scanning probe techniques, Rubén Pérez Pérez
- Colaboración Instituto de Fusión Nuclear, 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, Ángel Rubio
- INTI, Juan Luis Sampedro
- 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
- 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

» Overview



The LaPalma Supercomputer

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 Telescope 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

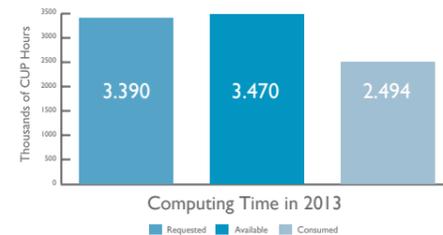
The Time Assignment Commission manages the 50 percent of the CPU time of LaPalma. Its members come from different divisions of the Instituto de Astrofísica de Canarias (IAC). For administration and management of the supercomputer node, the IAC makes available its IT support team and additionally has employed one engineer dedicated full-time to fulfil these functions.

The LaPalma Supercomputer Systems & Support Team: Antonio Jiménez Mancebo (PhD), Head of the I.T. Common Services (SIC); Carlos Martín Galán (Senior Engineer), Technician Responsible of SIC; Antonio Díaz China (Senior Engineer), System Administrator; Justo Luna López (Engineer), System Administrator; Ubay Dorta Guerra (Engineer), System Administrator and User Support; Antonio Dorta Lorenzo (PhD), User Support; Victor Plasencia Darías (Operator), User Support.



» Technical and Scientific Highlights 2013

Before 2013, the network connection between IAC facilities and mainland Spain was 625Mbps. Thanks to Project RedIRISNova, developed by the Spanish NREN (National Research and Education Network), IAC is now connected via a 10Gbps link to the mainland. LaPalma can use up to 4 Gbps of that link. In 2013 LaPalma provided roughly 3470k hours of CPU time for IAC researchers. Their projects consumed 72% of available time.



Key Publications 2013

Colloquiums • Mohamed, S., "Unwinding the secrets of a dying star", Colloquium at South African Astronomical Observatory (2013).

Journals • Beck, C.; Fabbian, D.; Moreno-Insertis, F.; Puschmann, K. G.; Rezaei, R., "Thermodynamic fluctuations in solar photospheric three-dimensional convection simulations and observations", *Astronomy & Astrophysics*, Volume 559, C1 (2013) • Mészáros, S.; Holtzmann, J.; García Pérez, A.; Allende Prieto, C. et al., "Calibrations of Atmospheric Parameters Obtained from the First Year of SDSS-III APOGEE Observations Based on Open and Globular Clusters", *The Astronomical Journal*, Volume 146, A133 (2013) • Moreno Insertis, F.; Galsgaard K., "Plasma Jets and Eruptions in Solar Coronal Holes: a 3D flux emergence experiment", *The Astrophysical Journal*, Volume 771, A20 (2013) • Parviainen, H.; Deeg, H.; Belmonte, Juan A., "Secondary Eclipses in the CoRoT Light Curves. A Homogeneous Search Based on Bayesian Model Selection", *Astronomy & Astrophysics*, Volume 550, A67 (2013) • Št pán, J.; Bueno, T., "PORTA: A 3D Multilevel Radiative Transfer Code for Modeling

the Intensity and Polarization of Spectral Lines with Massively Parallel Computers", *Astronomy & Astrophysics*, Volume 557, A143 (2013) • Sanromá, E.; Pallé, E.; García-Muñoz, A., "On the effects of the evolution of microbial mats and land plants on the Earth as a planet. Photometric and spectroscopic light curves of paleo-Earths", *The Astrophysical Journal*, V766, A133 (2013) • Schmieder, B.; Guo, Y.; Moreno-Insertis, F. et al., "Twisting solar coronal jet launched at the boundary of an active region", *Astronomy & Astrophysics*, Volume 559, A1 (2013)

Proceedings • Frinchaboy, P. M.; O'Connell, J.; Meszaros, S. et al., "SDSS-III/APOGEE: Science and Survey Calibrations and using Open Clusters", *American Astronomical Society Meeting Abstracts*, #221, #250.34 (2013)

Symposiums • Martínez González, M. J.; Manso Sainz, R.; Asensio Ramos, A.; de la Cruz Rodríguez, J.; Beck, C., "Observation of the magnetic field in solar tornadoes", *IAUS300 - Nature of prominences and their role in space weather*, Paris, France, 10-16 June 2013.

sdss3.org/instruments/telescope.php and obtains 300 stellar spectra simultaneously, which allows the completion of the project using only the bright time (when the moon is up) for three years, ending in June 2014. Thanks to using near-infrared light, which penetrates interstellar dust much better than optical light, APOGEE can measure the chemical composition of stars in the central parts of the Galaxy and throughout the Galactic disk.

Synthesis of Stokes profiles in 3D snapshots of solar magnetoconvection (PI.: Andrés Asensio Ramos) • A recent striking result in the study of the magnetism of the quiet Sun has been the discovery of dipolar structures emerging in the photosphere (Martínez González et al. 2007). In spite of their small size, they can be of importance for the energy balance in the solar atmosphere. Additionally, it has been found that the emergence of such dipolar structures is not distributed randomly on the solar surface (Martínez González et al. 2012). Clear voids that cannot be explained as random fluctuations of a Poisson point process are detected. The spatial distribution of such events follow a filamentary structure. We argue that these spatial statistical properties are a consequence of the specific mechanism that generates these fields in the very quiet Sun. The aim of the project is to use recent large-scale simulations of solar magnetoconvection (Stein 2012) to identify these structures in the simulations exactly as we do in the observations. This step of going through the observables is important to correctly identify the process responsible for the appearance of the polarimetric signals. This will help us identify the specific process of emergence and whether the simulations can explain the measured spatial statistics. We are currently analysing the results and we expect to publish a paper describing the results during 2014. (Martínez González, M. J., Pastor Yabar, A., Asensio Ramos, A., Manso Sainz, R., in preparation)

Inversion of spectropolarimetric data of chromospheric structures (PI.: Andrés Asensio Ramos) • Prominences, filaments and spicules are some of the chromospheric structures that we find lying at coronal heights in active stars like the Sun. These structures are made of cool plasma at temperatures around 10000 K embedded in the million K corona. It is thought that they are shaped and maintained by the magnetic field. During the last few decades, we have witnessed a slow increase in the number of spectropolarimetric observations of these objects. Only in the last few years, we have available the tools to observe them with high spatial and temporal resolution with enough polarimetric sensitivity to detect the four Stokes parameters. The Hazel code is an advanced inversion tool that allows us to obtain the thermodynamical and magnetic properties of such chromospheric structures. This code takes into account all the physical mechanisms that generate and modify the polarization in selected spectral lines. The aim of the project is to invert several maps that we have observed during the last two years with the Tenerife Infrared Polarimeter. The inversion process is computationally heavy and a supercomputer is needed in order to get the maps inverted. Additionally, the physical effects involved in the generation of the signals are prone to ambiguities and several such inversions are needed per map to capture all these ambiguities. The results have been submitted for publication. (Martínez González, M. J., Manso Sainz, R., Asensio Ramos, A., de la Cruz Rodríguez, J., Beck, C., submitted)

Smoothed Particle Hydrodynamic Simulations of the symbiotic binary, R Aquarii (PI.: Romano Corradi) • Jets are a common phenomenon in astrophysics. They are produced in young and old stars, interacting binaries with white dwarfs, neutron stars or black holes, and on scales of galaxies, AGNs, radio galaxies, and quasars. However, the physical processes by which the jets are launched operate on size scales that it is not possible to spatially resolve. In this respect, the highly evolved symbiotic binary star R Aqr displays what is perhaps the most propitious system to study, because it is one of the closest stellar jets (200 pc) and is bright and active. For this reason, we have embarked in an comprehensive study of R Aqr. Our multi-epoch imaging over several years reveals the evolution of the R Aqr outflows in real-time. Our goal is to support this accurate observational study with a detailed modelling of the system, taking advantage of the fully-tested Smoothed Particle Hydrodynamics code developed by S. Mohamed. The simulation allows

us to investigate the mass transfer processes in the binary system, to determine the mass accretion rate and hence the formation of the accretion disc which is supposed to be at the origin of the jet, and to determine the distribution of the circumstellar gas and dust through which the jet propagates. This is the first time that such a detailed comparison between observations and models is attempted. The models of R Aquarii that we have produced so far show significant departures from spherical symmetry of the circumstellar matter. Although the stars are separated by 15 AU, the initially spherical wind from the red giant star gets distorted by the gravity of the white dwarf companion. The slow moving wind material is focused through the inner Lagrange point and begins to form an accretion disk. The disk has not yet reached a steady state after 3 orbits and continues to grow; the average accretion rate is still increasing. Because the orbit is not circular, the amount of material transferred increases substantially at periastron (when the two stars are closest to each other). Some material is flung out from the binary, gets shocked and forms dense, gaseous spiral arms. The material between these spiral arms is cold and dense enough to condense and form dust grains. This results in the formation of dusty arcs seen in white in Fig. 1 surrounding the much hotter, dust-free circumbinary cavity.

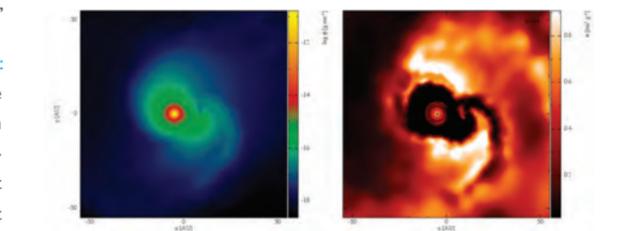


Fig. 1: A cross-sectional profile in the binary orbital plane of the gas density [left] and dust opacity [right].

Solar magneto-convection simulations and spectral synthesis for accurate chemical abundance determinations (PI.: Damian Fabbian) • Magnetic fields are ubiquitous in the photosphere of the Sun. Their presence influences the formation of spectral lines both directly and indirectly. Since the latter are commonly used to derive the abundance of chemical elements in the atmosphere of the Sun (and of stars in general), it is important to explore what influence magnetic fields have on abundance (i.e., chemical composition) estimates resulting from this method. This research project has used temporal snapshots from three-dimensional magnetohydrodynamic (3D MHD) "box in a star" radiation-convection simulations of the solar surface obtained via the parallel Stagger code by A. Nordlund (Nordlund 1982, Stein & Nordlund 1989). The resulting datacubes were fed as input to the non-LTE Stokes spectral synthesis code NICOLE (Socas-Navarro et al. 2013). We then compared the output theoretical line and continuum intensity profiles obtained for series of simulations with different amounts of magnetic flux, in order to study its effects on the formation of the solar spectrum.

The dynamics and magnetism of the solar atmosphere (PI.: 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. We use the radiation-MHD numerical code Bifrost which can be run in massively parallel mode over hundreds of CPUs using Message Passing Algorithms. The code contains LTE radiation transfer, scattering, optically thin radiation cooling and thermal (Spitzer) conduction. The processes studied in the 2013 campaigns involve the emergence of magnetic flux through a layer of convection cells of granular and mesogranular sizes, their passage through the photosphere and the rise into the corona, yielding a chromospheric jet, plasmoid production, a hot coronal jet and various attendant phenomena.

» Overview



The Atlante Supercomputer

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

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

Atlante was upgraded as a result of the installation of MareNostrum III at BSC-CNS, by virtue of the agreement between RES nodes. Atlante now offers 96TB of storage disk.

» Organisational Structure

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



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

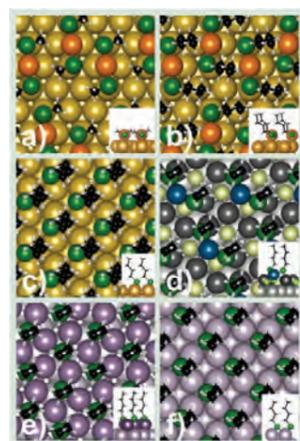
» Technical and Scientific Highlights 2013

In 2013 Atlante's local access granted 8 local projects corresponding to Canary Islands companies and researchers. They ran 796K hours of CPU time, related to the following projects and publications:

Key Publications 2013
Journals

- ▶ P. Carro, E. Pensa, C. Vericat, and R. C. Salvarezza. Hydrocarbon Chain Length Induces Surface Structure Transitions in Alkanethiolate Gold Adatom Self-Assembled Monolayers on Au(111). *The Journal of physical Chemistry C* 2013, 117, 2160-2165
- ▶ Julio C. Azcárate, Gastón Corthey, Evangelina Pensa, Carolina Vericat, Mariano H. Fonticelli, Roberto C. Salvarezza, and Pilar Carro. Understanding the Surface Chemistry of Thiolate-Protected Metallic Nanoparticles. *The Journal of physical Chemistry Letters* 2013, 4, 3127-3138

Key Projects 2013



Optimized structures for alkanethiols on different metal surfaces

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

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.

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 analyzed 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.

Dragon Airborne Power 10kW Prototype Simulation

Dragon Airborne Power has been actively pursuing the development of high-altitude wind power systems. To this end, the simulation of the external aerodynamic flow and energy-capturing process on a model of their first 10kW airborne turbine prototype was carried out using the finite-volume discretization of the Navier-Stokes equations through the Code Saturne flow solver on Atlante. This work has set the basic parameters of the design configuration in the form of calculated power levels, lift/drag/moment coefficients and stability derivatives. The use of these parameters is fundamental to the detailed structural and controls design being presently undertaken as a last step before prototype manufacture and operation.

» Overview

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

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

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

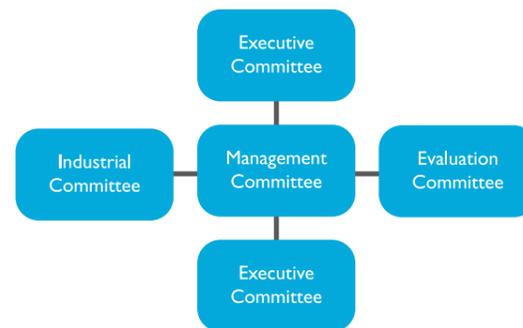
The Altamira node was upgraded in June 2012 with the installation of a new system at IFCA datacenter room. The system was presented on October 3rd, 2012. The current systems in the ALTAMIRA node is composed of 158 IBM-iDataPlex servers interconnected with Mellanox InfiniBand fabric. Also, ALTAMIRA has 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 2013

In 2013 the Altamira node executed applications corresponding to local users at the University of Cantabria with about a million hours of CPU.

Key Publications 2013

- ▶ Pablo Aguado-Puente; Javier Junquera; First-principles study of metal-induced gap states in metal/oxide interfaces and their relation with the complex band structure. *MRS Communications* 3.
- ▶ Abel García-Saiz; Dr. Pedro Migowski; Dr. Oriol Vallcorba; Prof. Javier Junquera; Prof. Jesús Angel Blanco; Prof. Jesús Antonio González; Dr. María Teresa Fernández-Díaz; Prof. Jordi Rius; Prof. Jairton Dupont; Prof. Jesús Rodríguez Fernández; Dr. Imanol de Pedro; A Magnetic Ionic Liquid Based on Tetrachloroferrate Exhibits Three-Dimensional Magnetic Ordering: A Combined Experimental and Theoretical Study of the Magnetic Interaction Mechanism. *Chemistry - A European Journal*.
- ▶ Harald Servat; Germán Llorit; Judit Giménez; Jesús Labarta; Detailed and simultaneous power and performance analysis. *Concurrency and Computation: Practice and Experience*.

Key Projects 2013

Genomic characterization of human tumours

Ignacio Varela leads a new research line in IBBTEC (Instituto de Biomedicina y Biotecnología de Cantabria) that uses the newly developed ultrasequencing technologies (NGS) to characterise at the genomic level human and mouse tumours in order to identify new molecular mechanisms involved on tumour progression and metastasis that could be used as therapeutic targets. This line is at the moment funded by the National Research Plan and a proposal for ERC funding is

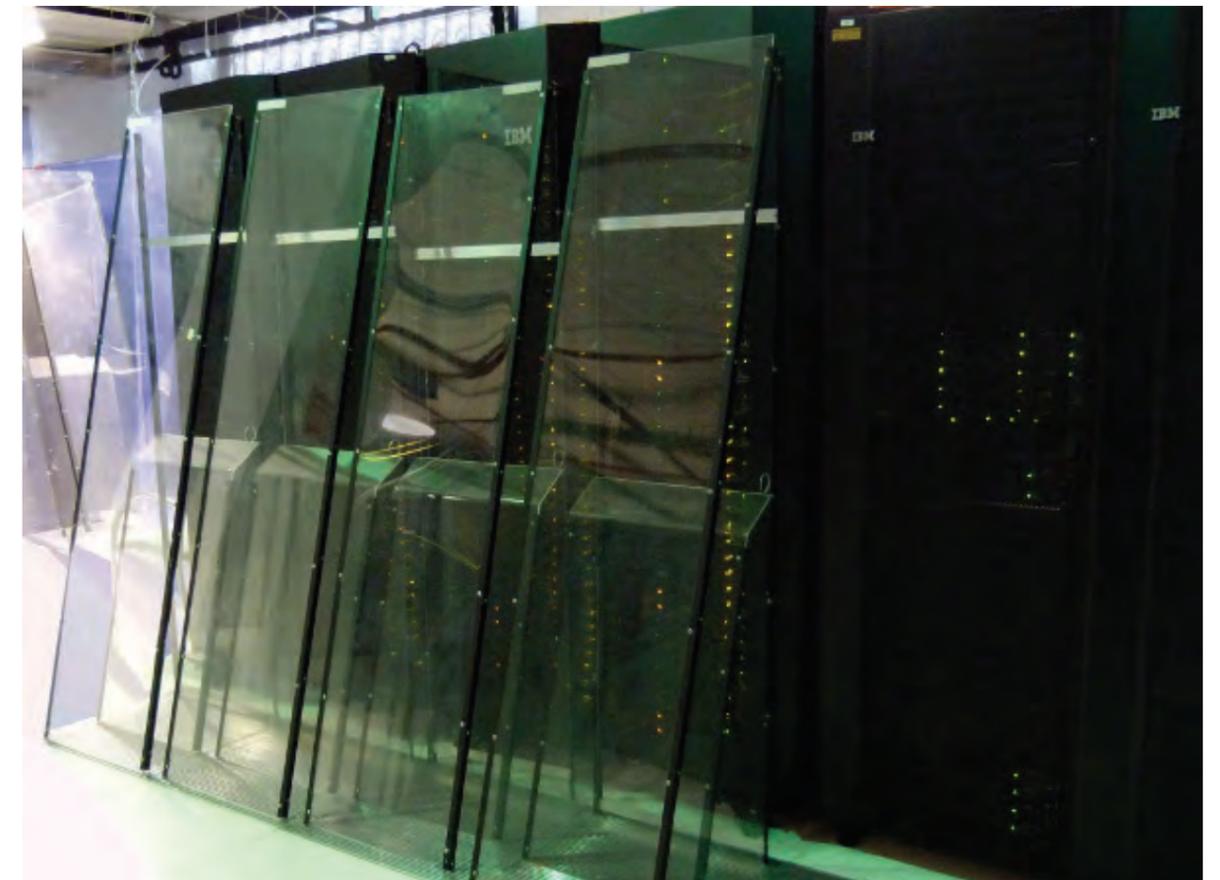
under evaluation. Altamira is used for the analysis of the NGS genomic data. This group also provides analysis support for NGS data to several collaborators in different institutions like IFIMAV (Spain), WTSI (UK), LRI (UK) or NCI (US).

Constraints on inflationary models of the universe based on CMB

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

RNA-seq analysis service

Rafael Zardoya leads 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 characterize 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.



The ALTAMIRA Supercomputer

» Overview



The Picasso Supercomputer

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.

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.



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



» Technical and Scientific Highlights 2013

In 2013 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 bigmem cluster for the assembly of genomes, and using also the rest of the system for other processes. Quantum mechanics, protein folding and custom made simulations, were the users write their own code, were also big users of the system, as can be seen in the publications list.

Key Publications 2013
Articles

- Javier Canales, Rocio Bautista, Philippe Label, Josefa Gómez-Maldonado, Isabelle Lesur, Noe Fernández-Pozo, Marina Rueda-López, Dario Guerrero-Fernández, Vanessa Castro-Rodríguez, Hicham Benzekri, [.....], Jean-François Trontin, Marie-Anne Lelu-Walter, Celia Miguel, María Teresa Cervera, Francisco R Cantón, Christophe Plomion, Luc Harvengt, Concepción Avila, M Gonzalo Claros, Francisco M Cánovas. "De novo assembly of maritime pine transcriptome: implications for forest breeding and biotechnology". *Plant Biotechnology Journal* 11/2013
- Julio F. Fernandez and Juan J. Alonso. Numerical results for the Edwards-Anderson spin-glass model at low temperature. *Physical Review B* 87, 134205 (2013)
- Rodrigo Prado Martins, Carmen Aguilar, James E Graham, Ana Carvajal, Rocio Bautista, M Gonzalo Claros, Juan J Garrido. Pyroptosis and adaptive immunity mechanisms are promptly engendered in mesenteric lymph-nodes during pig infections with *Salmonella enterica* serovar Typhimurium. *Veterinary Research* 12/2013; 44(1):120.

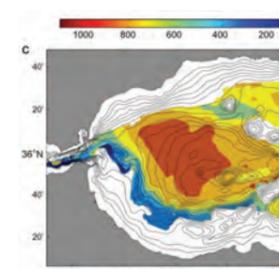
- Montero-Meléndez T, Llor X, García-Planella E, Perretti M, Suárez A. Identification of novel predictor classifiers for inflammatory bowel disease by gene expression profiling. *PLoS One*. 2013 Oct 14;8(10):e76235. doi: 10.1371/journal.pone.0076235. eCollection 2013. PubMed PMID: 24155895; PubMed Central PMCID: PMC3796518.
- Jesús García Lafuente, Elisa Bruque Pozas, José Carlos Sánchez Garrido, Gianmaria Sannino, Simone Sammartino, The interface mixing layer and the tidal dynamics at the eastern part of the Strait of Gibraltar, *Journal of Marine Systems*, Volumes 117–118, May 2013, Pages 31–42, ISSN 0924-7963.
- J. Casado, V. Hernández, J.T. López Navarrete, M. Algarra, D.A. da Silva, S. Yamaguchi, R. Rondao, J. Seixas de Melo, V. Navarro-Fuster, P.G. Boj, M. Diaz-García Amplified Spontaneous Emission In Pentathien-oacene Dioxides by Direct Optical Pump and by Energy Transfer: Correlation with Photophysical Parameters *Adv.Opt.Mat.* 1, pág. 588-599 (2013).

- R. Ponce Ortiz, H. Herrera, M. J. Mancheño, C. Seoane, J. L. Segura, P. Mayorga Burrezo, J. Casado, J.T. López Navarrete, A. Facchetti, T.J. Marks Molecular and Electronic Structure Basis of the Ambipolar Behavior of Naphthalimide-Terthiophene Derivatives. Implementation in Ofets 12458–12467 *Chem. Eur. J.*, 19, pág 12458-12467 (2013)
- J.L. Zafra, R. Andreu, E. Galán, J. Orduna, J. Garín, J.M. Ortiz, J.T. López Navarrete, J. Casado Interpretation of Infrared and Raman Spectra of Zwitterionic Push-Pull Dyes Based on Quinoidal Thiazole Thermomagnetic Molecular System Based on Ttf-Ptm Radical: Switching The Spin and Charge Delocalization *J.Mol.Struct.*, 1044
- J. Casado, P. Mayorga, F. J. Ramírez, J.T. López Navarrete, S. H. Lapidus, P.W. Stephens, H.-L. Vo, J. S. Miller, F. Mota, J. J. Novoa. Evidence for Multicenter Bonding in Dianionic Tetracyanoethylene Dimmers by Raman Spectroscopy. *Angew.Chem. Int Ed.*, 52, pág 6421-6425 (2013)
- M. Moreno Oliva, R. Juarez, M. Ramos, J.L. Segura, S. van Cleuvenbergen, K. Clays, T. Goodson III, J. Casado, J.T. López Navarrete Linear And Nonlinear Optical Properties of Ramified Hexaazatriphenylenes: Dipolar Versus Octupolar Contributions *J.Phys.Chem. C*. 117, pág. 626-632 (2013)
- Darío Guerrero-Fernández, Rafael Larrosa, M Gonzalo Claros. FQbin: a compatible and optimized format for storing and managing sequence data. *Current Bioinformatics*. 11/2013

Please, check the online version of this report to see other publications of Pablo Picasso Node.

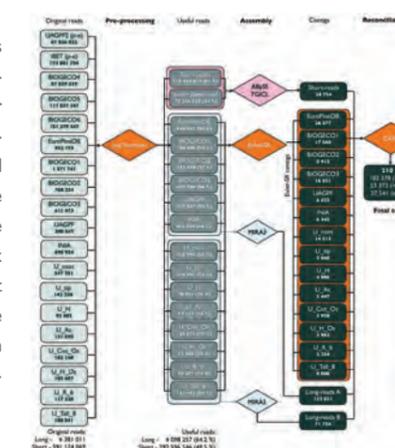
Key Projects 2013

2013 was a highly productive year, with numerous publications and very interesting research.

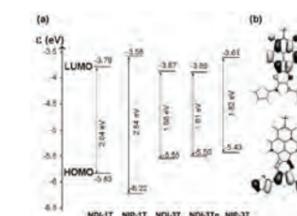


Physical oceanography research • The physical oceanography research group [1] of the University of Málaga continues doing work on the Strait of Gibraltar which is shown on this video: Internal waves in the Strait of Gibraltar. This group is also researching the behaviour of waves in the Málaga harbour.

Pine genome assembly • Maritime pine (*Pinus pinaster* Ait.) is a widely distributed conifer species in Southwestern Europe and one of the most advanced models for conifer research. In the current work, comprehensive characterisation of the maritime pine transcriptome was performed using a combination of two different next-generation sequencing platforms, 454 and Illumina. De novo assembly of the transcriptome provided a catalogue of 26 020 unique transcripts in maritime pine trees and a collection of 9641 full-length cDNAs. This also helps to assembly other less complex genomes, as a complete workflow has been developed for the Pine, which has one of the biggest genomes known. All the genome processing on Picasso has made necessary to work on the storage of genetic information, so GBytes of DNA can be stored compressed and also allow a fast random access. Also, work has been made in the processing of genomic data from a cluster, specifically boosting the performance of Blast+.



Properties of Materials • The properties (optical, magnetic, physical, ...) of materials were studied by different groups. For example, the search for organic ambipolar compounds that can efficiently transport both holes and electrons in a field effect transistor (FET) architecture is a topic of great current interest due to potential applications in complementary metal oxide-semiconductor (CMOS)-like circuits, sensors, and light-emitting transistors, here a new family of naphthalimide-fused thienopyrazine derivatives for ambipolar charge transport in organic field-effect transistors was found, and their performance in organic field-effect transistors was compared with twisted and planar naphthaleneamide monoimide-fused terthiophenes in order to understand the origin of ambipolarity in this new series of molecular semiconductors.



» Overview



The TIRANT Supercomputer

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

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.



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

» Technical and Scientific Highlights 2013

In 2013, Tirant offered more than 6,9 million CPU hours, of which 4,28 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 2013

- 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*, 2013, DOI:10.1021/ar400068w
- A. Pulido, B. Oliver-Tomas, M. Renz, M. Boronat, A. Corma. Ketonic decarboxylation reaction mechanism: a combined experimental and DFT study. *ChemSusChem* 2013, 6, 141-151
- 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. Submitted
- R. García-Meseguer, S. Martí, J. J. Ruiz-Pernía, V. Moliner, I. Tuñón. Studying the role of protein dynamics in an SN2 enzyme reaction using free-energy surfaces and solvent coordinates. *Nature Chemistry*, 5, 566-571 (2013)
- J. J. Ruiz-Pernía, L. Y. P. Luk, R. García-Meseguer, S. Martí, E. Joel Loveridge, I. Tuñón, V. Moliner, and R. K. Allemann. Increased Dynamic Effects in a Catalytically Compromised Variant of Escherichia coli Dihydrofolate Reductase. *Journal of the American Chemical Society*, 135, 18689-18696 (2013)
- K. Zinovjev, J. J. Ruiz-Pernía, I. Tuñón. Toward an Automatic Determination of Enzymatic Reaction Mechanisms and Their Activation Free

- Energies. *Journal Of Chemical Theory And Computation*, 9, 3740-3749 (2013)
- M. Della Morte, P. Hernández. A non-perturbative study of massive gauge theories. *JHEP*, 1311, 213 (2013)
- F.J. Salvador, J. Martínez-López, J.-V. Romero, M.-D. Roselló. Computational study of the cavitation phenomenon and its interaction with the turbulence developed in diesel injector nozzles by Large Eddy Simulation (LES). *Mathematical and Computer Modelling*, 57, 1656-1662 (2013)
- S. Molina, F.J. Salvador, M. Carreres, D. Jaramillo. A computational investigation on the influence of the use of elliptical orifices on the inner nozzle flow and cavitation development in diesel injector nozzles. *Energy Conversion and Management*, 79, 114-127 (2014)
- M. A. Aloy, C. Cuesta-Martínez, P. Mimica, M. Obergaullinger, C. C. Thöne, A. Ugarte Postigo, C. Fryer, K.L. Page, J. Gorosabel, D.A. Perley, C. Kouveliotou, H.T. Janka, J.L. Racusin. Interpreting Observations of GRBs with Numerical Simulations. *Numerical Modeling of Space Plasma Flows (ASTRONUM2012)*. ASP Conference Series Vol. 474, 33. (2013)
- C. M. Fromm, E. Ros, M. Perucho, T. Savolainen, P. Mimica, M. Kadler, A. P. Lobanov, M. L. Lister, Y.Y. Kovalev, and J.A. Zensus. Catching the Radio Flare in CTA 102. II. VLBI Kinematic Analysis. *Astronomy & Astrophysics*, Vol. 551, A32. (2013)

Contributed talks and posters 2013

- **Invited lecture:** M. Boronat "First principles design of highly selective heterogeneous catalysts", 3rd Workshop New trends in computational chemistry for industry applications, Barcelona (2013)
- **Oral contribution:** M. Boronat, A. Pulido, A. Corma "Theoretical insights into the origin of selectivity in the epoxidation of propene with O₂/H₂ mixtures over subnanometer gold and silver clusters", 11th European

Congress on Catalysis, Eurocapacat XI, Lyon (2013)

- **Oral contribution:** A. Pulido, B. Oliver-Tomas, F. Gonell, M. Renz, M. Boronat, A. Corma "Ketonic decarboxylation reaction mechanism: a combined experimental and DFT study", 11th European Congress on Catalysis, Eurocapacat XI, Lyon (2013)
- **Poster:** T. López-Ausens, M. Boronat, A. Corma Periodic DFT study of

the mechanism of ketonic decarboxylation of acetic acid over MgO(100 surface", 4th International Workshop of COST Action CM0903, UBIO-CHEM IV, Valencia (2013)

Key Projects 2013

Advanced scientific computing of astrophysical plasma Supernova remnants • This Group aims to obtain a deeper insight into the physical processes taking place in astrophysical magnetized plasmas involving a broad range of length and time scales. The projects follow three key lines of research: supernova physics and remnants, progenitors of black-body dominated gamma-ray bursts (GRBs) and the non-thermal emission of magnetized relativistic astrophysical plasma with applications to blazars and jets from tidal disruption events (TDEs).

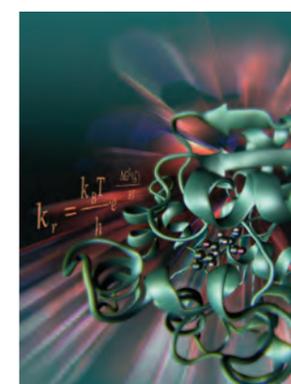


Image of the Nature Chemistry cover created by the group

Theoretical study of the DNA methyltransferase family by means of QM/MM simulations •

Knowing how enzymes work is key to controlling chemical processes in which these biological macromolecules are involved, with countless applications in the fields of medicine and industry. Led by Ignacio Tuñón, the work in 2013 focused on obtaining free energy surfaces, a map that allows the placement of the progress of a chemical reaction as a function

of two coordinates, one representing the chemical system and one representing the changes occurring on the enzyme.

A new algorithm for obtaining the lowest eigenvalue and eigenvector of a large matrix, based on the dressed Hamiltonians formalism

• On the basis of dressed hamiltonian formalism, Ignacio Nebot has devised a new algorithm for obtaining the lowest eigenvalue and the corresponding eigenvector of large matrices. The parallel version of the algorithm was implemented by using both OpenMP and MPI APIs. In both cases, the algorithm bottleneck is split over the available processors. The MPI implementation has been shown to be the most efficient one, and the calculations have been performed on the TIRANT HPC computer.

Study of the cavitation phenomena in Diesel injector nozzles • This project continued the study of the internal flow and the phenomenon of cavitation in Diesel injectors. There are 2 Diesel nozzles that cover almost the entire spectrum in commercial use: microSac nozzles and VCO nozzles. In 2013 the work focused on using the cavitation code already implemented and tested in OpenFOAM to study a VCO nozzle and compare the results with previously analysed microSac nozzles.

Testing new codes: First experiments • Simulations were performed of a new scenario that consists of the collision between a stellar wind and a pulsar wind, in the context of gamma-ray binary stars. This wind-wind collision, which involves a dense, slow stellar wind and a very diluted and relativistic pulsar wind, is thought to be the origin of the very-high-energy radiation detected with the Fermi gamma-ray satellite from this kind of binary star.

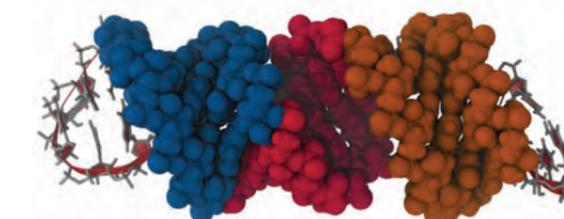
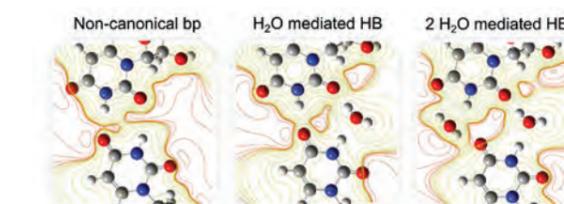
A non-perturbative study of massive gauge theories • This project considers a non-perturbative formulation of an SU(2) massive gauge theory on a space-time lattice, which is also a discretised gauged non-

• **Oral contribution:** S. Molina. Mathematical Modeling in Engineering & Human Behaviour 2013. Universitat Politècnica de València, Spain (September 2013)

linear chiral model. Results of an exploratory numerical simulation of the model were presented showing indications for the presence of a scaling region where both a triplet vector and a scalar remain light. The model could therefore provide an alternative to the Higgs mechanism of Electroweak Symmetry Breaking.

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

Myotonic Dystrophy type I (DMI) is caused by DMPK mRNA microsatellites formed during translation that contains expanded cytotoxic CUG repeats r(CUG). The biomedical importance of r(CUG) structures spurred efforts for the characterization of its tertiary structure and its implication in DMI pathogenic pathway. The group led by Ruben Artero used TIRANT-UV node of the RES to obtain a computational r(CUG) hairpin model.



Characterization of different UU non-canonical base pair conformation with direct hydrogen bonds or 1-2 water mediated hydrogen bonds

Parallel implementation of the MAGPACK package for the analysis of high-nuclearity spin clusters •

The group led by Modesto Clemente developed and optimized the parallel version of the integrated programs in the MAGPACK library, which allows for the calculation of different magnetic properties, both thermodynamic and optical, of high nuclearity spin systems.

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 • Homocoupling of aryl halides is an important reaction in synthetic organic chemistry, and it is of interest to develop an efficient solid catalyst able to replace the current homogeneous processes based on palladium complexes. This project aims to find the optimum gold particle size and morphology for catalysing the dissociation of the C-X bond in iodobenzene, bromobenzene and chlorobenzene.

Monte-Carlo simulations of neutron stars magnetospheres • The aim of this activity was to test a new numerical code that computes the X-ray emission spectrum from magnetised neutron stars using for the first time a self-consistent method. This code will be of significant importance in the understanding and interpretation of current observations of these astronomical objects. Due to the extreme physical requirements for the number of particles and photons, this problem can only be solved by means of supercomputers such as Tirant.

» Overview



The CAESARAUGUSTA Supercomputer

At the end of 2007, the supercomputer CAESARAUGUSTA joined the Spanish Supercomputing Network (RES), being one of its initial seven founding nodes. The system is managed by the HPC group at the Institute for Biocomputation and Physics of Complex Systems (BIFI) of the University of Zaragoza.

Until early 2013, CAESARAUGUSTA was a portion of the old Marenostrum, transferred by the Spanish Ministry of Science and the Barcelona Supercomputing Center to the University of Zaragoza. This supercomputer had 512 PowerPC processors and was located at the Faculty of Science of the University of Zaragoza.

In March 2013, the original system was replaced by a new supercomputer called MEMENTO, equipped with 3072 computing cores and 12TB of RAM memory. This machine was acquired together by BIFI and ZCAM (Zaragoza Scientific Center for Advanced Modeling) in 2012 with FEDER funds.

The portion of MEMENTO shared through RES has 1024 cores; 512 for RES users and 512 for local users. This represents a remarkable increase in the amount of resources shared by BIFI-UNIZAR in the project. In the RES context, this portion of the system is still referenced as "CAESARAUGUSTA". The current CAESARAUGUSTA is located at BIFI's premises in the Río Ebro Campus of the University of Zaragoza.

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

» Organisational Structure

CAESARAUGUSTA is maintained by technical staff of the 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 (portion of 512 cores) among applicant activities. This time is assigned by the Committee after evaluating the applications received. During 2013, the members of the local Access Committee were: Prof. Pablo Ibáñez Marín, Prof. Luis Ráñez García, and Prof. Alfonso Tarancón Lafita



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)

» Technical and Scientific Highlights 2013

In 2013 CAESARAUGUSTA's local Access Committee granted a total of 12 local projects, running 1.380.000 hours of CPU time. These activities have produced numerous scientific results and publications.

Key Publications 2013

Journals

- "[2n2 + 2n2] Cycloadditions: an alternative to forbidden [4 + 4] processes. The case of nitrene dimerization"; David Roca-Lopez, Tomas Tejero, Pierluigi Caramella, Pedro Merino; Org. Biomol. Chem. 2014, 12, 517-525
- "Stereoselective 1,3-dipolar cycloadditions of nitrones derived from amino acids. Asymmetric synthesis of N-(alkoxycarbonylmethyl)-3-hydroxypyrrolidin-2-ones"; Pedro Merino, Graziella Greco, Tomas Tejero, Ramon Hurtado-Guerrero, Rosa Matute, Ugo Chiacchio, Antonino Corsaro, Venerando Pistara, Roberto Romeo; Tetrahedron 2013, 69, 9381-9390
- "I. Genetic predisposition to early recurrence in clinically localized prostate cancer"; I. Borque A, Del Amo J, Esteban LM, Ars E, Hernández

C, Planas J, Arruza A, Larena R, Palou J, Herranz F, Raventós CX, Tejedor D, Artieda M, Simon L, Martínez A, Carceller E, Suárez M, Allué M, Sanz G, Morote J.; I. BJU International, 2013 Apr; 111(4):549-58.

• "Implementing the use of nomograms by choosing cut-off points in predictive models. 2012 updated Partin Tables versus a European predictive nomogram for organ-confined disease in prostate cancer"; 2. Borque A, Rubio-Briones J, Esteban LM, Sanz G, Domínguez-Escrib, Ramírez-Bachhaus M, Calatrava A, Solsona E.; BJU International, 2013, DOI: 10.1111/bju.12532

• "Linear combination of biomarkers to improve diagnostic accuracy in prostate cancer"; 3. Esteban LM, Sanz G, Borque A.; 3. Monografías Matemáticas García de Galdeano, 2013 38, 75-84.

mann rules. Instead, this type of reactions is concerted but not pericyclic as we have demonstrated in the case of dimerisation of nitrones. Studies on cycloaddition reactions leading to biologically active isoxazolidines have been studied with the aim of rationalising the mechanism of the reaction. Also, particular attention is focused on the mechanism of enzymatic reactions, e.g. transglycosylation reactions and protein-glycosylation reactions.

Key Projects 2013

Theoretical study of chemical and enzymatic reactions • Led by Pedro Merino (UNIZAR). This Project concerns investigations on several reaction mechanism regarding organic and enzymatic reactions including nucleophilic additions, cycloadditions and rearrangements. A new type of reactivity has been studied computationally, i.e. pseudopericyclic reactions, which seems to bypass the forbiddingness of the well-known Woodward-Hoff-

Calculations at this level intend to determine the reaction coordinate of the enzymatic reaction as well as the pathway in which the reagents lead to the products through transition states presumably stabilized by the aminoacids at the active site of the enzyme. Currently, the project is also focused to the study of electron localization function (ELF) and non-covalent interactions (NCI) analyses with the aim of understanding how the electrons move during bond formation along a chemical and/or enzymatic reaction. This research activity is conducted within the framework of National and International Projects in collaboration with researchers from BIFI (Dr. Ramon Hurtado-Guerrero and Dr. Victor Polo).

Overcoming data suppression in geographical and sectoral information through genetic algorithms • Led by Domingo Pérez Ximénez-de-Embún (UNIZAR). Suppressed data in regional and sectoral statistical databases represents a relevant challenge of research for social scientists. The objective of this project is to propose a new anti-suppression method using genetic algorithms which takes into account three dimensions: spatial units, sectors and time. The empirical application of the proposed method consists in imputing missing numbers for regional data released by the Bureau of Economic Analysis (BEA) and the County Business Patterns published by the US Census Bureau. The results obtained so far are promising and lead to consistent missing value imputations.



Laparoscopic radical prostatectomy

Algorithms for combining diagnostic tests that increase the discrimination capacity of predictive models in oncology • Led by Gerardo Sanz Saiz (UNIZAR). Management of prostate cancer is a complex decision-making issue. Validated, user-friendly predictive tools are extremely convenient in this decision process. In this context, it is very important to analyse the performance of different algorithms to build better predictive models in oncology. Discrimination is an important feature of a predictive model in medicine, it reflects how to distinguish between the different states of a disease. Through the use of high performance computing resources, the working group has analysed the building of models that achieve a greater ability to discriminate between different disease states. For this purpose, non parametric approaches have been implemented in R programming language. In addition, we have proposed a new methodology based on the use of density functions to choose thresholds to classify correctly patients, the clinical utility of predictive models have a strong dependence with this selection. We also have continued in the work to explore different measures to identify new markers that are statistically significant in prostate cancer recurrence. The use of these measures can be effective to build Risk Scores that combine markers in order to improve the predictiveness of models.

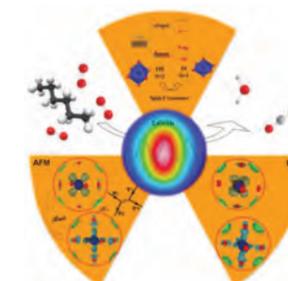
Design of group-6 organometallic systems for the activation and reduction of molecular nitrogen • Led by Miguel Baya García (ISQCH). The industrial production of ammonia is a chemical process of great importance today that requires a huge investment in energy and generates enormous volumes of pollutants. In contrast, nature is capable of accomplishing the reduction of nitrogen under mild conditions. The development of a novel environment-friendly technology that can assure the production of nitrogen derivatives from molecular nitrogen under less harsh conditions is a

major challenge for chemists.

Up to date, there are only two molecular systems that can catalyse the reduction of nitrogen to ammonia at the lab scale. Both are Molybdenum complexes stabilized by polidentate ligands. The current research project is a long term program whose final goal is to design group-6 (molybdenum and tungsten) organometallic systems which can coordinate nitrogen and activate the N-N bond for its subsequent transformation.

Towards a rational design of catalyst based on plasmonic metal oxides • J.

Gracia, M. Escuin, R. Mallada, N. Navascues, J. Santamaria (INA, UNIZAR); In the most efficient catalytic contactor conceivable, the energy must be exclusively and efficiently deposited on the active sites. We set the concepts in catalysis on the impact of correlated charge carriers for the selective deposition of electro-magnetic energy, and its preferential guidance towards chemical



Schematic Catalysis in Plasmonic metal oxides

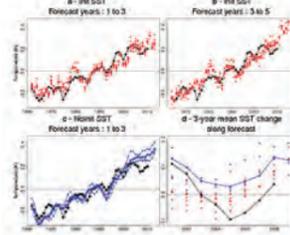
transformations. Outstanding dielectric losses at microwave frequencies emerge at the insulator to metal transition in Mott insulators from the long relaxation life of the charge carriers. Founded on theoretical principles, an exemplary justification for the optimization of LaCoO₃ based catalysts emerge with spin transitions in the Co atoms. The alteration of the Co spin state justifies a charge transfer, dielectric relaxation, and its frequency unifies enhanced dielectric losses and catalytic activity. Our understanding results in proficient catalysts under selective electromagnetic activation validated for the combustion of volatile compounds. Consequence of the self-energy of strongly correlated charge carriers and its distinctive response to electromagnetic fields correlated metals envision in future catalytic technologies.

Computational Modelling of Homogeneous Catalysts • Led by Francisco Javier Modrego Pérez (ISQCH). The project is developed in the research line "Catalysis and catalytic processes" within the ISQCH. By using computational chemistry methodology it is possible a detailed analysis of the reaction mechanisms and the homogeneous catalysis processes as a whole, getting results which are not amenable to experimental studies alone. The use of the supercomputing facilities at "CESARAUGUSTA" enables us to use realistic models of the molecules and processes avoiding simplifications in the model which are not always advisable. Complementing the experimental results with computational studies in a synergistic way leads to a deeper understanding of the catalytic processes allowing us to go beyond the trial and error approach in the development of new catalysts.

Magnetism of Tm atoms and monolayers on W(110) studied by x-ray magnetic dichroism • Led by César de la Fuente. We investigated the growth and magnetic properties of Tm atoms and monolayers deposited on a W(110) surface using scanning tunneling microscopy and x-ray magnetic circular and linear dichroism. The equilibrium structure of Tm monolayer films is found to be a strongly distorted hexagonal lattice with a Moiré pattern due to the overlap with the rectangular W(110) substrate. Isolated Tm adatoms on W present a trivalent ground state electronic configuration, contrary to weakly coordinated atoms on rough Tm films and gas-phase Tm. Both the Tm atoms and monolayer films exhibit large spin and orbital moments with out-of-plane uniaxial magnetic anisotropy. Temperature-dependent studies of magnetic ordering further show that Tm monolayers undergo a transition to antiferromagnetism at about 50K.

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

Abstract • The observed global mean near-surface temperature underwent a plateau during the early XXIst century. Most of this global warming slow down has been ascribed in previous literature to internally generated climate variability. Some authors also suggest substantial contributions by the minimum in solar activity that occurred during this period, and by the increase in atmospheric aerosol concentrations. This project aims to initialise near-term climate predictions every year from 1995 to 2005 and to compare them to uninitialised counterparts in order to assess the relative contributions of internally generated versus externally forced climate signal to the plateau.



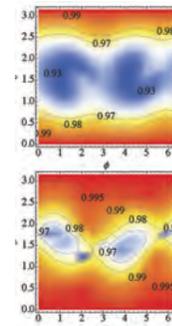
Ability to capture the warming slow-down

Results • The Climate Forecasting Unit (CFU) has produced retrospective climate predictions initialized every year from 1995 to 2011 from the best possible estimate of the observed climate state. The global mean near-surface temperature plateau observed in the last decade is reproduced with an error which does not exceed 0.03K in the first three forecast years of those climate predictions. This excellent performance of the EC-Earth forecast system has been published in Nature Climate Change. A thorough analysis of those climate predictions allowed for an attribution of the observed temperature plateau to an increased ocean heat absorption. More details are provided in the full report.

Publications • Guemas V., Doblas-Reyes F.J., Andreu-Burillo I., Asif M., 2013, Retrospective prediction of the global warming slowdown in the past decade. Nature Climate Change, doi : 10.1038/nclimate1863.

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

Abstract • We study the orbital dynamics of black hole binaries in general relativity, with special emphasis on simulating the gravitational wave signals emitted during the inspiral and coalescence of the black holes due to radiation reaction. It is foreseen that such signals will be observed by the advanced LIGO and Virgo detectors in the next five years (after the currently ongoing detector upgrades). However there is no clear picture yet of how to search for, and reliably identify, generic black hole binaries, due to our incomplete knowledge of the physically correct waveforms. Our work aims at providing this knowledge for stellar and intermediate mass black holes above 10 solar masses where the late merger and ringdown - the regions of largest spacetime curvature - can be observed through their gravitational waves.



Fitting factors of a non-precessing (top) and precessing (analytical) waveform model, plotted versus source sky angles theta and phi

Results • The most important result of our work on MareNostrum in 2013 was the construction of the first model for the complete gravitational wave signal from the inspiral, merger and ringdown for general precessing black hole binary systems. This model is based on previous work on a phenomenological description of the gravitational wave signal from non-precessing coalescing black hole binaries, which synthesizes results of supercomputer simulations and analytical perturbative calculations, and continues our family of increasingly accurate models for gravitational wave signals, which have become an essential ingredient of gravitational wave data analysis codes. Further refining this still very simple precessing model with a larger set of numerical simulations will be a major objective of our work in the next year. At the same time we will work with the gravitational wave data analysis community to use this model to improve current strategies for searching and identifying gravitational wave events, before the international advanced detector network will perform its first science run in 2015.

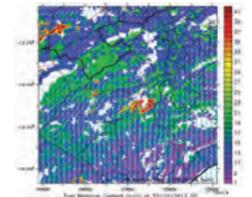
Publications • Mark Hannam, Patricia Schmidt, Alejandro Bohé, Leila Haegel, Sascha Husa, Frank Ohme, Geraint Pratten, Michael Pürrer. "Twist and shout: A simple model of complete precessing black-hole-binary gravitational waveforms", arXiv:1308.3271 [gr-qc], submitted to Physical Review Letters (2013) • Ian Hinder, et al. "Error-analysis and comparison to analytical models of numerical waveforms produced by the NRAR Collaboration", Classical and Quantum Gravity, 31 025012, (2014) (arXiv: 1307:5307 [gr-qc]) • Michael Pürrer, Mark Hannam, Parameswaran Ajith, Sascha Husa. "Testing the validity of the single-spin approximation in inspiral-merger-ringdown waveforms", Physical Review D, vol. 88, Issue 6, 064007 (2013)

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

Abstract • The activity is part of the project "Technologies for the comprehensive fighting of forest fires and for the conservation of our forests" (PROMETEO). The objective is to produce the best estimations of Fuel Moisture Content (FMC) as a key input parameter into wildfire simulations, using data assimilation techniques. This new FMC model has to be validated, however FMC measurements are not easy to obtain, so the FMC model validation will be developed

using FMC values as input to a fire forecast model applied to real fires. The results from the fire behaviour model runs with FMC input values calculated by our model, will be compared with real wildfires in Spain. Finally, we will simulate the impact of a fire on air pollution concentration using the WRF/Chem model developed by NCA.

Results • A new custom fuel moisture content model has been developed for the Iberian Peninsula. It was optimised based on results of many computational simulations. The new module allows each time step to calculate the fuel moisture content of dead fuels (1hr, 10hr, and 100hr) and live fuels. The fuel moisture content model is based on several moisture content algorithms and the system has capabilities to assimilate information from measurement networks and/or satellite data. A fire behaviour model (WRF-Fire) was run with the new customised FMC model to perform different sensitivity tests to the FMC input values based on real fires on the Iberian Peninsula and a preliminary model validation of the system was obtained. For the proposed simulations a computational mother domain with 86 x 71 grid cells and 15 Km resolution over the Iberian Peninsula was defined. One nested domain is required to scale the simulation down from the atmospheric mother domain to the atmospheric domain of 3 Km with 30 x 30 grid cells; this domain is centred on the fire ignition line. These precise simulations have a CPU time requirement which cannot be covered with common research clusters and must use a powerful supercomputer such as MareNostrum.

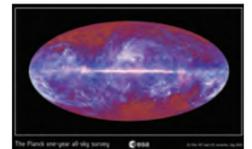


FMC (%) and wind vectors results over Valencia area, 200 m. resolution. Hourly values 30/10/2013 20:00.

Publications • Roberto San José, Juan Luis Pérez, Rosa Maria González, Julia Pecci, Marino Palacios. "The impact of a wildland fire on air pollution concentrations using WRF/chem/FIRE: An application over Murcia (Spain)". 33rd International Technical Meeting on Air Pollution Modelling and its Application. Miami, Florida 26-30 August, 2013 • R. San José, J.L. Pérez, R.M. González, J. Pecci and M. Palacios. "A customized FMC model for wildland fire simulations using WRF/Fire model over Spain". Third International Conference CEMEPE 2013 & SECOTOX. Skiathos, Grecia 24-28, June, 2013 • Roberto San José, Juan L. Pérez, and Rosa M. González-Barras. "Implementation Of A Fuel Moisture Content Model Into Wrf/Fire-Chem: A Real Fire Comparison In Murcia (Spain)". European Geosciences Union General Assembly 2013. Vienna, Austria 07-12 April, 2013 • R. San José, J.L. Pérez, R.M. González, J. Pecci and M. Palacios. "A customized FMC model for wildland fire simulations using WRF/Fire model over Spain". Third International Conference CEMEPE 2013 & SECOTOX. Skiathos, Greece 24-28, June, 2013.

Constraints on inflationary models of the universe based on CMB data, Enrique Martínez González, Instituto de Física de Cantabria

Abstract • The last decade has witnessed tremendous advances in cosmology, thanks to the unprecedented resolution maps of the Cosmic Microwave Background Radiation (CMB) anisotropies produced first by the NASA WMAP mission, and recently in 2013 by the ESA Planck mission. The mere existence of the CMB is a strong 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.



Results • In March 2013, the ESA released the initial 15.5 months of data from its Planck space telescope and the scientific results produced by the Planck collaboration were published in a series of 30 articles. The mission has produced the most detailed map ever created of the CMB anisotropies. The process, analysis and interpretation of this information require the use of significant high-performing computing resources. The goal of this project is the study of the anisotropies of the CMB radiation in order to understand the physics of the early universe, when space experienced an inflationary expansion in a short period of time. We have been developing, improving and optimizing novel estimators to detect imprints of different inflationary models on the CMB anisotropies. These imprints are usually characterized by non-Gaussian fluctuations. Some of our results, in particular regarding the Isotropy and Statistics, the search of primordial non-Gaussianities and the characterization of instrumental systematics have been published in the 2013 publications. We are improving and developing new algorithms to better and more optimally understand Planck data and future CMB experiments.

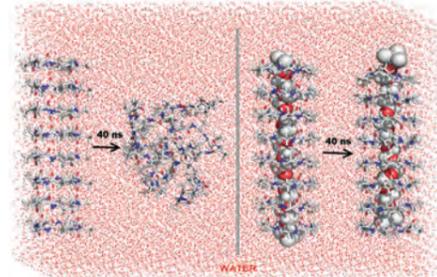
Publications • Overview of products and results, submitted to Astronomy & Astrophysics, (arXiv:1303.5062), 2013 • Low Frequency Instrument data processing, submitted to Astronomy & Astrophysics, (arXiv:1303.5063), 2013 • Constraints on primordial non-Gaussianity, submitted to Astronomy and Astrophysics, (arXiv:1303.5084), 2013 • Curto, A.; Tucci, M.; González-Nuevo, J.; Toffolatti, L.; Martínez-González, E.; Argüeso, F.; Lapi, A.; López-Cañiego, M.; "Forecasts on the contamination induced by unresolved point sources in primordial non-Gaussianity beyond Planck", Monthly Notices of the Royal Astronomical Society, 432, 728, 2013 • Casaponsa, B.; Barreiro, R. B.; Martínez-González, E.; Curto, A.; Bridges, M.; Hobson, M. P.; "Exploring local fNL estimators based on the binned bispectrum", Monthly Notices of the Royal Astronomical Society, 434, 796, 2013.

Transmembrane Ion Transport through alpha, gamma-Peptide Nanotubes, Rebeca García Fandiño, Universidad de Santiago de Compostela

Abstract • Self-assembling peptide nanotubes (SPNs) made from ALPHA,GAMMA cyclic peptides, consisting of alternating (1R,3S)-3-aminocyclohexane carboxylic acid and d-ALPHA-amino acid, have structural and functional properties that may be suitable for various applications in biology and materials science. From the structures obtained from X-ray crystallography, we have built models of SPNs inserted into a DOPC bilayer and we plan to investigate the transport of ions and water through these supramolecular channels using Molecular Dynamics calculations.

Results • We have used Molecular Dynamics (MD) simulations to investigate the stability and ion transport through cyclic peptides (CPs) containing g-amino acids self-assembled in lipid bilayers to form transmembrane nanotubes, and in chloroform and water to compare to the lipid environment. A marked destabilizing effect on the structure was observed in aqueous solution, suggesting that most of the water molecules that compete for the H-bonds are those that occupy the internal cavity. The introduction of organochloride molecules within the nanotubes is stabilized in water, and this property opens the door to a large number of possible future applications that are an important challenge in the field of molecular self-assembly, such as in drug delivery processes to control nanotube length by means of appropriate guests. A precise control of the nanotube length can be envisaged from the MD simulations of the encapsulation of a chlorated polymer inside its inner cavity, opening a very interesting possibility in this area. The size of these systems requires employing the supercomputing power of MareNostrum to complete the calculations in a reasonable period of time.

Publications • Rebeca García Fandiño; Juan R. Granja Guillén. From alpha, gamma-cyclic peptides to homo/hetero dimers and nanotubes in polar and non-polar solvents. Towards control of nanotube length: a computational study. *J. Phys. Chem. C*. 117, pp. 10143 - 10162. 2013 • Membrane-targeted Supramolecular Drugs from Peptide Nanotubes. XXXIV Reunión Bienal de la Real Sociedad Española de Química, Santander, Cantabria, Spain. 15-18/09/2013 • Juan R. Granja; Manuel Amorón; Rebeca García Fandiño; Arcadio Guerra; Nuria Rodríguez Vázquez. "Tomo QBIO-CI-04, Book of Abstracts, 64."



Stabilization of self-assembled peptide nanotubes via a organochloride polymer.

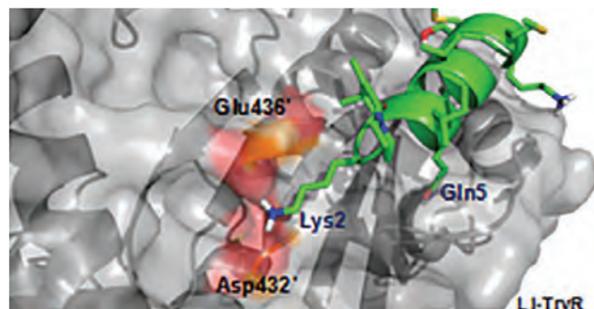
Targeting The Dimerization Interface Of Leishmania Trypanothione Reductase In The Search For New Drugs, Federico Gago, Universidad de Alcalá

Abstract • Trypanothione reductase (TryR) is an essential homodimeric flavoenzyme that is used by Leishmania parasites to maintain the dithiol of trypanothione in its reduced state. We have characterized the dimerisation interface of this enzyme and identified a "hot spot" region that can be targeted by short peptides able to disrupt both monomer association and catalysis. Molecular dynamics simulations will allow us to gain further atomic insight into the plasticity of the binding site and the determinants of binding affinity and inhibitory activity. In addition, the calculated trajectories for the free TryR monomer will provide us with a dynamic ensemble of structures that will be used in virtual screening experiments in the search for putative small-molecule dimerisation inhibitors.

Results • A novel mechanism of inhibition Leishmania infantum TryR was reported that is based on the perturbation of the dimerisation process of the enzyme, and thereby, of its catalytic activity. Mutagenesis studies as well as synthetic peptides led us to validate our design, which opens a new and promising strategy for new inhibitors. These results

represent, to the best of our knowledge, the first successful finding of a hot spot dimerisation region in TryR, a key enzyme for the survival of this parasite

Publications • Probing the dimerization interface of Leishmania infantum trypanothione reductase with site-directed mutagenesis and short peptides. Toro MA, Sánchez-Murcia PA, Moreno D, Ruiz-Santaquiteria M, Alzate JF, Negri A, Camarasa MJ, Gago F, Velázquez S, Jiménez-Ruiz A. *Chem-biochem*. 2013 Jul 8;14(10):1212-7. doi: 10.1002/cbic.201200744. Epub 2013 Jun 6. PMID: 23744811



Targeting protein - protein interactions as novel chemotherapeutic target for TryR of Leishmania infantum

Mechanistic and energetic analysis of binding interactions of ligands and proteins: Steered MD simulation of cofactor and anion dissociation from Helicobacter pylori and Anabaena PCC 7119 flavodoxins, Javier Sancho Sanz, Universidad de Zaragoza. Dept. Bioquímica, Biología Molecular y Celular de Zaragoza

Abstract • The mechanism of protein/ligand binding will be investigated using flavodoxin as target protein and the FMN cofactor and the chloride anion as ligands. Steered MD will be used to accelerate dissociation and characterize the lowest energy trajectories, paying special attention to understanding solvation/desolvation events. In the case of FMN dissociation, the simulation will be compared with a previous protein engineering analysis of the structure of the transition state of FMN/apoflavodoxin binding.

Results • Analysis of the classical simulations performed at 2BMV (Fld-Hp structure with an chlorine anion joined at the linkage site of cofactor FMN) enabled us to derive approximate statistics and the mechanism of disunion of the chlorine that appears to be linked at the point of union of cofactor FMN. For this, the state of solvation of the environment of this union site was considered and an analysis of the influence of the solvent on this mechanism was performed. The analysis of the simulations performed at IFLV (structure of Fld-Anabaena with its cofactor FMN) enabled an initial estimation of the union-dissociation energy curve via steered molecular dynamics.

The use of the BSC-CNS supercomputing cluster facilitated our increasing the number and run length of our simulations, with the benefit of better vision and statistics of the phenomena under investigation. This resulted in an analysis of the complex mechanism of union of FMN to the apoflavodoxina and obtained indications of the possible influence of linked protein anions at the union site of FMN phosphate.



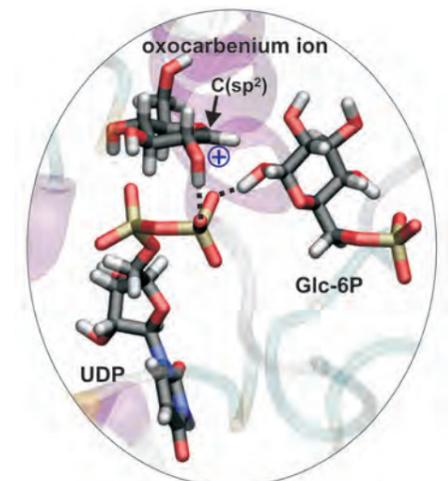
Initial position and force vector applied to the FMN phosphate in one of the SMD simulations on IFLV

Elucidating the catalytic mechanism of retaining glycosyltransferases, Carme Rovira, Parc Científic 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 prevents determination of whether this mechanism is feasible in the enzyme environment. In our project we plan to elucidate whether the front-face mechanism is feasible for some glycosyltransferases.

Results • By means of ab initio metadynamics dynamics techniques we have 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. 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 (Ardévoland Rovira, *Angew. Chem. Int. Ed.* 2011). In contrast, other glycosyltransferases operate via a double-displacement mechanism (Rojas-Cervellera et al. *Chem. Eur. J.* 2013). Glycosyltransferases are responsible for the structure of many carbohydrates and, therefore, the knowledge of their mechanism of action will help to modify their function, thereby improving the synthesis of known carbohydrates and new structures. It will also contribute to the design of inhibitors for those GTs that are involved in infectious diseases. The large-scale simulations needed to perform this project are possible only using high supercomputing facilities such as provided by MareNostrum.

Publications • V. Rojas-Cervellera, A. Ardévol, M. Boero, A. Planas, C. Rovira. "Formation of a Covalent Glycosyl-Enzyme Species in a Retaining Glycosyltransferase". *Chemistry - A European Journal*, 19, 14018-14023 (2013).

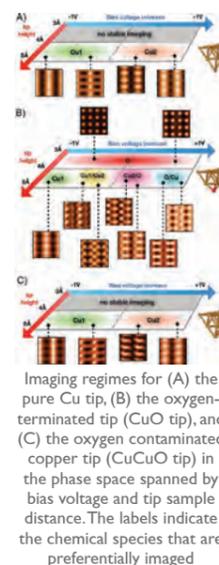


Molecular structure of the short-lived carbocation intermediate in the interior of the enzyme trehalose-phosphate synthase. This enzyme contributes to the synthesis of trehalose, a natural disaccharide used as food ingredient for its good preservative properties.

First-principles simulations of defects on metal oxides and graphene sensed by scanning probe microscopies, 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 characterization of the growth of graphene on metal step edges 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 powerful supercomputers such as those in the RES.

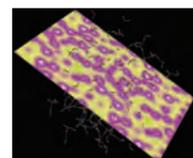
Results • The simulations allowed us to make important advances concerning i) the role of defects on high catalytically active oxide surfaces and ii) the characterization of edge states on graphene grown on metals. i) We have performed a comprehensive analysis of contrast formation mechanisms in scanning tunnelling microscopy (STM) experiments on a metal oxide surface with the oxygen-induced missing row reconstruction of the Cu(100) surface. Our results provide a conclusive understanding of fundamental STM imaging mechanisms, thereby providing guidelines for experimentalists to achieve chemically selective imaging by properly selecting imaging parameters. ii) Exotic extended nanostructures in graphene layers are an extremely hot topic in the field of Nanotechnology due to the exciting atomic properties generated at these nanoarchitectures and their possible use in new devices. In collaboration with the experimental group of Pr. J.A. Martín-Gago, we have provided evidence of the existence of 1D electronic states on graphene-metal heterostructures that are highly localized exclusively in one of the graphene sublattices and restricted to the crystallographic edges.



Publications • M. Z. Baykara, M. Todorovic, H. Mönig, T. C. Schwendemann, Ö. Ünverdi, L. Rodrigo, E. I. Altman, R. Perez, U. D. Schwarz. Atom-specific forces and defect identification on surface-oxidized Cu(100) with combined 3D-AFM and STM measurements. *Phys. Rev. B* 87 155414 (2013). DOI: 10.1103/PhysRevB.87.155414. Editors' Suggestion • Harry Mönig, Milica Todorovic, Mehmet Z. Baykara, Todd C. Schwendemann, Lucia Rodrigo, Eric I. Altman, Rubén Pérez, and Udo D. Schwarz. "Understanding Scanning Tunneling Microscopy Contrast Mechanisms on Metal Oxides: A Case Study" *ACS Nano* (2013) • P. Merino, L. Rodrigo, A. L. Pinardi, J. Méndez, M. F. López, P. Pou, R. Pérez, J.A. Martín-Gago. "Sublattice localized electronic states in atomically resolved Graphene-Pt(111) edge-boundaries." Submitted to *Nanoletters* (2013).

Study of bulk and nanoconfined liquid water from ab initio simulations, Emilio Artacho, CIC nanoGUNE Consolider and University of Cambridge

Abstract • Water is an extremely intriguing liquid that is vital to our understanding of numerous biological processes; its many anomalous properties are linked to its subtle nanoscale structure, and in particular to the hydrogen bond network that exists between individual water molecules. Furthermore, the mechanical, rheological and diffusive properties of nanoconfined water in biomolecular or nanotechnological systems can be very different from those of the bulk liquid. This project aims to understand the structure of both bulk and nanoconfined water from first principles simulations using density-functional theory; we employ the SIESTA code and make use of recently developed functionals that aim to accurately include the effect of van der Waals interactions, of great importance in the proper description of the structure of the liquid.



Electronic charge density for a 200-molecule liquid water ab initio molecular dynamics snapshot

Results • We have carried out ab initio molecular dynamics simulations of up to 200 molecules of bulk liquid water at different temperatures and pressures with several new fully non-local exchange-correlation functionals within a density-functional theory framework, that include long-range van der Waals interactions. Several important results have emerged from our post-processing analysis: 1. There are noticeable differences both in the radial distribution function and the pressure-volume equation of state for different implementations of the van der Waals interactions in DFT, although there is an overall noticeable improvement with respect to conventional semi-local functionals, in particular with respect to the equilibrium density, compressibility and diffusivity of the liquid; 2.

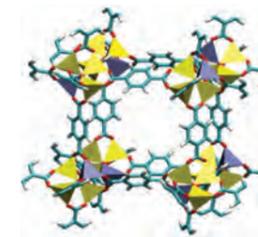
The two most successful van der Waals functionals reproduce almost perfectly the properties of water in the low- and high-density limits, respectively, providing some interesting insight into the proposed LDL/HDL split in liquid water at ambient conditions; 3. We have found evidence for the first time of the anomalous properties of liquid water (in the diffusivity and compressibility) from first principles simulations.

Publications • F. Corsetti, M.-V. Fernández-Serra, J. M. Soler, and E. Artacho. "Optimal finite-range atomic basis sets for liquid water and ice". *J.*

Phys.: Condens. Matter, 25, 43, 435504, October 2013 • F. Corsetti, E. Artacho, J. M. Soler, S. S. Alexandre, M.-V. Fernández-Serra. "Room temperature compressibility and diffusivity of liquid water from first principles". *J. Chem. Phys.*, 139, 19, 194502, November 2013.

Post-synthetic modification of Metal-organic frameworks: an ab initio theoretical study (1st. period), Nuria López, ICIQ

Abstract • Transmetalation procedures are an innovative way to change the nature of Metal-Organic Frameworks (MOF) after synthesis, thus achieving new structures that cannot be easily made from scratch with a high catalytic potential. Through Density Functional Studies we described in detail the underlying mechanism of substitution and singled out the key factors behind this mechanism, thus bridging the gap between theoretical and experimental knowledge of the phenomenon and improving the transmetalation strategies that are being studied by our experimental colleagues.



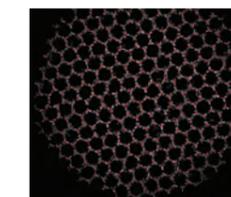
Transmetalated crystallographic unit cell of MOF-5, stoichiometry (Zn₃Ni(μ-O)(BDC)₃)₈

Results • For the first time, a general mechanism for the Ni-transmetalation (nickelation) of MOF lattices in N,N-dimethyl formamide (DMF) has been put forward. The complexity of this reaction is mirrored by its many different pathways, each of them properly explored and the intermediates fully characterized. Some of these intermediates are completely new structures not reported in the literature that deeply affect the pathways. The lowest energy path was taken as the most feasible and the transition states evaluated. Moreover, by means of ab initio molecular dynamics we attested the stability of the system in the presence of DMF at the liquid density, thus proving the importance of the flexibility of the metal core during the nickelation. The proposed mechanism accounts for the experimental results found in the literature. To extend the validity of this study, different solvents have been considered: N-methyl formamide (NMF), formamide, and acetonitrile. The new barriers found for the nickelation mechanism easily explain why, as seen in experiments, it is impossible to incorporate Ni to the metal core.

Publications • "How ligands improve the hydrothermal stability and affect the adsorption in the IRMOF family" L. Bellarosa, J. J. Sevilano, S. Calero, N. Lopez, *Phys. Chem. Chem. Phys.* 15, 17696 (2013) • "Strategies to simultaneously enhance the hydrostability and the alcohol-water separation behavior of Cu-BTC" *J. Phys. Chem. C* 117, 20706 (2013) • "The role of solvent in the ion-exchange mechanism of MOF-5 lattices", L. Bellarosa, C. Brozek, M. Dinca, N. Lopez. Submitted.

Ice crystallization, Carlos Vega, Parc Científic de Barcelona, Universidad Complutense de Madrid, Fac. Ciencias Químicas, Dep. Química Física I

Abstract • Among all the freezing transitions, that of water into ice is probably the most relevant to biology, physics, geology. When liquid water is cooled below 0 C, it becomes supercooled and transforms into ice via nucleation. Nucleation is the rare-event mechanism characterised by the stochastic formation of critical clusters that are very short-lived, one reason why experimental observations of ice nucleation are very troublesome. Depending on temperature and pressure some 16 crystalline phases of water have been identified. Even though computer simulations have proven to be a perfect tool to investigate ice nucleation from deeply supercooled water, not all simulation results reached the same conclusions. Our project aims to study water crystallisation into different ice polymorphs with several water model potentials.



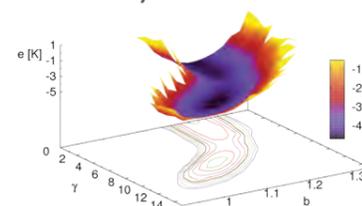
Spherical Ih-ice cluster containing about 5000 molecules

Results • We studied homogeneous ice nucleation by means of computer simulations using the TIP4P/2005 and TIP4P/ice water models. This is the first calculation of the size of the critical cluster and the nucleation rate at moderate supercoolings (14.5-35 K). Both models give similar results when compared at the same supercooling. To determine the size of the critical cluster, we use a numerical approach in the spirit coexistence methods. Next, we use Classical Nucleation Theory to estimate the interfacial free energy and the nucleation free-energy barrier. An extrapolation of the interfacial free energy to the melting temperature gives a value of 29 mN/m, in good agreement with experiments. We get free-energy barriers higher than 250 kT for supercoolings lower than 20 K, strongly suggesting that homogeneous ice nucleation for supercoolings lower than 20 K is impossible. According to this prediction, ice nucleation must necessarily be heterogeneous for supercoolings lower than 20 K. It would be of interest to consider other water models and to modify the shape or the structure of the inserted ice cluster. We foresee that all of these issues will be the subject of significant activity.

Publications • Sanz, C.; Vega, J. R.; Espinosa, R.; Caballero-Bernal, J. L.; F. Abascal, and C. Valeriani "Homogeneous Ice Nucleation at Moderate Supercooling from Molecular Simulation". *J. Am. Chem. Soc.*, 2013, 135 (40), pp 15008-15017 DOI: 10.1021/ja4028814 <http://pubs.acs.org/doi/abs/10.1021/ja4028814> • "The paper has also been chosen as a JACS Spotlight of the issue: "How does water start to freeze?" <http://pubs.acs.org/doi/pdf/10.1021/ja410682n> "On fluid-solid direct coexistence simulations: the pseudo-hard spheres model" *J. R. Espinosa, E. Sanz, C. Valeriani and C. Vega; J. Chem. Phys.*, 139 144502 (2013)

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

Abstract • Quantum effects in solids and liquids may play a role ranging from subtle to very significant. We study quantum effects in materials where such effects are most pronounced, including helium-4 and systems produced with trapped cold atomic clouds. In both cases the temperature is close to absolute zero and both the zero-point motion and quantum exchange effects are prominent. We use the BSC-CNS facilities to solve the Schrödinger equation for various systems such as cold trapped atomic gases, liquid and solid helium-4 at zero temperature. Quantum effects are very significant at such conditions. The approach allows to study the transition between the two phases and to investigate in detail how the transition is influenced by various factors. The goal is to determine the extent to which atomic exchanges influence the stability of quantum solids.



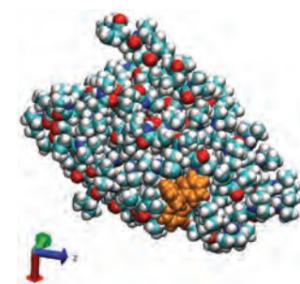
Energy of a bulk helium-4 ground state as a function of two variational parameters of the wavefunction. Two local minima correspond to the solid and liquid phases, and are found on the energy surface in the coexistence region

Results • The use of GPUs allows us to use previously inaccessible system sizes. Even for the largest systems, the execution times are so reasonable that we can search in large parameter spaces. This allows us to study the quantum solids and liquids in detail that was not previously possible. The GPU program is now made accessible to the public. Several results for cold atomic gases were published and are indicated in the literature list.

Publications • G.E. Astrakharchik, K.V. Krutitsky, P. Navez "Phase diagram of quasi-two-dimensional bosons in laser speckle potential" Phys. Rev. A 87, 061601(R) (2013) • G.E. Astrakharchik and I. Brouzos "Trapped one-dimensional ideal Fermi gas with a single impurity", Phys. Rev. A 88, 021602(R) (2013) • M.A. Garcia-March, B. Julia-Díaz, G.E. Astrakharchik, Th. Busch, J. Boronat, A. Polls "Sharp crossover from composite fermionization to phase separation in mesoscopic mixtures of ultracold bosons", arXiv:1307.3510 • Y. Lutsyshyn, "Fast quantum Monte Carlo on a GPU", eprint arXiv:1312.1282 (2013) • G.E. Astrakharchik, K.V. Krutitsky, P. Navez "Phase diagram of quasi-two-dimensional bosons in laser speckle potential" Phys. Rev. A 87, 061601(R) (2013) • G.E. Astrakharchik and I. Brouzos "Trapped one-dimensional ideal Fermi gas with a single impurity", Phys. Rev. A 88, 021602(R) (2013) • M.A. Garcia-March, B. Julia-Díaz, G.E. Astrakharchik, Th. Busch, J. Boronat, A. Polls "Sharp crossover from composite fermionization to phase separation in mesoscopic mixtures of ultracold bosons", arXiv:1307.3510.

GPU-accelerated simulations of all atomic and coarse grain models of soft matter systems, Jordi Faruado, ICMAB-CSIC

Abstract • Molecular Dynamics (MD) simulations are an essential tool to understand materials with atomistic detail but they require large amounts of computational power. In this activity, we take advantage of the acceleration provided by new graphical processing units (GPU) in MD simulations of soft materials. Thanks to this acceleration, we have been able to access simulations of processes which were otherwise not possible. The cases considered here include (a) the transport of ions across a protein nanochannel embedded in a lipid membrane (b) the self-assembly of amphiphilic molecules into nanoparticulate materials (bilayers, vesicles, polymeric nanogels) and (c) the solvation properties of complex hydrophobic-hydrophilic surfaces such as proteins.



Adsorption of a small hydrophobic molecule (orange) onto a self-assembled polymeric nanovesicle made of 5 PNIPAM chains (atoms shown with Van der Waals radius, color code corresponds to standard crystallographic conventions).

Results • The obtained results are the following: (a) We have successfully simulated the self-assembly process of different structures, starting from molecular components. This includes self-assembled monolayers and polymeric nanovesicles. (b) We have predicted the possibility of tuning the behaviour of protein channels by using trivalent ions. This opens the door to the possibility of designing single-molecule nanoscale diodes. In this case, extensive simulations of many configurations with different ionic concentrations and different applied fields were required. Both these simulations are computationally very demanding, these results were possible only thanks to the acceleration provided by GPU.

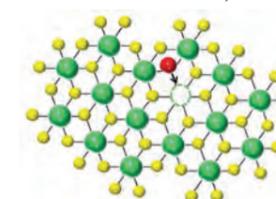
Publications • "Bioinspired catechol-terminated self-assembled monolayers with enhanced adhesion properties" by Mireia Guardingo, Elena Bellido, Rosa Miralles-Llumá, Jordi Faruado, Josep Sedó, Sergio Tatay, Albert Verdagué, Felix Busqué and Daniel Ruiz-Molina. Accepted to Small (October 2013).

Role of impurities and vacancies on the electronic and transport properties of magnetic semiconductors, Víctor Manuel García Suárez, University of Oviedo

Abstract • Electrically conducting ferromagnetic materials where the conduction electrons have a high mobility and are fully spin-polarized are desirable for realizing future thin film spin electronic devices. A comparative investigation will be carried out to study the electronic transport (MR, TMR) properties of defective ZnO, SnO₂, and TiO₂ systems.

These calculations will be a milestone not only towards theoretical condensed matter physics but also towards practical applications in the field of Spintronics. We will focus on native defects (cation and anion), light elements doped systems and the effect of native defects on the current-voltage (IV) characteristics.

Results • The magnetism and electronic structure of Li-doped SnO₂ were investigated using first-principles LDA/LDA+U calculations. We found that Li induced magnetism in SnO₂ when doped at the Sn site but became nonmagnetic when doped at the O and interstitial sites. The calculated formation energies showed that Li preferred the Sn site as compared with the O site, in agreement with previous experiments. The interaction of Li with native defects (Sn V_{Sn} and O V_O vacancies) was also studied, and we found that Li not only behaves as a spin polariser, but also a vacancy stabilizer, i.e., Li significantly reduces the defect formation energies of the native defects and helps the stabilization of magnetic oxygen vacancies. The electronic densities of states revealed that these systems, where the Fermi level touches the conduction (valence) band, are nonmagnetic (magnetic). We also found that the transport properties (metallic or insulator character) depended strongly on the doping site and type of vacancy. Sn-doping and Sn vacancies produced half-metallic behaviour.



Schematic representation of the structural relaxation in the LiO + VS_n system

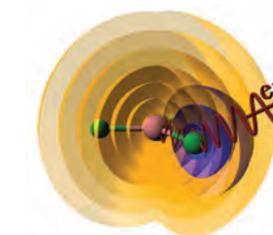
Publications • Gul Rahman, Naseem Ud Din, Víctor M. García-Suárez, and Erjun Kan. Physical Review B 87, 205205 (2013).

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

Abstract • Attosecond laser technology allows to explore the ultrafast electronic and nuclear dynamics induced by light. 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. We will focus on attosecond pulse train pump - infrared probe schemes, which involve high- and low-energy photons and different laser intensities. In this framework, we seek to perform numerical studies in molecules, a systematic study on the influence of laser parameters on autoionisation processes, and a study on single and double ionization of molecules. Our work will be carried out in parallel with experiments.

Results • We have performed ab-initio time-dependent calculations for describing the interaction of small molecules with ultrashort laser pulses. This was done with parallel codes, using MPI and PETSc, as well as the computational support available at Mare Nostrum. Main results: 1. We developed a new method to obtain accurate correlated electron- and nuclear-kinetic energy spectra for H₂⁺ ionization under strong infrared (IR) laser pulses [Silva2013]. For that we solved the time-dependent Schrödinger equation (TDSE) in a 2D grid. 2. Intramolecular photoelectron diffraction (IED) was found in the collective vibrational excitation caused by photoionisation of gas-phase molecules. For that we used density functional theory (DFT) time-dependent DFT [Kukk2013, Ueda2013]. 3. We studied the creation of oscillating dipoles in H₂⁺, by solving the TDSE in a 2D grid. We used ultrashort laser pulse pumps and low-frequency [Chang2013a] or static [Chang2013b] probes. 4. We introduced a simple semiclassical model to explain H₂ photoionisation spectra [Palacios2013]. We also studied electron localization involving doubly-excited states [Fischer2013]. For that we solved the TDSE with a full-dimensional method.

Publications • Silva, R. E. F., Catoire, F., Rivière, P., Bachau, H. & Martín, F. "Correlated electron and nuclear dynamics in strong field photoionization of H₂⁺" Physical Review Letters 110, 113001 (2013) • Kukk, E., Ayuso, D., Thomas, T. D., Decleva, P., Patanen, M., Argenti, L., Plésiat, E., Palacios, A., Kooser, K., Travnikova, O., Mondal, S., Kimura, M., Sakai, K., Miron, C., Martín, F. & Ueda, K. "Effects of molecular potential and geometry on atomic core-level photoemission over an extended energy range: The case study of the CO molecule". Physical Review A 88, 33412 (2013) • Ueda, K., Miron, C., Plésiat, E., Argenti, L., Patanen, M., Kooser, K., Ayuso, D., Mondal, S., Kimura, M., Sakai, K., Travnikova, O., Palacios, A., Decleva, P., Kukk, E. & Martín, F. "Intramolecular photoelectron diffraction in the gas phase" Journal of Chemical Physics 139, 124306 (2013) [Chang2013a] • Chang, B. Y., Shin, S., Palacios, A., Martín, F. & Sola, I. R. "Two-pulse control of long amplitude vibrations in H₂⁺" ChemPhysChem 14, 1405 (2013). [Chang2013b] • Chang, B. Y., Shin, S., Palacios, A., Martín, F. & Sola, I. R. "Ultrafast coherent control of giant oscillating molecular dipoles in the presence of static electric fields" Journal of Chemical Physics 139, 184306 (2013) • Palacios, A., Feist, J., González-Castrillo, A., Sanz-Vicario, J. L. & Martín, F. "Autoionization of molecular hydrogen: where do the Fano lineshapes go?" ChemPhysChem 14, 1456 (2013) • Fischer, A., Sperl, A., Cörlin, P., Scönewald, M., Rietz, H., Palacios, A., Goalez-Castrillo, A., Martín, F., Pfeifer, T., Ullrich, J., A. Senftleben & Moshhammer, R. "Electron localization involving doubly-excited states in broadband XUV ionization of H₂" Physical Review Letters 110, 213002 (2013).



Intramolecular electron diffraction in BF₃ [Ueda2013.]

Astronomy, Space & Earth Sciences 2013 Projects

- » **3D simulations of mixing in novae: the effect of the white dwarf composition and mass** - Leader Name: Jordi José, Leader Institution: UPC
- » **Building an improved catalog of gravitational waves from neutron star mergers** - Leader Name: José Antonio Font Roda, Leader Institution: Universidad de Valencia
- » **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 Martínez González, Leader Institution: Instituto de Física de Cantabria
- » **Dust Effects on the Spectral Energy Distribution of Galaxies** - Leader Name: Rosa Domínguez, Leader Institution: Univ. Autónoma Madrid
- » **Fuel moisture content models to forest fire behaviour forecast** - Leader Name: Roberto San José, Leader Institution: UPM Computer Science School
- » **Gaia: Simulation of Telemetry Stream** - Leader Name: Jordi Torra i Roca, Leader Institution: Universitat de Barcelona (UB), Departament d'Astronomia i Meteorologia
- » **Imaging fields for time reversal in seismology** - Leader Name: Daniel Stich, Leader Institution: Instituto Andaluz de Geofísica
- » **Impact of Charge and Spin on Black-Hole Collisions** - Leader Name: Ulrich Sperhake, Leader Institution: CSIC-IEEC Barcelona
- » **Impact Of Solar Forcing On Future Climate Change Using A Chemistry Climate Model – Final Stage** - Leader Name: Natalia Calvo Fernández, Leader Institution: Universidad Complutense de Madrid
- » **Implementation of a High-Res Ensemble Kalman Filter for the Western Mediterranean** - Leader Name: Victor Homar Santaner, Leader Institution: Universitat de les Illes Balears
- » **Initialization of seasonal-to-decadal climate predictions** - Leader Name: Francisco J. Doblas-Reyes, Leader Institution: Institut Català de Ciències del Clima
- » **Install and test run of the "Space Weather Modeling Framework" at RES** - Leader Name: Antonio Guerrero, Leader Institution: University of Alcalá
- » **Relativistic extragalactic jets: Interaction with stellar winds** - Leader Name: Manel Perucho Pla, Leader Institution: Universitat de València
- » **Simulations of dynamics of partially ionized solar atmosphere** - Leader Name: Elena Khomeiko, Leader Institution: Instituto de Astrofísica de Canarias
- » **Slow down of the global warming in the early XXIst century** - Leader Name: Francisco J. Doblas-Reyes, Leader Institution: Institut Català de Ciències del Clima
- » **The Magnetism of the Solar Atmosphere** - Leader Name: Fernando Moreno-Inserit, Leader Institution: Instituto de Astrofísica de Canarias
- » **The Marenstrum Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe** - Leader Name: Gustavo Yepes, Leader Institution: Universidad Autónoma 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)
- » **Weighing light with supermassive black holes** - Leader Name: Hirota Okawa, Leader Institution: Institute Superior Tecnico

Biology and Life Sciences 2013 Projects

- » **Catalytic mechanism of the Complex II family enzyme Succinate:quinone oxidoreductase (SQR)** - Leader Name: Marcel Swart, Leader Institution: Universidad de Girona
- » **Conformational transitions in the ATP-lid of HSP90: Free energy insights for drug design** - Leader Name: Xavier Barril, Leader Institution: ICREA & Universitat de Barcelona
- » **Development of novel treatments for myotonic dystrophy: in vivo drug discovery** - Leader Name: Jordi Teixidó, Leader Institution: Institut Químic de Sarrià (IQS, URL)
- » **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
- » **Genomic regulation of transcription in Human Pancreatic Islets** - Leader Name: Jorge Ferrer Marrades, Leader Institution: Centre Esther Koplowitz, IDIBAPS
- » **Investigating the Binding Conformational Flexibility of Non-Nucleoside Reverse Transcriptase Inhibitors through Metadynamics Simulations** - Leader Name: Agostino Bruno, Leader Institution: University of Naples
- » **Investigating the protomeric space of Hairpin DNA by CPMD simulations** - Leader Name: Paolo Carloni, Leader Institution: German Research School for Simulation Sciences GmbH
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- » **Microbial Oceanomics using Next-Generation Sequencing** - Leader Name: Ramiro Logares-Haurie, Leader Institution: Instituto de Ciencias del Mar, CMIMA, CSIC
- » **Molecular Dynamics Of Gpcrs In Lipid Rafts Of Cns Diseases** - Leader Name: Jana Selent, Leader Institution: Pompeu Fabra University
- » **Oligomerization of alpha-I-microglobulin triggered by heme binding** - Leader Name: Fco. Javier Luque Garriga, Leader Institution: Faculty of Pharmacy, University of Barcelona
- » **Probing the thermal stability of wild-type thioredoxin and selected mutants by means of unbiased molecular dynamics simulations** - Leader Name: Federico Gago, Leader Institution: Universidad de Alcalá
- » **Reverse-engineering embryo segmentation patterning in flies: exploring different scenarios** - Leader Name: Johannes Jaeger, Leader Institution: EMBL/CRG Research Unit in Systems Biology
- » **Simulation study of Genomic Selection for increasing heat tolerance of livestock** - Leader Name: Juan Pablo Sánchez Serrano, Leader Institution: IRTA
- » **Structural modelling 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 the nucleotide conformational switch in bacterial cell division proteins by all-atom simulations** - Leader Name: Pablo Chacón, Leader Institution: IQFR (CSIC)
- » **Targeting The Dimerization Interface Of Leishmania Trypanothione Reductase In The Search For New Drugs** - Leader Name: Federico Gago,

Leader Institution: Universidad de Alcalá

- » **The effect of the oncogenic mutations on the conformational landscape of B-RAF kinase** - Leader Name: Francesco Luigi Gervasio, Leader Institution: CNIO & UCL
- » **Thermodynamics and kinetics of ligand binding to retinol-binding protein I and II** - Leader Name: Fco. Javier Luque Garriga, Leader Institution: Faculty of Pharmacy, University of Barcelona
- » **Transmembrane Ion Transport through alpha, gamma-Peptide Nanotubes** - Leader Name: Rebeca García Fandiño, Leader Institution: Universidad de Santiago de Compostela
- » **Understanding the binding kinetics of Acetylcholine Binding Protein (AChBP) inhibitors** - Leader Name: Xavier Barril, Leader Institution: ICREA & Universitat de Barcelona

Chemistry and Material Sciences 2013 Projects

- » **A comparison of the exohedral reactivity of the endohedral metallofullerenes (EMFs) M@C_{2v}(9)-C₈₂ (M = Sc, Y, La, Ce, Gd, Lu, Er, Dy, Tb, Yb, Tm, Eu, Sm and Ti) in carbene addition** - Leader Name: Josep M. Luis, Leader Institution: Universitat de Girona
- » **A theoretical study on the adsorption and mechanical properties of the Immunoglobulin G (IgG)** - Leader Name: Rubén Pérez, Leader Institution: Universidad Autónoma de Madrid
- » **Ab initio calculation on graphene and two-dimensional transition metal dichalcogenides for sensing applications** - Leader Name: Blanca Biel, Leader Institution: Universidad de Granada
- » **Ab initio metadynamics simulations of the binding of peptides to gold nanoparticles** - Leader Name: Carme Rovira, Leader Institution: Universitat de Barcelona
- » **Ab initio molecular dynamics of organic ion-radical pairing in solution** - Leader Name: Juan José Novoa Vide, Leader Institution: University of Barcelona
- » **Ab initio study of organic molecule solvation in ionic liquid-water mixtures** - Leader Name: Thomas Schafer, Leader Institution: POLYMAT, UPV/EHU
- » **Ab-initio calculations of thermoelectric properties in nanostructures: silicene, germanene, Si/Ge heterostructure, and two-dimensional transition-metal-dichalcogenides** - Leader Name: Ángel Rubio, Leader Institution: University of the Basque Country UPV/EHU
- » **Ab-initio study of the magnetic behaviour in a Tm-monolayer on (110) W substrate** - Leader Name: César, Leader Institution: Universidad de Zaragoza
- » **Anomalous Thermodynamic Behaviour of Calcium Fluoride Under Pressure: Superionic versus Liquid Atomic Diffusion** - Leader Name: Claudio Cazorla, Leader Institution: Institute of Materials Science of Barcelona (ICMAB-CSIC)
- » **Benchmark Calculations on Few-Electron Harmonium Atoms** - Leader Name: Prof. Jerzy Cioslowski, Leader Institution: Institute of Physics, University of Szczecin
- » **Binding of glycosylated surfactants to concanavalin A** - Leader Name: Antoni Planas, Leader Institution: Laboratory of Biochemistry, IQS - Universitat Ramon Llull
- » **Catalysis modeling: gold nanoparticles supported on yttrium modified anatase as efficient WGS and CO oxidation catalysts** - Leader Name: Javier Fdez Sanz, Leader Institution: Universidad de Sevilla
- » **Conformational free energy landscapes of carbohydrates** - Leader Name: Carme Rovira, Leader Institution: Universitat de Barcelona

- » **CPMD study of the crystal thermal effects on the NCBDTA magnetic crystal: Vibrational thermal effect or phase transition?** - Leader Name: Juan Jose Novoa Vide, Leader Institution: University of Barcelona
- » **Characterization of supramolecular host-guest cages** - Leader Name: Marcel Swart, Leader Institution: Universidad de Girona
- » **Charge transfer and self-assembly of molecules on modified metal surfaces** - Leader Name: Manuel Alcamí, Leader Institution: UAM
- » **Chemical functionalization of carbon-based materials through reaction with benzyne. A comparison between the (2+2) and (4+2) cycloaddition pathways** - Leader Name: Miquel Solà, Leader Institution: Universidad de Girona
- » **De novo design of enzymes** - Leader Name: Kendall N. Houk, Leader Institution: University of California, Los Angeles (UCLA), Department of Chemistry and Biochemistry
- » **Design and Characterization of Advanced Photovoltaic Materials with High Efficiency** - Leader Name: Perla Wahnón, Leader Institution: Universidad Politécnica de Madrid
- » **DFT modeling of ethane dehydrogenation catalysts** - Leader Name: José Carlos Conesa, Leader Institution: Instituto de Catálisis y Petroleoquímica, CSIC
- » **Dielectric Losses Caused by Jahn-Teller Phonons in LaCoO₃ Perovskite Nanoparticles** - Leader Name: Jose Gracia, Leader Institution: UNIZAR
- » **Effect of epitaxial strain on the properties of BiMnO₃: a first-principles study** - Leader Name: Oswaldo Diéguez, Leader Institution: ICMAB-CSIC
- » **Electronic properties of the nanoscale interfaces based on the graphene and molybdenum monolayers.** - Leader Name: Joaquin Fernandez-Rossier, Leader Institution: International Iberian Nanotechnology Laboratory
- » **Electronic structure of semiconductors by means of quasiparticle calculations: relevance to photocatalysis** - Leader Name: Francesc Illas, Leader Institution: Universitat de Barcelona
- » **Electron-phonon coupling and CDWs in low-dimensionality crystals** - Leader Name: Pablo Ordejón, Leader Institution: CIN2 (CSIC-ICN)
- » **Elucidating the mechanism of formation of the enamine intermediate in proline catalyzed aldol reactions in water** - Leader Name: Jordi Ribas, Leader Institution: Universitat de Barcelona
- » **Exploring enzyme catalysis of a series of Directed Evolution ADH mutants** - Leader Name: Kendall N. Houk, Leader Institution: University of California, Los Angeles (UCLA), Department of Chemistry and Biochemistry
- » **First principles investigation of Ni/ceria nanocatalysts for water-gas shift reaction** - Leader Name: Maria Veronica Ganduglia-Pirovano, Leader Institution: Instituto de Catálisis y Petroleoquímica, CSIC
- » **First principles simulations of Scanning Probe Microscopies experiments on graphene heterostructures and metal oxides** - Leader Name: Ruben Perez, 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 simulations of defects on metal oxides and graphene sensed by scanning probe microscopies** - Leader Name: Rubén Pérez, Leader Institution: Universidad Autónoma de Madrid
- » **Formation of Molecular Hydrogen on Surfaces of Cosmic Dust** - Leader Name: Albert Rimola, Leader Institution: UAB
- » **Graphene heterostructures with 2D nanosheets** - Leader Name: Miguel Pruneda, Leader Institution: CIN2 (CSIC-ICN)
- » **High level QM/MM Free Energy Surfaces of enzyme catalyzed reactions by FEP methods** - Leader Name: Vicent Moliner, Leader Institution:

- Universitat Jaume I
- » **Ice crystallization** - Leader Name: Carlos Vega, Leader Institution: Universidad Complutense de Madrid, Fac.Ciencias Químicas, Dep.Química Física I
 - » **Ketonic decarboxylation over metal oxides: MgO and ZrO₂** - Leader Name: Mercedes Boronat, Leader Institution: Instituto de Tecnología Química UPV-CSIC
 - » **Magnetism and Transport Properties of Magnetic Molecules on Surfaces and Nanostructured Systems** - Leader Name: Eliseo Ruiz, Leader Institution: Universitat de Barcelona
 - » **MEMOIR: Multiferroic and magnetoElectric Metal Organic frameworks** - Leader Name: Alessandro Stroppa, Leader Institution: CNR-SPIN
 - » **Methane activation by metallic nanoparticles supported on MoC and Mo₂C** - Leader Name: Francesc Illas, Leader Institution: Universitat de Barcelona
 - » **Modelling silica supported organic nitroxide radicals with applications in NMR signal enhancement: effect of the solvent nature and silanol density on the surface** - Leader Name: Xavi Solans, Leader Institution: UAB
 - » **Molecular-level understanding of CeO₂ as catalyst for partial alkyne hydrogenation** - Leader Name: Maria Verónica Ganduglia-Pirovano, Leader Institution: Instituto de Catálisis y Petroleoquímica, CSIC
 - » **Multi-scale modeling of heme-proteins NMR chemical shifts** - Leader Name: Marcel Swart, Leader Institution: Universidad de Girona
 - » **Optical response, excitons and electronic correlations in TiO₂ nanomaterials: novel insights from a fully ab-initio many-body perturbation theory approach** - Leader Name: Ángel Rubio, Leader Institution: University of the Basque Country UPV/EHU
 - » **Optimization and Exploration of an Orbital Minimization Scheme for ab-initio molecular-dynamics simulation in the SIESTA code** - Leader Name: Alberto García, Leader Institution: ICMA-B-CSIC
 - » **Oxidative addition at Pd centers by explicit solvent ab initio molecular dynamics** - Leader Name: Agustí Lledós, Leader Institution: UAB
 - » **Performance of Time Dependent Density Functional Theory in the strong field photoionisation of noble gas atoms** - Leader Name: Ángel Rubio, Leader Institution: University of the Basque Country UPV/EHU
 - » **PNOF5-PT2: A new benchmark tool in computational chemistry** - Leader Name: Mario Piris, Leader Institution: EHU
 - » **Polyoxometallates on surfaces as new molecular electronic devices and electron storage systems** - Leader Name: Prof. Dr. Josep M. Poblet, Leader Institution: Universitat Rovira i Virgili
 - » **Post-synthetic modification of Metal-organic frameworks: an ab initio theoretical study (1st. period)** - Leader Name: Nuria López, Leader Institution: ICIQ
 - » **QM/MM metadynamics Studies on the Galactosidase Catalytic Mechanism** - Leader Name: J. J. Barbero, Leader Institution: CIB
 - » **Quantum nonlocal effects in plasmonic nanostructures: bridging the gap between fully atomistic approaches and the classical descriptions of their electronic response** - Leader Name: Ángel Rubio, Leader Institution: University of the Basque Country UPV/EHU
 - » **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
 - » **Regioselectivity of Bingel and Diels-Alder cycloadditions on non-IPR Endohedral Metallofullerenes** - Leader Name: Miquel Solà, Leader Institution: Universidad de Girona
 - » **Role of hopanoids in the mechanical properties of model bacterial membranes and function of mechanosensitive channels** - Leader Name: Juan M. Vanegas, Leader Institution: Sandia National Laboratories
 - » **Role of metal cations on the stability of protein motifs. An ab initio molecular dynamics study.** - Leader Name: Mariona Sodupe, Leader Institution: Universitat Autònoma de Barcelona
 - » **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: Centre d'Investigació en Nanociència i Nanotecnologia (CIN2)
 - » **Solvation dynamics - the very first steps** - Leader Name: Coen de Graaf, Leader Institution: Universitat Rovira i Virgili
 - » **Structure, stability and spectroscopic properties of charged PAH (Polycyclic Aromatic Hydrocarbons) and PAH clusters** - Leader Name: Manuel Alcamí, Leader Institution: UAM
 - » **Structure, stability and spectroscopic properties of positively charged polycyclic aromatic hydrocarbons** - Leader Name: Sergio Díaz Tendero, Leader Institution: UAM
 - » **Study of bulk and nanoconfined liquid water from ab initio simulations** - Leader Name: Emilio Artacho, Leader Institution: CIC nanoGUNE Consolider and University of Cambridge
 - » **Study of dopants in Silicon Quantum dots for Solar Cells Application (EU project FP7-NMP-245977)** - Leader Name: Albert Cirera Hernández, Leader Institution: Universitat de Barcelona
 - » **Study of the adsorption and reactivity of biomass-derived compounds on metallic surfaces in an aqueous environment: Ab Initio Molecular Dynamics studies on the structure of thick water layers. (1st. period)** - Leader Name: Nuria Lopez, Leader Institution: ICIQ
 - » **The Nature of Pd(0) precatalyst in Cross-Coupling Reactions** - Leader Name: Gregori Ujaque, Leader Institution: UAB
 - » **The Phase Diagram of Bismuth Ferrite by Ab Initio Calculations** - Leader Name: Claudio Cazorla, Leader Institution: Materials Science Institute of Barcelona -ICMAB-CSIC
 - » **Theoretical Characterization of the optimized geometry and energy levels in an hybrid nanostructure** - Leader Name: Pablo Palacios, Leader Institution: Universidad Politécnica de Madrid
 - » **Towards catalysts of new generation: Active sites of ionic Pt in nanostructured ceria** - Leader Name: Konstantin NEYMAN, Leader Institution: Departament de Química Física, Universitat de Barcelona
 - » **Transition metal chemistry with PNOF5** - Leader Name: Jesus Mari Ugalde Uribe-txeberria, Leader Institution: UPV/EHU
 - » **Ultrafast Electron Dynamics at alkali/ice structures adsorbed on Cu(111) from experiments and theory** - Leader Name: Angel Rubio, Leader Institution: University of the Basque Country UPV/EHU
 - » **Understanding the dynamics of water-silicate interactions at the nanoscale** - Leader Name: Stefan Bromley, Leader Institution: UB
 - » **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 a high-Reynolds-number homogeneous shear turbulence** - Leader Name: Javier Jiménez Sendín, Leader Institution: School of Aeronautics, Universidad Politécnica Madrid, 28040-Madrid, Spain
 - » **Direct Numerical Simulations of channel flows with regime transition due to coalescence in gas liquid bubbly flows** - Leader Name: Assensi Oliva, Leader Institution: Universitat Politècnica de Catalunya
 - » **Driving mechanisms of covalent and chiral self-assemblies of organic molecules on metal surfaces** - Leader Name: Andrea Floris, Leader Institution: King's College London
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c/ Jordi Girona, 31 – Torre Girona Building

08034 Barcelona (Spain)

info@bsc.es

www.bsc.es

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