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Annual Report
2015

**Barcelona
Supercomputing
Center**
Centro Nacional de Supercomputación

R E S

(11)

The 2015 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

BSC-CNS PATRONS

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Departament d'Empresa
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BSC-CNS GRATEFULLY ACKNOWLEDGES THE SUPPORT OF

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Barcelona Supercomputing Center
Centro Nacional de Supercomputación

2015 | Annual Report

BSC-CNS: Year in Review

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

In 2015, BSC-CNS celebrated its 10th birthday. Since the Centre was inaugurated in April 2005, the MareNostrum supercomputer has undergone three major upgrades and is now one of six Tier-0 nodes in the pan-European PRACE network servicing researchers worldwide, while the Centre has grown from 83 people in 2005 to over 447 today, and is firmly positioned amongst the very top supercomputing centres internationally in both research output and technical services.

Once again, the quality of BSC-CNS research staff and the professionalism of support staff were amply demonstrated by continued strong success in the highly competitive European H2020 programme. In 2015, BSC-CNS was successfully awarded grants for six Centre of Excellence projects, six Future and Emerging Technology (FET) projects and over a dozen projects in other H2020 programmes.

Mission

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

ETP4HPC Strategic Research Agenda

ETP4HPC is an industry-led think tank and advisory group of companies and research centres involved in HPC (Supercomputing) technology research in Europe. In November 2015, it released an update to the European High-Performance Computing (HPC) Technology Strategic Research Agenda (SRA). ETP4HPC issues and maintains this SRA as a mechanism to provide contextual guidance to European Researchers and Businesses and also to guide EU priorities for research in the Horizon 2020 HPC programme. This SRA delineates a roadmap for the achievement of European exascale capabilities focusing on the following areas: HPC System Architecture and Components, Energy and Resiliency, Programming Environment, System Software and Management, Big Data and HPC Usage Models, Balance Compute, I/O and Storage Performance, Mathematics and Algorithms for Extreme-Scale HPC systems and Extreme-Scale Demonstrators.

BSC-CNS played a key role in the development of the SRA and is a member of the ETP4HPC steering board.

The value of BSC-CNS as the National Supercomputing Laboratory and its success in spearheading Spain´s international standing in HPC development was recognised by the renewal of the Severo Ochoa Centre of Excellence Award by MINECO. The Ministry further reinforced the Centre by committing 34 million euro for the next MareNostrum upgrade, ensuring that BSC-CNS maintains its position as a PRACE hosting partner for the coming years, and together with the Generalitat of Catalonia and the Universitat Politècnica de Catalunya, renewed the consortium agreement funding BSC-CNS through to 2019.

At the national level, the Spanish Supercomputing Network (RES), which is coordinated by BSC-CNS, also grew significantly with the addition of five new nodes: Finis Terrae II (Galicia), Pirineus (Cataluña), Lusitania (Extremadura), Caléndula (Castilla y León) and Cibeles (Madrid). The RES nodes provide services to scientists from all disciplines throughout Spain, and BSC-CNS assists the nodes with technical expertise and organises trainings for both operators and users.

Barcelona is increasingly recognised as a global node for supercomputing excellence, with the number of high level scientific and training workshops taking place in the city increasing year on year. Highlights for 2015 included the Joint Laboratory for Extreme Scale Computing (JLESC) workshop in June 2015, where top researchers from six of the largest supercomputing centres in the world met in Barcelona to discuss the

software challenges for future supercomputers, which was followed by the JLESC Summer School on Storage, IO and Data Analytics, and the plenary meeting of Big Data and Extreme-scale Computing (BDEC), held in Barcelona in January. Also of great interest was the proof of concept trial of Fog computing architecture in collaboration with the City Hall of Barcelona and Cisco.

The year also saw further expansion of BSC-CNS collaboration with key IT industry leaders: new collaboration programmes were initiated with Lenovo, Cisco and Samsung, the existing collaboration with NVIDIA was renewed, and the joint research programmes with Intel and Microsoft were expanded. BSC-CNS collaborations with industry are not limited just to the IT sector; new HPC technologies and applications are being developed across a wide range of industries. In the energy sector, the extremely successful collaboration on subsea exploration with Repsol was renewed, and important developments were made on wind-farm modelling with Iberdrola. In the biomedical sector, BSC-CNS is improving drug design with AstraZeneca and Novozymes, while in climate and weather analysis and forecasting BSC-CNS is working with the World Meteorological Organization (WMO), the US National Oceanic and Atmospheric Administration (NOAA), the International Research Institute for Climate and Society (IRI), among others.

Mateo Valero - first European to receive the Seymour Cray Computer Engineering Award

The Seymour Cray Computer Engineering Award is one of the IEEE Computer Society's highest awards, presented to recognise significant and innovative contributions in the field of high-performance computing. The award honours scientists who exhibit the creativity demonstrated by Seymour Cray, founder of Cray Research, Inc., and an early pioneer of supercomputing.

Prof. Valero, Director of BSC-CNS, was selected as the recipient for the award in recognition of seminal contributions to vector, out-of-order, multithreaded, and VLIW architectures.

Patrons of BSC-CNS

BSC-CNS is a legally autonomous, public consortium, with three founding partners: the Spanish Ministry of Economy and Competitivity (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 (60%), DECO (30%), and UPC (10%).
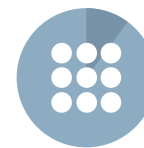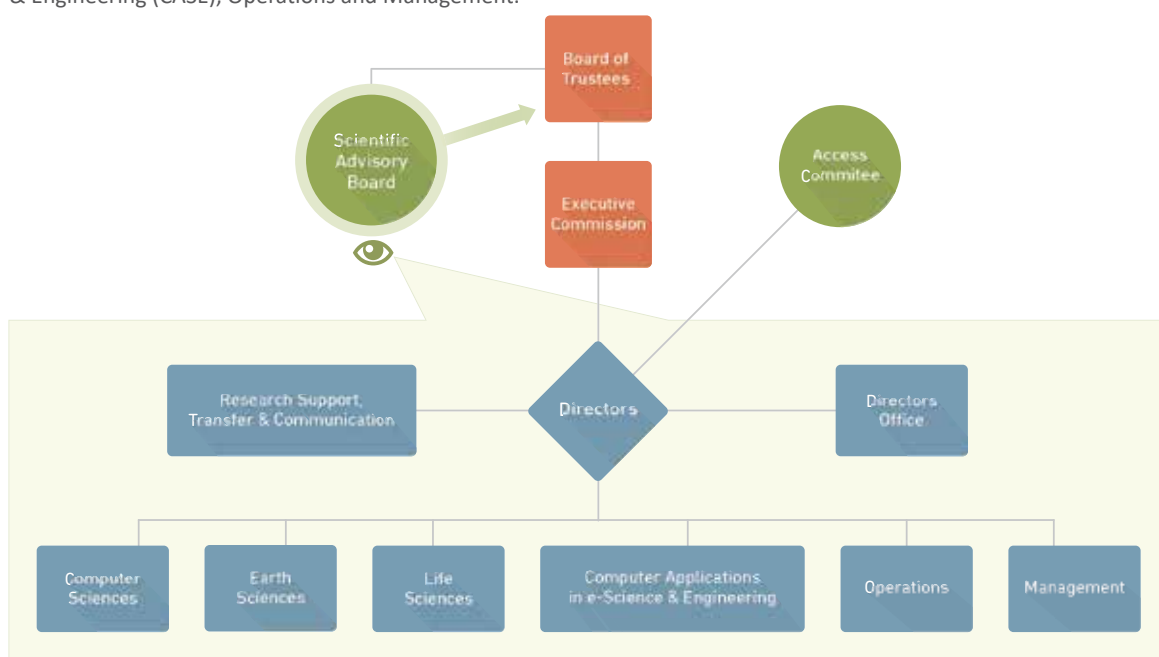
30% DECO   60% MINECO   10% UPC

Support and Research

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

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

The **Computer Sciences Department** pursued existing and new collaborations with IT market leaders (Intel, NVIDIA, Microsoft, IBM, Samsung, Xilinx, Qualcomm, and others), as well as with other international computing centres and key international research initiatives. The Department covers 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, as well as support for the efficient programming and management of BigData and Cloud architectures. Thanks in large part to the Severo Ochoa program, the Department has developed strong interactions with other BSC-CNS departments on multi-disciplinary projects requiring strong co-development of hardware and operating systems with new applications. Highlights of 2015 include the Department's participation in some 32 European projects and networks, two ERC grants, ongoing participation in key networks such as ETP4HPC, HiPEAC-3, EuroLab-4-HPC, the SCALUS Marie Curie training network, international alliances and standardisation efforts such as JLESC, BDEC and the OpenMP Architecural Review Board, industrial collaborations, and projects with the European Space Agency.

The **Earth Sciences Department** underwent a major organisational restructure in 2015 following the appointment of ICREA Prof. Francisco J. Doblas-Reyes as the new director in late 2014. Prof. Doblas-Reyes brought with him to BSC-CNS the majority of his research group from the Catalan Institute of Climate Sciences (IC3) and the Department is now organised in four main research areas: Atmospheric Composition, Climate Prediction, Earth System Services, and Computational Earth Sciences.

In addition to important roles in numerous international projects and organisations, including coordinator of the European project SPECS which aims to identify the main problems in climate prediction, the Department also maintains daily high-resolution operational air quality forecasts for Europe and Spain under the umbrella of the CALIOPE project, and also mineral dust forecasts for the Euro-Mediterranean region and East Asia. The Department hosts the Regional Centre for Sand and Dust Storm Warning System (SDS-WAS) covering Europe, northern Africa and the Middle-East, and the first WMO regional meteorological centre specialised in atmospheric sand and dust forecast, the Barcelona Dust Forecast Centre (BDFC).

The **Life Sciences Department** is tightly integrated in a collaborative effort with the Institute for Research in Biomedicine (IRB Barcelona) and the Centre for Genomic Regulation (CRG) under the Joint BSC-CRG-IRB Research Programme on Computational Biology. The Department initiated a number of new European projects in 2015, and continued extensive collaborations with major international initiatives such as the CAPRI life sciences community framework and the international PanCancer consortium. An important milestone was the formation during 2015 of the first BSC-CNS spin-off, Nostrum Drug Discovery, to commercialise drug discovery and design tools developed by researchers at the Department.

CASE Department research is primarily driven by the application needs of its collaborators, who come from all areas of science and technology. Current projects cover applications in diverse areas such as aerospace, fusion physics, biomechanics (cardiovascular and respiratory systems), geophysics, atmospheric flows, large scale social simulations and smart cities. During 2015, major industrial partnerships with Repsol and Iberdrola focused on applying supercomputing algorithms to solve complicated problems in subsea exploration and wind farm design, while scientific collaborations with the UK and USA seek to model the human respiratory system, and collaborations with the Spanish CNIC and LNCC in Brasil aim to perform full cardiovascular simulations of the heart. The Department also continued development of its visualisation capabilities, to facilitate graphic interpretation and visualisation of complex data resulting from its simulations.

The **Operations Department** ensures the continuous daily functioning of MareNostrum and other BSC-CNS facilities, as well as coordinating the RES and participation in the European PRACE network, managing remote access by users, both within Spain and internationally. A major activity in 2015 was the integration of five new RES nodes, bringing to 13 the total number of nodes in the Spanish network and a total computing capacity of 1500 TFlops. The Department also participated in a number of strategic projects at European level, such as PRACE 3rd and 4th Implementations, EESI2 to develop a vision of future European Petaflop machines, EUDAT to provide a pan-European solution for research data, RDA Europe to conduct cross-infrastructure experiments on global interoperability, and EXDCI to coordinate the development and implementation of a common strategy for the European HPC Ecosystem.

In Memoriam - Nacho Navarro

Nacho Navarro, leader of the Accelerators for HPC Group at BSC-CNS, passed away on February 28, 2016 at the age of 58. He was born and raised in Barcelona, studied at the Universitat Politècnica de Catalunya – Barcelona Tech (UPC) which he joined in 1985 as a lecturer before becoming Associate Professor. From 2001 onwards, he was also Visiting Research Professor at the Coordinated Science Laboratory at University of Illinois Urbana-Champaign. Although he would never acknowledge it thanks to his humble nature, Nacho Navarro was a truly remarkable person: highly intelligent, patient and incredibly kind, he always made time to listen and was ready to help. His profound humanity was evident in everything he did, shining a spotlight on others while putting himself last. He had friends all over the world about whom he cared deeply, and he touched a great number of people's lives.

Directors Office

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

2015 was a landmark year for BSC-CNS, marking 10 years of uninterrupted growth and advancement. What was a bright dream in 2005 has become a shining reality, with the Centre well established as an international reference and leader in its field, providing scientists from all disciplines across Spain and Europe with advanced supercomputing resources and applications, facilitating important advances in biomedicine, engineering, industry, climatology and even the social sciences. The Patrons of BSC-CNS have reaffirmed their commitment, extending the consortium agreement till the end of the decade and assuring the next upgrade of the MareNostrum Supercomputer, while the generosity of the Repsol Foundation is ensuring the Centre will have a home as the construction of the BSC-CNS building enters the next phase. This long-term commitment and stability enables the Centre to plan for the future and engage in long-term collaborative programs with confidence.

Most important of all, however, are the BSC-CNS staff, students, and collaborators, who through their efforts and talent have built the Centre to what it is today. The Directors extend their sincere gratitude to all who have contributed to the Centre during the past ten years, the BSC-CNS patrons, MINECO, DECO and UPC, and other key funding and support agencies such as the European Commission, Repsol, ICREA, CSIC and the European Research Council.
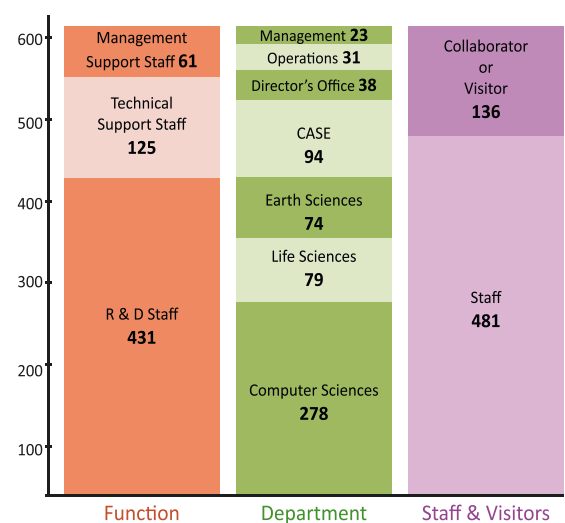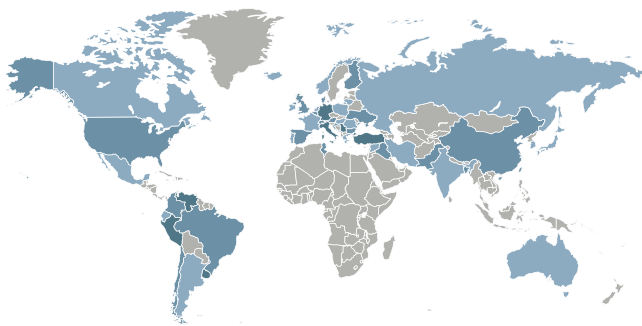
Scientific Output

The work carried out by the scientists at BSC-CNS resulted in some 134 journal, book and book chapter publications, 193 key conference presentations, and 17 PhD theses. Additionally, BSC-CNS researchers presented numerous workshops at both national and international levels, and the Centre hosted a number of key international events.

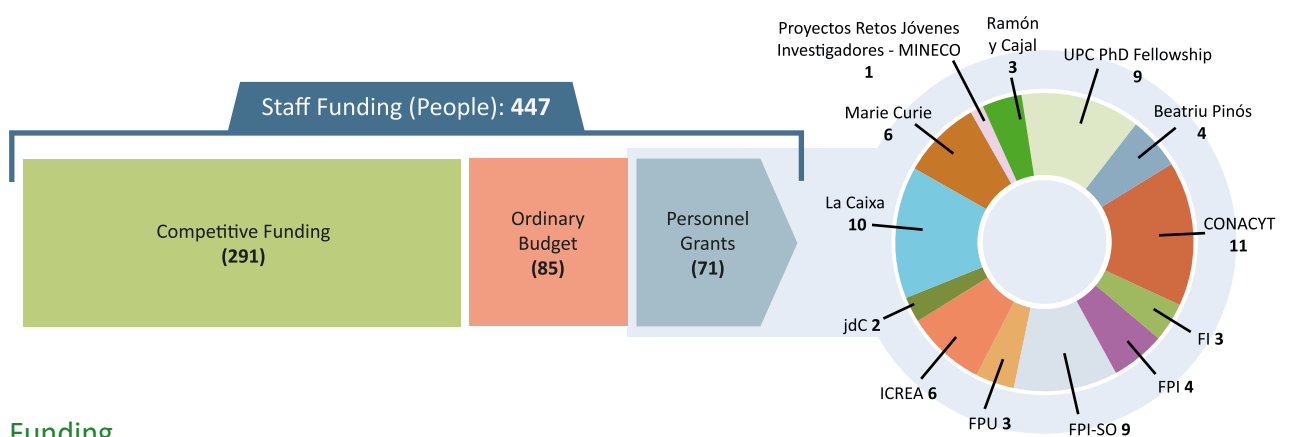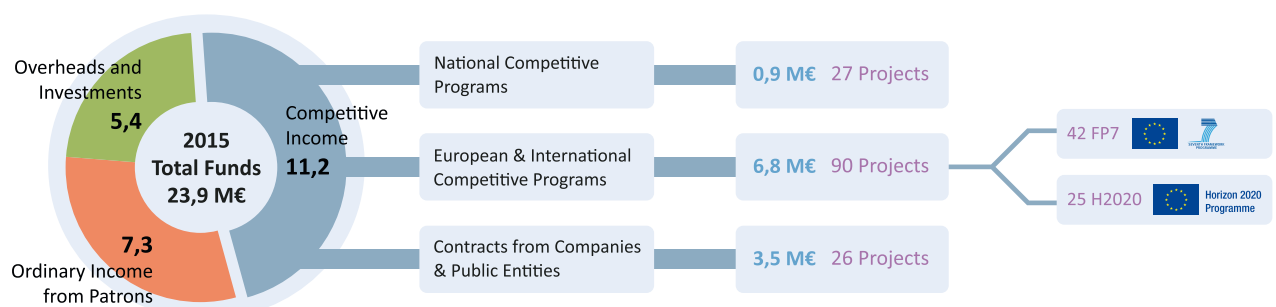| Publishing	Conferences & Workshops	Education
Journal Articles **122**	International Conferences **173**	PhD Theses Read **17**
	National Conferences **20**	Masters Theses Read **1**
Books **1**		
Book Chapters **11**	Workshops **23**	

People

During 2015, some 617 people (staff and visiting researchers) performed research or provided support at BSC-CNS, with over 53 countries represented.

Function	Department	Staff & Visitors
Management Support Staff **61**	Management **23** / Operations **31**	Collaborator or Visitor **136**
Technical Support Staff **125**	Director's Office **38**	
	CASE **94**	
	Earth Sciences **74**	
	Life Sciences **79**	Staff **481**
R & D Staff **431**	Computer Sciences **278**	

The chart below shows a snapshot of the sources of financing for the 447 staff contracted or ascribed to BSC-CNS as at 31st December 2015. The vast majority of BSC-CNS staff are funded by competitive projects or prestigious personal fellowships such as ICREA, Marie Curie, Ramón y Cajal, and many others.

Staff Funding (People): 447

Competitive Funding (291)

Ordinary Budget (85)

Personnel Grants (71)

Proyectos Retos Jóvenes Investigadores - MINECO **1**
Ramón y Cajal **3**
UPC PhD Fellowship **9**
Marie Curie **6**
Beatriu Pinós **4**
La Caixa **10**
CONACYT **11**
jdC **2**
FI **3**
ICREA **6**
FPI **4**
FPU **3**
FPI-SO **9**

Funding

2015 Total Funds 23,9 M€

Overheads and Investments **5,4**

Ordinary Income from Patrons **7,3**

Competitive Income **11,2**

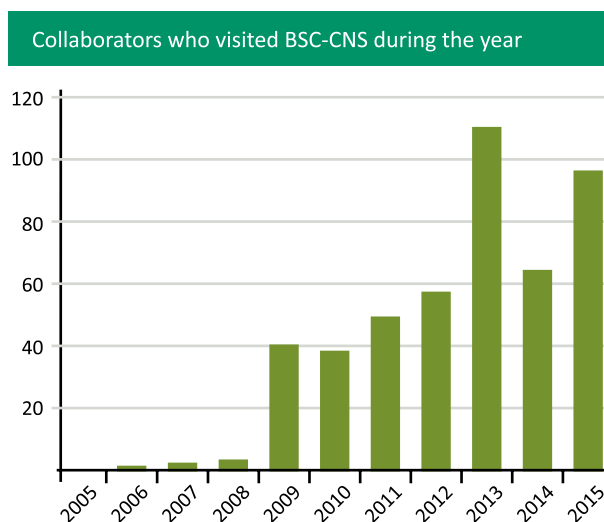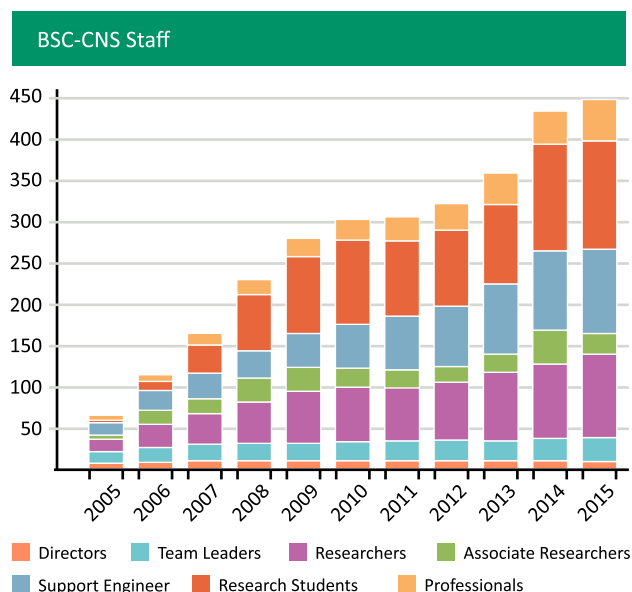|		
National Competitive Programs	**0,9 M€** 27 Projects	
European & International Competitive Programs	**6,8 M€** 90 Projects	42 FP7 / 25 H2020
Contracts from Companies & Public Entities	**3,5 M€** 26 Projects	

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 2015, the core staff of BSC-CNS totalled 447 people, including 85 permanent positions, 291 staff dedicated to specific projects and 71 staff funded by competitive personal grants. In addition, some 96 collaborating researchers from other public and private entities worked at BSC-CNS during the year. The evolution of staff and collaborators can be seen in the graphs below.

BSC-CNS Staff	Collaborators who visited BSC-CNS during the year

Legend: Directors · Team Leaders · Researchers · Associate Researchers · Support Engineer · Research Students · Professionals

Shared Staff and Human Resources Programmes

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

UPC

The Universitat Politècnica de Catalunya · BarcelonaTech (UPC) is a public institution dedicated to higher education and research, specialised in the fields of engineering, architecture and science. As a leading member of international networks of excellence, the UPC has a privileged relationship with global scientific and educational organisations and therefore is well positioned for attracting international talent. UPC participates in the governing Board of BSC-CNS, and in 2015 assigned 16 researchers and professors to BSC-CNS.

ICREA

Created in 2001, the Catalan Institution for Research and Advanced Studies (ICREA) is a foundation supported by the Government of Catalonia and governed by a Board of Trustees. Its aim is to promote research in any field of knowledge, facilitating the consolidation of collective research and the retention of talented research staff within the Catalan university and research centre system. ICREA, through a selection process based on scientific talent, hires senior scientists from around the world to work in and cooperate with local universities and research centres. BSC-CNS was proud to host 6 ICREA professors during 2015.

CSIC

The Spanish National Research Council (CSIC) is the largest public institution dedicated to research in Spain and the third largest in Europe. Belonging to the Spanish Ministry of Economy and Competitiveness through the Secretary of State for Research, Development and Innovation, its main objective is to develop and promote research that will help bring about scientific and technological progress, and it collaborates with Spanish and foreign entities in order to achieve this aim. BSC-CNS was proud to host 4 CSIC researchers during 2015.

The BSC-CNS Fellowship Programme

The BSC-CNS Training Fellowship programme invites applicants from relevant scientific disciplines to participate in several European research projects and collaborations with international industry such as IBM and Microsoft. These Training Fellowships are for PhD, Master and undergraduate students, and during 2015 BSC-CNS hosted 114 PhD Students who 11 of whom hold a Severo Ochoa La Caixa PhD fellowship, 18 Master students and 22 undergraduate students associated with several research projects.

BSC-CNS Governing Bodies

Members of the BSC-CNS Board of Trustees

President:

Mª Luisa Poncela, Secretary General of Science, Technology and Innovation, MINECO.

Vice President:

Antoni Castellà, Secretary General for Universities and Research, DECO.

MINECO Representatives:

Mª Luisa Castaño, Director General for Innovation and Competitivity.

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

DECO Representatives:

Josep Ma Martorell, Director General of Research.

Iolanda Font de Rubinat, Deputy Director General of Research.

UPC Representatives:

Enric Fossas, Rector.

Fernando Orejas, Vice Rector for Research Policy.

BSC-CNS Representatives:

Mateo Valero, Director.

Francesc Subirada, Associate Director.

Ernest Quingles, Manager.

Commission Secretaries:

Ramón Fernández Calvo, State lawyer.

Sue de Antonio Calvo, State lawyer.

Members of the BSC-CNS Executive Committee

President:

Mª Luisa Castaño, Director General for Innovation and Competitivity, MINECO.

Vice President:

Josep Ma Martorell, Director General of Research, DECO.

Representatives MINECO:

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

Representative DECO:

Iolanda Font de Rubinat, Deputy Director General of Research.

Representatives UPC:

Fernando Orejas, Vice Rector for Research Policy.

Esther Real, vicerector for Knowledge Transfer.

Representatives BSC-CNS:

Mateo Valero, Director.

Francesc Subirada, Associate Director.

Ernest Quingles, Manager.

Commission Secretaries:

Ramón Fernández Calvo, State lawyer.

Sue de Antonio Calvo, State lawyer.

Members of the Scientific Advisory Board

Achim Bachem

Chairman of the Board of Directors, Forschungszentrum Jülich.

Catherine Rivière

Présidente Directrice Générale, Grand Equipement National de Calcul Intensif, GENCI.

Horst D. Simon

Associate Laboratory Director for Computing Sciences, Lawrence Berkeley National Laboratory.

Guy Brasseur

Senior Scientist, Max Planck Institute for Meteorology, Germany.

Jack Dongarra

Electrical Engineering and Computer Science Department, University of Tennessee.

Janet Thornton

Director European Bioinformatics Institute, United Kingdom.

Satoshi Matsuoka

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

Thomas Zacharia

Executive Vice President of Research & Development, Qatar Foundation.

Paul Messina

Director of Science, Argonne Leadership Computing Facility, USA.

Manuel Peitsch

Chairman of Board of Directors, Swiss Institute of Bioinformatics.

Leonard Barrie

Bolin Centre for Climate Research, Stockholm University

Management Board

Management Board Chairman:

Mateo Valero, Director.

Management Board Vice-Chairman:

Francesc Subirada, Associate Director.

Members:

Jesús Labarta, Computer Sciences Director.

Eduard Ayguadé, Computer Sciences Associate Director.

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

Modesto Orozco, Life Sciences Director.

Sergi Girona, Operations Director.

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

Ernest Quingles, Management Director.

Access Committee

Core Team:

Julio Bravo, Agencia Nacional de Evaluación y Prospectiva.

Alfonso Tarancón, Universidad de Cantabria.

Joaquín Serrano, Ministerio de Ciencia e Innovación.

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

Biomedicine and Health Sciences Expert Panel:

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

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

Chemistry and Material Sciences Expert Panel:

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

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

Members of the BSC-CNS Executive Committee

Physics and Engineering Expert Panel:

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

Assistant: **Francisco Castejón**, CIEMAT.

Astronomy, Space and Earth Sciences Expert Panel:

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

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

RES Users Committee (CURES)

Physics and Engineering (FI) representatives:

Javier Jiménez Sendín, Fernando Martín García.

Chemistry and Material Sciences (QCTM) representatives:

Rubén Pérez, Núria López.

Biomedicine and Health Sciences (BCV) representatives:

Carme Rovira, Francisco Javier Luque.

Astronomy, Space and Earth Sciences (AECT) representatives:

Jordi Torra, Miguel Ángel Aloy.

BSC-CNS Staff and Collaborators during 2015

Directors Office

Director: **Mateo Valero Cortés** (UPC)

Associate Director: **Francesc Subirada Curcó**

Research Fellow: José María Baldasano Recio (UPC)

Director Assistant: Lourdes Cortada Agustí

Associate Director Assistant: Judith Camba Alvariño

European Relations

European Relations Senior Advisor Assistant: Amalia Elisabeth Hafner Táboas

European Relations Senior Advisor: Fabrizio Gagliardi

Latin America Relations

Latin America Relations Coordinator: Ulises Cortés García (UPC)

Severo Ochoa Programme

Severo Ochoa ProgrammeCoordinator: Josep Casanovas (UPC)

Research support, Transfer and Communication Group

Research support, Transfer and Communication Group Manager:
Eugene Griffiths

Project Management Office

Project Manager: Catherine Gleeson

Project Manager: Emma Torrella Amador

Project Manager: Ezequiel Mas Del Molino

Project Manager: Francesca Arcara

Project Manager: Guadalupe Moreno Beltrán

Project Manager: Isabel Martínez Beltrán

Project Manager: Maria Toth

Project Manager: Marina Azor Alastuey

Project Manager: Marta Rosselló Vallés

Project Manager: Pilar Callau Uson (Ending Date: 15/05/2015)

Project Manager: Xavier Salazar Forn

Project Manager Support: Isabel García Caparrós (Garantía Juvenil)

Strategy Support

Business Analyst: Marcin Ostasz

PRACE Project Manager: Oriol Pineda Martínez

Strategic Projects Senior Coordinator: Gina Michelle Alioto

Technology Transfer

Technology Transfer Manager : Anna Escoda Sabater

Communication

Communications Coordinator: Renata Giménez Binder

Communications Officer: María José Barroso Sáez

Communications Officer: Núria Masdeu Font

Communications Officer: Sara Ibáñez Leciñena

Dissemination Project Officer: Madeleine Gray

Marenostrum Visitors Officer: Oriol Riu Valentí (UPC)

Education & Training

RES Technical and Training Coordinator: Montserrat González Ferreiro

Education & Academic Programmes Coordinator: Maria Ribera Sancho
Samso (UPC)

Professional HPC Trainning: Evguenia Stoilova Alexandrova

Associate Researcher: Fermín Sánchez Carracedo (UPC)

Press & Protocol Relations

Press and Protocol Relations Manager: Gemma Ribas Maspoch

Computer Sciences Department

Computer Sciences Director: **Jesús Labarta Mancho** (UPC)

Computer Sciences Associate Director: Eduard Ayguadé Parra (UPC)

Computer Sciences Director Assistant: Núria Sirvent Pardell

Postdoctoral Researcher: Dario García Gasulla

Developer: Jonatan Moreno Vazquez

Undergraduate Student: Axel Brando Guillaumes

Undergraduate Student: Sergio Moyano Díaz

Associate Researcher: Julio Ramón Beivide Palacio (Universidad de Cantabria)

Visiting Collaborator: Ahsan J. Awan

Visiting Collaborator: Arnaud Legrand

Visiting Collaborator: Brice Videau

Visiting Collaborator: Hans Christian Hoppe

**Accelerators for High Performance Computing**

Accelerators for High Performance Computing Group Manager:
Nacho Navarro (UPC)

PhD Student: Diego Marrón Vida (BECA UPC)

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.
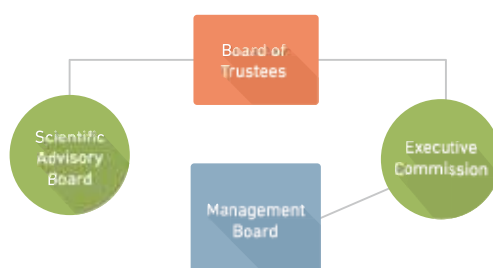
PhD Student: Ivan Tanasic

PhD Student: Javier Cabezas Rodríguez

PhD Student: Lluís Vilanova García

PhD Student: Marc Jordà Peroliu

PhD Student: Víctor García Flores (BECA UPC)

Master Student: Pau Farré González

Associate Research Student: Lluis Gifré (UPC)

Autonomic Systems and e-business Platforms

Autonomic Systems and e-Business Platforms Group Manager: Jordi Torres Vinyals (UPC)

Postdoctoral Researcher: Mario Macías Lloret

PhD Student: David Buchaca Prats

PhD Student: José Alejandro Cordero Rama (La Caixa)
(Ending Date: 22/06/2015)

PhD Student: Nicola Cadenelli

Developer: Alberto Huélamo Segura

Developer: Cesare Cugnasco

Developer: David Ortiz López (Ending Date: 02/09/2015)

Developer: Jordi Aranda Flores (Ending Date: 24/04/2015)

Developer: Josep Subirats Castell (Ending Date: 31/08/2015)

Developer: Mauro Canuto

Trainee Developer: Guillem Alomar Sitjes

Trainee Developer: Roger Hernández Domingo

Undergraduate Student: Josep Cugat Prieto (Ending Date: 31/05/2015)

Undergraduate Student: Mauro Gómez Parada

Associate Researcher: Jordi Guitart Fernández (UPC)

Associate Researcher: Jordi Nin Guerrero (UPC) (Ending Date: 04/05/2015)

Associate Researcher: Rubén Tous Liesa (UPC)

Associate Researcher: Yolanda Becerra (UPC)

Associate Research Student: Joan Capdevila Pujol (UPC - La Caixa)

Visiting Collaborator: Anastasios Gounaris

Computer Architecture / OS Interface (CAOS)

Computer Architecture / OS Interface (CAOS) Group Manager: Francisco Javier Cazorla Almeida (CSIC - UPC)

Senior Researcher: Eduardo Quiñones Moreno

Senior Researcher: Jaume Abella Ferrer (Ramón y Cajal)

Postdoctoral Researcher: Carles Hernández Luz (Proyectos Retos Jóvenes Investigadores - MINECO)

PhD Student: Gabriel Fernández Díaz

PhD Student: Javier Jalle Ibarra (Ending Date: 14/12/2015)

PhD Student: Leonidas Kosmidis (FPU-UPC)

PhD Student: María Astón Serrano García

PhD Student: Milos Panic (FPU)

PhD Student: Mladen Slijepcevic (La Caixa)

PhD Student: Qixiao Liu

PhD Student: Roberto Vargas Caballero

Developer: David Morales Sáez

Developer: Jaume Espinosa García (Ending Date: 30/04/2015)

Developer: Mikel Fernández Oreja

Master Student: David Trilla Rodríguez

Master Student: Enrique Díaz Roque

Master Student: Pedro Benedicte Illescas

Master Student: Suzana Milutinovic

Visiting Collaborator: Elvira Teran

Visiting Collaborator: Jaume Pujantell Trassera

Computer Architecture for Parallel Paradigms

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

Computer Architecture for Parallel Paradigms Group Manager: Osman Unsal

Postdoctoral Researcher: Adrià Armejach Sanosa

Postdoctoral Researcher: Ferad Hasanov Zyulkyarov

Postdoctoral Researcher: Georgios Passas (Ending Date: 30/09/2015)

Postdoctoral Researcher: Gulay Yalcin (Ending Date: 30/09/2015)

Postdoctoral Researcher: Nehir Sonmez (Ending Date: 31/10/2015)

Postdoctoral Researcher: Pablo Prieto Torralbo (Ending Date: 30/04/2015)

Postdoctoral Researcher: Santhosh Kumar Rethinagiri (Ending Date: 31/10/2015)

PhD Student: Azam Seyedi

PhD Student: Behzad Salami

PhD Student: Burcu Mutlu

PhD Student: Daniel Nemirovsky

PhD Student: Ivan Ratkovic (FPU-UPC)

PhD Student: Milan Stanic (FI)

PhD Student: Milovan Duric

PhD Student: Nikola Markovic (FPI-UPC)

PhD Student: Omer Subasi (FI-UPC)

PhD Student: Oriol Arcas Abella (Ending Date: 30/09/2015)

PhD Student: Timothy Hayes (FPU-UPC)

PhD Student: Vasileios Karakostas (FPU)

PhD Student: Vesna Nowack

Developer: Francisco Javier Arias Moreno

Associate Researcher: José Rubén Titos (UPC) (Ending Date: 30/09/2015)

Associate Researcher: Oscar Palomar Pérez (UPC)

Visiting Collaborator: Abraham Josafat Ruiz Ramírez

Visiting Collaborator: Cristóbal Ramírez

Visiting Collaborator: Eduardo Ramírez

Visiting Collaborator: Gorker Alp

Visiting Collaborator: José Luís Narváez

Visiting Collaborator: Kadir Tugberk

Visiting Collaborator: Naveed Ul Mustafa

Visiting Collaborator: Rasha Faqeh

Visiting Collaborator: Tatiana Martsinkevich

Data Centric Computing Area

Data Centric Computing Area Group Manager: David Carrera Pérez (UPC)

Postdoctoral Researcher: Jordà Polo Bardes

Postdoctoral Researcher: Nicolas Poggi Mastrokalo

PhD Student: Marcelo Carneiro Do Amaral

PhD Student: Nesrine Khouzami

Senior Developer: Juan Luis Pérez Rico

Developer: Álvaro Villalba Navarro

Developer: Davide Brini

Developer: Oscar Trullols Cruces

Trainee Developer: Aaron Call Barreiro

Undergraduate Student: Alejandro Montero Rivero

Associate Researcher: Josep Lluís Berral García (UPC)

Extreme Computing

Extreme Computing Group Manager: Vassil Nikolov Alexandrov (ICREA)

Postdoctoral Fellow: Javier Alfonso Espinosa Oviedo

Postdoctoral Fellow: Oscar Alejandro Esquivel Flores (CONACYT) (Ending Date: 21/10/2015)

Visiting Collaborator: Andrey Chernikh

Visiting Collaborator: Aneta Karaivanova

Visiting Collaborator: Diego Dávila

Visiting Collaborator: Dobromir Georgiev

Visiting Collaborator: Karssimir Georgiev

Visiting Collaborator: Krassimir Georgiev

Visiting Collaborator: Ostromsky Tzvetan Tomov

Visiting Collaborator: Raúl Ramírez

Visiting Collaborator: Sofiya Ivanovska

Visiting Collaborator: Svetlana Chuprina

H. A. Architecture simulation environments

Senior Researcher: Alejandro Rico Carro (Ending Date: 07/08/2015)

PhD Student: Nikola Rajovic

PhD Student: Ugljesa Milic (FPI-UPC)

Master Student: Constantino Gómez Crespo

Visiting Collaborator: Eisabet Valle Breix

H. A. Memory technologies

Senior Researcher: Petar Radojkovic

PhD Student: Darko Zivanovic

PhD Student: David Zaragoza Rodríguez

PhD Student: Kazi Asifuzzaman

PhD Student: Milan Pavlovic (Ending Date: 31/10/2015)

PhD Student: Milan Radulovic

H. A. Microserver architectures & system software

Senior Researcher: Paul Matthew Carpenter

PhD Student: Branimir Dickov

PhD Student: Karthikeyan Palavedu Saravanan (FI)

PhD Student: Luis Ángel Garrido Platero

PhD Student: Renan Fischer e Silva

Developer: Vishal Mehta

H. A. Mobile and embedded-based HPC

Senior Researcher: Filippo Mantovani

Developer: Daniel Ruíz Muñoz

Developer: Josep Oriol Vilarrubí Barri

Undergraduate Student: Luna Backes Drault (Ending Date: 07/08/2015)

Visiting Collaborator: Alice Valentini

Performance Tools

Performance Tools Group Manager: Judit Gimenez Lucas (UPC)

Senior Researcher: José Carlos Sancho Pitarch (Ramón y Cajal)

Postdoctoral Researcher: Claudia Andreina Rosas Mendoza

Postdoctoral Researcher: Damien Dosimont

Postdoctoral Researcher: Estanislao Mercadal Melià

Postdoctoral Researcher: Harald Servat Gelabert

Postdoctoral Researcher: Hugo Daniel Meyer

Postdoctoral Researcher: Michael Wagner

Postdoctoral Researcher: Vladimir Subotic

Developer: Eloy Martínez Hortelano

Developer: Germán Llort Sánchez

Developer: Juan González García (Ending Date: 04/03/2015)

Developer: Laura Auton García (Ending Date: 16/01/2015)

Developer: Milica Mrdakovic (Ending Date: 31/10/2015)

Developer: Pedro Antonio González Navarro

Trainee Developer: Arturo San Emeterio Campos

Undergraduate Student: Alejandro Velasco Jiménez

Undergraduate Student: Genís Moreno Reñe

Undergraduate Student: Juan Francisco Martínez Vera

Undergraduate Student: Marc Planas Bosch (Ending Date: 05/12/2015)

Associate Researcher: Ana Jokanovic (UPC)

Visiting Collaborator: Gonzalo Rodríguez

Visiting Collaborator: Michel Dagenais

Programming Models

Programming Models Group Manager: Xavier Martorell Bofill (UPC)

Senior Researcher: Isaac Juan Rudomin

Senior Researcher: Vicenç Beltran Querol

Postdoctoral Researcher: Antonio José Peña Monferrer

Postdoctoral Researcher: Josep Maria Pérez Cáncer

Postdoctoral Fellow: Benjamín Hernández Arreguin (CONACYT)
(Ending Date: 12/01/2015)

Postdoctoral Fellow: Israel Tabarez Paz (CONACYT)

PhD Student: Guray Ozen (UPC)

PhD Student: Javier Bueno Hedo

PhD Student: Lluc Álvarez Martí

PhD Student: Rajiv Nishtala

PhD Student: Sandra Macià Sorrosal

PhD Student: Tomasz Patejko

PhD Student: Víctor Hugo Pérez Valdez (CONACYT)

Senior Developer: Julián David Morillo Pozo

Developer: Alejandro Fernández Suárez (Ending Date: 31/07/2015)

Developer: Antonio Filgueras Izquierdo

Developer: Bence Kodaj (Ending Date: 21/06/2015)

Developer: Javier Teruel García

Developer: Roger Ferrer Ibáñez

Trainee Developer: Diego Caballero de Gea (FI)

Trainee Developer: Diego Nieto Muñoz

Trainee Developer: Florentino Sainz Manteca (Ending Date: 23/01/2015)

Trainee Developer: Jorge Bellón Castro

Trainee Developer: Marçal Solà Vélez

Trainee Developer: Sara Royuela Alcázar

Trainee Developer: Víctor López Herrero

Master Student: Albert Segura Salvador (Ending Date: 31/08/2015)

Master Student: Jaume Bosch Pons

Master Student: Miquel Vidal Piñol

Undergraduate Student: Artem Cherkashin

Undergraduate Student: Marcos Maroñas Bravo

Associate Researcher: Carlos Álvarez (UPC)

Associate Researcher: Daniel Jiménez (UPC)

Associate Researcher: Guillermo Miranda (UPC)

Associate Researcher: Julita Corbalán González (UPC)

Associate Researcher: Marisa Gil (UPC)

Associate Researcher: Sergi Mateo Bellido (UPC)

Visiting Collaborator: Alba De Melo

Visiting Collaborator: Kevin Sala

Visiting Collaborator: Marco D'Amico

Runtime Aware Architectures

Senior Researcher: Marc Casas Guix (Beatriu Pinós)

Senior Researcher: Miquel Moretó Planas (JdC)

Postdoctoral Researcher: Juan Manuel Cebrián González

PhD Student: Dimitrios Chasapis (FPI - SO)

PhD Student: Emilio Castillo Villar (FPU)

PhD Student: Luc Jaulmes (FPU)

PhD Student: Paul Caheny

PhD Student: Sicong Zhuang

PhD Student: Thomas Grass (FI-UPC)

PhD Student: Vladimir Dimic

PhD Student: Xubin Tan (UPC)

Developer: César Allande Álvarez

Developer: Francesc Martínez Palau

Master Student: Adrián Barredo Ferreira

Master Student: Calvin Bulla

Master Student: Cristóbal Ortega Carrasco

Master Student: Helena Caminal Pallares

Master Student: Isaac Sánchez Barrera

Master Student: Iulian Brumar

Undergraduate Student: Rafael López Martínez (Ending Date: 30/09/2015)

Undergraduate Student: Raúl Vidal Ortiz (Ending Date: 31/07/2015)

Associate Researcher: Gurindar Singh Sohi

Visiting Collaborator: Iiia Pietri

Visiting Collaborator: Josep Triviño Valls

Visiting Collaborator: Kevin Brown

Storage Systems

Storage Systems Group Manager: Antonio Cortés Rosselló (UPC)

Postdoctoral Researcher: Alberto Miranda Bueno

Postdoctoral Researcher: Anna Queralt Calafat

Postdoctoral Researcher: Jonathan Martí Fraiz

Postdoctoral Researcher: Ramón Nou Castell

Postdoctoral Fellow: Jaime Iván López Veyna (CONACYT)

Postdoctoral Fellow: Paola Garfias (CONACYT)

PhD Student: Rizk Allah Touma (Marie Curie)

Trainee Developer: Alex Barceló Cuerda

Trainee Developer: Daniel Gasull Moreira

Trainee Developer: Marc Siquier Peñafort

Associate Researcher: Juan José Costa Prats (UPC)

Visiting Collaborator: Andrés Pardo

Visiting Collaborator: Christos Ioannidis

Visiting Collaborator: David Gràcia Llobet

Unconventional Computer Architecture and Networks

Unconventional Computer Architecture and Networks Group Manager:
Mario Nemirovsky (ICREA)

Postdoctoral Fellow: Alexandro Castellanos Mier (CONACYT)
(Ending Date: 19/11/2015)

PhD Student: Damián Roca Marí (La Caixa)

PhD Student: Francesco Ciaccia (Ending Date: 31/05/2015)

Visiting Collaborator: Josué Vladimir Quiroga Esparza

Visiting Collaborator: Luis Expósito

Visiting Collaborator: Pavlos Maniotis

Workflows and Distributed Computing

Workflows and Distributed Computing Group Manager: Rosa Maria Badia
Sala (CSIC - UPC)

Senior Researcher: Daniele Lezzi

Senior Researcher: Raúl Sirvent Pardell

Postdoctoral Researcher: Enric Tejedor (Ending Date: 31/01/2015)

Postdoctoral Researcher: Francisco Javier Conejero Bañon

Postdoctoral Researcher: Jorge Ejarque Artigas

Postdoctoral Researcher: Pieter Bellens (Ending Date: 30/04/2015)

Postdoctoral Fellow: Fredy Juárez Pérez (CONACYT)

PhD Student: Francesc Lordan Gomis (FPI-UPC)

PhD Student: Jan Ciesko

PhD Student: Marta García Gasulla

PhD Student: Rahul Gayatri (Ending Date: 31/03/2015)
PhD Student: Vintoh Krishnan Elangovan (Ending Date: 31/03/2015)
Developer: Carlos Díaz Suárez
Developer: Kalliopi Chronaki
Trainee Developer: Roger Rafanell Mas (Ending Date: 20/02/2015)
Master Student: Cristian Ramón-Cortés Viladorrona
Undergraduate Student: Pol Álvarez Vecino
Undergraduate Student: Sandra Corella Pérez
Undergraduate Student: Víctor Antón Domínguez
Associate Researcher: Judit Planas Carbonell (UPC) (Ending Date: 03/11/2015)
Visiting Collaborator: Genoveva Vargas Solar
Visiting Collaborator: Timotheé Chaumier

Earth Sciences Department

Earth Sciences Director: **Francisco J. Doblas-Reyes** (ICREA)
Earth Sciences Director Assistant: Gabriela Tarabanoff
Associate Researcher: Mar Rodríguez Rodrigo (IC3)
Visiting Collaborator: Alan O ' Cais

Atmospheric Composition

Atmospheric Composition Group Manager: Oriol Jorba Casellas
Postdoctoral Researcher: Antonios Gkikas (Marie Curie)
Postdoctoral Researcher: Enza Di Tomaso
Postdoctoral Researcher: Marc Guevara Vilardell
Postdoctoral Researcher: María Teresa Pay Pérez (Beatriu Pinós)
Postdoctoral Researcher: Sara Basart Alpuente
Postdoctoral Fellow: Sergio Natan González Rocha (CONACYT)
PhD Student: Jaime Antonio Pérez-Benavides Acuña (FPI)
PhD Student: Lluís Vendrell Miguel (La Caixa)
PhD Student: Lorenzo Fileni (Ending Date: 02/10/2015)
PhD Student: Michele Spada
PhD Student: Víctor Manuel Valverde Morales (Ending Date: 30/09/2015)
PhD Student: Vincenzo Obiso (FPI - SO)
Associate Researcher: Carlos Pérez García-Pando (NASA)
Associate Researcher: Maria Gonçalves (UPC)
Visiting Collaborator: Florian Pantillon
Visiting Collaborator: Jorge Eduardo Pachón
Visiting Collaborator: Robert Banks

Climate Prediction

Cimate Prediction Group Manager: Virginie Guemas (Ramón y Cajal)
Postdoctoral Researcher: Chloé Prodhomme
Postdoctoral Researcher: Danila Volpi
Postdoctoral Researcher: Eleftheria Exarchou
Postdoctoral Researcher: Javier García Serrano (Marie Curie)
Postdoctoral Researcher: Neven Stjepan Fuckar (JdC)
Postdoctoral Researcher: Omar Bellprat Vilanova (ESA grant VERITAS)
Postdoctoral Researcher: Valentina Sicardi
PhD Student: Rubén Cruz García
Associate Researcher: François Massonnet (IC3)
Associate Researcher: Louis Phillipe Caron (IC3)
Associate Researcher: Martín Ménégoz (IC3)
Visiting Collaborator: Alberto Carrassi
Visiting Collaborator: Anna Lena Deppenmeier
Visiting Collaborator: Christopher Mehta
Visiting Collaborator: Claude Frankignoul
Visiting Collaborator: Constantin Ardilouze
Visiting Collaborator: Jara Imbers
Visiting Collaborator: Lauriane Batte
Visiting Collaborator: Martin King
Visiting Collaborator: Paolo Davinie
Visiting Collaborator: Ramiro Saurral

Visiting Collaborator: Scott Power
Visiting Collaborator: Tom Philp

Computational Earth Sciences

Computational Earth Sciences Coordinator: Josep Oriol Mula Valls
Computational Earth Sciences Coordinator: Kim Serradell Maronda
PhD Student: Oriol Tintó Prims
Senior Developer: Georgios Markomanolis (Ending Date: 18/02/2015)
Research Support Technician: Francesco Benincasa
Developer: Carles Tena Medina
Developer: Domingo Manubens Gil
Developer: Javier Vegas Regidor
Developer: Mario César Acosta Cobos
Developer: Miguel Castrillo Melguizo
Developer: Pierre Antoine Bretonnière
Trainee Developer: Jordi Cuadrado Borbonés (Garantía Juvenil)
Trainee Developer: Xavier Yepes Arbós
Associate Researcher: Muhammad Asif (IC3)
Associate Researcher: Nicolau Manubens Gil (IC3)

Earth System Services

Earth System Services Coordinator: Albert Soret Miravet
Postdoctoral Researcher: Doo Young Lee
Postdoctoral Researcher: Gustavo Arévalo Roa (Ending Date: 31/10/2015)
Postdoctoral Researcher: Nicola Cortesi
PhD Student: Verónica Torralba Fernández
Dissemination Project Officer: Isadora Jiménez García
Associate Researcher: Aida Pinto (IC3)
Associate Researcher: Daniel Ortega González (IC3)
Associate Researcher: Enric Terradellas (AEMET)
Associate Researcher: Melanie Davis Timea (IC3)
Associate Researcher: Nube González Reviriego (IC3)
Visiting Collaborator: Sergio Lozano
Visiting Collaborator: Sonia Jerez

Life Sciences Department

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

Computational Genomics

Computational Genomics Group Manager: David Torrents Arenales (ICREA)
Postdoctoral Researcher: Josep Maria Mercader Bigas (Beatriu Pinós)
PhD Student: Bernardo Rodríguez Martín (La Caixa)
PhD Student: Elías Rodríguez Fos
PhD Student: Marta Guindo Martínez
PhD Student: Marta Munar Ortiz (FI)(Ending Date: 16/09/2015)
PhD Student: Mercè Planas Fèlix (La Caixa)
PhD Student: Santiago González Rosado
PhD Student: Sílvia Bonàs Guarch (FI)
Research Support Technician: Ana Milovanovic
Research Support Technician: Friman Sánchez Castaño
Research Support Technician: Montserrat Puiggròs Maldonado
Undergraduate Student: Jordi Cardona Nadal (Ending Date: 15/09/2015)
Undergraduate Student: Judit Pinteño Artés (Ending Date: 30/08/2015)
Undergraduate Student: Laura Brandt (Ending Date: 30/08/2015)
Undergraduate Student: Sergi Alcaide i Portet (Ending Date: 15/09/2015)
Visiting Collaborator: Ester Cuenca León
Visiting Collaborator: Jordi Deu
Visiting Collaborator: Jordi Valls
Visiting Collaborator: Judit Pinteño Artés
Visiting Collaborator: Paula Cortés

Electronic and Atomic Protein Modelling

Electronic and Atomic Protein Modelling Group Manager: Víctor Guallar Tasies (ICREA)

Postdoctoral Researcher: Ignacio Soteras Gutiérrez (Beatriu Pinós)

Postdoctoral Researcher: Maria de Fatima Assunçao Lucas

Postdoctoral Researcher: Martin Ivanov Kotev

Postdoctoral Researcher: Ryoji Takahashi

Postdoctoral Researcher: Suwipa Saen Oon

PhD Student: Daniel Lecina Casas (FPI - SO)

PhD Student: Emanuele Monza (FI)

PhD Student: Gerard Santiago Morcillo (FPI)

PhD Student: Israel Cabeza de Vaca López

PhD Student: Jelisa María Iglesias Fernández (FPI - SO)

PhD Student: Pedro Hermosillas Casajus

PhD Student: Sandra Acebes Serrano (FPI)

PhD Student: Seyed Ali Hoseini (Ending Date: 30/04/2015)

PhD Student: Víctor Gil Sepúlveda

Research Support Technician: Pedro Riera Martorell

Developer: Jorge Estrada Collado

Visiting Collaborator: Adrie Westphal

Visiting Collaborator: Cristopher Grebner

Visiting Collaborator: Ferran Sancho Jodar

Visiting Collaborator: Gudrun Gygli

Visiting Collaborator: Joan Clark Nicolás

Visiting Collaborator: Maria Vittoria Cubellis

Visiting Collaborator: Marina Canellas

Visiting Collaborator: Pim Kolkman

Visiting Collaborator: Valerio Guido Giacobelli

INB-Computational Node 2

INB - Computational Group Manager: Josep Gelpi (Fundació Bosch Gimpera)

PhD Student: Víctor López Ferrando (LA CAIXA)

Research Support Technician: Dmitry Reptchevski

Research Support Technician: Laia Codó Tarraubella

Research Support Technician: Pau Andrió Balado

Research Support Technician: Romina Royo Garrido

Molecular Modelling and Bioinformatics

Life Sciences Director: Modesto Orozco López (Fundació Bosch Gimpera)

Senior Researcher: Josep Ramón Goñi Macià (Ending Date: 10/05/2015)

Postdoctoral Researcher: Robert Soliva

Research Support Technician: Núria Villegas Forn

Developer: Iván Navarro Parreño (Ending Date: 05/05/2015)

Undergraduate Student: Cristian García Montilla (Ending Date: 31/07/2015)

Associate Researcher: Patrick Aloy (IRB)

Associate Researcher: Roberto Mosca (IRB)

Associate Researcher: Xavier Salvatella (IRB)

Associate Research Student: Alexandra Emilia Balanceau (IRB)

Associate Research Student: Diana Camila Buitrago (IRB)

Protein Interactions and Docking

Protein Interactions and Docking Group Manager: Juan Fernández Recio

Postdoctoral Researcher: Iain Moal (Marie Curie) (Ending Date: 28/02/2015)

Postdoctoral Researcher: Lucía Díaz Bueno

Postdoctoral Fellow: Sergio Mares Samano (CONACYT)

PhD Student: Brian Jiménez García (FPI)

PhD Student: Chiara Pallara

PhD Student: Didier Barradas Bautista (CONACYT)

PhD Student: Luis Ángel Rodríguez Lumbreras

PhD Student: Miguel Romero Durano

PhD Student: Mireia Rosell Oliveras (FPI - SO)

Visiting Collaborator: Agustina Tamutyte

Visiting Collaborator: Imen Daoud

Visiting Collaborator: Jorge Luís Roel Touris

Visiting Collaborator: Mark Agostino

Visiting Collaborator: Nadia Arezki

Computer Applications in Science & Engineering Department

Computer Applications in Science and Engineering Director: **José María Cela Espín** (UPC)

CASE Director Assistant: Laura Gutiérrez Salamero

Postdoctoral Researcher: Mónica de Mier Torrecilla

Postdoctoral Researcher: Stephan Mohr

Postdoctoral Fellow: José Carlos Carrasco Jimenez (CONACYT)

Senior Developer: Georg Huhs

Visiting Collaborator: Lorenzo Chelleri

Visiting Collaborator: Maxime Morinière

Visiting Collaborator: Xavier Bergua

Data Pre&Post Processing

Data Pre&Post Processing Group Manager: Fernando Martín Cucchietti Tabanik

Postdoctoral Researcher: Artur García Sáez

Senior Developer: Mohammad Jowkar

Visualisation Technician: Guillermo Marin Getino

Developer: Abel Gargallo Peiro

Developer: David Fusté Vilella (Ending Date: 31/07/2015)

Developer: David García Povedano

Developer: Luz Calvo Flores

Visiting Collaborator: Rumyana Rumenova

Visiting Collaborator: Simos Kazantzidis

Environmental Simulations

Environmental Simulations Group Manager: Arnau Folch Duran

Postdoctoral Researcher: Ángel Coppola Owen

Postdoctoral Researcher: Matías Oscar Ávila Salinas

PhD Student: Alejandro Martí Donati (Marie Curie)

PhD Student: Georgios Chrysokentis (FPI)

PhD Student: Jordi Barcons Roca

Developer: Oddur Oskar Kjartansson (Ending Date: 15/07/2015)

Developer: Raúl De la Cruz Martínez

Fusion

Senior Researcher: Mervi Johanna Mantsinen (ICREA)

Postdoctoral Researcher: Shimpei Futatani (Ramón y Cajal)

PhD Student: Daniel Gallart Escola (La Caixa)

Developer: Albert Gutiérrez Milla

Developer: Xavier Sáez Pous

Geosciences Applications

Geosciences Applications Group Manager: Josep De la Puente Álvarez

Postdoctoral Researcher: David Modesto Galende

Postdoctoral Researcher: Eduardo José Sánchez Peiró

Postdoctoral Researcher: Jean Antoine Kormann

Postdoctoral Researcher: Otilio José Rojas Ulacio

Postdoctoral Researcher: Volodymyr Puzyrov

Postdoctoral Fellow: Armando Aguilar Meléndez

PhD Student: Octavio Castillo Reyes (CONACYT)

PhD Student: Prattya Datta (La Caixa)

Developer: Miguel Ferrer Ávila

Developer: Yevgeniy Gruver (Ending Date: 30/09/2015)

Visiting Collaborator: Aurelien Bain-Thouverez

Visiting Collaborator: Beatriz Martínez

High Performance Computational Mechanics

High Performance Computational Mechanics Group Manager: Mariano Vázquez (CSIC - UPC)

Postdoctoral Researcher: Daniel Mira Martínez

Postdoctoral Researcher: Jazmín Aguado Sierra

Postdoctoral Researcher: Mohammad Kouhi

Postdoctoral Researcher: Ruth Aris Sánchez

PhD Student: Alfonso Santiago (FPI - SO)

PhD Student: Margarida Moragues Ginard

PhD Student: Mariña López Yunta (FPI - SO)

PhD Student: Matías Ignacio Rivero (FPI - SO)

PhD Student: Miguel Zavala Ake (Marie Curie)

Senior Developer: Rogeli Grima Torres

Undergraduate Student: Laia Vilas Planas

Visiting Collaborator: Daniel Fernández

Visiting Collaborator: Federica Sacco

Visiting Collaborator: Joan Ferrer

Visiting Collaborator: José María De Vehí

Visiting Collaborator: Nathan Weinstein

HPC Software Engineering

HPC Software Engineering Group Manager: Mauricio Hanzich

Senior Developer: Albert Farrés Coma

Developer: Claudio Daniel Márquez Pérez

Developer: Juan Esteban Rodríguez Rodríguez

Developer: Natalia Gutiérrez Navarro

Developer: Samuel Rodríguez Bernabéu

Undergraduate Student: Benjamin Schmitt (Ending Date: 31/07/2015)

Physical and Numerical Modelling

Physical and Numerical Modelling Group Manager: Guillaume Houzeaux

Postdoctoral Researcher: Alberto Gambaruto (Marie Curie)

(Ending Date: 01/05/2015)

Postdoctoral Researcher: Beatriz Eguzkitza

Postdoctoral Researcher: Eva Casoni Rero

Postdoctoral Researcher: Xevi Roca Navarro (Marie Curie)

Postdoctoral Fellow: Juan Carlos Cajas García (CONACYT)

PhD Student: Cristóbal Augusto Samaniego

PhD Student: Edgar Olivares Mañas (La Caixa)

PhD Student: Paula Córdoba Pañella (La Caixa)

Senior Developer: Antoni Artigues Barceló

Developer: Hadrien Calmet

Visiting Collaborator: Adrià Quintanás

Visiting Collaborator: Benjamin Uekermann

Visiting Collaborator: Miguel Bárcena

Smart Cities

Senior Researcher: Jorge García Vidal (UPC)

Postdoctoral Researcher: Maria Cristina Marinescu

Senior Developer: Mónica Marrero Llinares

Developer: Sergio Mendoza Fariña

Social Simulation

Senior Researcher: Xavier Rubio Campillo

Postdoctoral Researcher: Jean Marc Montanier

PhD Student: María Coto Sarmiento

PhD Student: Simon Carrignon

Developer: Guillem Francès Medina

Developer: Guillem Laborda Cabo (Ending Date: 19/12/2015)

Developer: Jorge Caro Saiz (Ending Date: 31/07/2015)

Operations Department

Operations Director: **Sergi Girona Turell**

Operations Director Assistant: Núria Saavedra Hernández

Facility Management

Maintenance Technician: Albert Riera Muñoz

Maintenance Technician: Miguel Armenta Sánchez

Facility Management Consultant: Ramon Pallisa Munts (UPC)

System Administration

Systems Group Manager: Javier Bartolomé Rodríguez

IT Security & Networks Operator : Marcel Malet Abulí

Network Technician: Albert Benet Vila

Performance Technician: Alejandro Sánchez Graells (Ending Date: 09/10/2015)

Performance Technician: Carles Fenoy García (Ending Date: 31/03/2015)

System Administrator: Aníbal Moreno Gil

System Administrator: Felip Moll Marqués

System Administrator: Josep Manel Andrés i Moscardó

System Administrator: Marc López de Mantaras (Ending Date: 19/06/2015)

System Administrator: Oscar Yerpes Baena

System Administrator: Sergi Moré Codina

Helpdesk Technician: Antonio Espinar Sallares

Helpdesk Technician: Ferran Sellés Mompart

Helpdesk Technician: Pedro Gómez Bretones

User Support

User Support Group Manager: David Vicente Dorca

CNAG Support: Miguel Bernabéu Díaz

First Level User Support: Borja Arias Navarro

First Level User Support: Cristian Morales Pérez

PRACE Support: Janko Strassburg

Support Applications Consultant: Jorge Rodríguez Rey

Support Applications Consultant: Pablo Rodenas Barquero

Visualisation Technician: Carlos Tripiana Montes

Web Graphical Designer: Cristian Opi Muro

Web Graphical Designer: Laura Bermúdez Guerrero (Ending Date: 10/07/2015)

Webmaster: Martín Menes Rouco

Webmaster: Silvina Rusinek Milner (Ending Date: 12/05/2015)

Management Department

Management Director: Ernest Quingles Soteras

Business Administration Group Manager: Mercè Calvet Gómez

Administration

General Assistant: Aina Ribera Carrasquer

General Assistant: Aurora Rodríguez Velasco

General Assistant: Lisandra Souza do Nascimiento

Purchasing Officer: Cristina Vargas Cambilhon

Purchasing Officer: Neus Jiménez Ferrer

Receptionist: Carola Torra Miró (Ending Date: 16/10/2015)

Receptionist: Marta Carbonell Giménez

Support Purchasing Officer: Oriol Solani Calvet (Garantía Juvenil)

Finance and Accounting

Accounting Manager: Cristina Calonge Cortés

Economic Management Project Technical Support: Laia Traveset Solé

Economic Management Project Technical Support: Laura Viñas Alcoz

Support Accounting Technician: Alba Delclos Miret

Support Accounting Technician: Judit Soldevila García

Economic Management Project Technical Support: Carlos Melero Cabezas

Human Resources

Head of Human Resources: Marc González Vidal

HR Officer: Carla Santamaria Giménez

HR Senior Officer: Anna Martín Balbuena

HR talent Officer: Julio Gómez Navarro

HR Support Officer: Blanca Creus Freixas

Information Systems & Services

Information System & Services Coordinator: Toni Matas Figueras

Information System & Services Developer: Sergi Carrere Bach

Mission

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

Activities

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

Fostering Collaboration with Universities and Industry

BSC-CNS was closely involved in the design and delivery of the HPC Stream of the MIRI Master program, and offers annual MSc Scholarships under the BSC-CNS Severo Ochoa project. In 2015, 14 students were enrolled in the program.

Funded by AGAUR (Catalan government), development commenced of a MOOC "Introduction to Parallel Computing", in collaboration with Computer Architecture lecturers. The course will be delivered on the UCATx platform.

Mobility as a key success factor for education

The BSC-CNS mobility program, funded by the Severo Ochoa project, is available to BSC-CNS staff researchers, post-doctoral researchers and PhD students, as well as researchers from institutions collaborating with BSC-CNS. This programme supports collaboration and short-term visits worldwide in leading research and academic institutions and provides grants for visitors collaborating with BSC-CNS research groups. In the four mobility calls held to date, grants totalling nearly 70.000€ were awarded to 35 researchers from BSC-CNS and other institutions.

Training Courses

BSC-CNS is a PRACE Advanced Training Centre (PATC) and in 2015 delivered a programme of 13 courses with more than 300 attendees from across Europe. BSC-CNS courses were yet again very highly rated by the attendees and recognised as credited courses by the FIB Master programme MIRI.

Summer Schools

PUMPS Summer School, organised and delivered by specialists from the CUDA Center of Excellence (awarded by NVIDIA to BSC-CNS in association with UPC), held its 6th edition in 2015 with more than 80 attendees. The training was aimed at enriching the skills of researchers, graduate students and teachers with cutting-edge techniques and hands-on experiences in developing applications for many-core processors with massively parallel computing resources, such as GPU accelerators.

A number of project related courses and schools were co-organised and hosted by BSC-CNS in 2015, including: the Energy Consumption in Future ICT Devices school (at the Università di Perugia, supported by the EC under the FET Proactive Coordination Action ICT-Energy), T4 - Probabilistic Timing Analysis Tutorial (as part of AdaEurope 2015 in Madrid), and Simulation Methods Used for the In-flight Icing Certification of Aircraft, Rotorcraft and Jet Engines (co-hosted by CFD Lab, McGill University and NTI, Canada at BSC-CNS).

Workshops

The Education and Training team was involved in the organisation of three research workshops in 2015:

- PRACE Training Day at ICSC 2015.
- BRIDGE: Bridging the Talent Gap with Computational Science Methods, workshop at ICCS 2015.
- Best Practices for HPC Training, workshop at SC15.

Research Seminar Series & Doctoral Symposium

The Research Seminar programme is an initiative to improve communication, professional training and mobility of BSC-CNS staff and increase visibility of incoming mobility, thereby promoting collaborative research. During the 2014 - 15 academic year, 24 research seminars were held.

The 2nd BSC-CNS International Doctoral Symposium

For the first time, in 2015, the Doctoral Symposium was opened to participation by students from other institutions. The Symposium aims to provide a relaxed environment of collaboration and networking to share research results developed by PhD students and Postdoctoral researchers. Training sessions on research and career development skills are also offered.

A total of 33 oral presentations and over 20 posters were presented. The book of abstracts can be downloaded from the Symposium website link title.

The financial accounts for 2015 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 2015 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 2015
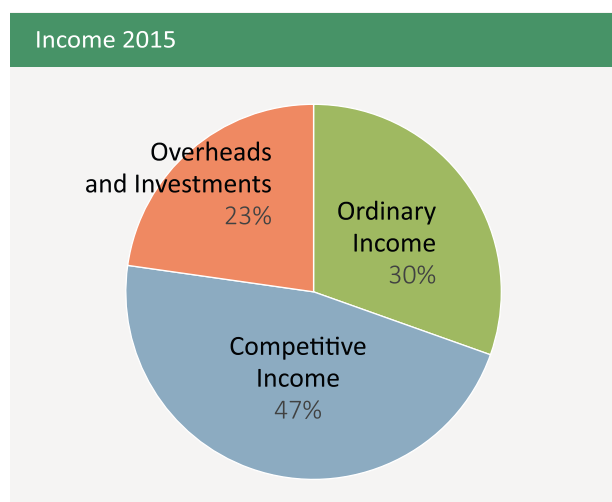
Income	Amount €
Ordinary Income	7.273.905
Ministry of Economy and Competitivity	5.808.530
Generalitat of Catalonia	1.465.375
Competitive Income	11.182.566
Spanish Government	734.277
Generalitat of Catalonia	214.868
European Commission	5.839.280
Private Companies	3.464.724
Other Institutions	929.419
Overheads and Investments	5.434.481
Applied Previous Reserves	2.424.921
Strategic Investments	1.511.379
Overheads/Capital Transfers	1.498.180
TOTAL INCOME	23.890.952

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.
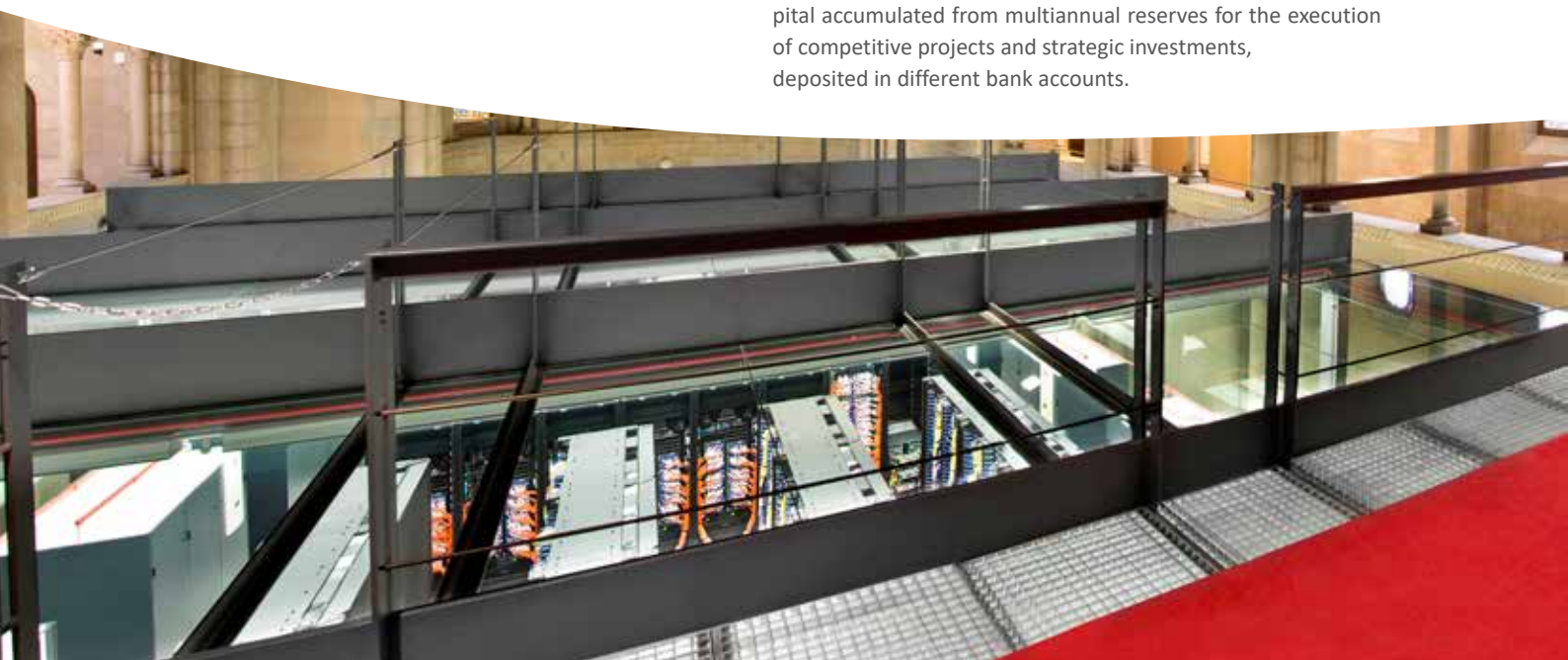
Breakdown of Competitive Income

The chart shows the evolution and breakdown of competitive income according to source. It demonstrates clearly the growth in recent years in funding from competitive European projects and Private Industry, and constant level of competitive funding from National competitive programs.

BSC-CNS Competitive and Industry Funding: 2007-2015
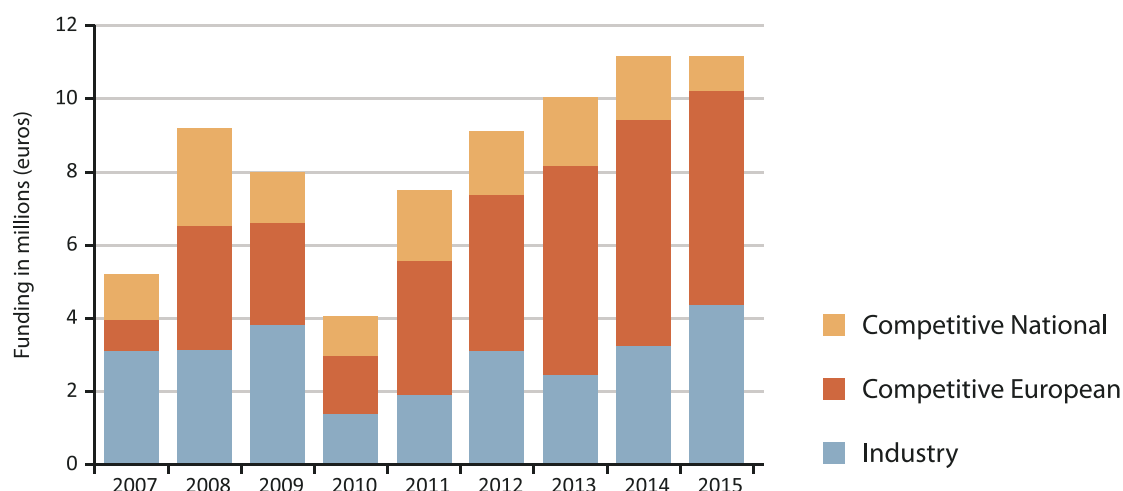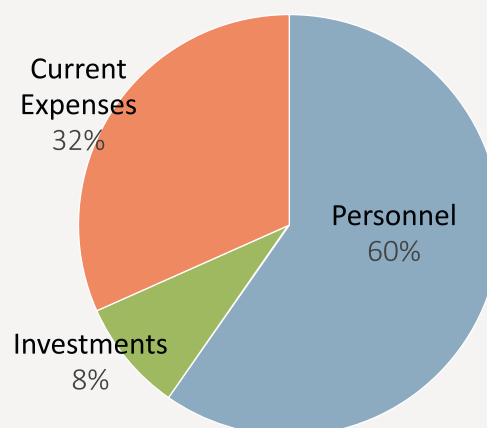

Expenses

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

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 11 public tender contracts were signed during the year.

Expenses 2015

Expenses	Amount €			
	Ordinary Budget	Strategic Budget	Projects Budget	Total
Personnel	4.073.433	302.504	9.889.583	14.265.520
Investments	262.226	1.515.951	280.363	2.058.530
Current Expenses	3.341.945	840.701	3.384.256	7.566.902
TOTAL EXPENSES	**7.677.605**	**2.659.146**	**13.554.201**	**23.890.952**

BSC-CNS – Severo Ochoa Center of Excellence

BSC-CNS was awarded the "Severo Ochoa Center of Excellence" by MINECO in 2011, commencing an ambitious research programme in 2012 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.

2015 was a year of consolidation of various important developments of the program, including the different scientific research activities, training and education activities, as well as the deployment of improved mechanisms in the management of Human Resources in Research and the empowerment of and networking between young researchers. Also during 2015, BSC-CNS elaborated its strategic vision for 2016-2019 which was presented to MINECO for renewing the Severo Ochoa award. The vision included strategic objectives linked to the scientific and technical activities of BSC-CNS, trading and human resources activities, internationalisation, exploitation and dissemination of scientific results and outreach.

In October 2015, MINECO once again awarded BSC-CNS the Severo Ochoa Centre of Excellence accreditation, following its assessment of the Centre's success during the previous accreditation period and the quality of the strategic research plan presented for 2016-2019. The board's Scientific Committee commended BSC-CNS on 'having positioned itself as a leading supercomputing centre of international renown' and for its 'excellent results in the period 2011-2015. The Centre's research programmes in Computer Architecture, Parallel Programming and Supercomputing are first class, matching the standard of the best centres in Japan, the United States and Europe'.

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

BSC-CNS Severo Ochoa Institution Building Activities

Acknowledging the typical difficulties of generalised cooperation at medium or large scale in research environments, specific actions were designed to break down barriers and increase cooperation both within individual departments and between different departments. This succeeded in fostering a deep spirit of interaction and cooperation between all groups at BSC-CNS, and is regarded as the program´s major success. Examples include formal monthly Executive Committees where young research team leaders define the progression of their transversal projects, and informal communication instruments like the "Severo Ochoa Cafes", proposed by the young researchers themselves.

Another key objective was to improve the overall positioning, reputation and activity of BSC-CNS at the international level via three key actions: 1) Active participation in those large international consortia that define strategies and research agendas; 2) Establishment of collaborations with other research groups worldwide to complement BSC-CNS research capabilities or to look for research alliances; and 3) Coordination and participation in collaborative EU projects.

The Education and Training Team was created with the objectives of improving the Centre's doctoral and post-doctoral capabilities and training courses, improving management processes and support facilities, designing a gender action plan and the extension of certification mechanisms to consolidate quality assessments for HPC training. Activities included organisation of Research Seminars, an annual Doctoral Symposium, summer schools, workshops, a Mobility Grants programme and scholarships for the HPC Masters at UPC.

BSC-CNS developed and implemented several policies and procedures for fostering research careers, with the major achievement being the award of the HRS4R logo in 2015. Communication and Outreach activities were also developed to showcase BSC-CNS activities in general society.

BSC-CNS Severo Ochoa Scientific Research Activities

Personalised medicine

Life Sciences developed a new framework for research on personalised medicine, focused on analysing the genomic basis of complex pathologies, such as diabetes, asthma or cancer. Method developments cover: i) methods for the determination of genomic alterations in cancer, including the development of Smufin, a fast and powerful method for determination of cancer genomic alterations and ii) linking genomic alterations with pathology, creating a new generation of procedures for Genome Wide Association Studies (GWAS), and further to perform target determination and finally link the target with potential drugs (SEABED infrastructure, PELE project).

Work also progressed on computational pipelines in synthetic biology to mine data in structural databases, and development of innocuous tags for visualisation of intracellular distribution of proteins. New computational methods for redesigning enzyme activity led to the definition of new proteins able to process new

compounds. Finally, structural predictive methods enabled the definition of protein-protein interactions and might emerge as a method for the novo design of biological networks.

Biomechanics (Alya-Red)

The CASE Department made important advances in developing the Alya Red simulation infrastructure, based on the in-house parallel multiphysics code Alya. Alya Red is a set of collaborative research projects to develop computational mechanics simulation tools specifically designed for biomedical research to run on supercomputers. The main goal is to contribute to the better understanding of biological systems by setting up a computational scenario where complex physiological models can be tested. Thanks to the Severo Ochoa program, the capabilities of the simulation infrastructure were improved to include blood flow, muscular electrical activity propagation, muscular mechanical action, electromechanical coupling and blood-muscle interaction. The team programmed and tested complex ventricular electrophysiology models and anisotropic active/passive tissues. The infrastructure advanced from electro-mechanics simulation of academic cases to coupled blood-electro-mechanics simulation of clinical geometries. Also of note is that it is now possible to couple Alya to an arterial network simulation tool developed by collaborators at the LNCC (National Laboratory for Cardiac Sciences) in Brazil.

### Air quality and high-resolution climate modelling

Earth Sciences applied the in-house global modelling system NMMB/BSC Chemical Transport Model (NMMB/BSC-CTM) at very high resolution. The NMMB/BSC-Chemical Transport Model was extended with a new global multicomponent aerosol coupled with a comprehensive chemical mechanism, and a new data assimilation capability. More recently the group worked on the coupling of NMMB/BSC-CTM with an ensemble-based data assimilation system (the LETKF scheme) in order to integrate surface and satellite observations into the model.

In collaboration with Computer Sciences, the NNMB/BSC-CTM and EC-EARTH codes were analysed in terms of performance bottlenecks and opportunities for optimisation were identified and addressed. The code was ported to the software stack of the Mont-Blanc prototype to show that it is possible to run operational codes on energy-efficient infrastructures and minimise their environmental footprint.

Software stack to support BigData and energy-efficient applications

Computer Sciences focused on the design of the software stack to support development of application workflows combining compute- and data-intensive applications. Two central components were developed: dataClay and pyCOMPSs.

- BSC-CNS proposed a new generation of object storage (dataClay) where objects are the persistent abstraction, as opposed to files, or databases. This will enable both the programmer and dataClay to take full advantage of forthcoming high-performance and byte-addressable storage devices, such as NVRAM or Storage Class Memories (SCM). DataClay stores object data, methods and behaviour policies
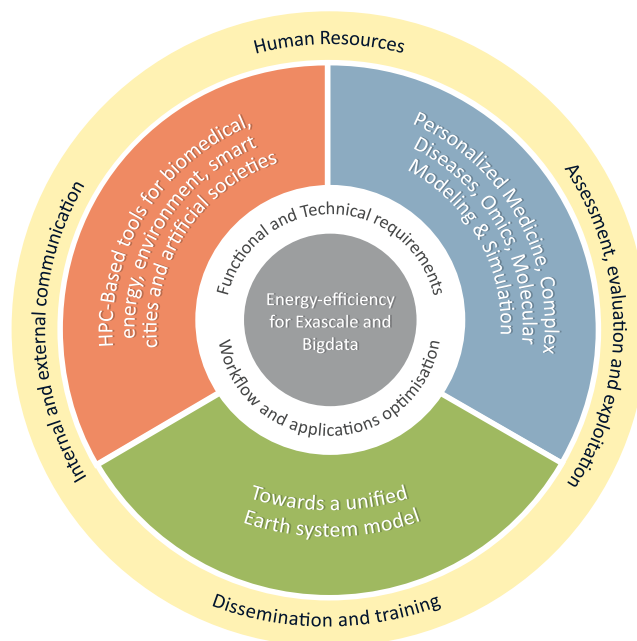
A picture is worth 1000 words: BSC-CNS's Severo Ochoa program

that define issues such as security, privacy, integrity, and life cycle. This integration of data and code enables very simple performance of computation close to the data, thus enabling the programmer or the middleware to decide where a given computation has to be executed. The object can easily be moved to different infrastructures and still behave as it was designed.

- PyCOMPSs programming model, a new Python binding for the COMPSs execution environment, whose aim is to support flexible computational workflows. BSC-CNS developed a framework to understand annotations of argument directionalities for method invocations and compute dependences at runtime. Tasks from the same computational workflow can be offloaded to different nodes within the local cluster or to external cloud resources in a transparent way. The research also studied the interoperability of the PyCOMPSs/COMPSs programming model with the dataClay library of self-contained objects and Hecuba framework for key-value databases. This leads to application scenarios for BigData, for example performing data analytics on simulation results or in-situ analysis.

The Department also studied state-of-the-art non-relational databases (Apache Cassandra) and developed a highly configurable tool (AENEAS) to evaluate the impact of different data models. A new research line was launched in designing Domain Specific Languages (DSL) for accelerator-based clustered architectures.

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 pro-actively transfer technology to industry, via direct R&D collaborations, development of spin-off companies, educational activities, and staff exchanges with private industry R&D laboratories.

During 2015, the Technology Transfer Office (TTO) conducted 24 corporate visits to MareNostrum, involving 554 companies and more than 700 IT, innovation, R&D and senior executives from the main industry clusters and sectors, including aeronautics, automotive, telecommunications, robotics, pharmaceutics, logistics, textile, and governmental IT related organisations.

Other activities coordinated by the TTO included the writing of 5 business plans based on BSC-CNS technologies in collaboration with ESADE students, a grant from Caixaimpulse to foster commercial application of SMUFIN, a reference free analysis and interpretation technology for genome sequencing, and the creation of the first BSC-CNS spin-off company, NOSTRUM BIODISCOVERY, supported by the Botín Foundation, which will work in the life sciences sector to improve the drug discovery process.

ACCIÓ **Generalitat de Catalunya** The activities related to the creation of Nostrum Biodiscovery and management of the BSC-CNS patent portfolio received the support of ACCIO (ref. VALUNI15-1-0010)

Computer Associates Technologies

The aim of the collaboration with Computer Associates Technologies (CA) is to enhance recommendation systems from CA using BSC-CNS research in Big Data Analytics and Cloud Computing. The main goal was to provide a decision support system, an open source IDE and run-time environment for the high-level design, early prototyping, semi-automatic code generation, and automatic deployment of applications on multi-Clouds with guaranteed QoS. BSC-CNS created an automatic text analysing tool able to extract QoS information about different cloud providers using public information obtained from different websites (such as stack overflow).

BSC-Cisco Collaboration

In 2015, a series of collaborative research projects were launched with CISCO to develop Fog Computing technologies for deployment at scale. BSC-CNS and other academic and industrial partners developed the Barcelona Fog Computing Proof-of-Concept project, to explore how Fog Computing could be leveraged across thousands of cabinets placed around Barcelona city, to gather information from city sensors as well as from cameras and traffic lights. In the Fog paradigm, the cabinets process some of the information locally and send other information to a central control hub through a secure platform which manages data from multiple sources, for multiple services.

European Space Agency

In 2015, the collaboration with the European Space Agency (ESA) was structured around four projects: 1) ESA NPI (Architectural solutions for the timing predictability of next-generation multi-core processors), where a number of memory controller and bus architectures were trialled to enable a Worst Case Execution Time (WCET) analysis of time-critical space applications in a multi-core execution environment; 2) ESA PROARTIS for SPACE, integrating software-randomisation techniques onto real space setups used by ESA

and its system providers; 3) ESA HAIR, developing several timing models that will be integrated as part of a virtual machine for the NGMP; and 4) ESA PMCs (Multi-Core Architectures - Cache Structure Optimisation for better RT Performance), focused on the analysis and proposal of a new performance monitoring counter support for the NGMP with the goal of better capturing how tasks interact and are delayed when accessing NGMP's hardware shared resources.

Fundación Botín

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

Iberdrola-BSC Research Collaboration

IBERDROLA and BSC-CNS are jointly developing a major R&D&I initiative known as the 'SEDAR Project (High Resolution Wind Simulation)'. SEDAR aims to develop a new computer model to improve estimates of electrical energy production in wind farms before their construction. Current models have significant limitations in their calculation times and the resolution of physical models, and this project seeks to overcome these shortcomings through the use of supercomputing techniques. The software developments in SEDAR are based on the Alya software platform developed at BSC-CNS. Current work focuses on introducing more complexity in the physical models simulated by Alya, with the objective to obtain a robust short-term power production forecast tool.

IBM-BSC Research Collaboration

During 2015, a number of Joint Study Agreements were executed with the IBM Watson Research laboratory: High-performance in-memory databases; Software-defined environments for HPC workloads; Adaptive resource management for Power; OmpSs @ P8/GPU; Deep learning and data mining; and Smart

Patents

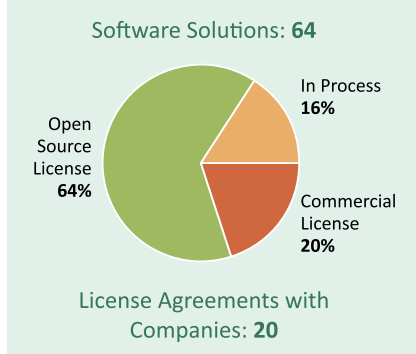Granted: **16** (14 EU, 2 USA)

Pending: **7**

In Preparation: **8**

New Contracts and Licenses (2015)

4,7M €*

*Value of new industry R&D contracts and software licenses signed during 2015.

Software

Software Solutions: 64

In Process
16%

Open Source License **64%**

Commercial License **20%**

License Agreements with Companies: 20

Spin-Off Companies

Launched 2015

Industry Visits to MareNostrum (2015)

24 visits

554 companies

712 attendees

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cities. Further JSAs with the Zurich Research Laboratory were also conducted: OmpSs programming model for asynchronous applications; and Applicable research to interconnection networks. The collaboration resulted in several joint papers and developments that influenced IBM products and prototypes. A new collaboration agreement was formed to create the BSC-IBM Deep Learning Center, to start in 2016.

## Intel-BSC Exascale Laboratory

The Intel-BSC Exascale Lab continued its research collaboration in novel programming models and performance tools. In particular, Extrae instrumentation was developed for OpenSHMEM and the Snipper simulator was integrated with Dimemas to support hierarchical multiscale machine modeling. The successful cooperation led to an extension of the collaboration agreement with new cooperation topics, including BSC-CNS involvement in the OpenHPC consortium, deployment of an SSF prototype at BSC-CNS for initial application evaluation, further development of BSC-CNS programming models and tools activities, development of instrumentation to analyse Lustre activity and big data infrastructures, extension of the memory tracking tools to provide guidance in the use of hybrid memory architectures that will be available in the KNL, and cooperation on the Rackscale architecture.

Microsoft-BSC Research Centre

Since 2014, the Microsoft-BSC Research Centre targets BigData topics, and in particular, the development of performance models for large scale data analytics frameworks. One of the goals is to explore and characterise upcoming platforms and hardware architectures for Big Data processing, and to reduce the TCO of running BigData Platforms. The Centre hosts the most comprehensive open public BigData benchmarking repository. The research compares not only software configuration parameters, but also contrasts current and newly available hardware including SSDs, InfiniBand networks, and Cloud services, while at the same time evaluating the TCO of each possible setup along with the running time to offer a recommendation. This analysis serves as a reference guide for designing new BigData solutions, exploring parameter relationships as well as reducing the TCO for existing data processing infrastructures.

NVIDIA-BSC/UPC Research Collaboration
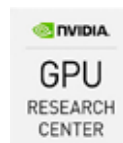
BSC-CNS, in association with the Universitat Politècnica de Catalunya (UPC), was designated by NVIDIA as a GPU Centre of Excellence (GCoE) in 2011. This acknowledges the broad-based research success of BSC-CNS in leveraging the NVIDIA CUDA technology and GPU computing. As part of GCoE training activities, during 2015, the Centre offered several courses in graduate and master programs at the Computer Sciences School (FIB) at UPC and as part of the PRACE Advanced Training Center (PATC), in addition to the renowned Programming and Tuning Massively Parallel Systems (PUMPS) Summer School held yearly in Barcelona since 2010. Research activities focused on: 1) Evaluation of low-power GPUs in platforms oriented to high-performance computing, including porting of several applications from CASE (Alya application), Earth Sciences (EC-Earth application) and Life Sciences (PELE application) Departments; 2) Task-parallel coupled simulation and visualisation of crowds in multi-node hybrid GPU/CPU platforms; 3) Development of software infrastructures to ease the development of applications on multi-GPU systems, and mechanisms and policies for scheduling multiprogrammed workloads; 4) Optimisation of applications in different domains in collaboration with the CASE (Transport-WARIS application) and Life Sciences (PELE application) Departments; and 5) Facial recognition and security video surveillance with the UPC start-up company HERTA Security.

Repsol-BSC Research Center

The Repsol-BSC Research Center (RBRC) was established in 2010 to tackle geophysical problems and a broad spectrum of other HPC challenges of interest for Repsol. The geophysical and computational developments at the RBRC have resulted in a unique software platform called Barcelona Subsurface Imaging Tools (BSIT). BSIT has enabled the development of a whole set of imaging applications which include state-of-the-art solutions for the most challenging problems in exploration geophysics. During 2015, the CS and CASE departments collaborated in the RESOLVER initiative to develop a high-level Domain Specific Language (DSL) to solve Partial Differential Equations (PDEs). Currently REPSOLVER is a multi-layer framework composed of an embedded compiler and a parallel/distributed runtime system based on OmpSs and MPI. RESOLVER was successfully used to solve several well-known problems in fluid mechanics and chemistry, such as 3D acoustic wave propagations or premixed flames.

SAMSUNG Collaboration

In 2015, the collaboration with Samsung focused on memory systems for high-performance computing, targeting three areas: 1) the analysis of application memory requirements in terms of capacity and bandwidth, analysing the impact of main memory latency on the overall performance; 2) the study of DRAM errors in production HPC workloads running on the MareNostrum supercomputer. In addition to the detection of DRAM errors, the system logs and correlates a number of statistics of interest such as the error type, time-stamp, physical position of errors, and the DIMM manufacturer; 3) analysis of the suitability of STT-MRAM for main memory of HPC systems, simulating HPC systems with the STT-MRAM main memory and the conventional DRAM, and comparing their performance on a set of production HPC applications.

Xilinx-BSC Research Collaboration

During 2015, the Programming Models group continued its collaboration with Xilinx towards easy programmability of the Xilinx Zynq platform. Using the OmpSs infrastructure on the Zynq board, the Group worked on extracting detailed traces from the execution of matrix multiplication and Cholesky and continued the development of the performance estimator tool to determine the proper combination of application kernels to be exploited on the FPGA. The Group also received early access to the SDAccel platform to generate OpenCL kernels for the FPGAs, and also the SDSoC platform to compile C/C++ kernels for the FPGAs.

Other Industry and Institutional Collaborations

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

Earth Sciences

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

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

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

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

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

EDP Renewables: BSC-CNS is working with EDPR in developing a pre-operational wind energy forecast based on seasonal predictions.

National Renewable Energy Centre (CENER): BSC-CNS is working with CENER within the context of the New European Wind Atlas assessing the predictability of climate predictions at different time scales.

Bodegas Torres: BSC-CNS is conducting a study on grape sustainability in western South America.

Life Sciences

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

In 2015, BSC-CNS received a Caixaimpulse grant to commercialise SMUFIN technology. SMUFIN is a computer protocol designed to identify disease causing mutations from disease genomes. In contrast to other existing methodologies, the innovative algorithm behind SMUFIN and its parallel implementation allow rapid and easy identification of practically all types of disease-causing mutations with high specificity in pathological genomes, including those that remain undetectable by other methods.

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

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

The BSC-CNS Life Sciences department has patented two biotechnological tools related with computational genomics, EDMD and SMUFFIN.

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

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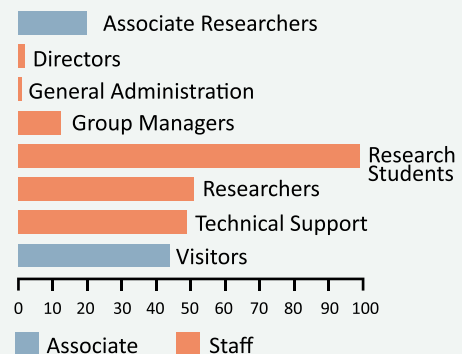
The scientific mission of the Computer Sciences Department is to influence the way computing machines are built, programmed and used. This is done through ideas, cooperation with manufacturers as technology transfer activities and "product-quality" open source developments that are usable by the scientific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

The Computer Sciences Department, led by Jesús Labarta and Eduard Ayguadé, is structured in 11 research groups. Although each group has its own specialised line of research, the teams often come together to collaborate on projects that require vertical integration, such as the Exascale EU projects Mont-Blanc (including MB2 and MB3) and DEEP/DEEP-ER, the RoMoL ERC project, the Human Brain Project (HPB) flagship and the national Severo Ochoa program. This vertical interaction is considered critical to the quality and success of the research, as feedback between the different groups enables application programmers to influence the direction of future systems architecture while better knowledge of architectures improves the design and implementation of novel programming models, execution environments and applications. The combination of broad coverage of all facets of computer systems design and programming, along with in-depth expertise in each area, is somewhat unique amongst supercomputing centres. This unique strength of the Computer Sciences Department has continued attracting leading computing companies to invest during 2015 in collaborative systems design R&D projects.

During 2015, some 214 staff and students and 64 collaborating researchers worked within the Department, organised in 11 research Groups; 4 focused on Computer Architecture (Heterogeneous Architectures, Computer Architecture for Parallel Paradigms, Operating System/Computer Architecture Interfaces and Unconventional Computer Architecture and Networks), 3 focused on improving productivity when programming and optimising parallel applications on large scale parallel systems (Programming Models, Performance Tools and Accelerators for HPC), 3 focused on APIs and resource management middleware for distributed heterogeneous architectures (Workflows and Distributed Computing, Autonomic Systems and e-Business Platforms and Storage Systems) and one on novel scalable mathematical methods and algorithms for large scale systems (Extreme Computing).

Computer Sciences Department Staff & Collaborators 2015

Bar chart categories: Associate Researchers, Directors, General Administration, Group Managers, Research Students, Researchers, Technical Support, Visitors. Scale: 0 10 20 30 40 50 60 70 80 90 100. Legend: Associate, Staff.

Impacting the Future of Computing

In collaboration with market leaders as well as other international computing centres, international research initiatives 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, 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.

Scientific Output

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), and also in prestigious journals in the area. 11 PhD thesis were defended during 2015 in the Computer Architecture Department at the Universitat Politècnica de Catalunya (UPC-BarcelonaTECH).

Key Projects and Networks

During 2015, the Computer Sciences Department participated in the following projects in national, European and industrial frameworks:

EU projects and networks:

● 32 projects: ASCETiC, Axiom, AXLE, BigStorage, BioExcel CoE, COMPOSE, DEEP, DEEP-ER, EUBrazil CloudConnect,

Communication & Dissemination 2015	
Publishing	
Journal Articles	32
Books	1
Book Chapters	3
Conference Presentations	
International	87
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Workshops	
Workshops	7
Education	
PhD Theses Read	11

EuroServer, ExaNoDe, EuroServer, Human Brain Project HBP, ICT-Energy, IOStack, LIGHTNESS, Mont-Blanc, Mont-Blanc2, Mont-Blanc3, NextGenIO, ParaDIME, parMERASA, POP CoE, PROXIMA, P-SOCRATES, RenewIT, RETHINK Big, SAFURE, SECURED, SKA-SDP, transPLANT and ARTEMIS VeTeSS:

- The HiPEAC-3 network of excellence.

- ETP4HPC: the European Technology Platform (ETP) for High-Performance Computing (HPC), in which the Computer Sciences Department is co-leading the Working Group on Programming Models.

- EuroLab-4-HPC: Foundations of a European Research Center of Excellence in High Performance Computing System, a two-year H2020 Coordination and Support Action (CSA) in which the Computer Sciences Department is leading the Research Work Package.

- The SCALUS Marie Curie Initial Training network.

European Research Council grants:

- RoMoL (Riding on Moore's Law) ERC grant (Mateo Valero).

- Hi-EST (Holistic Integration of Emerging Supercomputing Technologies) ERC grant (David Carrera).

International alliances and standardisation efforts:

- JLESC Joint Laboratory on Extrema Scale Computing, with participation of six of the leading supercomputing centres worldwide: Argonne National Laboratory (USA), The University of Illinois at Urbana-Champaign hosting NCSA (USA), BSC (Spain), INRIA (France), Jülich Supercomputing Center (Germany) and the Riken Advanced Institute for Computational Science (Japan).

- BDEC Big Data and Extreme-scale Computing, organising the 2015 plenary meeting in Barcelona (January 29-30).

- OpenMP Architectural Review Board, Language Committee, with special contributions to the Tasking working group.

Collaborations with IT companies:

- Intel Corporation with a multi-year agreement Intel-BSC Exascale Lab, on topics related to analysis of applications and performance prediction tools and programming models.

- NVIDIA through the GPU Center Of Excellence (GCoE), in association with the Universitat Politècnica de Catalunya (UPC-BarcelonaTECH).

- Microsoft Research through the BSC-Microsoft Research Centre agreement, on topics related to low-power vector architectures, architectural support for programming languages and analysis of Hadoop for MapReduce workloads.

- IBM Research through the following Joint Study Agreements: High-performance in-memory databases, Software-defined environments for HPC workloads, Adaptive resource management for Power, OmpSs @ P8/GPU, OmpSs programming model for asynchronous applications and Applicable research to interconnection networks.

- Samsung to evaluate memory behavior of HPC production applications and frequency and locality of memory errors.

- Xilinx Ireland to research OmpSs support for FPGA accelerators.

- CA to enhance recommendation systems by using Big Data analytics and Cloud computing.

- CISCO to develop Fog Computing technologies for deployment at scale.

- DENSO AUTOMOTIVE Deutschland GmbH (Germany) to investigate the programmability and predictability of many-core heterogeneous architectures for Advance Driving Assistant Systems (ADAS).

- The European Space Agency (ESA), with the following projects: NPI (Architectural solutions for the timing predictability of next-generation multi-core processors) PROARTIS for SPACE, HAIR, PMCs (Multi-Core Architectures - Cache Structure Optimisation for better RT Performance) and ITI (Parallel Programming Models for Space Systems).

Computer Sciences Projects 2015	58 Projects

41	4	13
EU and International	National	Industry

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.

- TIN Computación de Altas Prestaciones VII, together with the Universitat Politècnica de Catalunya, constitutes the basic research project of the Computer Sciences Department.

- TIN PROPHER targeting the design of high-performance and reliable time-randomised processor architectures.

Programming Models

Led by Xavier Martorell, the Group explores new programming models and their efficient implementation for current and future architectures. 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. A number of new features were included in both components. The Group had an important impact in the OpenMP standard, incorporating task priorities on the new OpenMP 4.5 specification (released November 2015), and contributing to task reductions based on taskgroups to be included in the upcoming OpenMP 5.0 specification. During 2015, the Group continued development of a framework to implement Domain Specific Languages (DSLs) for HPC systems; participated in three EU MontBlanc projects, DEEP, DEEP-ER and the Human Brain Project (HBP), as well as in the HiPEAC-3 Network of Excellence, initiated the AXIOM project, and continued research collaborations with Intel, IBM and Xilinx Research Labs.

Heterogeneous Architectures

This Group, led by the Department Directors, supported by three activity leaders, Paul Carpenter, Filippo Mantovani and Petar Radojkovic, aims to contribute to the design and evaluation of next generation HPC systems, capable of achieving the energy efficiency required by future Exaflop supercomputers. Development of prototype platforms represents an important step in the evaluation of new technologies for having both a development platform for HPC system software and a test bench for large scientific applications. During 2015, the Group successfully deployed the full Mont-Blanc prototype consisting of 1080 ARM-based compute nodes based on Samsung Exynos 5 dual SoC interconnected through Gigabit Ethernet with total power consumption below 3 kWatts; performed extensive studies of evaluation of the Mont-Blanc prototype as well as a reliability study of the mobile technology used in the prototype; continued the FP7 EuroServer project, evaluating the use of energy-efficient technologies from the mobile market for BigData processing; started its participation in the H2020 ExaNoDe project, contributing to the design and validation of the HPC nodes based on 3D-stacking and compute-chiplet/interposer/main-memory architecture, providing guidelines for the HPC node design, and defining methodologies for its validation and analysis of performance bottlenecks; continued the collaboration with Samsung in various fields of memory systems for HPC.

Unconventional Computer Architecture and Networks

Led by Mario Nemirovsky, UCAN conducts research on Internet of Things (IoT), Fog computing, Big Data, simulation techniques, and processor architectures. The convergence of Fog and IoT opens a vast research area that includes system architecture, virtualisation, mobility, connectivity (wired and wireless), and distributed computing among others.

The Group is working on a new simulation methodology, iQ, which performs rapid and accurate design space exploration to assist the processor design and optimisation. In parallel, new processor architectures and algorithms that can take advantage of Wireless Network-on-Chip (NoC), by using antennas at core-level to enable a natural broadcast network to communicate the cores are being developed.

Accelerators for HPC

The Group, led by Nacho Navarro (1958-2016), is the heart of the GPU Center of Excellence (GCoE) awarded by Nvidia, whose main aim is to leverage NVIDIA CUDA technologies and GPU computing. During 2015, the research activities focussed on the development of software infrastructures to ease the development of applications on multi-GPU systems, and mechanisms and policies for scheduling multiprogrammed workloads. The Group also contributed with optimisation of applications in different domains in collaboration with the CASE (Transport-WARIS application) and Life Sciences (PELE application) departments. Nacho Navarro also participated in the H2020 Axiom project as well as in the HiPEAC-3 Network of Excellence. His passing away in 2016 was keenly felt by all at BSC-CNS, who offer their condolences to his family and friends.

Computer Architecture for Parallel Paradigms

Led by Adrián Cristal and Osman Unsal, the group focused its research on the architectural support for novel programming models and execution environments for future multicore architectures. The group focuses its research on lowering the programmability wall raised by multicore architectures; research areas include low-power vector processors, reliability and accelerators for BigData. During 2015, the group finalized its work in two FP7 projects (ParaDIME and AXLE), while continued being involved in three ongoing FP7 projects (RETHINK big, ICT-Energy and MontBlanc 2).

Operating System / Computer Architecture Interface

The CAOS Group focuses its research activities on the convergence of embedded real-time and high-performance systems. During 2015, in the area of real-time systems the Group successfully completed the EU ARTEMIS VeTeSS project and several projects with the European Space Agency (ESA) continued participation in FP7 PROXIMA and P-SOCRATES projects, the RoMol ERC project, started two new projects with ESA, the MINECO PROPHER project, a bilateral project with the automotive Japanese company DENSO and the H2020 SAFURE project.

In the area of high-performance systems, the Group continued work on energy and CPU accounting and on adaptive prefetching techniques as part of a Joint Study Agreement with IBM.

Performance Tools

The Performance Tools Group, led by Judit Giménez, works on the design of tools to measure, analyse and predict the behaviour of parallel applications on parallel systems. All the tools developed are distributed as open source software. During 2015, the Group focused on advancing research targeting performance analytics and models as well as improving tools infrastructures and their integration. The POP H2020 Center of Excellence in the area of performance analysis and optimization was launched, and EU exascale projects Mont-Blanc/Mont-Blanc2 and DEEP/DEEP-ER continued. The Group is highly involved in the Intel-BSC Exascale Laboratory, an extensive collaboration with RIKEN (K-Computer) and contributes to JLESC and VI-HPS activities.

Storage Systems

Led by Toni Cortes, this Group explores appropriate solutions to the scalability of parallel storage systems in large installations (in which very large volumes of data need to be generated and accessed), new file-system approaches to increase their performance, and new approaches to store and manage Big Data. In 2015, the Group focussed on modifying Open Stack Swift to enable bandwidth differentiation to offer Software Defined Storage and on designing file-system solution for non-volatile memory architectures. In addition, the group has continued the development of a new storage abstraction based on self-contained objects by inspecting the code attached to the data to later implement prefetching policies, as well as by defining the concept of derived collections and special iterators to efficiently iterate over collections of persistent objects. During 2015 the research activities of the Group have been supported by the IOStack and NextGenIO EU projects, and the BigStorage ETN.

Computer Sciences General Support

Under the direct supervision of the Department Directors, Dario Garcia and Jonatan Moreno have been doing exploratory research on novel algorithms combining Deep Learning and Graph Mining, as part of the collaboration with IBM Research. In addition, Nuria Sirvent, the Department Secretary, has been taking care of the main adminstrative tasks and Director's agendas.

Autonomic Systems and eBusiness Platforms

Led by Jordi Torres and David Carrera, the Group performs high-level research in eBusiness applications and platforms executing on high-productivity multiprocessor architectures as well as distributed environments. The goal of the Group is to contribute in the continuous development of supercomputing systems enabling the convergence of big data technologies driving new insights based on the massive amounts of available data. The Group researches autonomic and intelligent resource management policies based on Self-Management strategies, new architectural proposals for memory/storage hierarchy including processing-in-memory techniques and novel key-value storage models to support Big Data workloads. Projects include ERC Starting Grant "HiEST", EU FP7 COMPOSE, RenewIT, ASCETiC, Euro-Server and LIGHTNESS projects; and collaborations with Microsoft, IBM Research, CA and Cisco.

Workflows and Distributed Computing

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 2015 focused on further development of the COMPSs programming model, specially in the Python binding, and in a more performant version of the runtime, its integration with new storage solutions such as dataClay and Hecuba, in a new version of the runtime for mobile devices, and other updates. The Group is also researching new technologies for low-cost energy efficient microservers. Finally, the Group has continued its participation in several EU FP7 projects (transPLANT, HBP, ASCETiC, EuroServer and EUBrazil CloudConnect) as well as in the Severo Ochoa Centre of Excellence, all of them related with extensions of COMPSs and porting of applications. Also, the group has started activities in new H2020 projects: the BioExcel CoE and NEXTGenIO, and collaborates in project SKA-SDP.

Extreme Computing

Led by Vassil Alexandrov, this Group focuses on development of novel scalable mathematical methods and algorithms for data and compute intensive problems on large scale systems and applying these to solving problems with uncertainty on such systems. The Group's main expertise is in the area of data and computational science, novel scalable mathematical methods and algorithms for large scale systems and exascale computing paradigm. In particular, scalable Monte Carlo and hybrid algorithms are developed for linear algebra, optimisation, computational finance, environmental models, computational biology, etc. The research also focuses on scalable, fault-tolerant and resilient algorithms for extreme scale (petascale and exascale) computing. In addition, the team led by Isaac Rudomin is working on the development of scalable algorithms for generation, simulation and visualization of large human crowds in heterogeneous clusters, as well as techniques for using real data in the development of such simulations.

Francisco J Doblas-Reyes, Director of the Earth Sciences Department

The Earth Sciences Department of BSC-CNS has the aim of modelling and understanding the behaviour of the Earth System, focusing its research activities on atmospheric processes and climate change modelling.
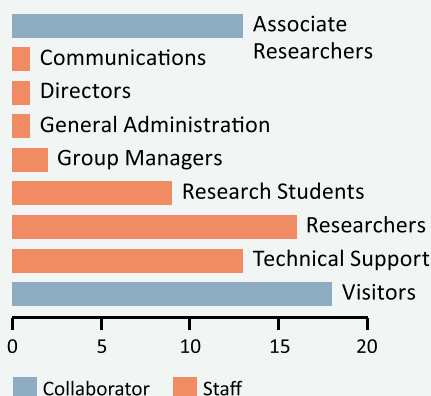
The goal of Earth Sciences is to apply the latest advances of High Performance Computing (HPC) and Big Data on Earth system modelling, putting the department at the forefront of the emerging problem of environmental forecasting. This very broad and ambitious objective is divided into four specific goals:

● Develop a modelling capability including the modelling of combined atmospheric processes, from urban to global scales, along with their impacts on weather, air quality, climate, health and ecosystems.

● Implement the most efficient climate prediction system to cover time scales ranging from a month to a few decades (subseasonal-to-decadal climate prediction) at global and regional spatial scales, while expanding at the same time our understanding of the climate system.

● Research the impact of weather, atmospheric chemistry, and climate on socio-economic sectors through the development of user-oriented services that ensure the transfer of developed technologies, and facilitate societal adaptation to a rapidly changing environment, especially for highly vulnerable communities.

● Use cutting-edge HPC and big data technologies to increase the efficiency, portability, and user-friendliness of the Earth system models, including pre-processing and post-processing of weather, atmospheric chemistry and climate data.

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

The Department is structured in four groups that represent the main topics of Earth Sciences research: Atmospheric Composition, Climate Prediction, Earth System Services, and Computational Earth Sciences. These groups are interrelated and work in a cooperative form. They are each led by a senior scientist and composed of a researcher, post-doctoral fellows and doctoral students. The technical support staff is shared by all the research groups. During 2015 some 46 staff, collaborators and visitors worked with the Department.

Earth Sciences Departments Staff & Collaborators 2015

Category	
Associate Researchers	
Communications	
Directors	
General Administration	
Group Managers	
Research Students	
Researchers	
Technical Support	
Visitors	

Collaborator   Staff

Scientific Output

The dissemination of research results obtained by the Earth Sciences Department is significant, having been presented in numerous ISI-JCR journals, European and international congresses and symposia organised during 2015, such as the Annual CMAS Conf., Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes; American Union Geophysical, European Geosciences Union General Assembly Meeting and other congresses organised by the European Meteorology Society (EMS), GLOREAM Conf., International Workshop on Air Quality Forecasting and Research.

Communication & Dissemination 2015

Publishing	
Journal Articles	17
Book Chapters	7
Conference Presentations	
International	43
National	13
Workshops	
Workshops	15
Education	
PhD Theses Read	1

Key Projects and Networks

- Continued IS-ENES2 project Infrastructure for the European Network for Earth System modelling - Phase 2, an FP7 Integrating Activity in the Capacities Programme.

- Continued the MACC-III (Monitoring Atmospheric Composition and Climate) FP7-project in collaboration with AE-MET, to establish the core global and regional atmospheric environmental services to be delivered as a component of Europe's GMES initiative.

- Continued the APPRAISAL project. Air Pollution Policies foR Assessment of Integrated Strategies At regional and Local scales, an FP7 Environment project.

- Initiated the CICYT project: Aerosol forecasting and assessment of radiative forcing on weather and climate applications with the online NMMB/BSC-CTM model. Funded by MINECO.

- Participated in the COST Action ES1004. European framework for online integrated air quality and meteorology modelling (EuMetChem) - focusing on a new generation of online integrated Atmospheric Chemical Transport (ACT) and Meteorology (Numerical Weather Prediction and Climate) modelling with two-way interactions between different atmospheric processes including chemistry (both gases and aerosols), clouds, radiation, boundary layer, emissions, meteorology and climate.

- Participated in the European Aerosol Research Lidar Network: EARLINET. The dataset generated is used to validate and improve models that predict the future state of the atmosphere and its dependence on different scenarios.

- Participated in AERONET (AErosol RObotic NETwork), an optical ground based aerosol monitoring network and data archive supported by NASA's Earth Observing System and expanded by federation with many non-NASA institutions.

- Hosted the World Meteorological Organization (WMO) SDS-WAS Northern Africa-Middle East-Europe (NA-ME-E) Regional Centre. The SDS-WAS mission is to enhance the ability of countries to deliver timely and quality sand and dust storm forecasts, observations, information and knowledge.

- Hosted the first WMO Regional Meteorological Centre specialised on Atmospheric Sand and Dust Forecast, the Barcelona Dust Forecast Centre (BDFC; http://dust.aemet.es). This centre will build and maintain a web portal to provide forecast products, related information, verification results and services on the internet; it is supported by the WMO.

- Participated in international initiatives such as the International Cooperative on Aerosol Prediction (ICAP) initiative, the Chemistry-Aerosol Mediterranean Experiment (ChArMEx), Air Quality Modelling Evaluation International Initiative (AQ-MEII), and the EURODELTA phase III.

- Participated in the Desert-dust Impact on Air quality through model - Predictions and Advanced Sensors ObservatioNs (Diapason) Project from Institute for Atmospheric Science and Climate of the National Research Council of Italy (CNR–ISAC; LIFE+ 2010 ENV/IT/391).

- Participated in a European modelling exercise to explore the impact of using finer grid horizontal resolution for policy support applications of the European Monitoring and Evaluation Programme (EMEP) model within the Convention on Long-Range Transboundary Air Pollution (CLRTAP) convention.

- Participated in the The Forum for Air quality Modelling (FAIRMODE) a joint response initiative of the European Environment Agency and the European Commission Joint Research Centre. It aims to bring together air quality modellers and users in order to promote and support the harmonised use of models by European Member States, with emphasis on model application under the European Air Quality Directive.

- Initiated the Marie Curie project: Effects of Mediterranean desert dust outbreaks on radiation, atmospheric dynamics and forecasting accuracy of a numerical mesoscale model (MDRAF).

- Coordinator of the European project SPECS which aims to identify the main problems in climate prediction and to investigate a battery of solutions from a seamless perspective.

- Participated in EUCLEIA, an EU project studying the attribution of weather and climate risks for Europe

Earth Sciences Projects 2015 — 24 Projects

18 — EU and International
4 — National
2 — Industry
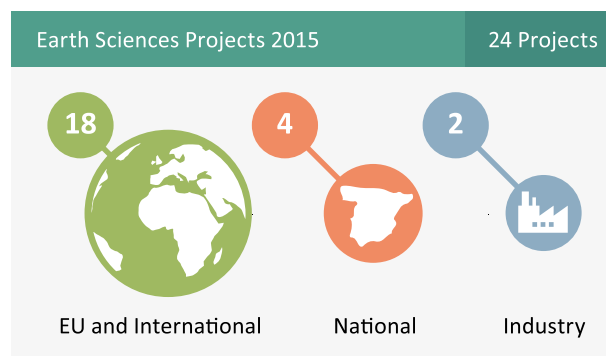
- Participated in EUPORIAS, to develop a number of fully working prototypes of climate services addressing needs of specific users.

- Leader of the MINECO project RESILIENCE, to strengthen the efficiency and security of the European energy network using best information from subseasonal-to-seasonal operational climate predictions in a coproduction process, with a special focus on the Iberian Peninsula and the North Sea region.

- Participated in the Spanish project NEWA whose main objective is the development of a new European Wind Atlas and improvement of advanced models towards the reduction of uncertainties to less than 3% for flat homogenous terrains.

Atmospheric Composition

The Atmospheric Composition Group aims to bet understanding of the chemical composition of the atmosphere and its effects upon air quality, weather and climate, while improving predictions from local to global scales. The goal is addressed through the development and use of the NMMB/BSC Chemical Transport Model (NMMB/BSC-CTM), an online multi-scale non-hydrostatic chemical weather prediction system that can be run either globally or regionally. The Group also develops and operates the CALIOPE system ("CALIdad del aire Operacional Para España"), which provides high-resolution short-term air quality forecasts for Europe, with a special focus over Spain and its main urban areas using the in-house HERMES emission model. The main research lines are:

Figure 1

Air Quality - Air quality is a major environmental and health problem affecting developed and developing countries around the world. This research focuses on the development and implementation of high resolution emission-meteorology-chemistry modelling systems to understand the physico-chemical processes taking place in the atmosphere.

Atmospheric Modelling - The evolution of the atmosphere governs a large number of processes that may impact directly to our society as severe-weather situations leading to high rainfall rates or atmospheric conditions that contribute to modify the air quality. This research aims to improve capabilities of mesoscale meteorological models for a deeper understanding of the mesoscale phenomena occurring in the atmosphere, with special attention to the boundary layer processes.

Mineral Dust - A large portion of atmospheric particulate matter is derived from desert and arid regions of the Earth and is distributed all over the globe. The most prominent example of this transport is the export of mineral dust from the Saharan desert. The main focus of this research line is to understand and model the atmospheric mineral dust cycle in order to assess and predict its impacts on air quality and climate.

Earth System Services

Knowledge and technology transfer, via tailored services, is essential to bridge the gap between science and its end users in key sectors of society (energy, urban development, infrastructure, transport, health and agriculture). Non-profit services are developed in-house (weather and atmospheric composition forecasting, and climate predictions) through projects in collaboration with public administrations, private contracts with companies or funding agencies, and spin-off companies that could exploit operational opportunities.

The overall aim of the Earth System Services Group is to demonstrate the ongoing value of climate prediction services, atmospheric composition and weather forecasting to society and the economy. The Group actively works in identifying user needs that will partly guide research in the Earth Sciences Department and aims to quantify the impact of weather, climate, aerosols and gaseous pollutants upon socio-economic sectors through the development of user-oriented services that ensure that the technologies developed are adapted and transfer to rapidly changing environments, especially for highly vulnerable populations.

Climate Prediction

The Climate Prediction Group aims at developing regional and global climate prediction capability for time scales ranging from a few weeks to a few decades into the future (sub-seasonal to decadal climate prediction).

This relies on expanding our understanding of the climate processes through a deep analysis of the strengths and weaknesses of state-of-the-art climate forecast systems in comparison with the most up-to-date observational datasets, and on exploiting these detailed analyses to refine the representation of climate processes in climate forecast systems and as well as their initialisation. Although the primary tool is the EC-Earth European climate model, frequent use is also made of large multi-model databases made available in the context of cooperative international projects (CMIP, SPECS, NMME, etc.) for process analysis.

The Group comprises a wide variety of expertise, both in terms of on climate processes and regions, from the stratosphere down to the deep ocean and from tropical to polar latitudes, as well as on climate modelling and data assimilation. The Group contributes to near-operational climate prediction exercises: on decadal and on seasonal time scales.

Climate Modelling

The horizontal resolution of coupled Global Circulation Models (GCM) is still too coarse to capture the effects of local and regional forcings in complex areas. The main focus of this research line is the development and testing of regional climate downscaling models for the generation of high-resolution regional climate information from coarse-resolution GCM simulations.
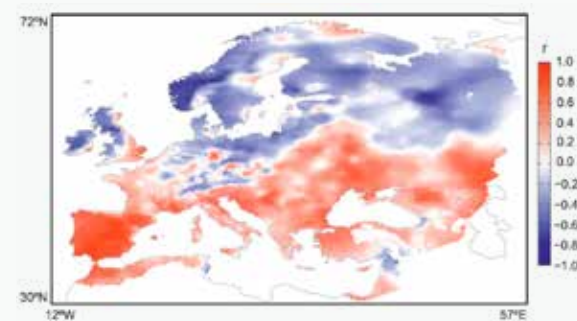

Figure 2

The Group has an interdisciplinary approach, collaborating closely with all research groups within the Department and with support groups at BSC-CNS (technology transfer, communications, visualisation, education and outreach).

Figure 3

Computational Earth Sciences

The Computational Earth Sciences Group is a multidisciplinary team with different IT profiles that interacts closely with all the other groups of the Department. The Group provides help and guidance to the scientists with technical issues and develops a framework for the most efficient use of HPC resources. In order to improve the use of the variety of computing resources available at BSC-CNS and in other HPC institutions, a solid software development, profiling and optimisation area is being created for Earth system model codes towards exascale computing, and to provide feedback on this to modellers around Europe. The Group develops a framework to disseminate the outputs generated by the Department among the research and service community.
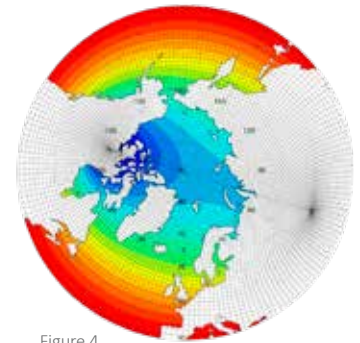

Figure 4

## WMO SDS-WAS NAMEE Regional Center

Activities were performed 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) and the Meteorological Centre specialised on Atmospheric Sand and Dust Forecast, the Barcelona Dust Forecast Centre (BDFC), hosted by AEMET and BSC-CNS. The web portal of the NA-ME-E Regional Centre provides National Meteorological and Hydrological Services (NMHS) with the necessary information to issue operational predictions and warning advisories related to the dust content in the atmosphere. During 2015, a new operational system were added to the list of 10 already existing operational dust forecast systems (BSC-DREAM8b, DREAM8-NMME-MACC, ECMWF-CAMS, NMMB/BSC-Dust, MetUM, GEOS-5, NGAC, EMA RegCM, DREAMABOL and NOA WRF-Chem) and was also included in the daily activities of NA-ME-E Regional Centre.

The current routine evaluation of dust predictions is focused on total-column dust optical depth and uses remote-sensing retrievals from sun-photometric (AERONET) and satellite (MODIS) measurements. Since the data sets of weather records have an excellent spatial and temporal coverage, maps of visibility reduction (by sand or dust to less than 5 km) reported in METAR or SYNOP bulletins are included in the website as an alternative way to monitor dust events in near-real time.

In 2015, the Regional Centre and BDFC organised, coordinated and participated in:

- Training course on the use of satellite products for agrometeorological applications (Addis-Ababa, Ethiopia, 23-27 March 2015) organised by the World Meteorological Organization (WMO), EUMETSAT and the Ethiopian National Meteorological Agency, as local organizer. Also Food and Agriculture Organization (FAO), Joint Research Centre (JRC) of the European Union, Royal Meteorological Institute of Belgium, University of Reading, State Meteorological Agency of Spain (AEMET).
- Side event on "Sand and Dust Storm. Forecast services" in the 17th Session of the World Meteorological Congress (Geneva, Switzerland, 8 June 2015).
- 1st Africa / Middle East Expert Meeting and Workshop on the Health Impact of Airborne Dust (Amman, Jordan, 6-2 November 2015) jointly organised by WMO, the World Health Organization (WHO), the United Nations Environment Program (UNEP), EUMETSAT and AEMET.
- 20th Session of the Conference of the Parties (COP12, Ankara, Turkey, 12-23 October 2015), organised by United Nations Convention to Combat Desertification (UNCCD).

The web portal of the BDFC operationally generates and distributes predictions for the NAMEE region. The dust forecasts are based on the NMMB/BSC-Dust model developed at BSC-CNS. In addition to the website, the operational products and activities are disseminating through Twitter and Newsletters.
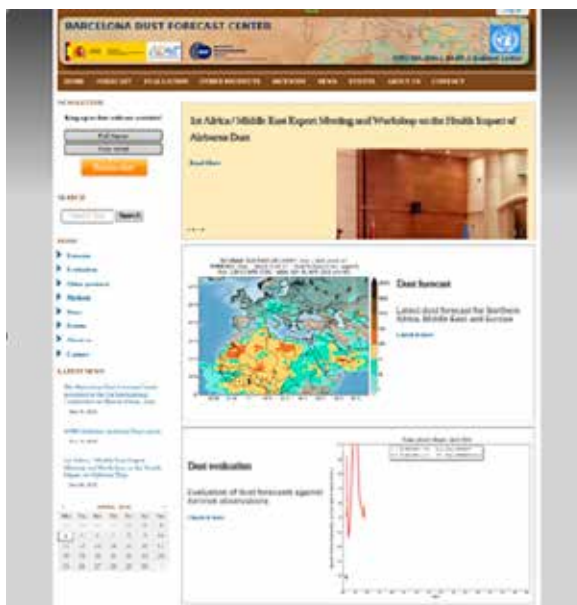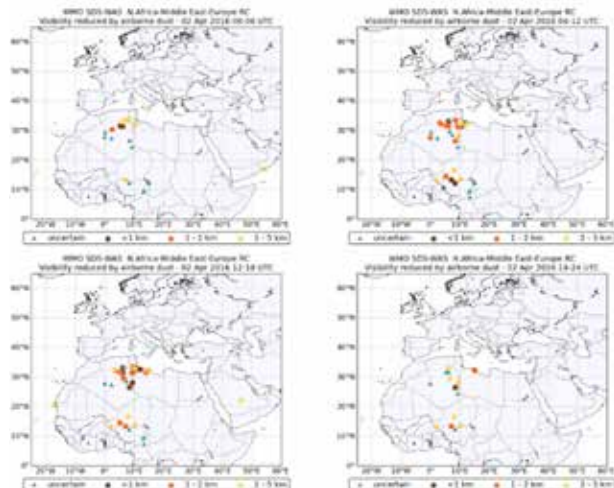
Modesto Orozco, Director of the Life Sciences Department

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

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

Developments of note in 2015 include the development of a Monte Carlo code for quickly and efficiently mapping DNA-ligand interactions (JCTC, 2015), development and testing of new docking and binding affinity prediction methods in the CAPRI community experiment framework, identification of eight new genetic variants associated with Type-2 Diabetes, analysis of more than 2500 whole genomes from cancer samples as part of the PanCancer consortium, major contributions within the MODEL project (Molecular Dynamics Extended Library) and the automatic servers MdWeb and NaFlex.
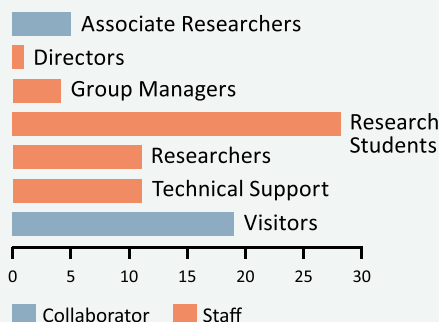
The Department is composed of 4 research groups and 2 research platforms:

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.

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 Bionformatics Laboratory (EBL), jointly run by BSC-CNS and IRB Barcelona, and the Computational Node (CN) of the National Institute of Bioinformatics, jointly run by BSC-CNS and INB.

Life Sciences Department Staff & Collaborators 2015

Associate Researchers · Directors · Group Managers · Research Students · Researchers · Technical Support · Visitors

0 5 10 15 20 25 30

Collaborator   Staff

Joint IRB-BSC-CRG Programme on Computational Biology

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

- Dr. Patrick Aloy, Group Leader, IRB Barcelona

- Dr. Xavier Salvatella, Group Leader, IRB Barcelona

- Dr. Juan Fernández Recio, Group Leader, Barcelona Supercomputing Center

- Dr. Victor Guallar, Group Leader, Barcelona Supercomputing Center

- Dr. David Torrents, Group Leader, Barcelona Supercomputing Center

- Dr. Roderic Guigó, Group Leader, CRG

- Dr. Cedric Notredame, Group Leader, CRG

- Dr. Yogi Jaeger, Group Leader, CRG

- Dr. Gian Gaetano Tartaglia, Group Leader, CRG

EU & National Projects

Highlights among 2015 projects include:

- ERC Advanced Grant PELE, a project to develop a software platform for "a la carte" drug design.

- eDRUG - the ERC market Proof-of-Concept for PELE

- SIMDNA - Multiscale simulation of DNA

- BIOEXCEL - A European Centre of Excellence in Biosimulation.

- Elixir-Excelerate - Fast-track ELIXIR implementation and drive early user exploitation across the life-sciences.

- MuG - a European project to develop a Virtual Research Environment for Multidimensional Genomics

- TransPLANT, an European project to develop a trans-national infrastructure for plant genomics

- ProCoGen, a European project to study confiner genomics

- BLUEPRINT, a European initiative to study haematopoietic epigenomes

- Marató TV3, to discover new inhibitors of the glutamate transporter

Life Sciences Projects 2015		25 Projects
12	7	6
EU and International	National	Industry
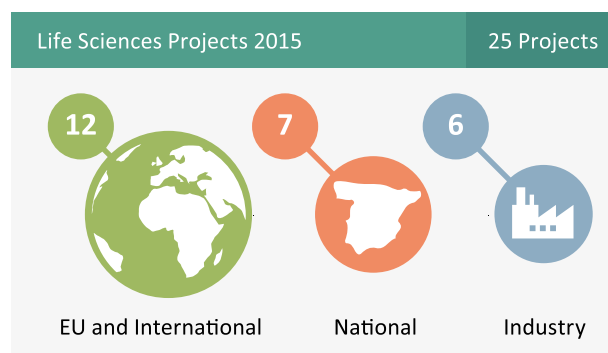
Scientific Output

The Life Sciences Department disseminates its results through major contributions to datasets and models utilised by the scientific community worldwide, and also through keynotes presentations at international conferences and publication in high impact journals, including Nature, Nature Methods, Nature Structure, J.Am.Chem.Soc., Angew. Chem. Int. Ed.Eng., Nucleic Acids Res., Structure, and others.

Communication & Dissemination 2015

Publishing	
Journal Articles	42
Conference Presentations	
International	12
National	3
Education	
PhD Theses Read	2

Protein Interaction and Docking (PID) Group

The main focus of the Group is the development, HPC-optimisation and application of computational methods for the study of protein interactions at the molecular level. The Group develops new computing tools to generate molecular models to understand how proteins interact to form specific complexes that are fundamental in biological processes, with the overall aim of advancing personalised medicine and drug discovery targeting protein-protein interactions.

In 2015, the Group focused on the development of novel computational methods for the structural and energetics characterisation of protein interactions, in particular with strong contributions to compile and analyze the most recent version of a standard benchmark set for the development, optimisation and validation of docking and binding affinity prediction methods, in a joint effort with renowned researchers in the docking field. Another important area of focus was molecular modeling of protein interactions of biomedical interest and for drug discovery. The Group studies the different members of the Heteromeric Aminoacid Transporters (HAT) family, which are involved in serious human pathologies.

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. Within this general objective the work centres on two topics: i) the study of nucleic acids with potential biomedical or biotechnological interest, in particular DNA in unusual conformations or in stressed conditions, and nucleic acids in chromatin; and ii) the study of protein dynamics, understanding the relationship between the essential dynamics of proteins and their functionality.

Work in 2015 focused on four main areas: (1) Development of methods for the high throughput study of dynamics in macromolecules via the MODEL project (Molecular Dynamics Extended Library), and the automatic servers MdWeb and NaFlex; (2) Development of Coarse Grained Methods for the study of protein dynamics, including Normal Mode Analysis, Brownian Dynamics, and Discrete Molecular Dynamics; (3) Study of unusual or stressed forms of DNA, and (4) Studies on the connection between physical properties, chromatin structure and biological functionality.

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 programme 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.

Major external collaborations during 2015 included: Development of new tools for molecular simulations and computer assisted drug design (U. Barcelona), Genomics studies of cancer (U. Oviedo, IDIBAPS), Bioinformatics for Plant Genomics (EBI), Data integration portals for large genomic projects (CNIO), and the European Elixir Bioinformatics infrastructure.

Electronic and Atomic Protein Modelling (EAPM) Group

The Electronic and Atomic Protein Modelling Laboratory is devoted to the development of computational algorithms to advance in the understanding of protein's biochemistry and biophysics. For these purposes, the Group applies and develops two different sets of techniques: Monte Carlo simulations on classical force fields, and mixed QM/MM (quantum mechanics/molecular mechanics) methods.

Work during 2015 focused on two main lines: Biochemical studies on enzyme engineering for industrial applications; and Biophysical protein-ligand software development and applications. Highlights include (1) the first complete in silico analysis where biophysical simulations produce free (unbiased) substrate diffusion, active site search and binding, and biochemical modelling permits a robust description of the chemical event, (2) a collaborative study with the pharmaceutical company Astra Zeneca to produce what is probably the most comprehensive mechanistic study in ligand binding in Nuclear Hormone Receptors, a very important pharmacological target.

Computational Genomics (CG) Group

The aim of the Computational Genomics Group is to investigate different biological processes of genomes and improve understandings of how the sequence and the structure of these macromolecu–les determine their basic functions. Efforts are focused in developing new approaches and methodology to identify the variation in the genome and transcriptome associated to disease and to interpret its molecular consequences, with the final aim of contributing to the generation of new diagnostic and treatment protocols within the developing field of precision medicine.

During 2015, the Group focused on three main areas: the identification and characterisation of risk genetic variants associated with Type 2 Diabetes, conducting a large study on the detection of genetic variants that confer risk to develop Type 2 Diabetes (T2D) via which eight new variants associated with risk factor were identified; active participation in the PanCancer initiative, as part of the International Cancer Genome Consortium (ICGC), conducting analysis of more than 2500 whole genomes from cancer samples covering several tumour types; and finally, analysis of the gut microbiome of patients with liver transplantation.

Experimental Bioinformatics Laboratory (EBL) Platform

The Experimental Bioinformatics Lab (EBL) is part of the collaborative research programme 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.

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, CASE collaborates with Spanish institutions such as CIEMAT, CSIC, IAC, CNIC, IMDEA and various universities, and also with institutions abroad like Imperial College, Oxford University, STFC in the UK; EDF, CERFACS and Ecole Centrale de Paris in France; University of Twente in the Netherlands; and George Mason University and Jackson State University in the USA. This is complemented with strong links with industrial partners such as REPSOL, Iberdrola or Siemens.

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

Computer Applications in Science & Engineering Department Staff & Collaborators 2015

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

● Alya: HPCM system. Fluid mechanics, Solid mechanics, Electric propagation, Combustion, Fluid-structure interaction, etc.

● FAll3D: Volcanos ash transport. Used in production in South American Volcanic Ash Advisory Centres (VAAC).

● NMMB-Ash: multi-scale meteorological model for the transport and deposition of volcanic particles.

● BSIT(Barcelona Subsurface Imaging Tools): Acoustic/Elastic/EM waves, Forward Modelling, RTM, FWI. Promoted by Repsol.

● SIESTA: Ab-initio molecular dynamics. CASE is a co-developer of this code.

● bigDFT: Ab-initio molecular dynamics. CASE is a co-developer of this code.

● Pandora: An HPC Agent-Based Modelling framework for social simulation.

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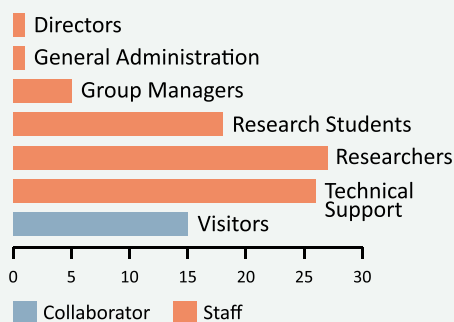
Scientific Output

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

● Development and optimisation of a solid mechanics module in Alya.

● Implementation of coupling strategies in a distributed memory environment (FSI).

● Coupling of Alya and Code_Saturne, the CFD code developed at EDF, France.

● Development of an implicit VMS compressible solver and preconditioning techniques.

● 3D Seismic inversion for large data sets using FWI from BSIT.

● Development of electromagnetic modelling (CSEM) on BSIT.

● BSIT kernel optimization for both Intel Sandy Bridge processors and Intel Xeon Phi co-processors.

Communication & Dissemination 2015	
Publishing	
Journal Articles	30
Book Chapters	7
Conference Presentations	
International	30
National	1
Workshops	
Workshops	1
Education	
PhD Theses Read	3
Masters Theses Reads	1

Key Projects

In 2015, the CASE Department carried out work under the scope of the following projects:

EU-funded projects:

CASE has been actively involved in the PRACE 3IP and PRACE 4IP projects, mainly concerning the optimisation on massively parallel supercomputers of Alya code, which is part of the European Unified Benchmark Suite.

CASE has been also the coordinator of the H2020 project High Performance Computing for Energy (https://hpc4e.eu) and participated in the 7FP project New European Wind Atlas (NEWA) (http://euwindatlas.eu) and the Initial Training Networks COPA-GT (http://copagt.cerfacs.fr) and NEMOH (http://www.nemoh-itn.eu). It is member of three Centers of Excellence (CoE) funded by the European Union under the Horizon2020 program, namely Novel Materials Discovery (NOMAD) Laboratory (https://www.nomad-coe.eu), Materials design at the Exascale (MaX) (http://www.max-centre.eu) and Energy oriented Centre of Excellence for computing applications (EoCoE) (http://www.eocoe.eu). Also, important contributions were made to applications work packages of DEEP-ER.

Enterprise-funded projects:

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

Nationally funded projects:

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

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

CASE has established strong national and international collaborations, all of them fostered by the Severo Ochoa Programme. In summary, CASE collaborates with: the National Centre for Cardiology Research (CNIC) to work on ventricular arrhythmias,

performing full cardiovascular simulations from the heart up to the cerebral arteries by coupling Alya with ADAN, the arterial network created at the LNCC in Brazil; with Imperial College and St Mary's hospital (UK) on respiration and sniff simulations; and with Jackson State University (USA) on coupling real patient large airways to generic models for small airways, in order to carry out simulations of almost the complete respiratory system.

CASE Projects 2015 — 38 Projects

21 EU and International · 8 National · 9 Industry

Other collaborations:

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

- CINES, France: asynchronous and dynamically load balanced code coupling.
- Technical University of Munich, Germany: multi-code coupling strategies.
- STFC, UK: multi-code coupling strategies.
- EDF, France: multi-code coupling strategies.
- NCSA, USA: performance studies of Alya code on Blue Waters supercomputer and scalability of direct solvers. Prediction of the reacting flow field of industrial combustion systems using Alya.
- CERFACS, France: collaboration framework to conduct high-fidelity numerical simulations of gas turbine engines.
- University of Twente, Netherlands: development of a turbulent combustion model using tabulated chemistry in the flamelet regime.
- Lancaster University, UK: performance assessment of biomass-derived fuels for combustion applications.
- CIEMAT, Spain: analysis and development of the thermochemical structure of turbulent flames.
- Siemens AG, Germany: analysis of the effects of fuel split and heat losses in practical combustion systems.
- Oxford University, UK: numerical prediction of separated flows in a full-aircraft configuration.

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 recent years, the Group dedicated a lot of resource to upgrade the Alya high performance computational mechanics (HPCM) code, including implementation of direct and iterative solvers (PASTIX, MAPHYS) in collaboration with INRIA Bordeaux; Hybrid MPI+OpenMP; Dynamic load balancing (MPI+OpenMP+DLB); and implementation of MPI3.

Computational Fusion Physics

Fusion Group researches the development of nuclear fusion as a future energy source, focusing on the numerical modelling of experiments in magnetically confined fusion devices in preparation for ITER (www.iter.org) operation. The overall objective is to enhance the modelling capabilities by code development, validation, integration and optimisation, with the ultimate goal of helping improve the performance of ITER and future fusion reactors.

In 2015, research was conducted on the physics of fast ions; modelling of pellet injection into the fusion plasma; fusion code implementation within the EUROfusion Code Development Work Package (WPCD) for integrated fusion modelling; development and optimisation of the gyrokinetic particle-in-cell (PIC) code EUTERPE; and also participation in the EUROfusion High Level Support Team (HLST) to provide expertise to scientists from the EUROfusion Research Units for the development and optimisation of supercomputing codes.

The activities covered modelling for several present-day tokamaks such as JET (UK), ASDEX-Upgrade (Germany) and DIII-D (USA), and were oriented on the objectives of EUROfusion (www.euro-fusion.org).

High Performance Computational Mechanics (HPCM)

The HPCM Group conducts application R&D in different science and technology domains where simulations are needed, driven by direct interaction with users and industry.

Usually the core problem requires modelling of physical processes which then must be solved by intensive numerical calculation. The principal application fields that have been developed to date are:

- Alya applications: biomechanics; building, energy and environment; dynamic structural behavior of complex aerospace problems; vehicle dynamics; combustion processes and heat transfer in combustors; and simulation of chemical reactions in biodiesels inside batch reactors.
- Fall3D applications: atmosphere science (volcanic ash transport).
- SIESTA and bigDFT applications: ab-inito DFT and TDDFT molecular dynamic simulations.
- Other applications: plasma physics.

HPC Software Engineering (HPCSE)

HPCSE is responsible for providing tools and methodology for proper software engineering processes, and is responsible for the good HPC performance of the different codes developed by CASE. HPCSE is also the interlocutor of the CASE department for all HPC application related projects, actively participating in Aurora, DEEP-ER, Montblanc and HPC4E projects.

Computational Social Sciences and Digital Humanities

Since 2009, the Group is working on specialised applications for use in social sciences and policy analysis. It is developing a new simulator capable of executing Agent-Based Models of human societies in an HPC environment, in order to explore the emergence of behavioural patterns in human societies, interactions between societies and their relationship with environment and landscape, impacts 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.

Smart and Resilient Cities Initiative

Availability and integration of data is fundamental in smart cities. The Group works on semantic models applied to problems such as urban planning and sustainability, energy efficiency, and sustainable transport. One example is the Group´s participation in the H2020 lighthouse project GrowSmarter (http://www.grow-smarter.eu) that proposes 12 solutions for low energy districts, integrated infrastructures, and sustainable urban mobility. The Group also works on identifying information in large collections of texts with applications for e-governance and homeland security.

Environmental Simulations (ES)

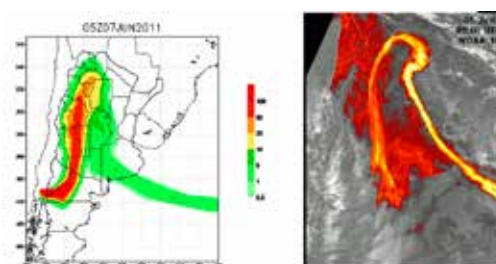This Group has three main areas of activity:

Atmospheric Transport

Modelling of atmospheric transport, with particular emphasis on volcanic ash. Research lines include: Volcanic Ash Transport and Dispersal Models (VATDMs); 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; feedback effects of large-magnitude eruptions on regional meteorology; and code optimisation.

Meteorological Modelling

Modelling different aspects of weather. Research lines include: Mesoscale Numerical Weather Prediction (NWP); data assimilation and downscaling from mesoscale NWP models to local-scale; high-resolution wind field modelling in complex terrains using CFD with Alya; modelling of the atmospheric boundary layer including turbulence and thermal effects.

Wind energy

Numerical modelling of wind farms is a crucial aspect in terms of both wind farm design and management. Applications using ALYA Green for high-resolution wind field modelling include: modelling of on-shore and off-shore wind farms; modelling of wind turbines using actuator disks and the HERMESH method; wind resource assessment; forecast of short-term wind farm power production; and tailored modelling postprocess using GoogleEarth to facilitate visualisation and standard data interchange.

Comparison between forecasted ash cloud column mass (ton km-2) and split windows satellite image during the 2011 Cordón-Caulle eruption in Chile"

Geosciences Applications (GA)

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

The Group´s 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 addition, the Group investigates 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).

The final objective is to merge all developments in the BSIT geophysical imaging toolkit (www.bsc.es/bsit).
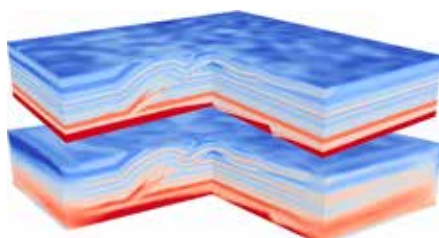
Inverse model using Full Waveform Inversion

Data Pre & Post Processing (DPPP)

- The DPPP 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 using pure data visualisation as the medium; and publication of results from a scientist to other experts in the field.
- Key activities in 2015 included:
- Collaboration with the international music festival Sónar to create "We Know What You Did Last Sónar".
- The short documentary Sniff was premiered at Imagine Science Film Festival, and later published in the Supercomputing visualisation showcase.
- Work commenced on the European Centers of Excellence NOMAD and EoCoE.
- Collaboration with the Life Sciences department to produce a graphical interface for the PELE molecular dynamics simulation software.
- An interface was developed for a numerical optimisation framework for Repsol.
- Numerous short videos and static images were produced for scientists of BSC-CNS and the RES for use in scientific publications and webpages.

Sergi Girona, Operations Department Director

The key mission of the Operations Department is to ensure the continued availability and accessibility of RES systems 24 hours a day, 7 days a week and to provide support to all the users of the RES and PRACE. Further core objectives are to manage upgrades to the MareNostrum and other RES nodes; facilitate access to RES facilities, including online electronic applications, remote access, and porting of code; manage the environmental aspect of the BSC-CNS installations; manage the technical aspects of integration of the MareNostrum in the PRACE, EUDAT and European HPC network ; and ensure that RES staff receive appropriate training and skills development in order to be able to professionally carry out their duties in an environment of constant technological change and advancement.
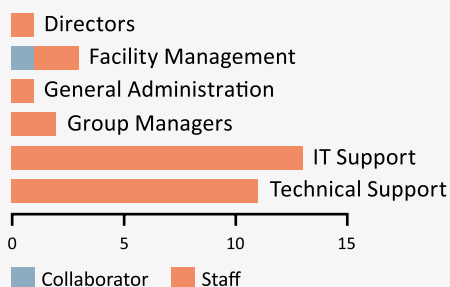
Led by Sergi Girona, the Operations Department ensures the continuous daily functioning of RES supercomputers and remote access by users, both within Spain and internationally. In addition to all the routine maintenance and operations tasks, Department staff are also heavily involved in planning and designing new systems and support facilities. Furthermore, the entire Department participates in European projects such as PRACE, EESI-2 and EUDAT.

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

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

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

Operations Department Staff & Collaborators 2015

Directors
Facility Management
General Administration
Group Managers
IT Support
Technical Support

0   5   10   15

Collaborator   Staff

Key Projects

The Operations Department was involved in the following projects during 2015:

- **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 3IP:** In the PRACE Third Implementation Phase, the Operations Department is involved in WP2, WP5, WP6 and WP7, and coordinates the participation of BSC-CNS in the project.
- **PRACE 4IP:** In the PRACE Four Implementation Phase, the Operations Department is involved in WP2, WP5, WP6 and WP7, and coordinates the participation of BSC-CNS in the project.
- **EESI2:** The objective of this Support Action, co-funded by the European Commission, is to build a European vision and

roadmap to address the challenges of the new generation of massively parallel systems composed of millions of heterogeneous cores which will provide multi-Petaflop performances in the next few years and Exaflop performances in 2020.
- **EUDAT2020:** The EUDAT project aims to contribute to the production of a Collaborative Data Infrastructure (CDI). The project's target is to provide a pan-European solution to the challenge of data proliferation in Europe's scientific and research communities.
- **RDA-EUROPE:** The RDA-EUROPE is a project focuses on coordinating a series of cross-infrastructure experiments on global interoperability with a selected group of projects and communities. One of its main functions is support of the RDA initiative.
- **EXDCI:** The EXDCI's objective is to coordinate the development and implementation of a common strategy for the European HPC Ecosystem.

User Support

User Support is responsible for direct user support providing detailed knowledge of programming models, libraries, performance tools and applications, including code optimisation and parallel model building, porting, creation of scripts, and tutorials on specialised topics. It is also responsible for management of the BSC-CNS website, intranet, graphic design, and the SC virtual reality and 3D visualisation equipment.

Some 7403 support requests were handled during 2015.

Highlighted Projects

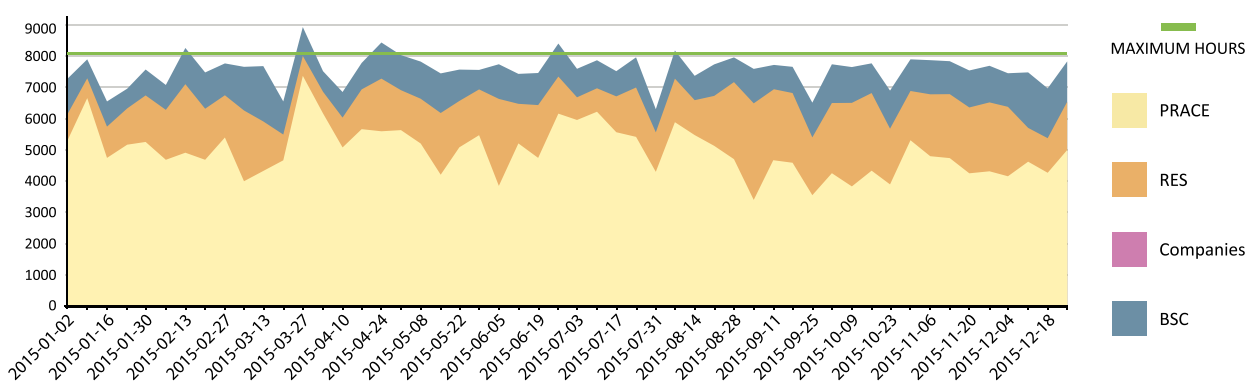**SPMA-Support Performance Monitoring Applications**

During 2015, the User Support group deployed SPMA on MareNostrum 3. SPMA stands for Support Performance Monitoring Application. It consists of a set of benchmarks which run daily on MareNostrum 3 and show the current behaviour of the machine. There are two sets of benchmarks: one for HPC applications such as WRF, GROMACS, CPMD, NAMD, AMBER and VASP; and another one for GPFS, which shows some metrics about bandwidth and current use of the filesystems.

These graphs are available to RES users through the RES Area (www.res.es) as well as to BSC users through BSC's Intranet.

MareNostrum Performance 2015

MareNostrum was in full production during the entire year with a total of 48128 cores. The observed system utilisation was approximately 93%. In addition to BSC-CNS internal groups, more than 230 external groups accessed the MareNostrum system during 2015.

MareNostrum Weekly Performance in Computing Hours (Thousands)

Jobs are accounted at the end of execution, which may produce a figure exceeding total capacity in some weeks.

System Administration

System Administration Group is responsible for general operation, upgrades, system administration, security, resource management, networking, helpdesk 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.

Minotauro hardware updated

During December 2015, the Minotauro GPU supercomputer was upgraded with 39 new nodes

Minotauro new node:
- 2 Xeon E5-2630v3 Haswell processors
- 128 GB of main memory
- 2 NVIDIA K80 GPU
- 120 GB SSD local storage

This upgrade introduces more than 200 Teraflops of the latest GPU computing technology, enabling the execution of applications related to BigData, Deep Learning and cognitive computing.

Facility Management

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

Highlighted Projects

● Rack Liquid Cooling Package

Rack 42 units with a cooling capacity of until 40KW. The fan modules and the water module contain their own electronic controls (1 x RLCP fan and 1 x RLCP water), which are connected to the CMC III PU via a CAN bus.

Highlight features include: Collection and real-time monitoring of all facility parameters, and alarm notification.

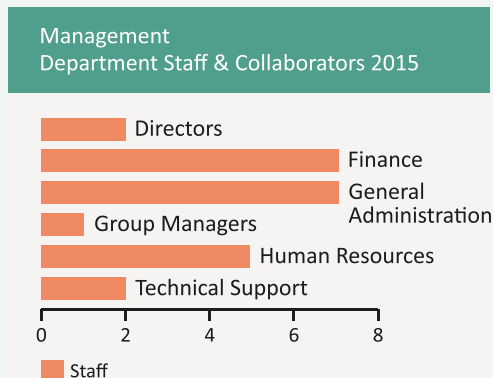Ernest Quingles, Management Department Director

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 helping them to achieve funding opportunities, applying and managing competitive projects, initiating and developing systems and processes to increase the efficiency and effectiveness of staff and the quality of work, and developing electronic management tools.

The Management Department, led by Ernest Quingles, aims to provide administrative and management services to all the other departments, and is supported by Mercè Calvet, as Associate Manager, in order to manage and coordinate all units of the business administration area. Due to the continued growth of BSC-CNS and constantly changing needs resulting from the range of activities carried out by the Centre, the Management Department maintains a somewhat flexible internal structure, with work teams being formed to tackle different issues.

The Management Department integrates all units related with the business administration area that is structured as follow: Finance & Accounting, Administration & Purchasing, Information System & Services and Human Resources.

Management Department Staff & Collaborators 2015

Bar chart showing staff numbers by category: Directors, Finance, General Administration, Group Managers, Human Resources, Technical Support, with axis from 0 to 8.

Staff

Finance & Accounting

The Finance & Accounting Group is responsible for financial resources management of all activities of BSC-CNS (expenses, budgets, audits, bank relations, suppliers, receiving payments and control budget deviations). According to existing financial legislation and accountancy norms, they manage and safeguard the Centre´s funds and assets, with support from the Administration Group. 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 had to increase the role of controller and began working on the automation of certain data analysis and exploitation processes, as well as introducing a semiannual review of financial indicators. In 2015, the Group continued working on a SAP B1 tool with a system upgrade for better reporting capabilities and new finance queries.

The Group also worked on process improvement in electronic management to provide finance services according to new regulations applicable to research centres, such as electronic invoicing and evaluation of digital signature systems.

Activities of note recorded during the year include: the creation of the first spin-off company with participation of BSC-CNS, the return of the last installment of the loan granted for the first upgrade of the MareNostrum, investments in equipment Exascale for Big Data granted by European Development (ERDF) funds and execution of works of the new building thanks to funding from sponsors the Repsol Foundation.

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Information System & Services

During 2015, the newly established Information System & Services unit was consolidated; the team comprises the Coordinator of the unit, two senior Engineers and one Engineer officer, who provide support and keep the IT systems maintained and updated.

In particular, the unit focused on improving the budget reservation system for Purchasing and Human Resources, enabling future budget provisioning of up to 5 years; the accounting of the Centre´s flexible compensation scheme and other minor upgrades through a new wizard tool, which enhances pre-existing procedures. Other improved services include a new refurbished Professional Development tool, tailored to suit current employee needs.

General Administration & Purchasing

The General Administration Group is responsible for activities such as organisation of official meetings, including those of the Access Committee, the Executive Commission, the Board of Trustees and other institutional events, for example, the meeting of international Scientific Advisory Board of the BSC-CNS in 2015.

The Group worked on process improvement in management of travel services, space allocation and new offices requirements, purchasing services and execution of public tender processes as well as providing general administrative support, logistic and reception services, such as the development of a new information services section for suppliers and customers on the BSC-CNS website, and the integration of inventory data in a centralised system with the implementation of an asset labeling system.

The staff structure of the purchasing unit was strengthened during the year, in order to meet growing needs for internal assistance due to project activities and public tender requirements, and to work on increasing the efficiency of the services. This also enabled the incorporation of best management practices in the selection and hiring of suppliers with social value.

During the year, BSC-CNS issued 10 public calls in order to accept 4 supply tenders, 5 services tenders and 1 works tender. The works tender was for the continuation of the 2nd phase construction of the new BSC-CNS building. A total of 97 administration contracts were signed during the year.

In 2015, the HR Group helped BSC-CNS achieve the HR Excellence in Research (HRS4R) recognition, awarded in April 2015 by the EU. The HR vision embodied in the award is that BSC-CNS recognises that researchers from all areas and levels, and also support staff, are all essential contributors and key players for scientific success at national and international levels. BSC-CNS wants to promote a challenging work environment which provides equal opportunities, ethics & integrity, work-life balance, career prospects and the best-practice working conditions.

Human Resources

The Human Resources Group is responsible for managing recruitment processes, hiring and training, job descriptions, labour relations and collective bargaining, compensation and benefits, HR development programs, planning careers and internal promotions, employee branding and health & safety, among other responsibilities related to this area.
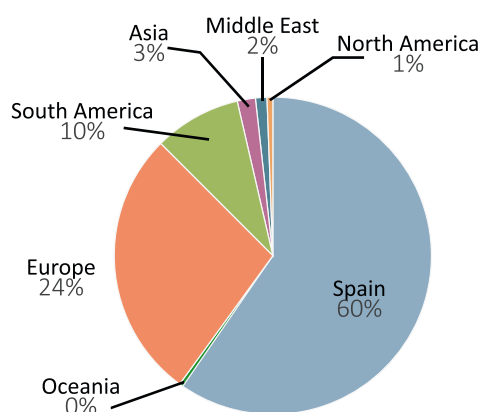
During 2015, the HR Group consolidated in a structure with two main areas, HR Development (Recruitment, Training, HR Development projects) and HR Management (Personnel Administration, HR Controlling), both coordinated by the Head of Human Resources.

The BSC-CNS action plan was approved by the Executive Board on February 2015. It is an extensive and ambitious project, whose highlights include the creation of advisory committees formed by researchers, boosting the equal opportunities and gender policies, strengthening the activities in outreach and public engagement, and maintaining and improving the career development system.
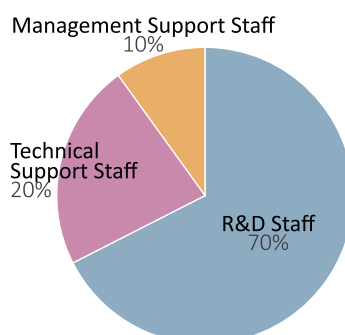
The HR team, following these commitments, continued work on a professional development system for all BSC-CNS staff. The web tool, which was implemented in 2013, was refurbished to be more user-friendly, and helped manage the BSC-CNS Staff Professional Development Plan (Annual staff evaluation, monitoring of the Plan's development, and keeping it aligned with annual goals of the department as well as of the entire Centre).

Other HRS4R projects included the Folks BSC platform for ex-BSC-CNS staff to keep in contact, new recruitment procedures focused on gender equality, a new induction program, and others, all of which are published on the BSC-CNS website. In October of 2015, BSC-CNS hosted the Euraxess Roadshow, which promotes scientific careers in Europe and opportunities at BSC-CNS, with conferences and other activities open to the general public. BSC-CNS continues to attract researchers from all over the world: at the end of 2015, 32% of BSC-CNS staff were from abroad (from a total of 44 countries) and BSC-CNS had 73 external fellowships.
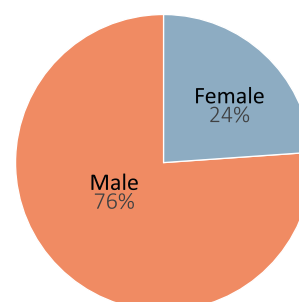
2015 Personnel by Region of Origin

Asia 3%
Middle East 2%
North America 1%
South America 10%
Europe 24%
Oceania 0%
Spain 60%

2015 Personnel by Function

Management Support Staff 10%
Technical Support Staff 20%
R&D Staff 70%

### 2015 Personnel by Gender

Female 24%
Male 76%

The Research Support, Transfer and Communication Area is led by Eugene Griffiths, who reports directly to the BSC-CNS Director and Associate Director.

The area is made up of: the Project Management Office, the Communication Unit, the Technology Transfer Office and the Strategy Support Unit.

Project Management Office

The Project Management Office (PMO) is staffed by nine 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 taking care of the 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.

BSC-CNS Projects	143 Projects
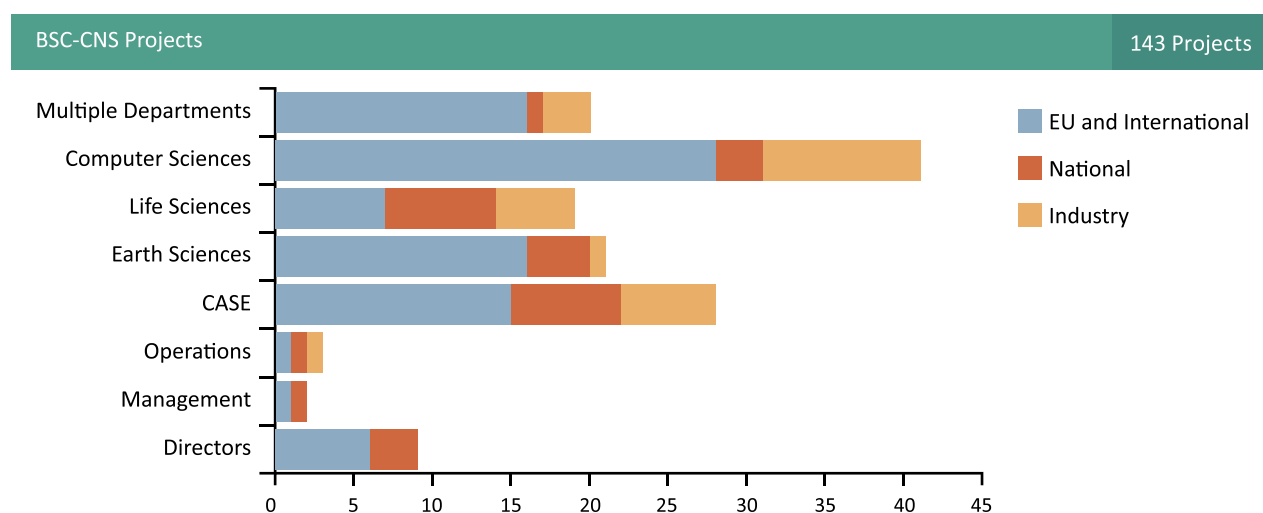
In particular, BSC-CNS project managers help researchers understand and fulfil the requirements of the European Union's Horizon 2020 funding program. In 2015, BSC-CNS participated in 143 projects (excluding personnel grants), with a total BSC-CNS grant of over 56 million euros. 77 projects were funded by the extremely competitive FP7 and H2020 programs of the European Commission. Of these European projects, 7 were led by BSC-CNS, in which BSC-CNS coordinated partners based throughout Europe and overseas. 27 projects were funded by Spanish National or Catalan funds. A total of 26 research projects were funded by private companies, representing total financing of over 12 million euros.

In addition to managing active projects, the Project Management Office assists BSC-CNS researchers in submitting new project proposals for research projects and personnel grants to help ensure continued future funding of BSC-CNS activities. In 2015 they assisted with more than 200 project proposals. Highlights of 2015 for the PMO included: 42 H2020 projects running or in negotiation during the course of the year (BSC's success rate of 33% was well above the average for the programme); the merger with Francesco Doblas Reyes's group from IC3 and the transfer of various European and national projects; the successful submission of the second proposal to the Severo Ochoa programme, whose grant will last until the end of 2019; the start of the Performance Optimisation and Productivity Centre of Excellence on HPC Applications, a project coordinated by BSC; the approval of the Hi-EST ERC grant for David Carrera; New contracts with Lenovo, Cisco, Samsung widening of participation with Intel and Microsoft; successful completion of the Mont-Blanc and PROARTIS projects, both coordinated by BSC-CNS; and the start of the first coordinated European project for the CASE department.

Strategy Support

The Strategy Support Unit works on coordinating activities linked to prioritising and road-mapping future research (including The European Technology platform for High Performance Computing-ETP4HPC, and the EC-funded RETHINK big project on roadmapping for big data technologies), and provides support in the definition of the organisation and management of international research infrastructures, such as PRACE, among others. Highlights of 2015 included funding being secured for BSC-CNS to continue as a PRACE hosting partner; the update of The Strategic Research Agenda of the ETP4HPC, and BSC-CNS being renewed as a member of the ETP4HPC steering board.

Technology Transfer Office

The Technology Transfer Office helps to transfer knowledge and technology developed at the centre to industry worldwide, and promotes the use of HPC by local industry in order to increase its competitiveness. The Technology Transfer Manager works with researchers to identify technology with commercial potential, protect this technology in the most appropriate way; promote and license BSC-CNS know-how and technology through agreements with companies and the foundation of spin-off companies; and promote consultancy services and research agreements.

Highlights for 2015 included the creation of the first Spin-off at BSC-CNS, Nostrum Biodiscovery, which will work on improving the drug discovery process. The office also helped researchers to find funding for transfer activities, and organised visits to Mare Nostrum for over 500 companies. More information can be found in the Technology Transfer section of this report.
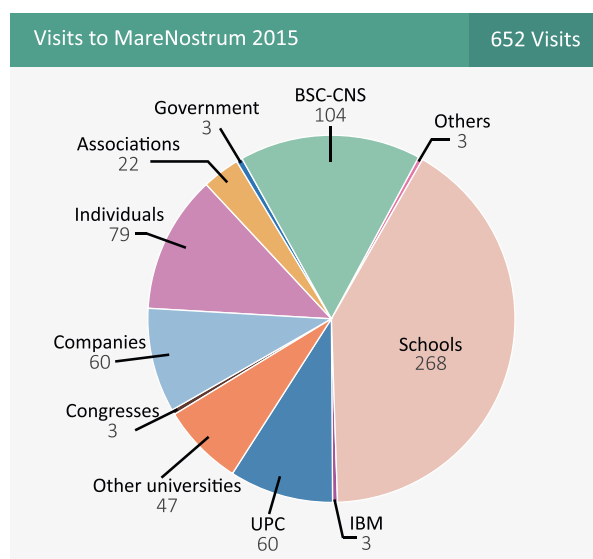
Communication Area

The 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 2015, BSC-CNS received a total of 10,052 visitors from national and international groups, including schools, universities, research centres, industry and non-profit organisations.

Visitors to the MareNostrum are given a tour of the supercomputer and a talk about the Centre, its technology and its research lines.
Most visits are tailored depending on the target audience and often incorporate videos and a visit to the BSC-CNS collection of "antique" supercomputers.

Visits to MareNostrum 2015	652 Visits

Government 3
BSC-CNS 104
Associations 22
Others 3
Individuals 79
Companies 60
Congresses 3
Other universities 47
Schools 268
UPC 60
IBM 3

BSC-CNS in the Media

BSC-CNS sent out 26 press releases in Spanish, Catalan and English, and identified 450 unique media impacts, all posted on the "BSC in the media" section of the BSC-CNS website. Efforts are made to promote and track BSC-CNS appearances in local, international, general, specialised, on and off line media.

Web and Social Media

In 2015, the Communication team invested considerable effort in strengthening BSC-CNS's web presence and social media networks. The website had more than 1,700,000 visits. 135 articles were published on the corporate website and 1000 posts were made on Facebook, Twitter and Linkedin.

The number of Facebook fans and Twitter followers increased by nearly 50%. The YouTube channel had more than 450 subscribers and more than 20,000 views in 2015 alone. BSC Folks, a new website for former employees of BSC-CNS, was also launched in collaboration with the Human Resources department.

Internal Communication

Three issues of the BSC-CNS Newsletter were published in 2015. The team also coordinated the development of the BSC-CNS social plan in collaboration with the HR department, provided support for Education & Training dissemination activities, organised the BSC-CNS 10th Anniversary event and disseminated information of interest for BSC-CNS staff internally.

Events, Seminars and Workshops

In 2015, BSC-CNS hosted and organised the following events:
- BDEC workshop, 28-30 January.
- ETP4HPC General Assembly, 5 March.
- Bull User group for eXtreme computing, 23-25 March
- 7th ICAP working group meeting, 16-19 June
- JLESC workshop, 29 Jun- 1 July.
- PUMPS Summer School, 6-10 July.
- FDL 2015, 14-16 September.
- WISE workshop, 20-22 October.

Participation in International Supercomputing Conferences

The Communications team prepared and supported the BSC-CNS presence at the exhibitions of the International Supercomputing Conference 2015 and SC15, and the exhibition of the SEG Annual Meeting, 18-23 October 2015.

Dissemination of European and National Projects

The Communications team also carried out BSC-CNS dissemination tasks for 31 European and National projects.

PRACE, Mont-Blanc, HiPEAC, EXDCI, HPC4E and RethinkBig were the projects with most dissemination time assigned in 2015.

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- Diego Caballero, ""SIMD@OpenMP: A Programming Model Approach to Leverage SIMD Features"", Supervised by: Xavier Martorell Bofill, Alejandro Duran González, 2015
- Javier Bueno, ""Run-time support for multi-level disjoint memory address spaces"", Supervised by: Xavier Martorell Bofill, 2015
- Javier Cabezas, ""On the programmability of multi-GPU computing systems"", Supervised by: Nacho Navarro, Wen-mei Hwu, 2015
- Jorge Ejarque, ""Semantic Resource Management and Interoperability between Distributed Computing"", Supervised by: Rosa M Badia, 2015
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- Judit Planas, ""Programming Models and Scheduling Techniques for Heterogeneous Architectures"", Supervised by: Eduard Ayguadé, Rosa M Badia, 2015
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- Lluc Álvarez, ""Transparent Management of Scratchpad Memories in Shared Memory Programming Models"", Supervised by: Xavier Martorell Bofill, Marc Casas, Miquel Moretó, 2015
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- Alba Cánovas, Rainer Zah, "Comparative Life-Cycle Assessment of Residential Heating Systems, Focused on Solid Oxide Fuel Cells", Sustainability in Energy and Buildings, 22, 659-668, 2015

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- Chloé Prodhomme, Francisco Doblas - Reyes, Omar Bellprat, "Understanding the 2003 and 2010 heat waves", Poster, Reading, UK, 2015

- D. Manubens, J. Vegas, F. Doblas-Reyes, "Autosubmit: a versatile tool to manage Weather and Climate Experiments in diverse Supercomputing Environments", Poster, Reading, UK, 2015

- D. Volpi, "Opportunities for seasonal forecasting application in fisheries", ICAWA conference, Dakar, Senegal, 2015

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- Eleftheria Exarchou, Chloé Prodhomme, Virginie Guemas, Francisco Doblas-Reyes, "Impact of the initialization with different ocean reanalysis on forecast bias", EC-Earth meeting (Poster), Reading, UK, 2015

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- F. Benincasa, "Dust forecast services", Amman, Jordan, 2015

- F. J. Doblas-Reyes, "Climate prediction in a user-driven context", Bergen, Norway, 2015

- F. J. Doblas-Reyes, "Polar-lower latitude linkages", Geneva, Switzerland, 2015

- F. J. Doblas-Reyes, "Seasonal-to-decadal forecasting with EC-Earth at IC3/BSC", EC-Earth meeting, Reading, UK, 2015

- F. J. Doblas-Reyes, "SPECS: Climate Predictions for Climate Services", 17th Meeting of the Working Group on Seasonal-to-Interannual Prediction, Norrköping, Sweden, 2015

- Francisco Doblas-Reyes, "Some comments from WGSIP", AGCI Workshop, Aspen, USA, 2015

- Francisco Javier Doblas-Reyes, "Weather, seasonal and decadal forecasts for the energy sector", Geneva, Switzerland, 2015

- Francisco Javier Doblas-Reyes, "What are the global impacts of Arctic climate changec ", Brussels, Belgium, 2015

- François Massonnet, Martin Vancoppenolle, Detelina Ivanova, Olivier Lecomte, Paul Hezel, Thierry Fichefet, "Process - oriented diagnostics in the polar regions . Part 1: Quantifying model complexity for the simulation of Arctic sea ice", EMBRACE/WCRP conference (Poster), Dubrovnik, Croatia, 2015

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- Miguel Castrillo, "CALIOPE Mobile. European Air Quality Forecast at hand", Open Geospatial Consortium Joint Session on Citizen GEOSS, Mexico, 2015
- Neven S. Fuckar, Virginie Guema, Matthieu Chevallier, Michael Sigmond, Felix Bunzel, Rym Msadek, Francisco J. Doblas-Reyes, "On the anatomy of the NH sea ice extent and impacts of different bias correction methods in a set of CMIP5 coupled climate models", Workshop on CMIP5 Model Analysis and Scientific Plans for CMIP6 (Poster), Dubrovnik, Croatia, 2015
- Neven S. Fuckar, Virginie Guemas, Nat C. Johnson, François Massonnet, Francisco J. Doblas-Reyes, "Determination of Arctic sea ice variability modes on interannual time scales via K-means cluster analysis", EGU meeting (poster), Vienna, Austria, 2015
- Oriol Tintó Prims, Miguel Castrillo, Harald Servat, Germán Llort, Kim Serradell, Oriol Mulla Valls, Francisco J. Doblas-Reyes, "Optimization of an ocean model using performance tools", CS15-Poster, Austin, US, 2015
- Oriol Tintó-Prims, Miguel Castrillo, Kim Serradell, Oriol Mula-Valls, Anna Cortés, Francisco J. Doblas-Reyes, Francisco Javier Doblas-Reyes, Jesús Labarta, "Understanding Scientific Application's Performance using BSC performance tools", International Conference on Computational Sciences, Reykjavik, 2015
- P.A. Bretonnière, A. Stephens, "SPECS data repositories: status and upload", SPECS 4th GA , Norrköping, Sweden, 2015

- R. Banks, J. M. Baldasano, "Impact of WRF PBL schemes on boundary-layer simulations using lidar, modelling, and observations during Spring 2015: Towards improvement of an air quality forecast system", Meteorology and Climate – Meteorological Aspects of Air Quality (MAC-MAQ) conference, Sacramento, USA, 2015
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- Sara Basart, "Dust prediction models", 1st Africa/Middle-East Expert Meeting and Workshop on the health impact of airborne dust, Amman, Jordan, 2015
- Sara Basart, Oriol Jorba, Carlos Pérez García-Pando, Catherine Prigent, J. M. Baldasano, "Modelling mineral dust emission over North Africa and Middle East using high-resolution surface properties from satellite retrievals", European Aerosol Conference (EAC2015) Poster, Milan, Italy, 2015
- T. Fichefet, H. Goosse, F. J. Doblas-Reyes, J. Baeseman, A. Bradley, François Massonne, T. Jung, "The Year of Polar Prediction", Frascati, Italy, 2015
- V. Torralba, F. J. Doblas-Reyes, M. Davis, N. González-Reviriego, "State-of-the-art seasonal forecasts for the wind energy sector", EUPORIAS General Assembly (Poster), Winterthur, Switzerland, 2015.

National Conferences

- Albert Soret, "Ciudades como centros de modelización científica ", Barcelona, 2015
- F. J. Doblas-Reyes, "El proyecto SPECS y la multidisciplinaridad en la investigación en servicios climáticos", Madrid, Spain, 2015
- F. J. Doblas-Reyes, "Impact of resolution and initialisation in climate seasonal predictions", 9th RES Users' Conference, Barcelona, Spain, 2015
- Francisco Doblas-Reyes, Melanie Davis, Verónica Torralba-Fernandez, Aida Pinto-Biescas, "Climate Services for energy ", Tortosa, Spain, 2015
- Francisco Javier Doblas-Reyes, "Climate information for the next 30 years ", Tortosa, Spain, 2015
- Francisco Javier Doblas-Reyes, "Climate prediction and climate services", Granada, Spain, 2015
- Francisco Javier Doblas-Reyes, "Framing climate services research", Tortosa, Spain, 2015
- Francisco Javier Doblas-Reyes, "How to predict future climates ", Barcelona, Spain, 2015
- Javier Vegas, Domingo Manubens, "Autosubmit: investigando el clima con Python", PyConES Python conference, Valencia, Spain, 2015
- Miguel Castrillo, Oriol Tintó-Prims, Harald Servat, Kim Serradell, George S. Markomanolis, "Applying clustering and folding techniques to study performance issues on the NEMO global ocean model", HPC Knowledge Meeting'15, University of Barcelona, Spain , 2015
- Oriol Tintó-Prims, Miguel Castrillo, Kim Serradell, Oriol Mula-Valls, Francisco J. Doblas-Reyes, Anna Cortés, "Entendiendo el rendimiento de aplicaciones científicas de clima", Jornadas Sarteco, Córdoba, 2015
- Virginie Guemas, "Ocean prediction activities at BSC-IC3", Barcelona, Spain, 2015

- Virginie Guemas, Francisco Javier Doblas-Reyes, "Climate prediction and climate services ", Barcelona, Spain, 2015.

PhD Theses

- Michele Spada, "Development and evaluation of an atmospheric aerosol module implemented within the NMMB/BSC Chemical Transport Model (NMMB/BSC-CTM)", Supervised by: Oriol Jorba Casellas, Jose M. Baldasano, 2015

Workshops

- C. Prodhomme, F. Doblas-Reyes, O. Bellprat, E. Dutra, "Predict and understand heat waves: A case study of summer 2003 and 2010", HEPEX workshop, Norrköping, Sweden, 2015
- C. Prodhomme, F. J. Doblas-Reyes, "Seasonal prediction of seasonal extremes ", Madrid, Spain, 2015
- F. J. Doblas-Reyes, "Predictability and prediction in the SPECS project", AGCI Workshop, Aspen, USA, 2015
- F. J. Doblas-Reyes, "Predicting climate extreme events in a user-driven context", WCRP Workshop on Understanding, Modelling and Predicting Weather and Climate Extremes, Oslo, Norway, 2015
- F. J. Doblas-Reyes, "WGSIP experience: Land, ocean, cryosphere initialization ", Paris, France, 2015
- Francisco Javier Doblas-Reyes, "Climate prediction for climate services", Offenbach, Germany, 2015
- Francisco Javier Doblas-Reyes, "Decadal predictability and prediction in a complex international context", CLIVAR-ICTP, Trieste, Italy, 2015
- Francisco Javier Doblas-Reyes, "Near-term predictions and projections as sources of climate information", C3S Climate Projections Workshop, Reading, UK, 2015
- J. García-Serrano, "Drivers of mid-latitude seasonal forecasts", Madrid, Spain, 2015
- J. García-Serrano, "Predictability of the Euro-Atlantic climate from Arctic sea-ice variability", WCRP Workshop on Understanding, Modelling and Predicting Weather and Climate Extremes, Oslo, Norway, 2015
- Miguel Castrillo, "CALIOPE Mobile. European Air Quality Forecast at hand", Workshop of Open Data projects cluster, Brussels, Belgium, 2015
- Miguel Castrillo, Oriol Tintó-Prims, Kim Serradell, "BSC tools to study the computational efficiency of EC-Earth components", EC-Earth Meeting, Reading, United Kingdom, 2015
- Miguel Castrillo, Oriol Tintó-Prims, Kim Serradell, "BSC tools to study the computational efficiency of EC-Earth components", JLESC Workshop, Barcelona, 2015
- Oriol Tintó-Prims, Miguel Castrillo, Kim Serradell, Oriol Mula-Valls, Anna Cortés, Francisco J. Doblas-Reyes, Francisco Javier Doblas-Reyes, Francisco Javier Doblas Reyes, Jesús Labarta, "Understanding Scientific Application's Performance", 2nd International BSC Doctoral Symposium, 2015
- Virginie Guemas, "Are we ready for hot and cold extremesc", Barcelona, Spain, 2015

Life Sciences 2015 Publications

Journals

- Albesa-Jové, David, Mendoza, Fernanda, Rodrigo-Unzueta, Ane, Gomollón-Bel, Fernando, Cifuente, Javier O, Urresti, Saioa, Comino, Natalia, Gomez, Hansel, Romero-García, Javier, Lluch, José M, Sancho-Vaello, Enea, Biarnés, Xevi, Planas, Antoni, Merino, Pedro, Masgrau, Laura, Guerin, Marcelo E, "A Native Ternary Complex Trapped in a Crystal Reveals the Catalytic Mechanism of a Retaining Glycosyltransferase", Angewandte Chemie International Edition , 54, 34, 9898-9902, 2015
- Alonso, Arnald, Domènech, Eugeni, Julià, Antonio, Panés, Julián, García-Sánchez, Valle, Mateu, Pilar Nos, Gutiérrez, Ana, Gomollón, Fernando, Mendoza, Juan L, García-Planella, Esther, Acosta, Manuel Barreiro-de, Muñoz, Fernando, Vera, Maribel, Saro, Cristina, Esteve, Maria, Andreu, Montserrat, Chaparro, María, Manyé, Josep, Cabré, Eduard, López-Lasanta, María, Tortosa, Raül, Gelpí, Josep Lluís, García-Montero, Andres C, Bertranpetit, Jaume, Absher, Devin, Myers, Richard, Marsal, Sara, Gisbert, Javier P, "Identification of Risk Loci for Crohn's Disease Phenotypes Using a Genome-wide Association Study.", Gastroenterology, 148, 4, 794-805, 2015
- Arcella, Annalisa, Dreyer, Jens, Ippoliti, Emiliano, Ivani, Ivan, Portella, Guillem, Gabelica, Valérie, Carloni, Paolo, Orozco, Modesto, "Structure and dynamics of oligonucleotides in the gas phase.", Angewandte Chemie International Edition, 54, 2, 467-471, 2015
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- Octavio Castillo, Josep de la Puente, Vladimir Puzyrev, José María Cela, "Edge-elements for geophysical electromagnetic problems: a new implementation challenge.", PRACEdays15 Conference, http://upcommons.upc.edu/handle/2117/85917, 2015
- Octavio Castillo, Josep de la Puente, Vladimir Puzyrev, José María Cela, "Parallel and numerical issues of the edge finite element method for 3D controlled-source electromagnetic surveys", Proceedings of the International Conference on Computing Systems and Telematics, 2015
- S. Futatani, J. A. Morales, W. J. T. Bos, "Dynamic equilibria and MHD instabilities in toroidal plasmas with non-uniform transport coefficients", Proceeding of 42nd European Physical Society Conference on Plasma Physics, Lisbon, Portugal, June 2015, 2015
- Samuel Rodriguez, Vladimir Puzyrev, Mauricio Hanzich, Santiago Fernandez, "Efficient sparse matrix-vector multiplication for geophysical electromagnetic codes on Xeon Phi coprocessors", Second EAGE Workshop on High Performance Computing for Upstream, Dubai, 2015
- Vladimir Puzyrev, Josep de la Puente, "Performance of Parallel Linear Solvers in Electromagnetic Geophysics", SIAM Conference on Mathematical and Computational issues in the Geosciences, Stanford, USA, 79-87, 2015
- Vladimir Puzyrev, Natalia Gutierrez, Juan Esteban Rodriguez, Mauricio Hanzich, Josep de la Puente, "Electromagnetic Modeling Using a Massively Parallel Software Framework", 77th EAGE Conference & Exhibition, Expanded Abstract, 2015
- Xavier Sáez, Alejandro Soba, Edilberto Sánchez, Mervi J. Mantsinen, José María Cela, "Performance analysis of a particle-in-cell plasma physics code on homogeneous and heterogeneous HPC systems", Proceedings of Congress on Numerical Methods in Engineering, Lisbon, Portugal, 43101, 2015
- Yevgeny Gruver, Vladimir Puzyrev, Josep de la Puente, "Improving Hankel transform filters for parallel electromagnetic modeling tools", 77th EAGE Conference & Exhibition, Expanded Abstract, We-P4-10, 2015
- Zavala-Ake, M, Mira, Daniel, Vázquez, Mariano, Houzeaux, Guillaume, "A Multiphysic implementation for conjugate heat transfer and compressible-low Mach coupling", The 18th International Conference on Finite Elements in Flow Problems, Taipei, Taiwan, 2015

National Conferences

- Xavier Sáez, Alejandro Soba, Mervi J. Mantsinen, "Plasma Physics Code Contribution to the Mont-Blanc Project", Book of abstracts of the 2nd BSC International Doctoral Symposium, Barcelona, Spain, 83–84, 2015

PhD Theses

- Chiara Scaini, "Modelling strategies for volcanic ash dispersal and management of impacts on civil aviation", Supervised by: Arnau Folch, 2015
- Cristóbal Samaniego, "Parallel Algorithms for Fluid and Rigid Body Interaction", Supervised by: Guillaume Houzeaux, Mariano Vazquez, 2015
- Raúl de la Cruz, "Leveraging Performance of 3D Finite Difference Schemes in Large Scientific Computing Simulations", Supervised by: José María Cela, 2015

Master Thesis

- Dani Gallart, , Mervi J. Mantsinen, , Yevgen Kazakov, "Computational Analysis of Ion Cyclotron Resonance Frequency Heating for DEMO", Supervised by: Mervi Mantsinen, 2015

Workshops

- Octavio Castillo, O. Castillo, Josep de la Puente, J. de la Puente, Vladimir Puzyrev, V. Puzyrev, J.M. Cela, "HPC and edge elements for geophysical electromagnetic problems: an overview", BSC Doctoral Symposium (2nd: 2015: Barcelona), 2015

Education and Training 2015 Publications

Journals

- Nia Alexandrov, V Alexandrov, "Computational Science Research Methods for Science Education at PG Level", Procedia Computer Science, 51, International Conference On Computational Science, ICCS 2015 – Computational Science at the Gates of Nature, 1685-1693, 2015

International Conferences

- Raul Ramirez-Velarde, Nia Alexandrov, Raul Perez-Cazares, "Mathematical Modelling Based Learning Strategy", Procedia Computer Science, , 51, Proceedings of ICCS'15 , 1694-1704, 2015

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 with a total capacity of 24 Pflop/s (including one at BSC-CNS) distributed across the continent, providing outstanding computing services to enable world-class research on world-class systems. The systems are installed at centres in France, Germany, Italy and Spain. Through PRACE, scientists and technologists from Europe and around the world are provided access to world-class supercomputers with capabilities comparable to those available in the USA and Japan. These leadership class systems help the continent's scientists and engineers to remain internationally competitive.

BSC-CNS played a key role in the creation of the PRACE Research Infrastructure at all levels, with Sergi Girona serving as Chairman of the Board of Directors, significant technical contributions, and leadership of the organisational design.

BSC-CNS and PRACE

In 2015, BSC-CNS secured a commitment from the Spanish Ministry of Economy and Competitiveness (MINECO) to invest 34 million euros to upgrade the MareNostrum supercomputer. This upgrade will allow BSC-CNS and Spain to continue participating in PRACE at the highest possible level.

BSC-CNS is one of the six selected PRACE Advanced wTraining Centres (PATC) and conducted 15 PATC training activities in 2015, and was ranked amongst the best performing PATC centres according to quality assessment and user feedback.

In the 4th PRACE Implementation Project, run during 2015, BSC-CNS continued many of the PRACE 1st to 3rd implementation phase activities on organisational aspects, community code enabling support, and best practice for HPC system commissioning.

PRACE Summer of HPC Training Week 2015 hosted by BSC

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

The 2015 3rd edition of the Summer of HPC started with a training week hosted by BSC-CNS. A total of 24 European undergraduates and early stage postgraduate students participated. Two of these students were then hosted by BSC-CNS and trained in data visualisation applied to scientific and HPC environments, as well as data and imaging streaming technologies.

Spanish participation in PRACE

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

Some of the projects with Spanish participation are:

- *Direct Numerical Simulation of Equilibrium Adverse Pressure Gradient Turbulent Boundary Layers, Prof. Javier Jiménez Sendín (UPM), 17 million hours on SuperMUC@LRZ@GCS*
- *Large-scale radiation damage cascades from first principles, Prof. Emilio Artacho (CIC nanoGUNE), 36 million hours on Hermit@HLRS@GCS*
- *INFLUM2 - Effects of selective mutations on the ligand binding and unbinding to the M2 proton channel of influenza virus, Prof F. Javier Luque (UB), 22 million hours on MareNostrum@BSC*
- *NEMERTE - Numerical Experiment on the Mediterranean model response to Enhanced Resolution and TidE, with the participation of IMEDEA, 17 million hours on Fermi@CINECA*
- *Identification of somatic variations in PanCancer genomes using SMUFIN, a reference-free approach, Prof. David Torrents, 6 million hours on MareNostrum@BSC*
- *DNA crystal simulations: a step towards the understanding of the crowded cellular environment, Prof. Modesto Orozco (IRB), 22 Million hours on MareNostrum@BSC*
- *EXCOMM - EXtreme scale domain decomposition solvers for COMputational Mechanics, Prof. Santiago Badia (CIMNE-UPC), 10 million hours on Fermi@CINECA*
- *COMPHOTOCAT - Computational design of TiO2 based nanoparticles for improved photocatalytic activity towards water splitting under visible sunlight, Prof. Francesc Illas (UB) 62 million hours on MareNostrum@BSC*
- *SANDGRAIN - UnderStANDing the effects of wall-surface rouGhness on the flow past ciRculAr cylINders, Prof. Assensio Oliva (UPC), 31 million hours in Fermi@CINECA*
- *EBAPAM - Emergent behavior and active patterns in active materials, Prof. Ignacio Pagonabarraga (UB), 22 million core hours in MareNostrum@BSC*
- *Charge and Spin Hall Kubo Conductivity by Order N Real Space Methods, Prof. Stephan Roche (ICN), 20 million hours in MareNostrum@BSC*

# Minimal Composite Higgs

Leader Name: Claudio Pica
Leader Institution: CP3-Origins, IMADA, U. of Southern Denmark

Names and affiliations of the project participants:

- Francesco Sannino, CP3-Origins, FKF, U. of Southern Denmark
- Ari Hietanen, CP3-Origins, IMADA, U. of Southern Denmark
- Michele Della Morte, CP3-Origins, IMADA, U. of Southern Denmark
- Rudy Arthur, CP3-Origins, IMADA, U. of Southern Denmark
- Vicent Drach, CP3-Origins, IMADA, U. of Southern Denmark
- Martin Hansen, CP3-Origins, IMADA, U. of Southern Denmark

Summary of activity:

The project focuses on the minimal realisation of two popular proposals for beyond Standard Model (BSM) physics in which the Higgs boson is in a composite state: Technicolor and the so-called "composite Higgs" models. The simplest realisation is based on the SU(2) gauge theory with 2 Dirac fermions in the fundamental representation. A Higgs-like state is present in the model which, depending on how the model is embedded in the SM Electroweak sector, can be either the Technicolor scalar state or the extra Goldstone bosons or a
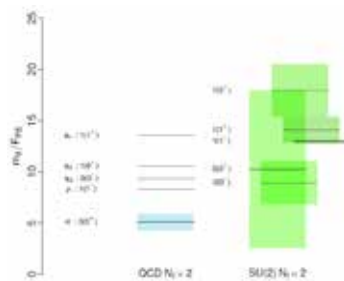
Summary of the spectrum and comparison with QCD.

mix of these two possibilities. Numerical simulations were used to understand the spectrum quantitatively by Lattice Gauge Theory.

Description of the results and benefits derived from the use of supercomputing:

Results include: the first measure of the lattice spacing for the numerical simulations with high accuracy needed for an accurate continuum extrapolation of all the following results; for the first time, the necessary non-perturbative renormalization constants (RI'-MOM scheme) were determined; a reliable continuum estimate of the low energy constants related to chiral symmetry breaking, such as the pion decay and chiral condensate; and a reliable continuum estimate of the lightest vector resonances in the model.

MareNostrum is particularly well suited for these large simulations, as the machine is perfectly tuned for large job sizes. On a related note, user support at BSC-CNS is outstanding.

List of publications:

- "SU(2) Gauge Theory with Two Fundamental Flavours: a Minimal Template for Model Building", Rudy Arthur et al. arXiv:1602.06559 [hep-lat]. (submitted)
- "Template Composite Dark Matter : SU(2) gauge theory with 2 fundamental flavours", Vincent Drach, et al. arXiv:1511.04370 [hep-lat]. Proceedings of the 33rd International Symposium on Lattice Field Theory.

High Resolution Ensemble Climate Modelling (HiResClim II)

Leader Name: Francisco J. Doblas-Reyes
Leader Institution: IC3/BSC

Names and affiliations of the project participants:
- Sophie Valcke (CERFACS)
- Klaus Wyser (SMHI)
- Wilco Hazeleger (KNMI).

Summary of activity:

HiResClim aims to make major advances in the science of estimating climate change and formulating climate predictions, by addressing the dual requirements of increased climate model resolution and increased number of ensemble realisations of future climate conditions over a range of time scales and for a set of plausible socio-economic development pathways. The project considered two state-of-the-art coupled models, EC-Earth and ARPEGE-NEMO HR. IMAGES ILLUSTRATING THE RESULTS OBTAINED:
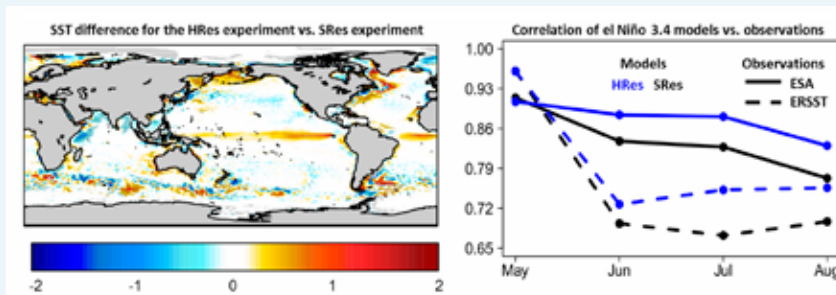
The figure shows how the results of the summer hindcast performed with EC-Earth 3.0.1 coupled model differ by the resolution used. The map highlights the differences between the Standard resolution (SRes, ~1º in the ocean and ~70km in the atmosphere) and the High Resolution simulation (HRes, ~0.25º in the ocean and ~40km in the atmosphere). The plot shows how the skill of the HRes simulation is systematically higher than SRes in the Niño 3.4 region. (Prodhomme et al., Journal of Climate, under review).

Description of the results and benefits derived from the use of supercomputing:

The spin-up, pre-industrial climate simulations encountered technical problems and the lack of stability of the EC-Earth model prevented EC-Earth from completing a pre-industrial run. The high-resolution predictions made in the project have been compared to lower resolution predictions performed using national HPC allocations. Results for the decadal and seasonal integrations showed differing improvements in

predictions for precipitation, arctic sea ice, sea surface temperature and other variable, that largely justify the cost of the resolution increase.

List of publications:

- "Decadal prediction with a high resolution model", Monerie, et al. (Submitted)
- "Benefits of resolution increase for seasonal forecast quality in EC-Earth", Prodhomme, et al. (Submitted)

Unraveling the effects of selective mutations on the ligand binding and unbinding to the M2 proton channel of influenza virus INFLUM2

Leader Name: F. Javier Luque
Leader Institution: University of Barcelona (Spain)

Names and affiliations of the project participants:
- Jordi Juárez-Jiménez, University of Barcelona (Spain)
- Salomé Llabrés, University of Barcelona (Spain)
- M. Massetti, University of Bologna (Italy)
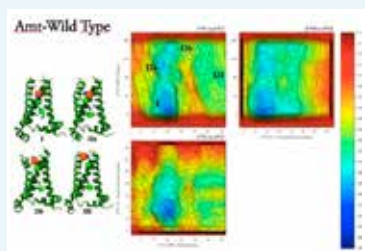- A. Cavalli, University of Bologna (Italy)

Summary of activity:

The M2 proton channel of influenza A virus is an integral membrane involved in the acidification of the viral interior, a step necessary for the release of the viral genetic material.

This project investigated the binding mode of amantadine to the wild type M2 channel and its V27A mutated variant using extended molecular dynamics simulations in conjunction with multiple-walker metadynamics.

Figure 1. Free energy surface for the acces of amantadine to the wild type M2 channel. Representative structures at selected points are also shown.

Description of the results and benefits derived from the use of supercomputing:

The results led to a proposal of a mechanism for the binding/unbinding of amantadine to the wild-type M2 channel, which involves the adoption of two distinct binding modes. Furthermore, the results showed that the relative stability of the binding modes and the barrier for ligand exchange between them is very sensitive to mutations in the channel. The results provide a basis to explain the differences in inhibitory potency of amantadine toward wild type and V27A M2 channels. This information will be valuable for the design of novel inhibitors for different M2 channels.

List of publications:

- "New polycyclic dual inhibitors of the wild typa and the V27A mutant M2 channel of the influenza A virus with unexpected binding mode", Matias Rey-Carrizo, et al. European Journal of Medicinal Chemistry 2015, 96, 318-329.
- "On the Binding Mechanism of Amantadine to the M2 Proton Channel", Salomé Llabrés, et al. (Submitted)

Multi-scale simulations of Cosmic Reionization

Leader Name: Ilian T. Iliev
Leader Institution: Astronomy Centre, Department of Physics & Astronomy, Pevensey II Building, University of Sussex, Falmer, Brighton BN1 9QH, United Kingdom

Names and affiliations of the project participants:

- Hannah Ross
- David Sullivan
- Peter Thomas
- Kyungjin Ahn
- Romain Teyssier
- Garrelt Mellema
- Dominique Aubert
- Pierre Ocvirk
- Paul Shapiro
- Hyunbae Park
- Jun-Hwan Choi
- Anson D'Aloisio
- Karl Joakim Rosdahl

Summary of activity:

Understanding the nature of the first galaxies and how they affect the progress, duration and observational signatures of cosmic reionization requires detailed modelling of complex interactions. The aim of this project is to combine a unique set of simulations of cosmic reionization covering the full range of relevant scales, from very small, sub-galactic scales, for studying the detailed physics of radiative feedback, all the way to very large cosmological volumes at which the direct observations will be performed.
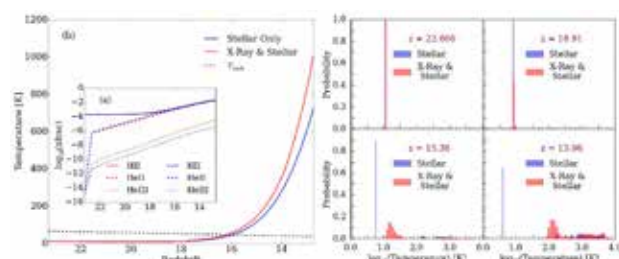

Figure 1. (left panels) The volume-weighted mean temperature evolution vs. redshift for stellar-only sources (blue) and stellar and X-ray sources (red). (inset) Ionised fraction evolution for each of species (as labelled) is shown, using the same colour notation. (right panels) Histograms of the temperature at several stages of the evolution, as labelled, showing the different heating profiles of the intergalactic medium.

Description of the results and benefits derived from the use of supercomputing:

Comprehensive results were obtained on the radiative feedback effects on small scales, on the early inhomogeneous X-ray background and its corresponding heating of the neutral intergalactic medium, and some results on the other processes that affect the formation of the first stars and galaxies. These results will be used to provide sub-grid models for the ionizing sources and small-scale structures, and applied in large-scale simulations to study the progress of reionization and derive a variety of expected observational signatures. Such work is critical in preparating for future large experiments like the Square Kilometer Array, James Webb Space Telescope, Euclid Observatory and others, and for reliable interpretation of their results. Using large-scale computing resources like PRACE is invaluable in enabling such science.

Ensemble-based approach for global ocean forecasting (ENS4OCEAN)

Leader Name: Simona Masina
Leader Institution: Centro Euro-Mediterraneo sui Cambiamenti Climatici (CMCC), Italy (Spain)

Names and affiliations of the project participants:
- J Andrea Storto
- Dorotea Iovino
- Giovanni Aloisio
- Italo Epicoco
- Pier Giuseppe Fogli
- Silvia Mocavero

Summary of activity:

With the goal of developing a realistic global eddying ocean/sea-ice system, CMCC implemented GLOB16, the highest spatial resolution implemented to date in a global domain within the NEMO modeling framework. The project produced the first numerical hindcast covering the Argo period, 2003-onwards, creating a reference simulation for oceanic process studies at very fine resolution, enabling:

- detailed analysis of the main ocean/sea ice processes in a large range of spatial scales and at time scales from few-days to decade,
- detailed investigation of the capability of the model components (ocean and sea-ice) to accurately represent small-scale physical processes.
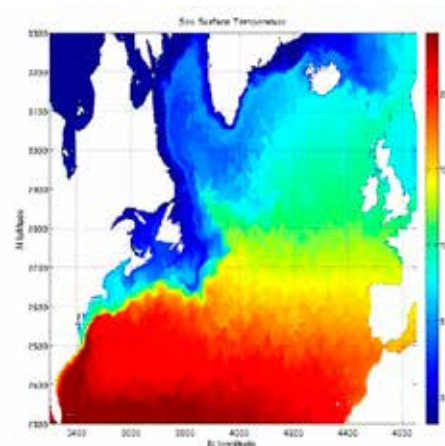
Description of the results and benefits derived from the use of supercomputing:

The simulation confirms that high resolution is required to resolve narrow boundary currents and energetic mesoscale eddies, which are ubiquitous in the world ocean, and high-resolution global simulations add value compared to regional models, because eddies and unstable jets can transfer eddy energy across ocean basins and from one basin to the adjacent ones. GLOB16 provides a unique opportunity to investigate the variability of the Atlantic Meridional Overturning Circulation (AMOC), which plays a major role in the North Atlantic heat budget.

Due to the high computational cost and the huge amount of data produced, this research would have been almost impossible without PRACE supercomputer infrastructure

Sea surface temperature (in °C) in a sector of the Atlantic Ocean, averaged in the period 27th – 31st December 2013.

Influence of the Injector Geometry on Primary Breakup Modelling

Leader Name: Heinz Pitsch
Leader Institution: Institute for Combustion Technology, RWTH Aachen University

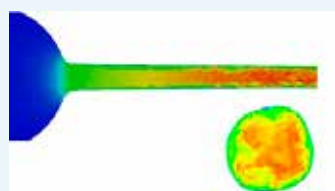Names and affiliations of the project participants:
- Mathis Bode, Institute for Combustion Technology, RWTH Aachen University

Summary of activity:

A variety of flows encountered in industrial configurations involve liquid and gas. Systems to atomize liquid fuels, such as diesel injection systems, are one example. The performance of a particular technical design depends on a cascade of physical processes, originating from the nozzle internal flow, potential cavitation, turbulence, and the mixing of a coherent liquid stream with a gaseous ambient environment. This mixing stage is critical, however, how design parameters influence surface density and ultimately drop size distribution is not clear, and predictive models do not exist. This is partly caused by the complexity of the process and the difficulties of performing experiments characterizing the atomization process. Therefore, this project addresses the understanding and accurate modeling of the effect of the injector geometry on the primary breakup in turbulent spray formation.

Description of the results and benefits derived from the use of supercomputing:

Several simulations with respect to the Spray A case specified by the Engine Combustion Network were performed with the high-fidelity scientific code CIAO. Two different Reynolds numbers and two different geometries (pipe and exact) were considered. The nozzle inflow simulations were analyzed with respect to the velocity profile, velocity fluctuations and generated turbulent kinetic energy at the nozzle exit. One

Instantaneous velocity field of simulation with exact Spray A geometry and realistic Reynolds number.

result was the smaller amount of turbulent kinetic energy in the simulation with exact injector geometry compared to the one with generic pipe geometry. Although the post-processing is not complete, first data was presented at the Engine Combustion Network Workshop 3 and shared with other modeling groups so they can benefit from the unique quality of the data. Without the access to PRACE computing resources, simulations with the performed resolution would not have been possible.

List of publications:

- M. Bode et al., "A New Euler/Lagrange Approach for Multiphase Simulations of a Multi-Hole GDI Injector," SAE Technical Paper 2015-01-0949, 2015, doi:10.4271/2015-01-0949.
- M. Bode et al., "Numerical study of the impact of cavitation on the spray processes during gasoline direct injection," ICLASS 2015, 13th Triennial International Conference on Liquid Atomization and Spray Systems, Tainan, Taiwan, 2015.
- M. Bode et al., "Direct numerical simulations of novel biofuels for predicting spray characteristics," ICLASS 2015, 13th Triennial International Conference on Liquid Atomization and Spray Systems, Tainan, Taiwan, 2015.
- Internal Flow Modeling Presentation, Engine Combustion Network 4rd Workshop, Kyoto, Japan, 2015.

Atomistic simulations of heterogeneous media on the Intel Xeon Phi

Leader Name: Daniele Coslovich
Leader Institution: Université de MontPellier, France

Names and affiliations of the project participants:
- Dwigth Smite

Summary of activity:

The goal of the project was to develop a molecular dynamics code able to simulate large-scale heterogeneous materials, such as porous media. The code was meant to perform well on multi- and many-core architectures, such as Intel Xeon Phi co-processors. The code was developed in Fortran 90 using OpenMP for parallelisation, with particular attention to achieve vectorisation of the main loops in order to exploit the vector capabilities of the Intel Xeon Phi. The results show that the code scales reasonably well on both Xeon and Xeon Phi architectures for large system sizes. However, despite the efforts, performance on the Intel Xeon Phi remains inferior, in absolute terms, to that on conventional multi-core Intel Xeon. The conclusion is that more aggressive optimisations are needed to harvest the computing power of the Intel Xeon Phi for this specific application.

List of publications:

- Dynamique moléculaire sur architecture SIMD. Dwight Smite, Master thesis, Universite Montpellier 2
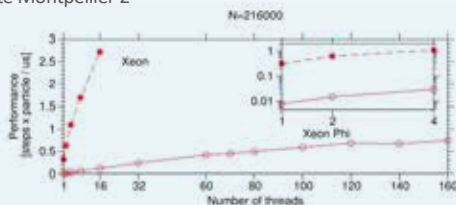
Description of the results and benefits derived from the use of supercomputing:

The molecular dynamics code (mdpar) developed during this preparatory access PRACE project on Marenostrum is distributed under the GNU general public license and is available at https://gitlab.info-ufr.univ-montp2.fr/daniele.coslovich/mdpar

The code can simulate simple systems (fluids, solids) based on Lennard-Jones interactions but generalisation to different forcefields would be straightforward. The code is particularly well suited to simulate heterogeneous large-scale materials. For large systems the parallel efficiency is good (>75%) up to 16 cores on the Intel Xeon and up to 60 threads on the Intel Xeon Phi.

Although the main goal of the project was achieved, despite efforts to vectorise and fully parallelise the code, the performance on the Intel Phi remains below expectations as it corresponds approximately to that of 4 cores of a standard Xeon node. Thus, at least for this specific application, optimisation on the Intel Xeon Phi still requires a substantial investment in developer time.

The computing facilities at Marenostrum enabled the code to be developed and tested directly on Intel Xeon Phi. These co-processors are still relatively expensive, "niche" products even within the HPC world and it is not easy to find clusters that feature them. Their availability on Marenostrum was the main enabling factor for this project.

Three-Dimensional Simulations of Core-Collapse Supernova Explosions of Massive Stars Applying Neutrino Hydrodynamics

Leader Name: Hans-Thomas Janka
Leader Institution: Max Planck Institute for Astrophysics (MPA)

Names and affiliations of the project participants:
- Alexander Summa, Max Planck Institute for Astrophysics (MPA)
- Tobias Melson, Max Planck Institute for Astrophysics (MPA)
- Andreas Marek, Max Planck Computing and Data Facility (MPCDF) University

Summary of activity:

The project is concerned with a problem of fundamental importance in stellar astrophysics: Why and how do massive stars explode at the end of their lives as so-called supernovae? Supernovae are the brightest and most powerful explosions in the universe. With the computer time granted by PRACE on MareNostrum, for the first time successful model calculations of the complex and extremely complicated physical processes that lead to supernova explosions were achieved. It was demonstrated that neutrinos (weakly interacting, nearly massless elementary particles, of which huge numbers are created in the supernova core by interactions of energetic particles) may initiate the explosion. These computer simulations thus bring us considerably closer to the solution of a 50 year old astrophysics problem.

Description of the results and benefits derived from the use of supercomputing:

The successful computations of supernova explosions on MareNostrum provide further theoretical support of the long-standing theory that neutrinos radiated from the innermost core of a dying star are responsible for the spectacular explosive ejection of the outer stellar layers with velocities up to 10 percent of the speed of light.

This theoretical concept is not yet proven. A major problem is that the physical conditions in the center of exploding stars are too extreme to explore all relevant physical processes by laboratory experiments. Moreover, the innermost regions of a supernova are inaccessible by direct observations with telescopes, because the "heart" of a dying star is obscured by many solar masses of dense, opaque matter. Only neutrinos and gravitational waves can bring information directly from the center of the exploding star. The computer simulations on MareNostrum are crucial for most precise predictions of the neutrino bursts and gravitational waves that can be expected in future observations of supernovae.

List of publications:

- Melson T. et al., "Neutrino-driven supernova of a low-mass iron-core progenitor boosted by three-dimensional turbulent convection", Astrophys. Journal Letters 801, L24 (2015); arXiv:1501.01961
- Melson T. et al., "Neutrino-driven explosion of a 20 solar-mass star in three dimensions enabled by strange-quark contributions to neutrino-nucleon scattering", Astrophys. Journal Letters 808, L42 (2015); arXiv:1504.07631
- Summa A. et al., "Progenitor-dependent explosion dynamics in self-consistent, axisymmetric simulations of neutrino-driven core-collapse supernovae", Astrophys. Journal, submitted (2015), arXiv:1511.07871

Identification of somatic variations in Pan-cancer genomes using SMUFIN, a reference-free approach

Leader Name: David Torrents
Leader Institution: Joint BSC-CRG-IRB Research Programme in Computational Biology, Barcelona Supercomputing Center (BSC-CNS)

Names and affiliations of the project participants:
- Santiago Gonzalez
- Montserrat Puiggròs

Summary of activity:

The analysis of genomic DNA is a key step in any study related to genetic diseases. BSC-CNS is developing and applying tools for the analysis of genome sequences in the context of cancer genomics. In particular, the SMUFIN tool for identification of somatic variation in cancer genomes. This PRACE project analysed more than 2000 complete genomes derived from more than 20 types of cancer types. The results of this analysis are now being interrogated in by several research groups to answer specific questions regarding the formation and progression of tumors.
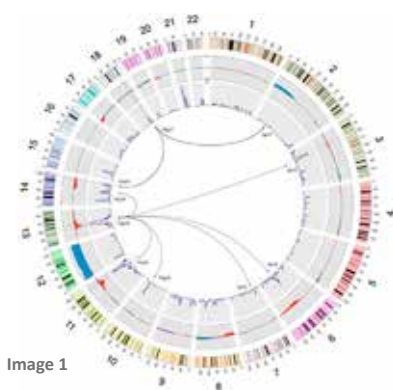

Image 1

Description of the results and benefits derived from the use of supercomputing:

The use of PRACE HPC resources at BSC-CNS enabled an extensive analysis of genomic variation in cancer that aids in the understanding of tumor biology. In the context of the ICGC-CLL consortium, 148 whole genomes from CLL patients were analysed using SMUFIN and the somatic variation associated with genome structure was characterised. In particular, chromosome translocations and catastrophic events reorganizing tumor chromosomes, such as chromoplexy and chromotripsis. Regions in the genome that are recurrently rearranged in CLL were identified, pointing to events that impact on pathology, such as time to treatment. This analysis also allowed reconstruction of a complex karyotype, which is the result of chromoplexy and chromothripsis occurring in the same tumor. This work was published in Nature (Puente et al, Nature 2015).

In addition to this activity, the PRACE supercomputer was to identify mutations in more than 2500 PanCancer genomes. All these samples were analysed using SMUFIN and the results are currently being interpreted in order to identify mutational patterns associated with tumor formation and progression. In addition to providing information on the underlying molecular basis of cancer, the mutation set generated with SMUFIN is a valuable resource for further studies of cancer genetics.

List of publications:

Xose S. Puente, et al. Non-coding recurrent mutations in chronic lymphocytic leukaemia. Nature 2015; doi:10.1038/nature14666

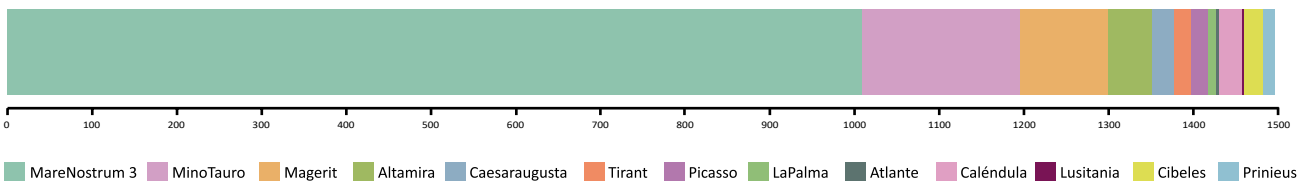Location of the nodes of the Spanish Supercomputing Network (RES)

RES

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

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.

In March 2015, the Spanish Supercomputing Network (RES) signed a new Agreement that integrates the existing nodes with five new ones, which are: Centro de Supercomputación de Galicia (CESGA), Fundación Centro de Supercomputación de Castilla y León (FCSCL), Consorci de Serveis Universitaris de Catalunya (CSUC), Universidad Autónoma de Madrid (UAM), and Fundación Computación y Tecnologías Avanzadas de Extremadura (COMPUTAEX).

With the incorporation of these new members, the RES now comprises a total of 13 nodes. BSC-CNS continues its role as the main node and manager of the network, while the governing Council (in which all the nodes are represented) provides overall governance.

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.


MareNostrum 3 ▪ MinoTauro ▪ Magerit ▪ Altamira ▪ Caesaraugusta ▪ Tirant ▪ Picasso ▪ LaPalma ▪ Atlante ▪ Caléndula ▪ Lusitania ▪ Cibeles ▪ Prinieus

The objetives of the RES are:

1. To provide unified and optimal services to the users of supercomputation for R&D in Spain by applying homogeneous criteria for access to these services.
2. To provide specific services of calculation, support and other associated services in the field of supercomputation for projects with and for industry.
3. To improve efficacy, sharing and performance of the resources available in the network (calculation, storage, parallelisation, etc.) with the aim of optimising resources and gaining added value for the nodes.
4. To jointly manage the shared resources: monitoring of systems, queue management, register of performance, evaluation indicators, support to parallelisation, usage of HPC in industry, assessment and industrial partnership, among others.

5. To promote and execute actions of common interest for the entities that own the nodes, by means of common plans such as:
   - Training and dissemination and divulgation.
   - Elaboration and presentation of projects.
   - Mobility of researchers and technicians between nodes.
   - Other actions of common interest.
6. To respond to evaluation assessments requested by the Spanish Ministry as well as to participate in any initiatives that might be requested either at national or international level.
7. Any other actions that may boost the use of supercomputing in R&D in Spain.
8. To meet all organisational, structural and technical requirements to be certified as a national distributed ICTS (Singular Scientific-Technological Infrastructure) of distributed character.

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

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

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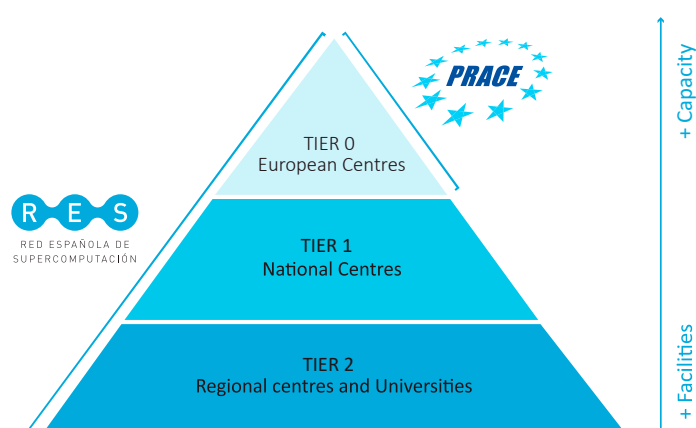
Access protocol and allocations in the RES

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

The Expert Panels
• Astronomy, Space and Earth Sciences
• Life and Health Sciences
• Mathematics, Physics and Engineering
• Chemistry and Materials Science and Technology

Each panel is composed of a coordinator, an assistant, and eight reviewers.

Access Committee Core Team
• Francisco Herrada, MINECO.
• Julio Bravo, ANEP.
• Alfonso Tarancón, BIFI-Universidad de Zaragoza.
• Jordi Torres, BSC-CNS.

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

More than 119.5 million hours were awarded by the Access Committee in the 3 calls for applications that took place during 2015. In addition to internal research activities of the RES nodes, more than 124 external research projects made use of the RES system in 2015.

It is important to note that many scientific projects often request several periods of access during the year (each access lasts 4 months) in order to perform different work activities. As specified in the Access Protocol, each request is treated separately and must pass the evaluation procedure of the Access Committee. Consequently, the number of activities reported by the RES is higher than the number of projects registered for the year.

Access requests and usage of RES resources

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

The chart below shows the evolution of requested, awarded and consumed TFLOP since the RES was founded in 2006. It clearly shows that demand is consistently higher than the resources offered, and that all capacity upgrades are quickly absorbed, as can be clearly seen during the first and second MareNostrum upgrades in 2008 and 2013.

Access requests and usage of RES resources
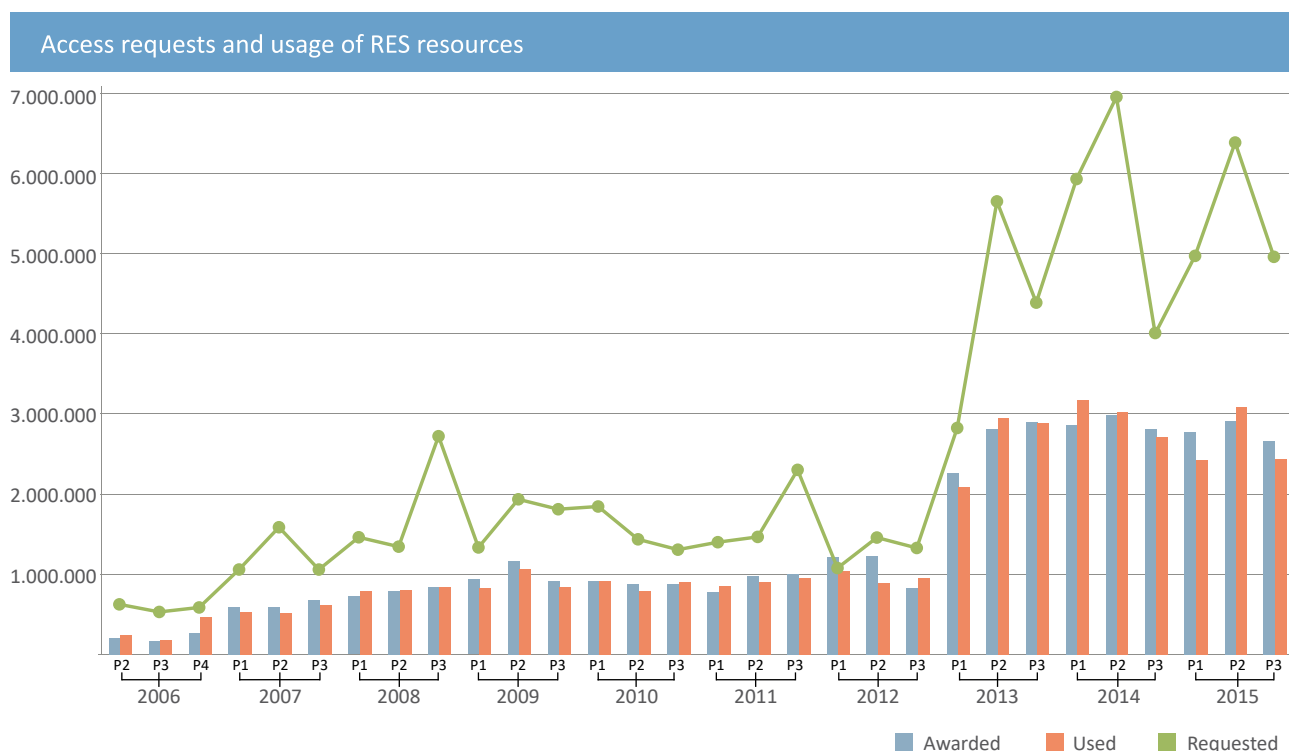
CURES, the RES Users Committee

CURES Members

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

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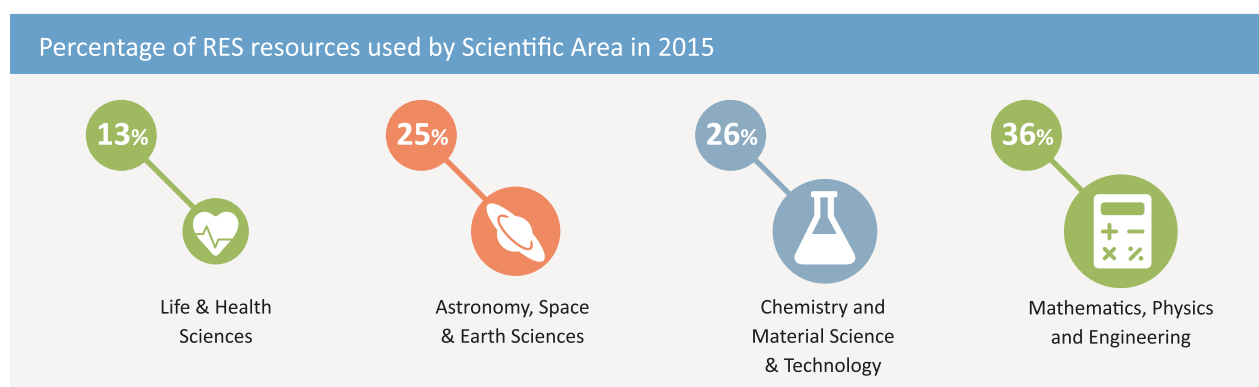
CURES aims to promote the effective use of the facilities by sharing information on experiences in using the different systems, suggesting new research and technology directions in scientific computing and, above all, voicing user concerns.

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

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

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.

Percentage of RES resources used by Scientific Area in 2015

13%	25%	26%	36%
Life & Health Sciences	Astronomy, Space & Earth Sciences	Chemistry and Material Science & Technology	Mathematics, Physics and Engineering

The different research activities carried out on RES supercomputers during 2015 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.

9th RES Users Conference

The 9th RES Users Conference took place on the 23rd September 2015 in Barcelona, Spain.

The goal of the meeting was to promote available resources and services, to explain procedures for requesting time and reviewing of proposals, to disseminate the results obtained using the RES, and to offer a discussion forum among users, the CURES, and RES coordinators.

Five different sessions were held: Resources and services offered by the RES and PRACE; The challenge of using PRACE supercomputer; Effects of Science on the society wellbeing; Increasing the knowledge on Earth and Cosmology Sciences; and Industrial applications and fundamental research.

Planned to coincide with the Users Conference, the 4th Annual HPC Advisory Council Spain Conference was held the next day, co-organised by BSC-CNS and the HPC Advisory Council, a network of experts from some of the leading global HPC companies.

Further information at: www.bsc.es/res-and-hpcac-2015

The Magerit Supercomputer

CeSViMa (Centro de Supercomputación y Visualización de Madrid) is located in the Campus de Excelencia Internacional de Montegancedo, one of the sites of the Parque Científico y Tecnológico de la Universidad Politécnica de Madrid (UPM). CeSViMa, which is a member of the Red Española de Supercomputación (RES), Red Española de e-Ciencia (Spanish Network of e-Science) and Red de Laboratorios e Infraestructuras de la Comunidad de Madrid (Laboratory and Infrastructures Network of Madrid), focuses on three main objectives:

- High Performance Computing
- Advanced Interactive Visualisation
- Massive Storage

CeSViMa's supercomputer is called Magerit (the ancient recorded name of Madrid). The current second generation of this supercomputer is a cluster of 245 nodes PS702, that provides 3920 cores and 200 TB of storage inter-connected by a very high bandwidth switch. The nodes are interconnected with a high bandwidth and low latency infiniband network.

Organisational Structure
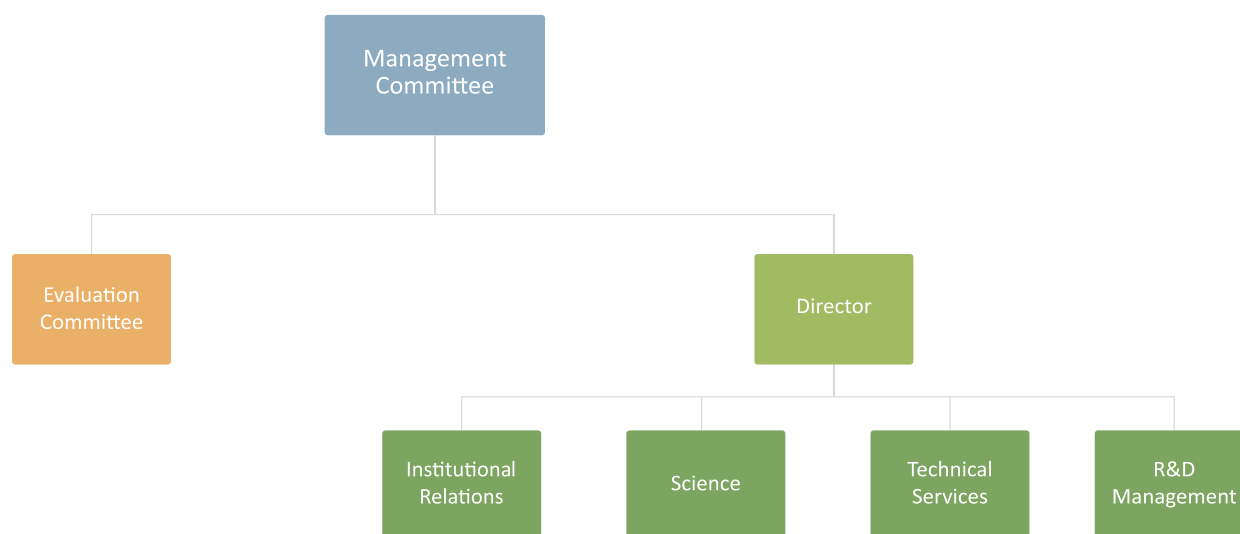
Technical Performance 2015

In 2015, UPM reserved 6.867.840 hours for RES projects on Magerit. The RES assigned 5.602.000 hours to 20 groups that used a total of 6.178.903 hours (89.97% of the reservation).

Training and Other Activities 2015

During 2015, 21 guided visits of the Magerit supercomputer were conducted involving some 850 visitors.

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%. Installed in a controlled environment room of 32 square meters, the supercomputer has two terabytes of principal memory in addition to its 38.5 TB of hard disk data storage.

Organisational Structure

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

The IAC IT support team is responsible for administration and management of the supercomputer node, with one engineer dedicated full-time to fulfil these functions.
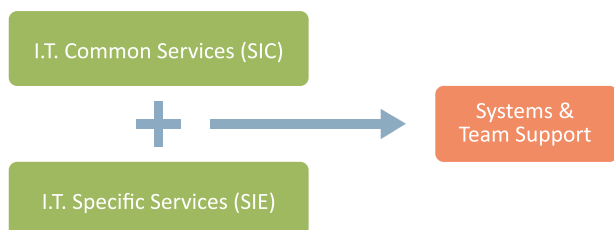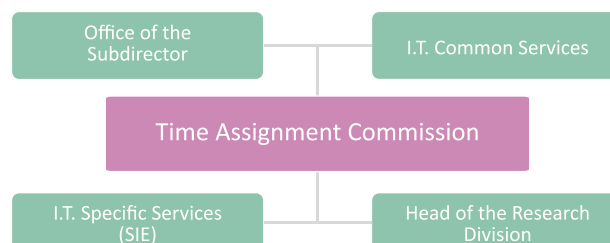
The LaPalma Supercomputer Systems & Support Team:
Antonio Jiménez Mancebo (PhD), Head of the I.T. Common Services (SIC); Carlos Martín Galán (Senior Engineer), Technician Responsible of SIC; Antonio Díaz Chinea (Senior Engineer), System Administrator; Justo Luna López (Engineer), System Administrator; Ubay Dorta Guerra (Engineer), System Administrator and UserSupport; Antonio Dorta Lorenzo (PhD), User Support; Victor Plasencia Darias (Operator), User Support.

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

Technical Performance 2015

In 2015 LaPalma provided more than 3.4 million of CPU hours to RES users. The consumed time represented the 85% of the available time.

Training and Other Activities 2015

In December a group of students from Eusebio Barreto Lorenzo Secondary School (Los Llanos de Aridane, La Palma) visited the LaPalma Supercomputer facilities. They were introduced to supercomputing concepts and its importance not only for science but also for our daily lives.

The Atlante Supercomputer
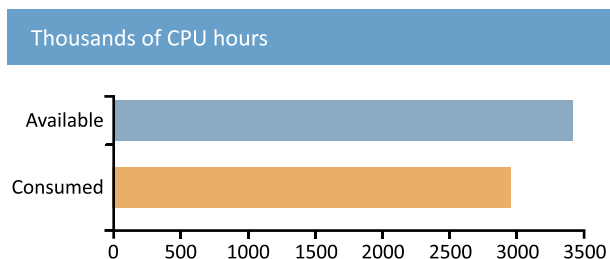
Atlante supercomputer joined the RES on February 16th 2009, becoming its 8th member and the 2nd member from the Canary Islands. It is managed by Instituto Tecnológico de Canarias (ITC), a public company of the Canary Islands Regional Government, that promotes industrial development of the region, fostering 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. and offers 96TB of storage disk.

Organisational Structure

Mª Belén Esteban Sánchez
(System Administrator and User Support)

The technical staff of Atlante comprises a computing engineer from ITC (María Belén Esteban Sánchez), who is responsible for system management and user support, and a group manager (José Manuel Pérez Pérez).

A local Access Committee allocates the 80% of local CPU time amongst users from the Government of Canary Islands, private companies and R&D groups, while the remaining processing time is provided to the RES network.

Technical Performance 2015

In 2015 Atlante provided 1 million of CPU hours to its users. RES users consumed 55% of the total.

Remaining hours were consumed by users from Universidad de Las Palmas de Gran Canaria, Universidad de La Laguna and other private entities.

Accounting Atlante 2015

ITC 0%
ULPGC 1%
ULL 35%
Government - Companies 9%
RES 55%
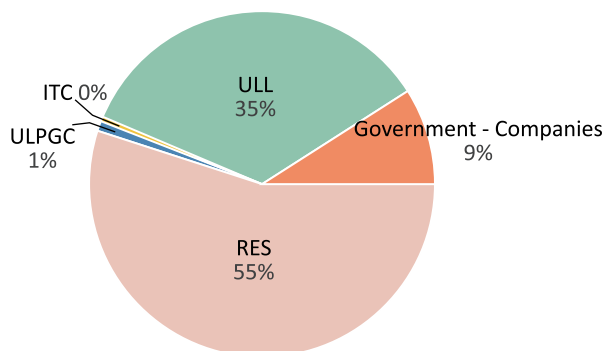
Training and Other Activities 2015

In 2015 Atlante facilities were visited by groups of students of Computer Science at Universidad de Las Palmas de Gran Canaria and IES 7 Palmas.

They were introduced to supercomputer concepts and the use of high performance computing in science and technology.

The Altamira Supercomputer

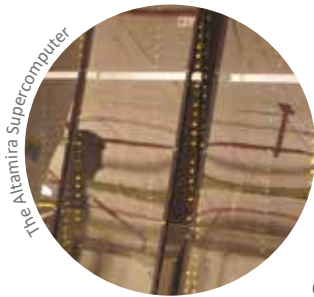The Altamira node of the RES at the University of Cantabria is located in the Juan Jorda Building and is jointly managed by the IFCA Distributed Computing Team and the Computer Architecture Group (ATC) of the University of Cantabria.
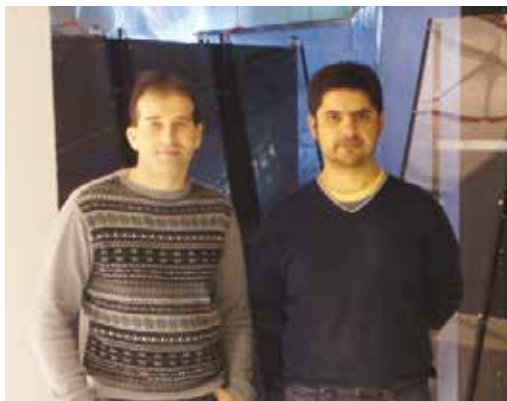
IFCA (Instituto de Física de Cantabria) is a joint centre of the University of Cantabria and CSIC with research lines in astrophysics, high energy physics and distributed computing. It participates in several national and European computing projects.

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 2012 with the installation of a new system at IFCA datacenter room. The main 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 system administration and user suppor

Miguel Angel Nuñez and Luis Cabellos.

Executive Committee

Industrial Committee — Management Committee — Evaluation Committee

Exectutive Committee
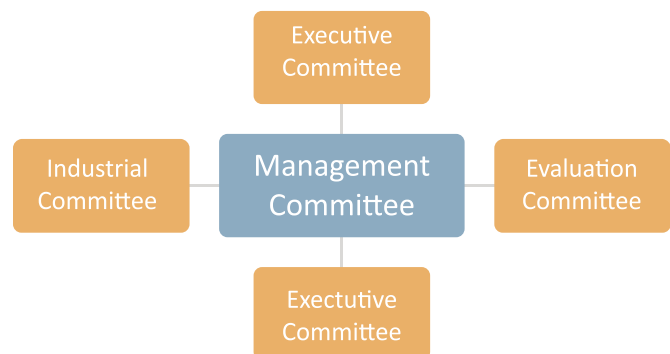
Technical Performance 2015

During 2015, RES projects consumed 2.575 million hours of computing time in Altamira, representing about 19% of all consumed time in Altamira during the year.

Training and Other Activities 2015

The Altamira node is utilised by students in the Masters of Physics, Instrumentation and Environment of the University of Cantabria. In total, around 600 people have guided visits of the Altamira supercomputer each year, including technicians, students, seniors, and also the press.

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 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, totaling 63 TFLOP/s. All these resources share a 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.

In November 2015 an Illumina genome sequencer was installed at Picasso, creating a new and important source of data. It is used for cutting-edge research on genomics focused mainly on humans, but also for some research activities relating to animals and plants. The architecture of the Picasso computer was designed to optimise genomic data processing and other tasks requiring large amounts of memory. Thanks to the availability of RAM in Picasso´s seven "fat" nodes with 2TB of RAM each, tasks like the assembly of new genomes and the 3D reconstruction from images taken by microscopes of a virus were accomplished.

Organisational Structure

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

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

The SCBI is an independent service with its own staff dedicated to administration of machines and user support, but also giving higher level support to researchers in the development of computational solutions for problems in several areas, especially biological research. There is also strong cooperation with the Computer Architecture Department of UMA whose main research areas are analysis, design, and evaluation of high performance architectures, from the application level to the lower hardware levels.

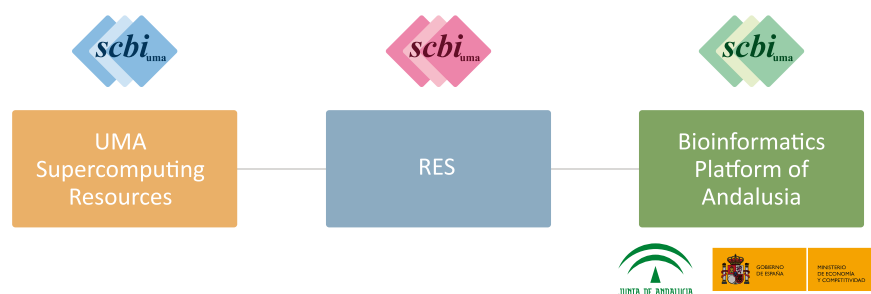## Technical Performance 2015

In 2015, some 30% of Picasso resources were made available to RES users, who used more than three million hours of computing time with more than 30.000 jobs processed.

Training and Other Activities 2015

In order to better process genomic data, in 2015 the Picasso team developed several software pipelines, which are continuously evolving.

This was accomplished by installing several hundred genomic applications, details of which can be seen on the Picasso software web page.
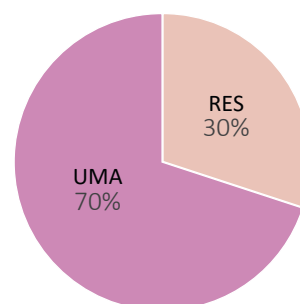
Allocation of Picasso computing time 2015 - 30% RES, 70% UMA

The Tirant Supercomputer

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

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

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

Organisational Structure

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 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.

Left to right: Alejandro Soriano - System Analyst and Josep Vicent Sala - System Analyst

Technical Performance 2015

During 2015, a total of 6,784,459 computing hours were used, of which 4,400,785 were consumed by users of the University of Valencia.

Training and Other Activities 2015

Tirant has been conducting guided visits of Tirant facilities since 2009. In 2015, 20 visits were conducted totaling 334 people.

The CAESARAUGUSTA Supercomputer

The Institute for Biocomputation and Physics of Complex Systems of the University of Zaragoza (BIFI-UNIZAR) is a research organisation that promotes interdisciplinarity to develop competitive research in computation applied to physics of complex systems and biological systems. The Institute has developed intense research activity in several fields of computation: high performance computing, cloud & grid computing, special purpose computers (FPGA-based) and volunteer computing.

CAESARAUGUSTA is a founding node of the Spanish Supercomputing Network (RES). The current version of the supercomputer ("Caesaraugusta II", locally also known as "Memento"), is located at BIFI's premises in the Río Ebro Campus of the University of Zaragoza and is managed by the High Performance Computing group of the Institute. It is equipped with 3072 computing cores (AMD64), 12TB of RAM memory, 72TB of raw storage and Infiniband QDR interconnection network (40Gb/s), offering an overall raw performance (Rpeak) of 25,8 TFLOPS (Rmax is 20 TFLOPS). The portion of Caesaraugusta II publicly shared through the RES during 2015 was equal to 768 cores; 512 for RES users and 256 for local ("CeSAr") users.

Organisational Structure

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

Caesaraugusta is maintained by technical staff of the Computing Area at BIFI, namely the HPC group. This includes hardware and software administration as well as first level user support, all of which are coordinated with the BSC-CNS Operations Department.

There is also a local Access Committee which periodically (each four months, coinciding with the RES schedule) evaluates applications and allocates the CPU time reserved for CeSAr projects among applicant activities. During 2015, the members of the local Access Committee were: Prof. Pablo Ibáñez Marín, Prof. Luis Rández García, and Prof. Alfonso Tarancón Lafita.

Technical Performance 2015

During 2015, a total of 20.221.991 hours of CPU time were consumed on Caesaraugusta, representing 76,74% of the theoretical maximum utilisation of the system.

In particular, RES users consumed **3.269.915 hours**, while CeSAr activities consumed 1.104.150 hours. The remaining 15,847,926 hours were consumed by BIFI members and their collaborators. All these activities produced numerous scientific results and publications.

Training and Other Activities 2015

During the last year, the following dissemination activities were carried out:

ORAL CONTRIBUTIONS

1. Giner Gracia A. Accounting of HPC resources at BIFI. VII National Conference BIFI2015. Zaragoza (España). February 2015.

2. Losilla Anadón G. ETP4HPC: the European Technology Platform for High-Performance Computing. VII National Conference BIFI2015. Zaragoza (España). February 2015.

OTHER

A guided visit of EINA-UNIZAR's computer science students to our data center took place on December 22nd.

Accounting Caesaraugusta II / Memento 2015 (CPU Hours)

BIFI-ZCAM 15.847.926

RES 3.269.915

CeSAr 1.104.150
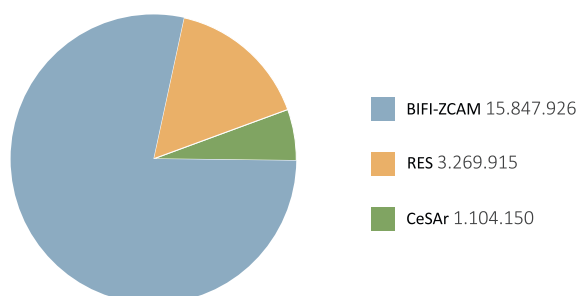
FinisTerrae-II Supercomputer

In total, the newly installed FinisTerrae II system has 7.712 cores, 44,8 TB memory and 1,5 PB in disc. Its peak performance reaches 238 TFLOPS. It was acquired in 2015 and will be fully operational by the beginning of 2016. FinisTerrae II is composed of 306 computing nodes, each of these has two Haswell 2680v3 processors, 128 GB memory and one 2TB disc, 4 nodes have GPUs, each of these has 2 NVIDIA Tesla K80 GPU, 2 Haswell 2680v3 processors, 128 GB memory and a 2TB disc, 2 nodes have Intel Xeon Phi, each with 2 Intel Xeon Phi 7120P processors, 2 Haswell 2680v3 processors, 128 GB memory and a 2TB disc. It also has a FAT node with 8 Haswell 8867v3 processors, 4096 GB memory and 24 discs with a capacity of 1,2 TB each.

This system has a high performance interconnect Mellanox Infiniband FDR@56Gbps with Fat-tree topology and a Lustre parallel file system with a capacity of 768TB (750TB net) and 20GB/s of I/O.

Organisational Structure

Fundación Pública Galega Centro Tecnolóxico de Supercomputación de Galicia (CESGA) is the main Centre for computing, storage, visualisation, high performance communications and advanced services of the Galician scientific community, university academic system, and Spanish National Scientific Research Council (CSIC). CESGA is a non-profit institution whose trustees pertain to the Regional Government of Galicia and to CSIC.

CESGA's mission is to contribute to the advancement of Science and Technical Knowledge, by means of research and application of high performance computing and communications, as well as other information technologies resources, in collaboration with other institutions, for the profit of society. In 2008, CESGA was recognised by the Ministry of Science and Innovation of the Government of Spain as a Singular Scientific Technological Installation (ICTS).

In March 2015, CESGA joined the Spanish Supercomputing Network (RES). CESGA will start providing access to computing capacity to RES users through the FinisTerrae-II system from the second quarter of 2016.
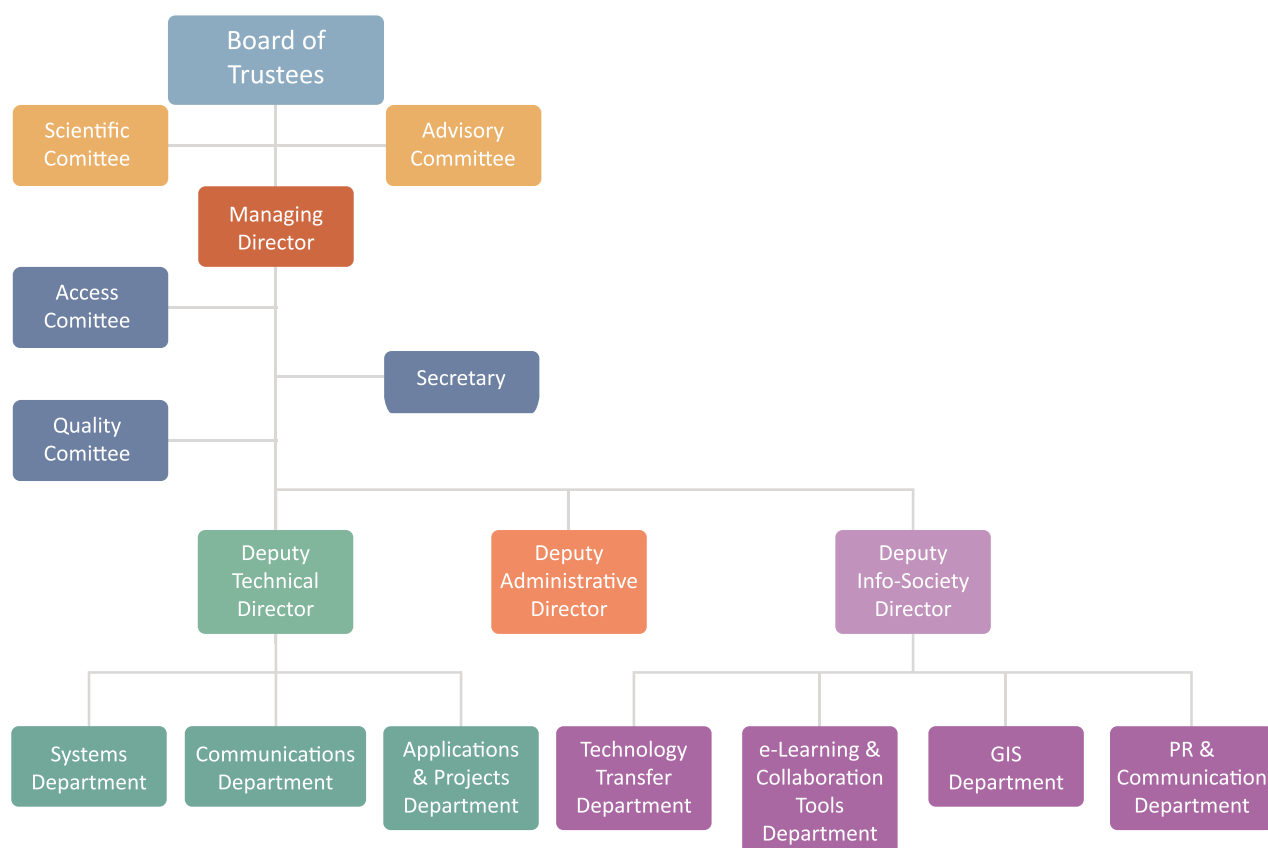
Cesga Team as of January 2015

Technical Performance 2015

CESGA will only start to provide RES services during 2016 once the new supercomputer is operational.
In 2015, CESGA directly provided more than 20 million CPU hours to a user community of well over 300 researchers. The user community mostly came from Galician research institutions and from CSIC centres and laboratories from all over Spain. In the last ten years, CESGA's users reported an average annual production of over 200 scientific publications per annum.

Throughout the year 2015, CESGA provided regular daily operational services to the Galician Weather Forecast Service (MeteoGalicia), to the Copernicus Iberia-Biscay-Ireland Marine Forecasting Centre (IBI-MFC) through a Puertos del Estado (Spanish Port Authority) led collaboration with Mercator-Ocean, MeteoFrance, Marine Institute, and AEMET (Spanish Weather Forecast Service), and to an international weather forecasting company.

CESGA also provided daily computing capacity for Fundación Pública Galega de Medicina Xenómica (FPGMX), the institution responsible for research, genomic analysis and clinical support services for SERGAS (Galicia's Public Health Service).

Training and Other Activities 2015

One of CESGA's main goals is the promotion of high performance computing, storage, and communications systems for numerical modelling, simulation, and data analysis among small and medium enterprises (SME) in order to increase their competitiveness. In 2015, over 35 SMEs benefited from the use of CESGA's systems, knowledge and experience both through everyday services to SMEs, and through European projects such as CloudPYME2, Fortissimo, Fortissimo2, and SESAME NET.

View of SGI Altix UV 1000 (Pirineus)

The Altix UV 1000 (Pirineus) is a shared-memory machine, with 6.14 TB of memory on a single operative system, a peak performance (Rpeak) of 14.30 Tflop/s and an estimated maximum performance (Rmax) of 12.61 Tflop/s. It consists of 224 64-bit Intel Xeon X7542 processors (2.66 GHz/6 core), resulting in a total of 1344 processing cores, and 112 TB of disk storage. This system is a multiprocessor with a shared-memory design which offers a flexible and competitive work environment for many applications.

Amongst its advantages is the fact that the degree of parallelism is not limited to the number of processors of the nodes and that it does not present restrictions on memory, which is shared efficiently by the large bandwidth and very low latency of the internal communications. The internal network is built using a NUMAlink topology that allows all processors to work sharing a single memory space, which can be up to tens of petabytes.

The operating system is a Linux SLES distribution by Novell, as this is the only version of Linux which currently offers a scalable kernel up to 2048 cores. The server works with the standard SLES distribution, which ensures compatibility with any application. The Altix UV 1000 was acquired with financing from the former Ministry of Science and Innovation, using funds from the European Regional Development Funds (ERDF) and the Generalitat of Catalonia.

Organisational Structure

President
Andreu Mas-Colell

Exec. Comm. President
Lluís Jofre

Managing Director
Miquel Puig

The Consorci de Serveis Universitaris de Catalunya (CSUC[1]) provides shared academic, scientific, library, knowledge transfer and management services to R&D entities to improve effectiveness and efficiency by enhancing synergies and economies of scale.

CSUC provides extensive computing services [2] not only to academic researchers but also to industry, with a wide range of scientific software available. It also manages the Drug Design Service (SDF) which helps pharmaceutical laboratories and research groups to develop new medicines in a more efficient way. Supercomputers with different architectures and numerous specialised programs are available at CSUC facilities to satisfy the very diverse needs of scientific computing.

CSUC provides technical and scientific support to users, so that they can receive the maximum benefit of HPC related technologies. Its key members are the Generalitat of Catalonia and ten Catalan universities (UB, UAB, UPC, UPF, UdL, UdG, URV, UOC, URL and UVic-UCC).

Administration & Finance
Miquel Huguet

ICT Services
Xavier Peiró

Libraries, Information & Documentation
Lluís Anglada

Joint Procurement
Elena Parpal

Administration & Secretariat
Carme Monsterrat

System & Networks
Caterina Parals

Services & Applications

Library Support
Marta Tort

Digital Library
Núria Comellas

Budget & Contracts
Ma. José Miranda

Operations & Security
Jordi Guijarro

HPC & Applications
Ricard de la Vega

Library & Documentary Applications
Ramon Ros

Communication & Marketing
Teresa Via

Communications
M. Isabel Gandia

e-Administration
Albert Portugal

GEPA Facility
Santi Balagué

Repositories
Sandra Reoyo

Customers & Projects
Gorka Roldan

Quality & Support
Joan Cambras

CCUC
Joana Roig

Technical Performance 2015

CSUC was incorporated into the RES during 2015, serving its first user group in November 2015. The total computing capacity of Pirineus node in 2015 was 7.347.984 hours, of which RES usage from October to December 2015 was 165.885 hours.

The Lusitania II supercomputer, named after the ancient Iberian Roman province, joined the RES on 29th April 2015. The Lusitania I was initially established in 2009, located in Trujillo (Cáceres) at CénitS (the Extremadura Supercomputing, Technological Innovation and Research Center).

Its goal is to promote and provide HPC resources and services as well as advanced communications to the research communities and companies or institutions that request it and thus contribute through technological improvements and innovation, improving the competitiveness of enterprises. CénitS is managed by COMPUTAEX (Computing and Advanced Technologies Foundation of Extremadura), a non-profit public foundation dependent on the Regional Government of the Autonomous Community of Extremadura

Lusitania II is a 128 core SMP-ccNUMA system with 2 HP SuperDomes SX2000 nodes equipped with 64 dual-core Intel Itanium2 Montvale (1.6GHz, 18MB Cache) processors running at 1.6GHz with 18MB cache, both of them with 1TB memory on a single image, SX2000 chipsets designed to take advantage of Itanium2 Montvale CPUs, and high availability, together with 2 Enterprise Virtual Arrays (EVAs) 8100 x [(208 FATA disks x 1TB) + (128 FC disks x 450GB)] = 265TB. In addition, the backup system on tape library HP Storageworks EML 245e has capacity for 245 tapes of LTO-4 Ultrium technology, offering capacity of 392 TB in 2:1 compression.

Lusitania II also has several cloud computing nodes (3 HP ProLiant servers with 2 Intel Xeon Quad Core processors; 4 HP ProLiant Gen6 servers with 2 Intel Xeon 5600 and 128 GB of memory; 8 HP ProLiant Gen8 servers with 2 AMD Opteron processors with 128 GB of memory; and 1 Fujitsu Primergy RX350 S8 server with 2 Intel Xeon E5 2620v2 processors and 256 GB of memory, as well as computing accelerating units (2 NVIDIA Tesla M2070Q and an Intel Xeon Phi 3120P Co-Processor).

External connectivity is provided through a 10Gbps connection with the Extremadura Scientific Technology Network, connecting major cities and technology centers in the region. CénitS is also interconnected with RedIRIS and the European GÉANT network.

One of its most important characteristics is that the supercomputer is installed inside a mobile container. This is to ensure that CénitS engineers can continue their research in the field of mobility, monitoring and modularity of Data Processing Centers, with the objective of improving their sustainability and efficiency.
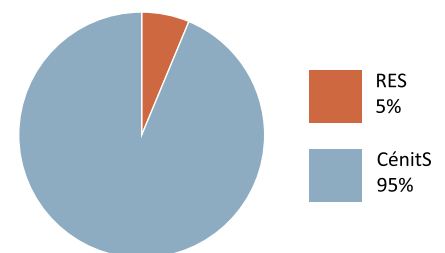
Organisational Structure
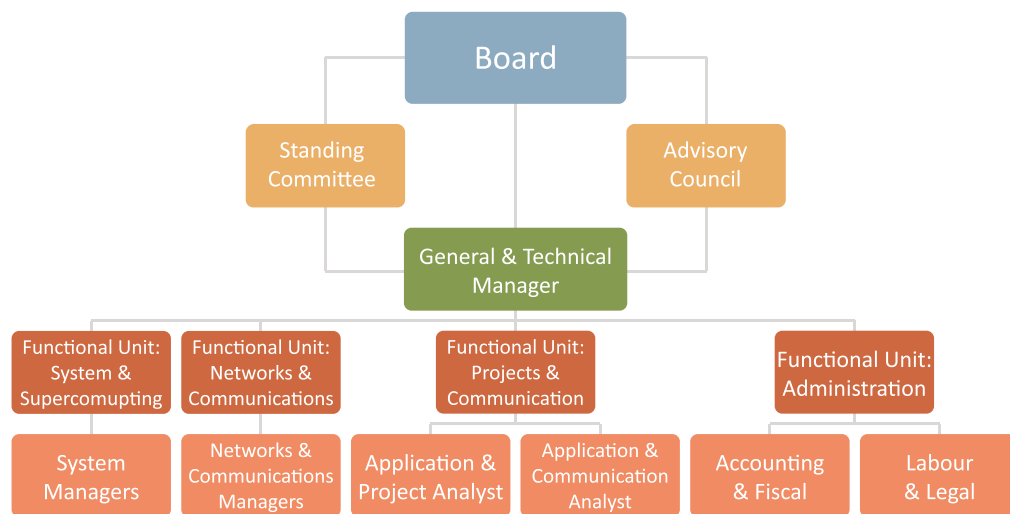
Staff 2015

Technical Performance 2015

Lusitania II began providing resources to RES users from October 2015. In total, RES users consumed 5% of the maximum available computing hours in 2015. The remaining 95% was consumed by local users. All these activities produced numerous scientific results and publications.

RES 5%

CénitS 95%

Training and Other Activities 2015

During 2015, CénitS received 14 visits from nearly 350 students and visitors. In addition, CénitS successfully participated in The European Researchers' Night, which took place on 25th September at the School of Technology of the University of Extremadura and all over Europe. During this event, CénitS staff showed how researchers contribute to society in an interactive and engaging way, and promoted research careers to young people and their parents.

CénitS staff also contribute strongly to the ICT Masters programme at the University of Extremadura, and during 2015, attended sixteen events on behalf of CénitS, related to research and innovation activities.

Caléndula Supercomputer

The Caléndula supercomputer, located in León, is run by the Foundation of Supercomputing Center of Castilla y León (FCSCL), a public research centre dependant of the Community of Castilla y León. Its main activity is to support the improvement of R&D&I activities in the region.
Caléndula currently comprises several parallel computing systems integrated into a single heterogeneous MPI cluster architecture, regularly upgraded from the original systems installed in 2008 to the latest updates at the end of 2015. It currently has a calculation capacity of 130 TeraFlops.

Organisational Structure

The strategic policy of the Centre focuses on four lines: Supercomputing, project development, boost of cloud technologies and the consolidation of the Regional Network of Science and Technology. Apart from that, the Centre runs also its own research lines such as: Energy Efficiency, Technologies in Cloud for Public Administrations and the Federation of Identities, Infrastructures and Execution of Workflows.
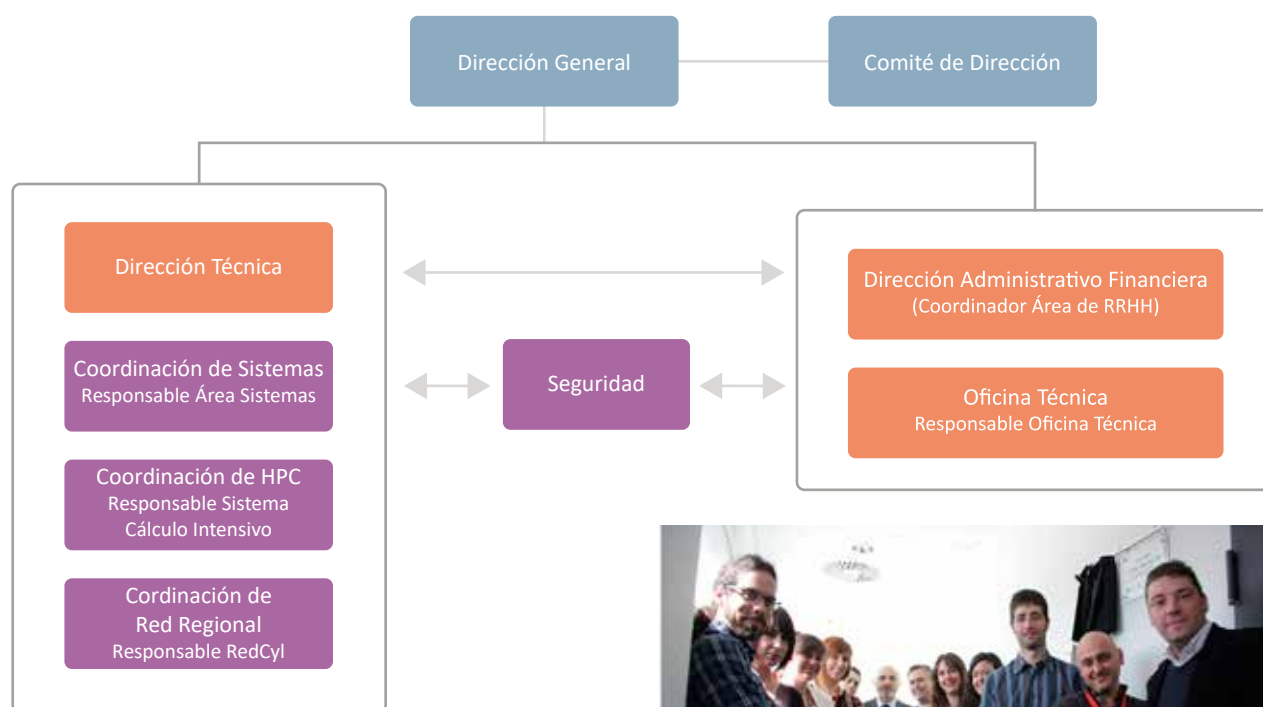
Technical Performance 2015

Since joining the RES during the third quarter of 2015, Caléndula provided more than 2 million CPU hours for RES users, which is 50% of the available computing power. The rest was used by local users.

Training and Other Activities 2015

FCSCL´s training programme included a number of outreach and communication actions with participation in around thirty conferences, scientific committees, scientific-technical workshops and various working groups.

The Centre also ran a series of training courses and other training collaborations such as participation in Masters courses, technology campus and a number of courses organised by entities outside the FCSCL. The Centre also participated in various national, European and public administration projects.

Cibeles Supercomputer

Cibeles Node is hosted by the Center for Scientific Computation (Centro de Computación Científica - CCC) which belongs to the Autonomous University of Madrid (Universidad Autónoma de Madrid - UAM). This University, together with 10 centres of the Spanish Research Council (CSIC) located at the same campus, and two Centres of the Madrid Research Institute (Instituto Madrileño de Investigación Avanzada – IMDEA), form the Campus of International Excellence (CEI) UAM + CSIC.

The CCC computing facilities are available for all the Campus members, covering many different disciplines (material chemistry, physics, economy, biology, etc.) that can benefit from HPC, offering computing and hosting services together with system management.
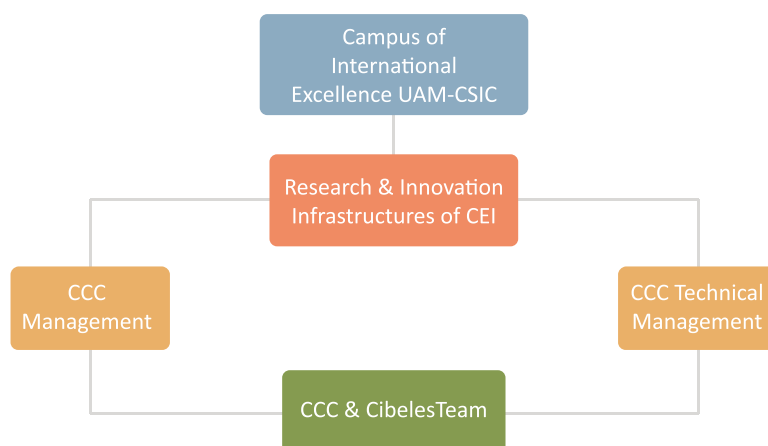
The supercomputer is named after Cibeles, the Goddess of Mother Earth and a symbol of earth, agriculture and fertility. Cibeles was used historically to represent Madrid, and one of its most famous squares is also named after her.

The Cibeles node is provisionally made up of a cluster of 448 Intel cores Xeon E5-2630v3 with a peak performance of 17.2 Tflops interconnected by Infiniband. It will be upgraded in 2016.

The Cibeles node of the RES consists of 28 servers with double processor Intel(R) Xeon (R) CPU E5-2630 v3 @ 2,40 GHz, 32 GB RAM memory. These nodes are connected to a network of high speed and low latency FDR-Infiniband 56 Gbps. This is networked to storage filesystems for users, projects, software, and scratch, integrated in a Lustre environment of 167 TB size.

Organisational Structure

The CCC-UAM has about 500 computers (more than 7000 calculation cores). Those servers come from CCC-UAM own resources as well as cooperation agreements, and are managed by CCC staff and used by the International Excellence Campus researchers.

Campus of International Excellence UAM-CSIC

Research & Innovation Infrastructures of CEI

CCC Management

CCC Technical Management

CCC & CibelesTeam

Technical Performance 2015

Since the node was included in the RES infrastructure only on 1st November 2015, the computing capacity contributed to the RES in 2015 was only 161.280 hours. This will increase significantly in 2016.

Training and Other Activities 2015

Members of staff attended several PATC courses covering topics such as parallel programming and an introduction to CUDA programming

Astronomy, Space & Earth Sciences
Projects in Astronomy, Space and Earth Sciences 2015

- » **Coalescence of Black Hole Binary systems** - Leader Name: Sascha Husa, Leader Institution: Universitat de les Illes Balears

- » **Constraints on inflationary models of the universe based on CMB data** - Leader Name: Enrique Martinez Gonzalez, Leader Institution: Instituto de Fisica de Cantabria

- » **Development and Consolidaton of Geo-Spatial Sustainability Services for Adaptation of Environmental and Climate Change Urban Impacts (Decumanus)** - Leader Name: roberto san jose, Leader Institution: UPM Computer Science School

- » **Environment Driven Galaxy Evolution (EDGE)** - Leader Name: Claudio Dalla Vecchia, Leader Institution: Instituto de Astrofisica de Canarias

- » **European framework for online integrated air quality and meteorology modelling** - Leader Name: roberto san jose, Leader Institution: UPM Computer Science School

- » **Gaia: Data Processing and Simulation of Telemetry Stream** - Leader Name: Jordi Torra i Roca, Leader Institution: Universitat de Barcelona (UB), Departament d Astronomia i Meteorologia

- » **Gaia: Data Processing and Simulation of Telemetry Stream** - Leader Name: Jordi Torra i Roca, Leader Institution: Universitat de Barcelona (UB), Departament d Astronomia i Meteorologia

- » **Impact of land surface initialisation in climate seasonal predictions** - Leader Name: Francisco J. Doblas-Reyes, Leader Institution: Institut Català de Ciències del Clima

- » **Impact of ocean resolution and initialisation in climate seasonal predictions** - Leader Name: Francisco J. Doblas-Reyes, Leader Institution: Institut Català de Ciències del Clima

- » **Impact of sea ice initialization on seasonal climate prediction** - Leader Name: Neven Stjepan Fuckar, Leader Institution: Catalan Institute of Climate Sciences (IC3)

- » **Merger and gravitational wave signal of non-precessing black holes with large spins** - Leader Name: Sascha Husa, Leader Institution: Universitat de les Illes Balears

- » **Modeling the coalescence of magnetized neutron stars** - Leader Name: Carlos Palenzuela, Leader Institution: Universidad de las Islas Baleares (UIB)

- » **Numerical simulation of turbulent optical parameters around telescopes** - Leader Name: Joan Baiges, Leader Institution: CIMNE

- » **Simulations of dynamics of partially ionized solar atmosphere** - Leader Name: Elena Khomenko, Leader Institution: Instituto de Astrofísica de Canarias

- » **Simulations of dynamics of partially ionized solar atmosphere** - Leader Name: Elena Khomenko, Leader Institution: Instituto de Astrofísica de Canarias

- » **The Marenostrum Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe** - Leader Name: Gustavo Yepes, Leader Institution: Universidad Autonoma de Madrid

- » **The Marenostrum Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe** - Leader Name: Gustavo Yepes, Leader Institution: Universidad Autonoma de Madrid

- » **The MICE project -2. Volume and mass resolution effects on small-scale dark matter clustering** - Leader Name: Pablo Fosalba, Leader Institution: ICE (IEEC-CSIC)

- » **The Small-Scale Magnetic Activity of the Quiet Solar Photosphere** - Leader Name: Javier Trujillo Bueno, Leader Institution: Instituto de Astrofísica de Canarias (IAC)

- » **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)

- » **Urban climate atlas and health impact DECUMANUS premium services** - Leader Name: roberto san jose, Leader Institution: UPM Computer Science School

- » **Wind-wind interaction in gamma-ray binaries and long term evolution of extragalactic jets** - Leader Name: Manel Perucho Pla, Leader Institution: Universitat de València

Biology and Life Sciences
Life and Health Sciences Projects 2015

- » **A molecular-dynamics study of the temperature dependence of polypeptide-hydration thermodynamics -** Leader Name: Xavier Daura, Leader Institution: Institut de Biotecnologia i de Biomedicina - Universitat Autonoma de Barcelona

- » **Allosteric regulation of the SHIP2 phosphatase by its C2 domain.** - Leader Name: Daniel Lietha , Leader Institution: Spanish National Cancer Research Center (CNIO)

- » **Assessing the inherent conformational flexibility of F1-ATPase alpha subunit: a molecular dynamics simulation study** - Leader Name: Xavier Barril, Leader Institution: ICREA & Universitat de Barcelona

- » **Binding of novel activators to AMPK and theoretical study of the activation mechanism (II)** - Leader Name: Fco. Javier Luque Garriga, Leader Institution: Faculty of Pharmacy, University of Barcelona

- » **Computing signals of positive selection in the pattern of somatic mutations in tumors** - Leader Name: Nuria Lopez-Bigas, Leader Institution: University Pompeu Fabra UPF

- » **Development of novel treatments for myotonic dystrophy: in vivo drug discovery** - Leader Name: Jordi Teixidó, Leader Institution: Institut Químic de Sarrià (IQS, URL)

- » **Discovery of new EGFR inhibitory peptides with improved Blood-Brain Barrier (BBB) permeability** - Leader Name: Ernest Giralt Lledó, Leader Institution: Institute for Research in Biomedicine (IRB)

- » **Evidence of Conformational Selection in a Glycosyltransferase Structure?** - Leader Name: Antoni Planas, Leader Institution: Laboratory of Biochemistry. IQS - Universitat Ramon Llull

- » **Heterochiral Proteins?** - Leader Name: Ernest Giralt Lledó, Leader Institution: Institute for Research in Biomedicine (IRB)

- » **High-resolution structures of whole viruses by cryo-electron microscopy techniques** - Leader Name: Nicola GA Abrescia, Leader Institution: Center for Cooperative Research in Biosciences (CIC bioGUNE)

- » **Identification of somatic variation in ICGC-PanCancer Genomes** - Leader Name: David Torrents Arenales, Leader Institution: BSC

- » **Implication of conformational changes in the activation loop of MNK1/2 in breast cancer** - Leader Name: Roger Estrada, Leader Institution: Institut Químic de Sarrià

- » **In silico evolution of the gap gene network: how to turn one fly into another** - Leader Name: Johannes Jaeger, Leader Institution: EMBL/CRG Research Unit in Systems Biology

- » **In-silico Protein Engineering with BindScan. Epoxide Hydrolase Benchmark.** - Leader Name: Xevi Biarnés, Leader Institution: Institut Químic de Sarrià

- » **Interactions between Peptides and Membranes Studied by all-atom free Energy Calculations** - Leader Name: Carmen Domene, Leader Institution: University of Oxford

- » **Lipid-dependent binding of neutralizing and nonneutralizing antibodies to the membrane-proximal external region of HIV gp41** - Leader Name: Jordi Villà-Freixa, Leader Institution: Polytechnic School, University of Vic - Central University of Catalonia

- » **Microbial Oceanomics using Next-Generation Sequencing (454/Illumina)** -

Leader Name: Ramiro Logares, Leader Institution: ICM-CSIC

» **Modulation of immune receptors function as a novel therapeutic strategy for acute CNS damage** - Leader Name: Jordi Villà-Freixa, Leader Institution: Polytechnic School, University of Vic - Central University of Catalonia

» **New strategies in GPCR drug discovery** - Leader Name: Leonardo Pardo, Leader Institution: Universitat Autonoma Barcelona

» **New strategies in GPCR drug discovery** - Leader Name: Leonardo Pardo, Leader Institution: Universitat Autonoma Barcelona

» **Probing Conformational Selection in a Glycosyltransferase Structure by Bias-Exchange.** - Leader Name: Antoni Planas, Leader Institution: Laboratory of Biochemistry. IQS - Universitat Ramon Llull

» **Rare genetic variants in Alzheimer's disease (AD): use of next-generation sequencing for a comprehensive analysis of genes related to AD** - Leader Name: Jordi Clarimón, Leader Institution: Sant Pau Research Institute

» **Standardized and comparable ecological and biotechnological metagenome analysis of Ocean Sampling Day's marine ocean microbes** - Leader Name: Antonio Fernandez-Guerra, Leader Institution: Oxford e-Research Centre

» **Study of the role of EGFR activating mutations in the development of drug resistance in non-small cell lung cancer treatment** - Leader Name: Jordi Teixidó, Leader Institution: Institut Químic de Sarrià (IQS, URL)

» **The Quasi-Bound State: application to binding mode prediction** - Leader Name: Xavier Barril, Leader Institution: ICREA & Universitat de Barcelona

» **Towards the design of isoform-selective adenylyl cyclase inhibitors for the study of signaling cascades: a molecular simulation study** - Leader Name: Pietro, Leader Institution: UAB

» **Translocation of ADP/ATP: Mechanism of the membrane protein carrier** - Leader Name: Fco. Javier Luque Garriga, Leader Institution: Faculty of Pharmacy, University of Barcelona

» **Uncovering the molecular mechanisms of O-glycosylation -** Leader Name: Carme Rovira Virgili, Leader Institution: University of Barcelona

» **Uncovering the molecular mechanisms of O-glycosylation: enzyme s**pecificity - Leader Name: Carme Rovira Virgili, Leader Institution: University of Barcelona

Chemistry and Material Sciences
Chemistry and Material Sciences Projects 2015

» **Ab initio molecular dynamics of photovoltaic organic self-assembled monolayers adsorbed on metal surfaces** - Leader Name: Sergio Diaz Tendero, Leader Institution: UAM

» **Acid Gas Removal by Ionic Liquids: a Computational Approach** - Leader Name: Santiago Aparicio, Leader Institution: Universidad de Burgos

» **Activation and conversion of CO2 through novel catalysts based on Au and Cu nanoparticles supported on molybdenum carbides** - Leader Name: Francesc Illas, Leader Institution: Universitat de Barcelona

» **Active centers in realistic metal oxide surfaces characterized with first-principles simulations and scanning probe microscopies** - Leader Name: Rubén Pérez, Leader Institution: Universidad Autónoma de Madrid

» **Alkane oxidation over CeO2 nanoparticles: role of defects** - Leader Name: Avelino Corma Canós, Leader Institution: Instituto de Tecnología Química UPV-CSIC

» **Analysis of the ultrafast charge transfer in organic photovoltaic devices based on endohedral metallofullerenes** - Leader Name: Antonio Rodríguez Fortea, Leader Institution: Universitat Rovira i Virgili

» **Characterization of Cu active centers in Cu-zeolite catalysts for the selective reduction of NOx** - Leader Name: Mercedes Boronat, Leader Institution: Instituto de Tecnologia Quimica UPV-CSIC

» **Competition between phonons and electron-hole pair excitations in ab-initio molecular dynamics simulations of gas/surface reactivity** - Leader Name: Maite Alducin Ochoa, Leader Institution: Centro de Fisica de Materiales, centro mixto CSIC-UPV/EHU

» **Computational exploration and design of new epoxide hydrolase variants** - Leader Name: Kendall N. Houk, Leader Institution: University of California, Los Angeles (UCLA), Department of Chemistry and Biochemistry

» **Conferring natural enzymes new synthetically useful functionalities** - Leader Name: Kendall N. Houk, Leader Institution: University of California, Los Angeles (UCLA), Department of Chemistry and Biochemistry

» **Conformational free energy landscapes of carbohydrates** - Leader Name: Carme Rovira Virgili, Leader Institution: University of Barcelona

» **Conformational free energy landscapes of carbohydrates. Implications for catalysis in carbohydrate-active enzymes.** - Leader Name: Carme Rovira Virgili, Leader Institution: University of Barcelona

» **Design and characterization of the physical properties of distorted nanographenes** - Leader Name: Blanca Biel, Leader Institution: Universidad de Granada

» **Determination of chemical ordering in large bimetallic particles from density-functional calculations** - Leader Name: Konstantin Neyman, Leader Institution: Uni Barcelona

» **Dynamics and Stability of Novel Polymersome Formulations for Drug Delivery** - Leader Name: Xevi Biarnés, Leader Institution: Institut Químic de Sarrià

» **Electronic and magnetic properties of molecules adsorbed on semi-infinite surfaces including spin-orbit coupling** - Leader Name: Jorge Iribas Cerdá, Leader Institution: ICMM-CSIC

» **Existence of the liquid-liquid critical point in supercooled water** - Leader Name: JOSE LUIS FERNANDEZ ABASCAL, Leader Institution: Universidad Complutense de Madrid

» **First principle simulations of gas storage on nano-structured materials** - Leader Name: JORNET SOMOZA, Joaquim, Leader Institution: Universitat de Barcelona

» **First-principles investigation of intrinsic screening mechanisms in ferroelectric thin film** - Leader Name: Emilio Artacho, Leader Institution: CIC nanoGUNE Consolider and University of Cambridge

» **First-principles simulations of metal oxide surface chemistry and defects aided by scanning probe microscopies** - Leader Name: Rubén Pérez, Leader Institution: Universidad Autónoma de Madrid

» **First-principles study of Na insertion/extraction in the (Fe,Mn)PO4-Na(Fe,Mn)PO4 system for cathode material in Na-ion batteries** - Leader Name: Javier Carrasco, Leader Institution: CIC Energigune

» **Flow-induced anisotropy in metallic glasses** - Leader Name: Daniel Crespo, Leader Institution: Universitat Politècnica de Catalunya

» **Fluorescence markers for amyloid detection. Insights from molecular dynamics simulations.** - Leader Name: Mariona Sodupe, Leader Institution: Universitat Autònoma de Barcelona

» **Fragmentation and reaction dynamics of charged and excited molecules in gas phase** - Leader Name: Manuel Alcami, Leader Institution: UAM

» **Fragmentation of biomolecules from selected valence-hole states.** - Leader Name: Manuel Alcami, Leader Institution: UAM

» **High voltage sulphate cathodes Li2Fe(SO4)2 for batteries: evaluation of stability and Li diffusion using first principles** - Leader Name: Javier Carrasco, Leader Institution: CIC Energigune

» **Homogeneous versus heterogeneous catalyst: Catalytic Reduction in Surfactant Coated Nanoparticles (2nd period)** - Leader Name: Feliu MASERAS, Leader Institution: Institute of Chemical Research of Catalonia (ICIQ)

» **Hydration force in the supercooled regime of water: a Molecular Dynamics study** - Leader Name: Giancarlo Franzese, Leader Institution: Universitat de

Barcelona

- » **Ice crystallization** - Leader Name: Carlos Vega, Leader Institution: Universidad Complutense de Madrid, Fac.Ciencias Quimicas, Dep.Quimica Fisica I
- » **In silico speciation of Pd catalyst in water by first principles simulation** - Leader Name: Andras Stirling, Leader Institution: Institute of Organic Chemistry of the Hungarian Academy of Sciences
- » **Interfacial level alignment across the photodissociation coordinate of water and methanol on rutile TiO2(110).** - Leader Name: Annapaola Migani, Leader Institution: CSIC-ICN2
- » **Looking for High Conductance Molecules** - Leader Name: Eliseo RUIZ, Leader Institution: Universitat de Barcelona
- » **Looking for High Conductance Molecules** - Leader Name: Eliseo RUIZ, Leader Institution: Universitat de Barcelona
- » **Markov State Models for enzyme design** - Leader Name: Sílvia Osuna, Leader Institution: UdG
- » **Maximum Aromaticity as the key property to unravel the Relative Stabilities of Endohedral Metallofullerenes** - Leader Name: Miquel Solà, Leader Institution: Universidad de Girona
- » **Metal oxides beyond the common limits: complex reactivity, surface dynamics, and doping** - Leader Name: Nuria Lopez, Leader Institution: ICIQ
- » **Modelling 2D Transition Metal Dichalcogenide Heterostructures** - Leader Name: Angel Rubio, Leader Institution: Universidad Pais Vasco/CSIC/FHI
- » **Modifying the properties of graphene supported on ruthenium** - Leader Name: Fernando Martín, Leader Institution: Universidad Autónoma de Madrid
- » **Molecular dynamics simulations of manipulation and irradiation of graphite and graphene** - Leader Name: Maria José Caturla Terol, Leader Institution: Universidad de Alicante
- » **Molecular-level understanding of hydrogen activation on copper-ceria catalysts for methanol synthesis** - Leader Name: Maria Veronica Ganduglia-Pirovano, Leader Institution: Instituto de Catalisis y Petroleoquimica, CSIC
- » **New Frontiers on Scanning Probe Microscopies: charge density distribution, subsurface resolution and atomic manipulation with the force and the electric current studied by First Principles simulations.** - Leader Name: Pablo Pou Bell, Leader Institution: Universidad Autónoma de Madrid
- » **Optoelectronic properties of defects in semiconductors through GW simulations. Case of Silicon.** - Leader Name: Iván Santos, Leader Institution: Universidad de Valladolid
- » **Oxygen induced step-doubling transition of the vicinal Pt(997) surface.** - Leader Name: Annapaola Migani, Leader Institution: CSIC-ICN2
- » **Oxygen intercalation in graphene on metals with ab initio DFT and STM simulations** - Leader Name: Rubén Pérez, Leader Institution: Universidad Autónoma de Madrid
- » **Quantum Effects in the Diffusion of Atomic Hydrogen on Interstellar Silicate Surfaces** - Leader Name: Albert Rimola, Leader Institution: UAB
- » **Rational design of noble-metal free catalysts for the dry reforming of methane** - Leader Name: Maria Veronica Ganduglia-Pirovano, Leader Institution: Instituto de Catalisis y Petroleoquimica, CSIC
- » **Simulation of selective protein channels embedded in electroactive polymeric membranes** - Leader Name: David Zanuy Gomara, Leader Institution: upc
- » **Structure and reactivity of Au nanoparticles supported on MoC, improving catalysts for the low temperature water gas shift reaction** - Leader Name: Francesc Illas, Leader Institution: Universitat de Barcelona
- » **Synthesis-structure-activity relationships for surfactant coated metal nanoparticles** - Leader Name: Nuria Lopez, Leader Institution: ICIQ
- » **Towards more realistic modelling of industrially important Pd/CeO2 and Pt/CeO2 catalysts** - Leader Name: Konstantin Neyman, Leader Institution: Uni Barcelona

- » **Towards new oxynitride phases for cathodes in Li-ion batteries** - Leader Name: Javier Carrasco, Leader Institution: CIC Energigune
- » **Towards realistic models of stoichiometric and doped TiO2 nanoparticles relevant to photocatalysis: Atomic and electronic structure from Density Functional Theory and Quasiparticle GW calculations** - Leader Name: Francesc Illas, Leader Institution: Universitat de Barcelona
- » **Turning Metal-Organic Frameworks into active, stable and selective Catalytic Materials (1st. period)** - Leader Name: Nuria Lopez, Leader Institution: ICIQ
- » **Understanding Polytypism in Group IV Nanowires from an Ab initio perspective** - Leader Name: Michele Amato , Leader Institution: Université Paris-Sud
- » **Understanding the nature of the driving force of the phase transitions in switchable phenalenyl-base molecular materials** - Leader Name: Juan Jose Novoa Vide, Leader Institution: University of Barcelona
- » **Understanding the nature the phase transitions in switchable molecular materials containing TCNQ- ions** - Leader Name: Juan Jose Novoa Vide, Leader Institution: University of Barcelona
- » **Understanding the water-gas shift reaction for hydrogen production on model Ni/ceria catalysts** - Leader Name: Maria Veronica Ganduglia-Pirovano, Leader Institution: Instituto de Catalisis y Petroleoquimica, CSIC
- » **Wacker-type oxidation of olefins: the effect of solvent in anti-Markovnikov addition** - Leader Name: Gregori Ujaque, Leader Institution: Universitat Autònoma de Barcelona
- » **Zirconia Nanoparticles for Catalytic Applications: Size, Shape and Composition from Density Functional Theory** - Leader Name: Francesc Illas, Leader Institution: Universitat de Barcelona

Physics and Engineering
Mathematics, Physics and Engineering Projects 2015

- » **3D Elastic Full Waveform Inversion: Toward Reflection Based Inversion** - Leader Name: Jean Kormann, Leader Institution: BSC-CNS
- » **A SPH based model to analyze ship induced sediment transport in Harbors using GPU cluster** - Leader Name: Ramon Gómez Gesteira, Leader Institution: Universidade de Vigo
- » **Advanced turbulence models for buoyancy driven flows** - Leader Name: Assensi Oliva, Leader Institution: Universitat Politècnica de Catalunya
- » **CFD of the flow inside a Gerotor Pump with Dynamic Mesh and Contact Point** - Leader Name: Robert Castilla, Leader Institution: Universitat Politècnica de Catalunya
- » **Complex structures in complex active materials** - Leader Name: Ignacio Pagonabarraga, Leader Institution: University of Barcelona
- » **Development of turbulent combustion models for premixed combustion based on tabulated chemistry for Reynolds-Averaged Navier-Stokes (RANS) and large-eddy simulation (LES)** - Leader Name: Daniel Mira, Leader Institution: Barcelona Supercomputing Centre
- » **Diffusion Monte Carlo simulation of quantum gases and solids.** - Leader Name: Grigory E. Astrakharchik, Leader Institution: Departament de Fisica i Enginyeria Nuclear, Universitat Politecnica de Catalunya
- » **Diffusion Monte Carlo simulation of quantum gases and solids.** - Leader Name: Grigory E. Astrakharchik, Leader Institution: Departament de Fisica i Enginyeria Nuclear, Universitat Politecnica de Catalunya
- » **Direct Numerical Simulations of 3D flows over flapping wings** - Leader Name: Manuel Garcia-Villalba, Leader Institution: Universidad Carlos III de Madrid
- » **Direct Numerical Simulations of Compressible Turbulent Flows at Moderate Reynolds Numbers: Compressible Flow around a NACA0012 airfoil with**

incidence - Leader Name: Assensi Oliva, Leader Institution: Universitat Politècnica de Catalunya

» **Direct numerical simulations of Taylor-Couette flow for the Princeton experimental setup.** - Leader Name: Francisco Marques Truyol, Leader Institution: UPC

» **Electro-chemical reactivity of defects and grain boundaries in 2D materials** - Leader Name: César González Pascual, Leader Institution: Universidad de Granada

» **Electrostatic microinstabilities and zonal flows in stellarator plasmas.** - Leader Name: Edilberto Sánchez, Leader Institution: Laboratorio Nacional de Fusion-CIEMAT

» First-principles modelling of grain boundaries in W - Leader Name: César González Pascual, Leader Institution: University of Granada

» **Flow topology in turbulent natural convection: direct numerical simulation and advanced turbulence modeling** - Leader Name: Assensi Oliva, Leader Institution: Universitat Politècnica de Catalunya

» **GPU codes for plasma physics simulations** - Leader Name: Jose E. Roman, Leader Institution: Universitat Politècnica de València

» **HPC - EUNISON: High Performance Computing Algorithms for the EUNISON project.** - Leader Name: Joan Baiges, Leader Institution: CIMNE

» **Improving the scalability of balancing substructuring domain decomposition methods for computational fusion** - Leader Name: Santiago Badia, Leader Institution: Universitat Politècnica de Catalunya & Centre Internacional de Mètodes Numèrics en Enginyeria

» **Large eddy simulations of the flow past a circular cylinder. Flow control mechanism by means of surface-roughness.** - Leader Name: Assensi Oliva, Leader Institution: Universitat Politècnica de Catalunya

» **Large-scale classical simulations of quantum system using the Trotter-Suzuki decomposition** - Leader Name: Peter Wittek, Leader Institution: ICFO-The Institute of Photonic Sciences, Spain

» **Molecular dynamics simulation study of the influence of cholesterol on ionic adsorption in biological membranes** - Leader Name: Jordi Marti, Leader Institution: Universitat Politècnica de Catalunya

» **Molecular Kondo Project - III** - Leader Name: Juan José Palacios Burgos, Leader Institution: Universidad Autónoma de Madrid

» **Multi-physics coupled simulations: interaction of turbulence with radiation. Application to direct numerical simulation of turbulent Rayleigh-Bénard convection in a radiatively participating medium.** - Leader Name: Assensi Oliva, Leader Institution: Universitat Politècnica de Catalunya

» **Nanoporous silicon for thermoelectric applications** - Leader Name: Riccardo Rurali, Leader Institution: Institut de Ciència de Materials de Barcelona (ICMAB) Consejo Superior de Investigaciones Científicas (CSIC) Campus de Bellaterra

» **Non-linear MHD modelling of pellet injection for ELM control in fusion plasmas** - Leader Name: Shimpei FUTATANI, Leader Institution: Barcelona Supercomputing Center

» **Numerical Simulation of Mixing Layers with variable density** - Leader Name: Oscar Flores, Leader Institution: Universidad Carlos III de Madrid

» **Particle-In-Cell simulations of laser-plasma interactions: From very intense to relativistic regime** - Leader Name: Javier Honrubia, Leader Institution: Universidad Politécnica de Madrid

» **Polymers for thermoelectric energy conversion** - Leader Name: Roberto DAgosta, Leader Institution: Universidad del Pais Vasco

» **Prediction of stabilization mechanisms for lean-premixed flames in a downscale stage can combustor using large-eddy simulation.** - Leader Name: Daniel Mira, Leader Institution: Barcelona Supercomputing Centre

» **Random Field Ising Model in four spatial dimensions and beyond** - Leader Name: Victor Martin Mayor, Leader Institution: Universidad Complutense de Madrid

» **Segregated Runge Kutta and Block precondtioners based on multilevel domain decomposition for the incompressible Navier Stokes equations.** - Leader Name: Santiago Badia, Leader Institution: Universitat Politècnica de Catalunya & Centre Internacional de Mètodes Numèrics en Enginyeria

» **Self assembly in active suspensions** - Leader Name: Ignacio Pagonabarraga, Leader Institution: University of Barcelona

» **Simulation of damage failure mechanisms in composites structures using high-performance computing technologies.** - Leader Name: Eva Casoni, Leader Institution: BSC-CNS

» **Study of STM conductivity throught Rare Earth Adatoms.** - Leader Name: Cesar, Leader Institution: Universidad de Zaragoza

» **Theoretical study of Majorana single-charge transistor using numerical renormalization group** - Leader Name: Alfredo Levy Yeyati, Leader Institution: Universidad Autónoma de Madrid

» **Time-resolved evolution of vorticity and momentum cascades in statistically stationary homogeneous shear turbulence** - Leader Name: Javier JIMENEZ Sendin, Leader Institution: School of Aeronautics, Universidad Politecnica Madrid, 28040-Madrid, Spain.

» **Understanding and optimizing turbulent transport simulations in stellarator plasmas with the GENE gyrokinetic code** - Leader Name: Jose Miguel Reynolds, Leader Institution: Universidad Carlos III de Madrid

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» **XUV/X-ray laser pulses for ultrafast electronic control in molecules** - Leader Name: Fernando Martín, Leader Institution: Universidad Autónoma de Madrid

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