SUMMARY
2016

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

WHO WE ARE

Barcelona Supercomputing Center – Centro National de Supercomputación (BSC) is the leader in supercomputing in Spain and a reference centre in this field internationally.

We are specialised in High Performance Computing. Our mission is: to offer infrastructure and supercomputing services to Spanish and European scientists; to generate knowledge and technology in Computer Sciences, Life Sciences, Earth Sciences and Engineering, and to transfer this knowledge and technology to society.

We are a Severo Ochoa Centre of Excellence, a Singular Scientific and Technical Infrastructure (ICTS), first-level members of the PRACE (Partnership for Advanced Computing in Europe) European research infrastructure and we manage the Spanish Supercomputing Network (Red Española de Supercomputación).

BSC is a public consortium formed of:

GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA, INDUSTRIA Y COMPETITIVIDAD

Generalitat de Catalunya
Departament d'Empresa i Coneixement

UPC
UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

OUR COMMITMENTS

Scientific and technical excellence

- To perform excellent, internationally-competitive research in Computer Sciences, Life Sciences, Earth Sciences and Engineering, using supercomputing as the main tool
- To promote cooperation between multi-disciplinary groups
- To attract and retain national and international talent
- To innovate by applying computing to unconventional fields

Support to e-science

- To provide competitive access to supercomputing infrastructures for researchers from a wide range of disciplines
- To support and train the scientific community in the use of supercomputing technologies

Wealth creation

- To collaborate with the private sector to promote the use of supercomputing as a tool for innovation and competitiveness
- To transfer cutting-edge supercomputing technologies to society
- To disseminate the benefits of supercomputing for companies and society
- To ensure the efficient management of public supercomputing resources

BSC in numbers

RESEARCH

33 Research groups

4 ERC Projects in progress

7 ICREA researchers

71 Researchers with personal scholarships

83 Projects in progress

17 Projects begun in 2016

#3 European Research Ranking

99 Articles in magazines — **66** In Q1

94 Articles in conference proceedings — **15** In A and A* conferences

2 Books published

10 Book chapters

279 Open access publications

21 Doctoral theses

31 Events organised

Conferences **2**

Workshops **9**

Severo Ochoa seminars **9**

Other events **11**

TECHNOLOGY TRANSFER

9 Patents approved or pending approval

1 Spin-off created

5 Joint centres with companies

18 Licensed or transferred technologies

2 Patents

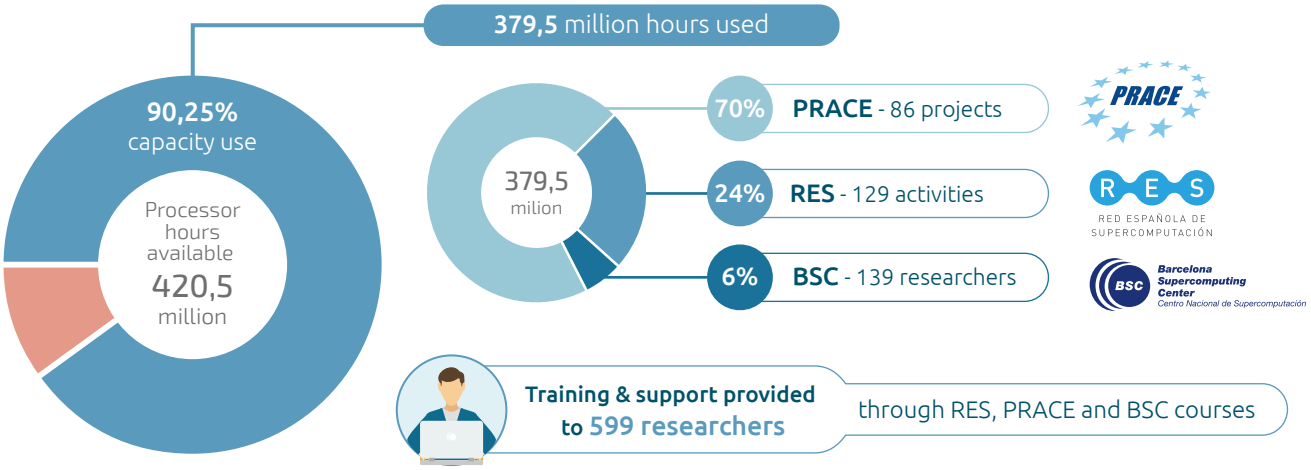
16 Software

Bilateral collaboration with companies

26 In progress

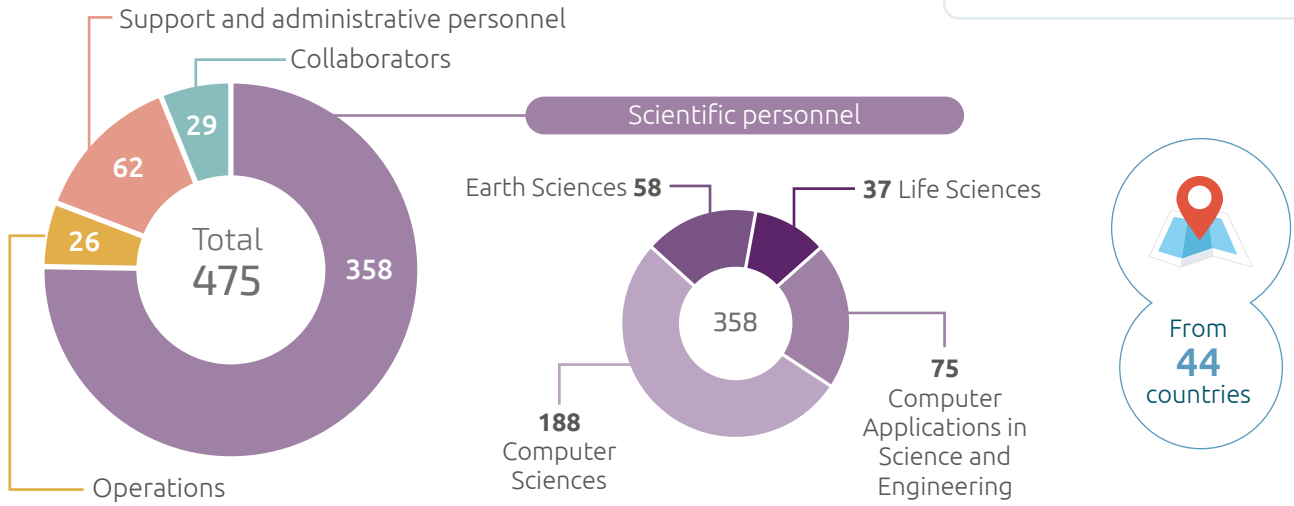
16 started in 2016

SUPERCOMPUTING

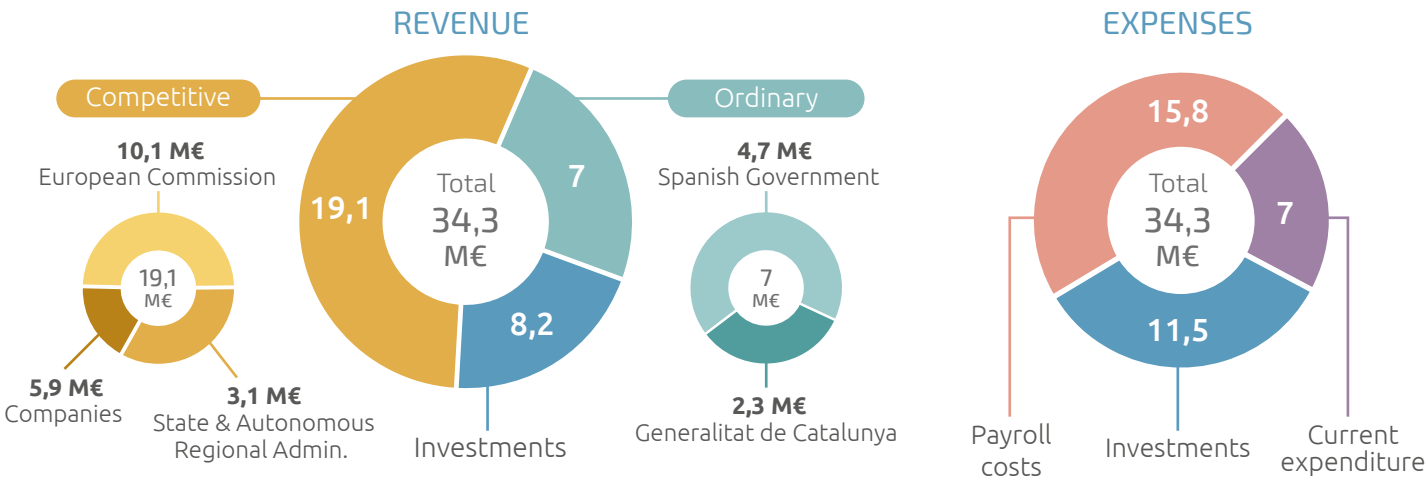


PEOPLE

Data as of 31st of December 2016



RESOURCES



UPC contributes, in terms of assigned staff and room space, the equivalent of 10% of regular income

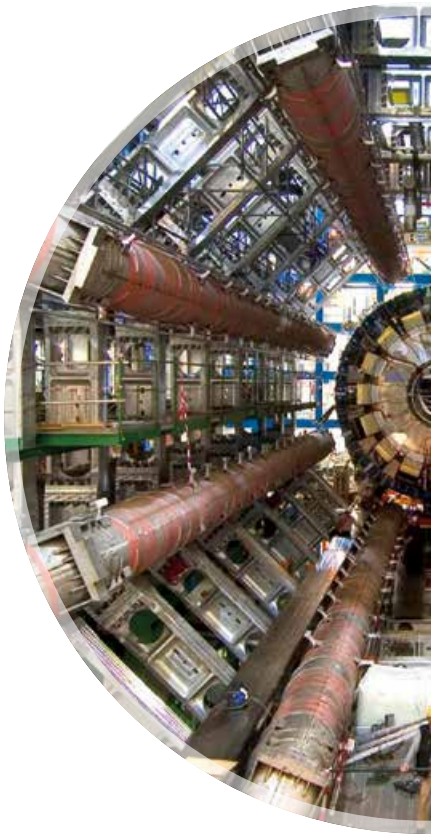
Infrastructures and services

From the handcrafted telescopes used by Galileo, to the particle accelerator in Geneva, scientific instruments have undergone huge technological advances.

As a consequence, the types of questions which science tries to answer have also changed. We want answers to questions about phenomena that can no longer be observed by a simple view nor with the help of optical instruments.

What is supercomputing?

Supercomputing enables scientific experiments by simulating "in silico" the behaviour of the object under study. Bringing together all the knowledge about the object of a computer simulation and experimenting with it, can reduce costs, avoid suffering and enable experiments to be conducted that could not be performed in the real world, because they would be too expensive, too dangerous or, simply, impossible.

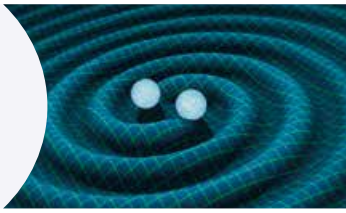


Supercomputers are also needed to analyse large amounts of data, such as those provided by scientific instruments (e.g. particle accelerators, large telescopes, interferometers or genome sequencing platforms) and the ever-growing number of devices that make up the Internet of Things.

High-performance computing has already become a great accelerator of science and engineering. It is used, and is increasingly being considered as essential, by the majority of scientific disciplines.

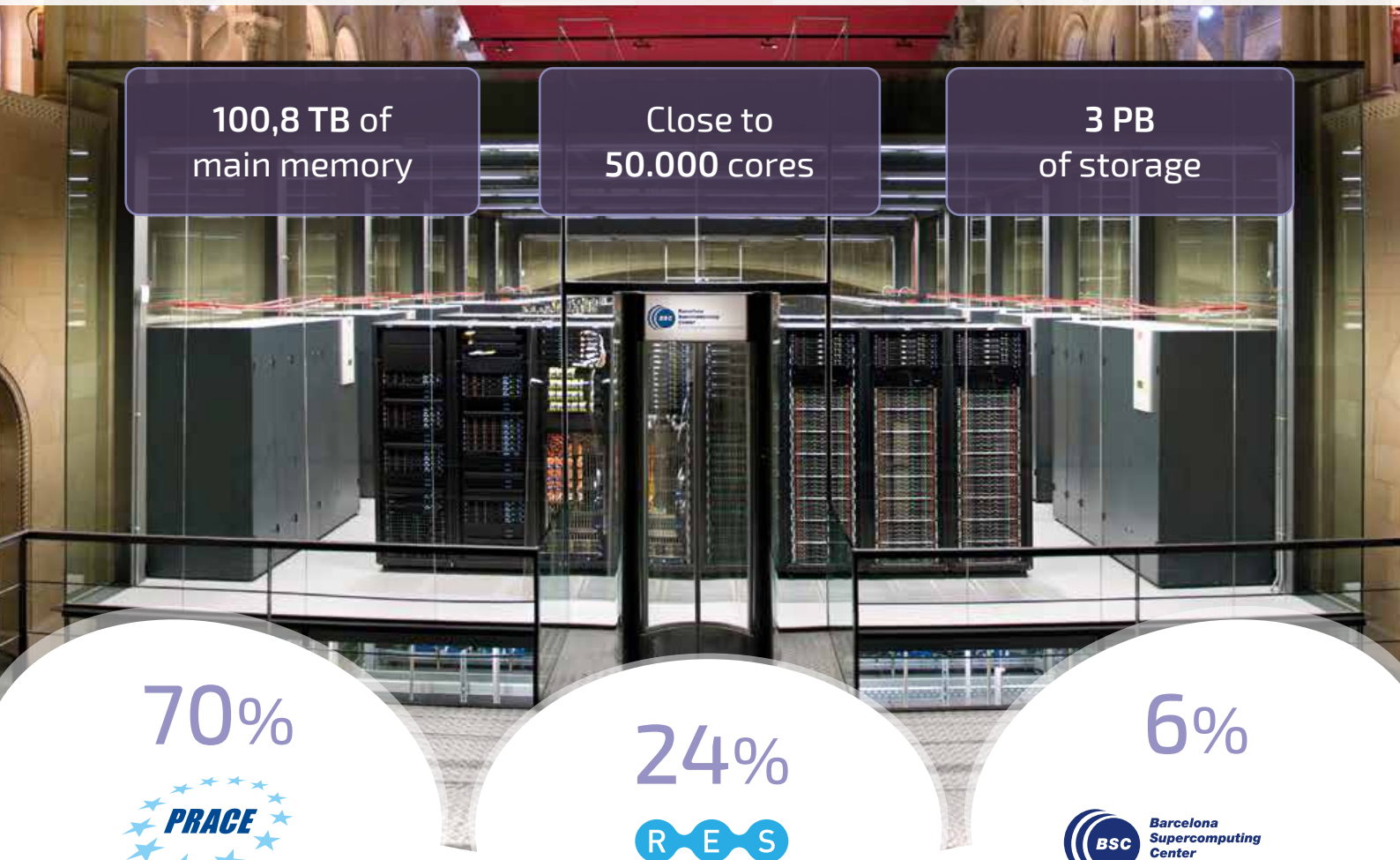
MareNostrum helps to detect gravitational waves

MareNostrum has collaborated in the detection of gravitational waves, one of the most celebrated scientific discoveries of 2015 and 2016. More than 16 million processor hours of the BSC supercomputer were used to run numerical simulations for the project, with data coming from the LIGO interferometers.



MareNostrum 3 Supercomputer

More than 10^{15} floating-point operations per second (1.1 Petaflops)



100,8 TB of main memory

Close to **50.000** cores

3 PB of storage

70%

PRACE

Access: prace-ri.eu/hpc-access

24%

RES

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

Access: bsc.es/res-intranet

6%

BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

1.1 Petaflops are 1,100 trillion (1.1 x 10^{15}) floating-point operations a second

Visit us and learn more about MareNostrum - Book your visit: visits@bsc.es

10.318 visitors from schools, universities, research centres and companies in 2016.

GOBIERNO DE ESPAÑA · MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD
UNIÓN EUROPEA
Infraestructura cofinanciada por el Fondo Europeo de Desarrollo Regional "Una manera de hacer Europa"

Infraestructuras Científicas y Técnicas Singulares

MareNostrum is the generic name that BSC uses to refer to the different updates made to its most emblematic supercomputer.

Meet MareNostrum 4

In 2016, we started to install the MareNostrum 4 supercomputer, which will become fully operational in the first half of 2017.

Top performance: 13,7 Pflops - 12 times more powerful than MareNostrum 3

General purpose computing: 11,1 Pflops 3.456 nodes with Intel Xeon V5 processors

Emerging technologies for the assessment of the Exascale (1018) systems for 2020:
3 systems with more than 0.5 Pflops each,
with Intel KNL/KNH, IBM Power + NVIDIA GPU, ARMv8

Storage: 15 Petabytes of GPFS, Elastic Storage System
Network: IB EDR/OPA, Ethernet
Operating system: SuSE

Exascale supercomputers, which are currently in the research stage, will be capable of performing one quintillion (10^{18}) floating-point operations per second.

Other BSC infrastructures

MinoTauro supercomputer

Heterogeneous cluster with NVIDIA GPUs.
343.74 Teraflops top speed.

Big Data infrastructures

Total capacity of 24.6 Petabytes
of storage of scientific data.

Research

BSC renews the distinction as a Severo Ochoa Centre of Excellence

The Ministry of Economy and Competitiveness renewed BSC's recognition as a Severo Ochoa Centre of Excellence. The Scientific Committee commended BSC for ***"having positioned itself as a leading and internationally recognised centre in supercomputing"*** and for its "*excellent results in the 2011-2015 period. The centre's research programmes in Computer Architecture, Parallel Programming and Supercomputing are first class, up there with the best from Japan, the USA and Europe*".

Awards

Xevi Roca receives a European Research Council Starting Grant

Xevi's project aims to create new simulation methods that respond to the challenges of the aviation sector. Roca has been working in the field of aviation simulation geometry since 2004. His research integrates the time dimension to the geometry of dynamic performance simulations and improves its efficiency, accuracy and robustness.

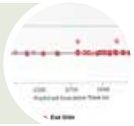
David Carrera is awarded the ICREA Academia distinction

The leader of Data-Centric Computing at BSC added this recognition to the ERC Starting Grant that he was awarded for the Hi-EST project: Holistic Integration of Emerging Supercomputing Technologies. Carrera´s research areas relate to Big Data, from applications management to the features of the behaviour of data centres.

Carlos Pérez García-Pando returns to the BSC with an AXA Chair

Carlos has worked at the NASA Goddard Institute for Space Studies, the International Research Institute for Climate and Society and the Department of Applied Physics and Applied Mathematics of Columbia University. He returned to BSC to take up the AXA Chair on Dust Storms and to lead the Atmospheric Composition Group.

New lines of research



Applied learning methods

Exploration of the use of learning techniques in different domains, from the optimising of data centres, to cancer genomics. The initiative uses the most advanced techniques in Machine Learning, Deep Learning and neural networks. Lead researcher: David Carrera

Supercomputing for Artificial Intelligence

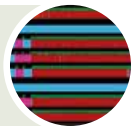
Research into the convergence of artificial intelligence and HPC, and its application to current challenges. Lead researcher: Jordi Torres

FPGA accelerators for deep neural networks

Research into, and implementation of neural network architectures and their respective learning algorithms in FPGAs. Lead researchers: Osman Unsal and Adrián Cristal

Disaggregated Computing

Neural and computing architectures for disaggregated memory systems. Lead researcher: Mario Nemirovsky

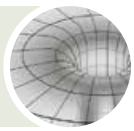


Development of OmpSs on FPGAs for the Internet of Things

OmpSs deployment on systems with small processing capabilities and memory capacity, with the need to process a variable amount of information coming from external sensors. Lead researcher: Xavier Martorell

Biochips

Generation of heart tissue from stem cells in order to obtain parameters that allow for customised simulations. Lead researcher: Mariano Vázquez. Collaboration with Michigan University



Mesh curves adapted for space-time flow simulations

Integration of the time dimension to the geometry of dynamic performance simulations in order to improve their efficiency, accuracy and robustness. Lead researcher: Xevi Roca. ERC Starting Grant

Biogas combustion Features

Combustion process analysis of biogas mixtures and the study of its application in industrial systems using high performance simulations. Lead researcher: Daniel Mira, within the HPC4E project

Noteworthy publications

Emergent Behaviours in the Internet of Things: The Ultimate Ultra-large-scale system

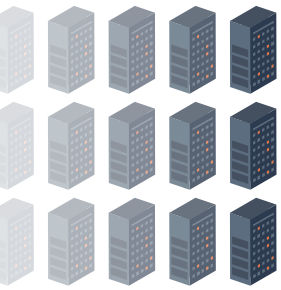
The article explores emergent hierarchical behaviours to solve complexity and orchestration problems in ultra-large-scale systems.

Authors: Damián Roca, Daniel Nemirovsky, Mario Nemirovsky, Rodolfo Milito, Mateo Valero. (IEE Micro, Dec. 2016)

Future Vector Microprocessor Extensions for Data Aggregations

This publication proposed extensions to vector processor instruction sets for database applications. It was presented at the International Symposium on Computer Architecture.

Authors: Timothy Hayes, Oscar Palomar, Osman S. Unsal, Adrián Cristal, Mateo Valero. (ISCA 2016)



Large-Memory Nodes for Energy Efficient High-Performance Computing

In this article, BSC researchers demonstrated that extending scalability in large memory nodes can acheive savings of up to 52% of the energy consumed by HPC systems.

Authors: Darko Zivanovic, Milari Radulovic, Germán Llort, David Zaragoza, Janko Strassburg, Paul Carpenter, Petar Radojkovic, Eduard Ayguadé. (**Best Paper MEMSYS'16**)

Reconstructing the plinian and co-ignimbrite sources of large volcanic eruptions: A novel approach for the Campanian Ignimbrite

The article describes a simulation that reconstructs in detail, the super volcanic eruption that slowed the expansion of modern humans in Europe.

Authors: Alejandro Marti, Arnau Folch, Antonio Costa, Samantha Engwell. (Nature Scientific. Feb. 2016)

Noteworthy publications

Attribution of extreme weather and climate events overestimated by unreliable climate simulations

This article attracted a lot of attention for its innovative approach to addressing the problem of attributing climatic anomalies to climate change caused by humans.

Authors: Francisco J. Doblas-Reyes i Omar Bellprat. (Geophysical Research Letters, 43)

Geophysical Research Letters
AN AGU JOURNAL

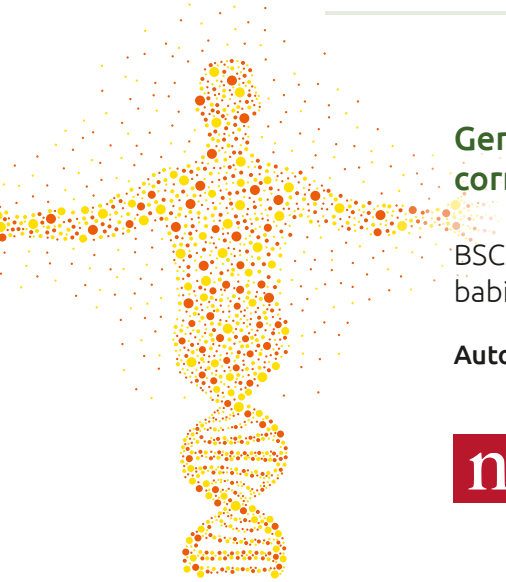
Using climate models to estimate the quality of global observational data sets

The quality of the models used to study climate change are constantly evaluated by comparing their predictions with the data provided by different climate monitoring systems.

The authors of the article, all from BSC, put forward an innovative proposal to study the reliability of these data.

Authors: François Massonnet, Omar Bellprat, Virginie Guemas, Francisco J. Doblas-Reyes (Science, 6311)

Science
AAAS



Genome-wide associations for birth weight and correlations with adult disease

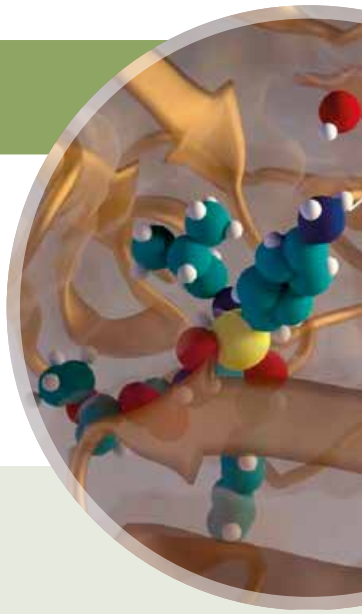
BSC was involved in this study on how genes influence the weight of babies and the diseases they may develop over their life course.

Autors: Momoko Horikoshi et al. (Nature, Oct. 2016)

nature

Technologies developed

BSC and IrsiCaixa create a bioinformatics method to predict the effectiveness of antiretroviral drugs against HIV mutations



- The method has been effective in predicting the resistance of viruses with genetic mutations in a protein of HIV-1 to the drugs Amprenavir and Darunavir.
- It makes predictions based on the features of each genetic mutation and the changes that this mutation causes to the proteins that act as therapeutic targets.
- The entire analysis can be performed in less than 24 hours using relatively small computers, which is available to any laboratory.

The comparative exercises financed by the National Institute of General Medical Sciences of the USA were "particularly impressed" with the results of the PELE software

The PELE software, produced by BSC to simulate the coupling of molecules in therapeutic targets, was given a prominent mention in the "CSAR Benchmark Exercises".

New version of Smufin, the BSC's software for detecting genetic alterations

BSC has developed a new version of Smufin (Somatic Mutations Finder), the BSC's computational method for detecting the genetic alterations responsible for causing tumours, was developed.

Smufin makes it possible to quickly, accurately and simply, detect the genomic changes responsible for the onset and progression of tumours.

The new version was implemented through hardware/software co-design and includes improvements in order to run on modern disaggregated hardware architectures with accelerators and non-volatile memory.

- **PARSECSs:** BSC made public PARSECSs, a suite of parallel reference based on tasks to help the scientific community to better develop, evaluate and understand task-based programming models, "runtime" systems and future multi-core architectures.
- **MUSA:** New multi-scale simulation approach to simulate next-generation HPC systems with thousands of cores. Musa is capable of modelling the communication network, the micro architecture details and the interactions of the system software, providing a quick simulation speed with high precision.
- **COMPSs 2.0:** A new version of COMPSs was made available, the task-based programming model that improves the performance of large-scale applications based on automatically parallelising their execution. The new version includes features such as integration with both persistent storage solutions and with the OmpSs programming model, including support for heterogeneous devices (GPUs).
- **Improvements to real time systems:** In the PROXIMA project BSC demonstrated that measurement-based probabilistic timing analysis simplifies the synchronisation of software in the presence of complex processors, and is beneficial for real-time systems used in the aviation and automotive industries.

Technology transfer

Launch of Nostrum BioDiscovery, a spin-off based on supercomputing to speed up pharmaceutical development

In July 2016, BSC and IRB Barcelona presented Nostrum BioDiscovery, a biotech company which uses computational simulation to speed up the discovery and launch to market of new pharmaceutical drugs and biotechnology molecules. The creation of this spin-off was made possible thanks to the collaboration of the Fundació Bosch i Gimpera of the University of Barcelona, the Institució Catalana de Recerca i Estudis Avançats (ICREA) and the Fundación Botín, which acted as a catalyst by providing support and advice and contributed to part of the start-up capital.

Agreement with CaixaBank to explore the application of cognitive computing to financial innovation

In May 2016 CaixaBank and BSC began collaborating on the development of advanced Deep Learning systems applied to banking services. The agreement aims to provide the financial institution with new tools to improve its service to customers and optimise operational efficiency.

BSC starts a three-year joint research collaboration with Lenovo

Lenovo and BSC initiated a three-year collaboration agreement to undertake joint research projects. The agreement includes using BSC performance analysis platforms, developing resource management environments based on the monitoring of performance and power consumption, analysing the feasibility of virtualised environments in HPC, and optimising Spark/Hadoop environments in supercomputing architectures.

IBM-BSC Deep Learning Centre is born

BSC and IBM renewed their collaboration and created the IBM-BSC Deep Learning Centre, in which research and development projects in the Deep Learning field will be carried out, paying special attention to the creation of new algorithms to improve and expand the cognitive capabilities of Deep Learning systems. In addition, research will be done into flexible computing architectures –essential for Big Data tasks– such as data centric systems and applications.

Strategic alliance for technological research and collaboration with CISCO

BSC and CISCO signed an agreement making them into technological and research partners. The aim is to reinforce their collaboration by sharing knowledge, synergies and technical and human resources to research and design advanced solutions in cutting edge technological areas, including the Internet of Things, Fog Computing/Smart Cities and computing platforms for data centres.

BSC's dust storm forecasting system will be used to improve the safety of business flights

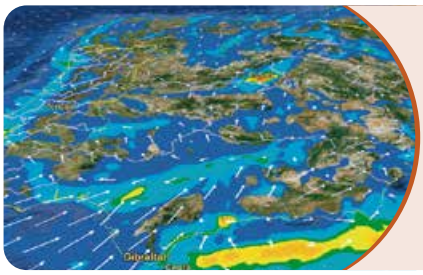
The dust and sand storm forecasting system will be incorporated into the planning tools of ARINCDirect flights offered by Rockwell Collins, an American company whose systems and electronic devices are used by aviation companies all over the world.

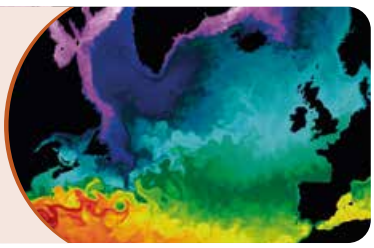
Collaboration with Vortex Bladeless for an innovative wind power system

BSC started collaboration with Vortex Bladeless S.L. to simulate the operation of an innovative wind power device. The aerodynamics simulations and fluid-structure interaction of the device will be done using the Alya code, developed by BSC.

The CALIOPE system incorporated into the proposal for Intelligent Cities of Vodafone Spain

Vodafone incorporated BSC's air quality forecasts into its portfolio of services for Smart Cities. The CALIOPE system forecasts will form part of the "Vodafone Connected City", the intelligent solutions service for public administrations.





Optimisations of NEMO

Optimisations of NEMO, the global European oceanographic model, created by BSC were included in the latest versions of NEMO 3.6 and EC-Earth 3.2. models. These modifications will help save hundreds of millions of hours in climate and ocean simulation around the world.

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