Barcelona Supercomputing Center
Centro Nacional de Supercomputación

SUMMARY **2022**

Who we are

The Barcelona Supercomputing Center – Centro Nacional de Supercomputación (BSC) is the leader in supercomputing in Spain and an international centre of reference in this field.

We are a multidisciplinary research centre of reference. We host high-performance computing infrastructures, which are at the service of the international scientific community.

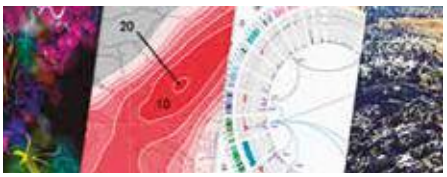
We are Tier-0 members of the European HPC infrastructure PRACE, we manage the Spanish Supercomputing Network (RES), a Singular Scientific and Technical Infrastructure (ICTS) that distributes HPC and data management resources, and support the international biomedical community, coordinating the Elixir and INB-ISCIII infrastructures.

Created in 2005 based on the experience of fruitful collaborations between the public authorities and private companies, such as CEPBA and CIRI, we have quickly grown from a staff of 60 people to around 800, thanks to the continuous commitment of our trustees and our ability to raise competitive funds from companies and public institutions.

We have installed four consecutive versions of the MareNostrum supercomputer and we are currently preparing the fifth version.

BSC's missions

Supercomputing services for Spanish and European researchers



R&D in Computer, Life, Earth and Engineering Sciences

Knowledge transfer (education, tech transfer and public engagement)

BSC is a public consortium made up of:

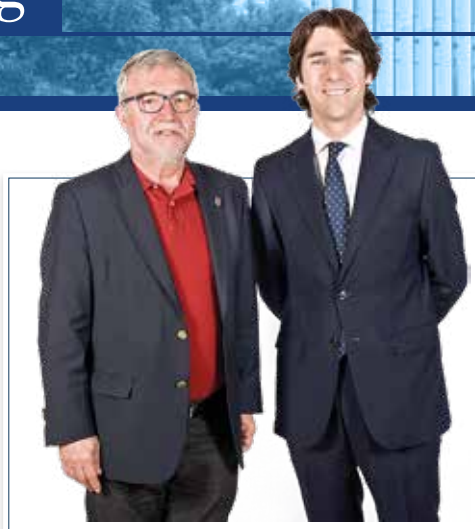
Generalitat de Catalunya
Departament de Recerca i Universitats

Gobierno de España
Ministerio de Ciencia e Innovación

Universitat Politècnica de Catalunya
BarcelonaTech

Where **we are**, where **we are going**

If we had to define 2022, we could use a word that, seen with the perspective that the pandemic and all its repercussions have given us, now makes much sense. This word is none other than a reunion. For us, it has been a year of reunion for all the people who are part of the centre with colleagues who, for various reasons, remained in their countries or places of origin, awaiting the arrival of the normality that would allow them to return to presence.



Mateo Valero and **Josep M. Martorell**
Director and associate director of BSC

The year 2022 has also been the year of reunion with the Severo Ochoa Centre of Excellence accreditation, which BSC had already held on two occasions (2012-2015 and 2016-2020). Last November, the State Research Agency (AEI) announced the resolution of the 2021 call to grant this type of accreditation, which includes 56 Spanish research institutions. This announcement represents the recognition of the project proposed by BSC for the 2023-2026 program, which combines actions to strengthen the centre's leadership in Open Hardware and Software and in the co-design of HPC applications, as well as efforts to promote diversity, education, technology transfer and dissemination of results.

Under the premise that equal opportunities are an essential criterion for attracting and retaining talent in a context where diversity is a source of incalculable value, one of the critical pieces of BSC project for the Severo Ochoa 2023-2026 program is the equality plan. This roadmap includes a series of actions and measures to guarantee effective equality of treatment and opportunities between women and men who develop their professional careers at our centre, eliminating any direct or indirect discrimination due to sex.

This year has also been crucial for our institution since, thanks to the efforts made by our centre, the Spanish, Portuguese and Turkish governments, as well as the EuroHPC Joint Undertaking, the MareNostrum 5 acquisition contract was signed in the middle of the year. A few months later, around December, the first components of what will be one of the most powerful supercomputers in the world started arriving at our house.

We also received another piece of good news from the supercomputing consortium of the European Union. BSC was selected as one of the six centres hosting the first EuroHPC quantum computer. The new quantum computer will be installed at BSC. It will have the potential to significantly increase the impact of research and innovation by enabling solutions that exceed the capabilities of current supercomputers.

Another adjective that also defines this year for us is intense. After several months of intense and fruitful negotiations with Intel last May, BSC and Intel announced our agreement to jointly create a leading laboratory to develop a new generation of supercomputers that will break the zettascale barrier. This agreement includes the design of microprocessors or chips with technology based on open hardware of the RISC-V type. This joint laboratory, the first in Europe to design this type of chip, will allow us to contribute to our continent's digital sovereignty strategy.

The intensity, excellence and dedication with which our researchers work and the important support structure at their disposal have borne fruit in consolidating the outstanding position of our centre as a national and international institution in the participation, management and coordination of competitive public and private projects. At the national level, the BSC-CNS is the fourth institution to return funding from the Horizon Europe framework program, the largest funding program in the world for research and innovation. At a European level, we are the institution that participates in more s of Excellence in supercomputing applications, while, at an international level, BSC is part of the main HPC initiatives and associations of worldwide reference.

Undoubtedly, it has also been a year of intense work for two of the most emblematic projects in natural language processing. While AINA went out on the streets to capture voices that helped generate the first corpus of Catalan and managed to go from 6,665 in 2021 to 30,888 in 2022, MarIA trained its model with more than 135 billion words in Spanish, the equivalent of 360,000 Don Quixotes. We must also remember that these two projects are part of the Strategic Project for Economic Recovery and Transformation (PERTE) of the New Language Economy of the Spanish government's Recovery Plan.

The unique capabilities of our centre have led us to be a key element in the Destination Earth (DestinE) initiative of the European Union (EU), which will develop the so-called digital twins of the Earth to help to predict the effects of climate change and increase its resilience.

We do not doubt that 2022 has been the year of reunion and the arrival of very positive news for our centre. We are sure that 2023 will be a year full of challenges, which we will face with the same enthusiasm and strength as always, and opportunities, which we will try to make the most of to keep moving forward and help meet the significant challenges that we have to face on a global level as a society and, in turn, put our grain of sand in scientific progress.

The three BSC trustees have appointed new representatives to BSC's Governing Board

Raquel Yotti
President
Secretary General of Research

Joaquim Nin
Vice-president
Secretary General of Research and Universities

Gonzalo Arévalo Nieto
Director General of Research Planning

José Ignacio Doncel
Deputy Director General of Large Scientific and Technical Facilities

Joan Gómez Pallarès
Director General of Research

Lluís Juncà
Director General for Innovation, Digital Economy and Entrepreneurship

Daniel Crespo
Rector

Jordi Llorca
Vice-Rector for Research

Generalitat de Catalunya
Departament de Recerca i Universitats

GOBIERNO DE ESPAÑA MINISTERIO DE CIENCIA E INNOVACIÓN

UPC UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH

BSC in numbers

Research

Data as of December 31, 2022

63 Research groups

7 ERC projects in progress

10 ICREA researchers

70 Researchers with personal fellowships

Horizon Europe **€19.5 M**

3rd highest return of any Spanish organisation in Horizon Europe

150 H2020 & Horizon Europe projects in progress

21 Horizon Europe projects begun in 2022

16 H2020 & Horizon Europe projects coordinated by BSC

BSC participated in 12 of the 15 European centres of excellence for HPC applications

We participated in **12**

We led **4**

325 Articles in peer-reviewed journals

244 in Q1

23 Doctoral theses

214 Open-access publications

57 Papers in conference proceedings

25 In A and A* conferences

1 Book published

8 Chapters in published books

Technology transfer

Data as of December 31, 2022

Technologies transferred or licensed

5 Patents

4 Methodologies

21 Software

11 Spin-off created

Billateral collaborations with companies

37 In progress

11 Started in 2022

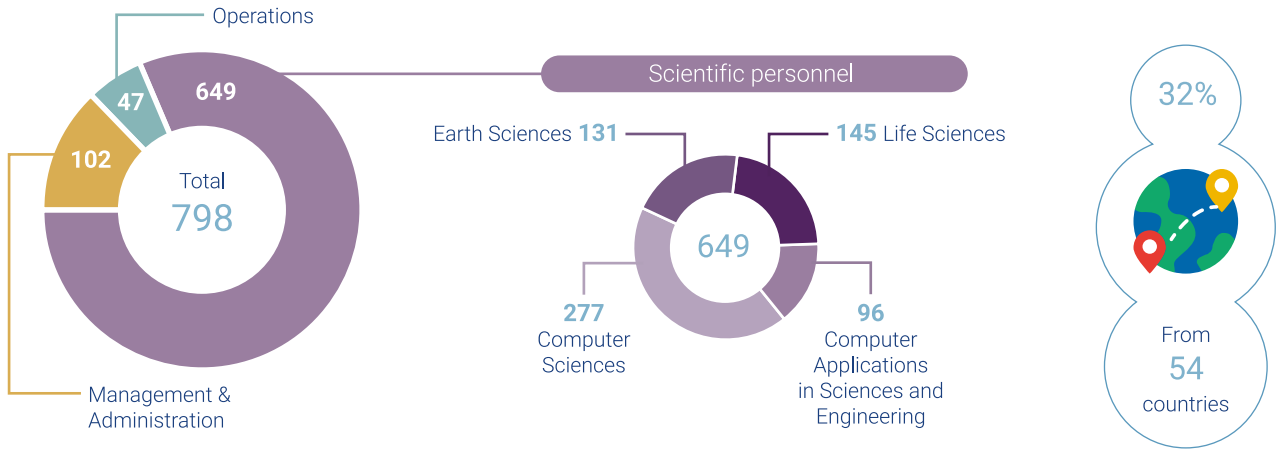
31 Patents approved or pending approval

Supercomputing

Data as of December 31, 2022

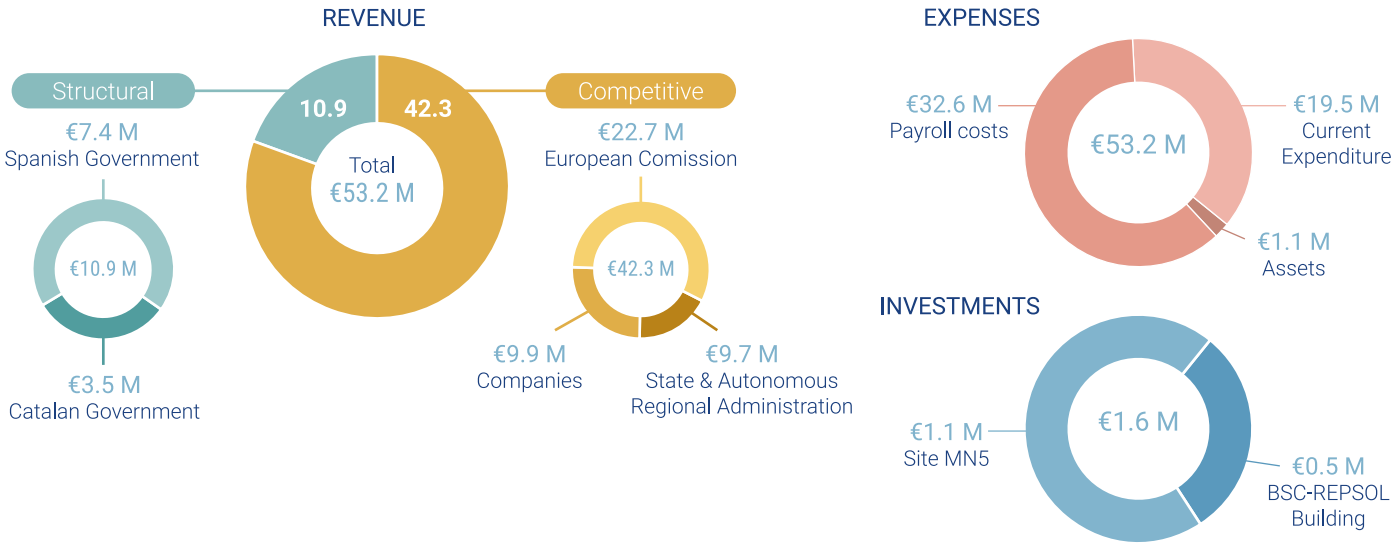
People

Data as of December 31, 2022



Resources

2022 executed budget



UPC contributes, in terms of assigned staff and room space, the equivalent of 10% of structural funds.

Revenue and expenses according to finance criteria. Investments according to budgetary criteria. Estimated data prior to the end of the 2022 financial year and the formulation of the annual accounts.

BSC and INTEL to set up a joint laboratory to develop zettascale supercomputers

During the 2022 ISC conference in Hamburg, the Barcelona Supercomputing Center (BSC) and Intel announced an agreement to jointly set up a pioneering laboratory to develop a new generation of supercomputers that will break the zettascale barrier.

This agreement includes the design of microprocessors or chips with technology based on RISC-V open-source hardware. The joint laboratory will enable Europe to be autonomous in the creation of these types of chips, which can be used worldwide in the design of self-driving cars or devices for artificial intelligence applications.

Mateo Valero, the director of BSC, emphasized during the announcement that "one of the objectives of this laboratory is for future European supercomputers, such as MareNostrum 6 in 5 years' time and many others worldwide, to incorporate technology developed there. This laboratory will also help to create an innovation hub for new companies and jobs."

Jeff McVeigh, the vice-president and general manager of the Supercomputing Group at Intel, said: "High-performance computing is the key to solving the world's most challenging problems, and Intel has an ambitious goal to accelerate this field into the zettascale era. BSC shares our vision, with the same emphasis on sustainability and an open-source approach. We are excited to be embarking on this new journey."

This joint laboratory will receive investment of up to €400 million over 10 years. These funds will come from Intel and from the Spanish Government through PERTE Chip within the framework of the Recovery, Transformation and Resilience Plan, approved by the Cabinet at the end of May.

BSC implements a new equality plan to apply gender equity criteria

Last September, BSC presented its new Equality Plan, which includes a series of actions and measures to guarantee effective equality of treatment and opportunities between women and men who develop their professional careers at BSC, eliminating any type of direct or indirect discrimination based on sex.

The new priority objective of BSC's Equality Plan is to adopt a joint policy to guarantee real and effective equality of opportunities between women and men at BSC, for which it proposes 44 specific actions in eight work areas: Organizational Culture, Recruitment and Hiring, Training, Promotion and Personal Development, Remuneration, Joint Responsibility for Exercising Personal, Family and Work Life Rights, Inclusive Communication and Prevention and Action against Sexual Harassment and Sex-based Harassment.

Several strategic objectives have been established in each work area: consolidate the value of equality in the organization; reduce segregation in staff recruitment and professional promotion processes; ensure equal opportunities through training; guarantee equal pay for men and women; provide a professional, personal and family life balance; and guarantee a workplace free of discrimination and sexual harassment.

The Equality Plan 2022-2026 is the result of collaborative work and the time and effort dedicated by the Human Resources department, the Works Council, the Equity Committee, the Women in Science initiatives of each scientific department, as well as all BSC staff who have actively participated in the working sessions.

European Commissioner for Research Mariya Gabriel visits BSC's facilities

Last May, Mariya Gabriel, the European Commissioner for Innovation, Research, Culture, Education and Youth, visited the facilities and infrastructures of the Barcelona Supercomputing Center, together with Diana Morant, the Minister of Science and Innovation; Pere Aragonès, the President of the Catalan Government.

The visit was also attended by Raquel Yotti, the Secretary General for Research at the Ministry of Science and Innovation; Gemma Geis, the Catalan Government Minister for Research and Universities; Victoria Alsina, the Catalan Government Minister for Action Abroad and Open Government; Daniel Crespo, the Rector of Universitat Politècnica de Catalunya, and Laia Bonet, Deputy Mayor for the 2030 Agenda, Digital Transition, Sport and Territorial and Metropolitan Coordination of Barcelona City Council.

Both the commissioner and the other esteemed guests were able to see first-hand the chapel that houses the centre's current supercomputer, MareNostrum 4, as well as the facilities that will house the future MareNostrum 5, which will come into operation in 2023.

During the visit, Gabriel highlighted the key role of this "strategic infrastructure" in driving innovation across Europe and helping researchers find solutions to contemporary challenges.

The National Library of Spain commissions BSC to back up its entire digital collection, which could reach 4 petabytes by the end of 2023

BSC has entered into a strategic collaboration with the National Library of Spain (BNE), which archives Spain's bibliographic and documentary heritage. Under the agreement, our centre will provide initial storage space of 5 PB in the Agora infrastructure. The goal is to host a full backup copy of the library's digital data. The current collection includes 400,000 deposited titles, 115,000,000 digitized pages and 17,122 million collected URLs. It is currently estimated at 2.4 Petabytes, although the initial forecast for the end of 2023 is to reach 4 Petabytes of filled storage.

As part of this collaboration, BSC and the BNE will facilitate access to these digital resources through calls for data exploitation projects by the Spanish Supercomputing Network (RES) to promote their use as a means of cultural, social and economic enrichment. There will thus be controlled access for data mining and research support, in accordance with the BNE's conditions and legal obligations. The data will always be kept in BSC's Agora infrastructure.

BSC achieves Severo Ochoa Centre of Excellence accreditation

The Ministry of Science and Innovation awarded BSC the Severo Ochoa Centre of Excellence accreditation. This is the highest national award for Spanish research institutions that stand out for the quality and impact of their research and for their scientific leadership at the national and international level.

Severo Ochoa Centre of Excellence accreditation is accompanied by €4 million in government funding over four years (2023-2026). The aim is to support ongoing projects, enable the opening of new lines of research, and help the centre raise its international scientific profile. This is the third time BSC has received this accreditation. It previously obtained it in the 2012-2015 and 2016-2020 periods.

The centre achieved the accreditation for a third time in 2022, to carry out a series of measures aimed at continuous improvement during the period 2023-2027.

The specific objectives of the Severo Ochoa programme are:

- Improve the capacity of high-level research centres to organize and carry out their research.
- Improve their ability to attract, recruit, train and retain talent.
- Create and/or consolidate their relationships with other excellent research centres.
- Disseminate research results to the general public.

MareNostrum 5 procurement agreement signed

The European High Performance Computing Joint Undertaking (EuroHPC JU), the European supercomputing initiative created in 2018, and Atos, the selected supplier, signed the procurement agreement for MareNostrum 5, EuroHPC's new pre-exascale supercomputer, in June.

The MareNostrum 5 supercomputer will have a peak performance of 314 PFlops (per second) or 314 thousand trillion operations per second and more than 200 PB of storage and 400 PB of active archive. This supercomputer will be specially designed to support European medical research in the design of new drugs, vaccine development, virus spread simulations, as well as artificial intelligence applications and big data analysis.

Moreover, the new machine's first components began to arrive at BSC's facilities at the end of December.

BSC selected to host one of Europe's first quantum computers

Spain is one of six European countries selected by the EuroHPC JU to host and operate one of the first EuroHPC quantum computers. The new infrastructure will be installed at BSC and will be integrated into the MareNostrum 5 supercomputer, the most powerful in Spain and among the most advanced in Europe, in collaboration with Instituto de Física de Altas Energías (IFAE) and the International Iberian Nanotechnology Laboratory (INL) in Portugal.

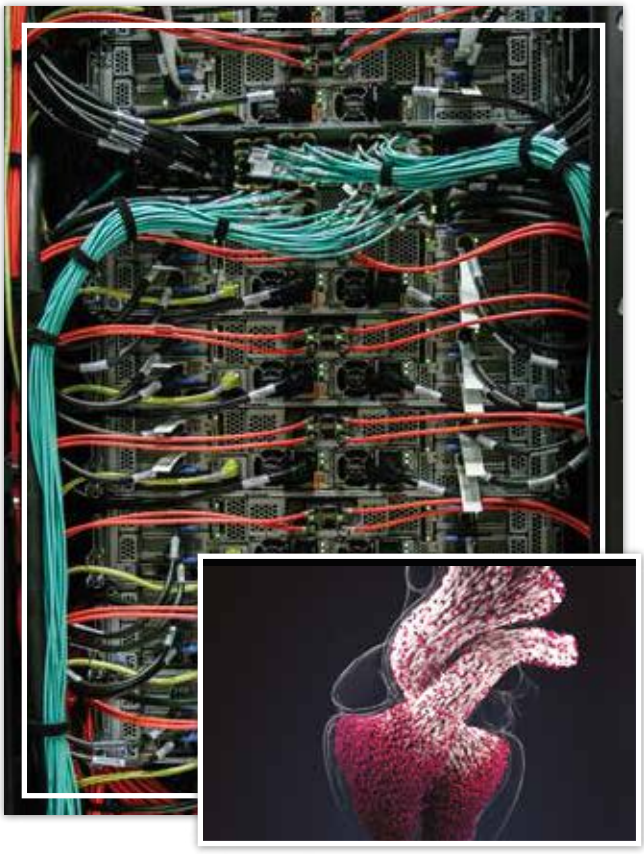
The new quantum computer to be installed at BSC will have the potential to considerably increase the impact of research and innovation by enabling solutions that exceed the capabilities of today's supercomputers. Spain's investment will be €12.5 million, co-financed 50% by the EU and the Secretariat of State for Digitalization and Artificial Intelligence (SEDIA), from the Ministry of Economic Affairs and Digital Transformation.

At the **service** of **science**

From Galileo's handcrafted telescopes to the particle accelerator in Geneva, scientific instruments have undergone an enormous technological evolution.

They have also changed the kinds of questions science seeks to answer. We want to answer questions about phenomena that cannot be observed with the naked eye or with the help of optical instruments.

What is supercomputing?



Supercomputing allows us to carry out scientific experiments by simulating the behaviour of the object os study in silico. Bringing together all the knowledge about this object in a computer simulation and experimenting with it makes it possible to cut costs, avoid animal suffering and perform experiments that could not be done in the real world, because they would be too expensive, too dangerous or simply impossible.

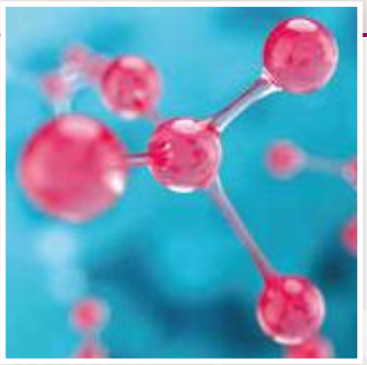
Supercomputers are also necessary to analyze large amounts of data, such as those provided by large-scale modern scientific instruments (particle accelerators, large telescopes, interferometers, genome sequencing platforms, etc.) or the ever-increasing number of devices in the Internet of Things.

It has been demostrated for years now that supercomputing is also the great ally of artificial intelligence, since its great calculation capacity aids the training of algorithms and drawing of conclusions from large amounts of data.

High-performance computing has already become a great accelerator for science and engineering. Most scientific disciplines use it to expand their frontiers of knowledge.

Research in MareNostrum 4

MareNostrum 4 provided 1,207 million processor hours in 2022 (292,460 Exaflops). 80% of these were allocated to researchers who gained access to the supercomputer through the Spanish Supercomputing Network (RES) or the Partnership for Advanced Computing in Europe (PRACE).



Elena Beatriz Martín Ortega
Segregation assessment in the manufacturing process of metal powder cored-wire

Núria López
Dynamic behavior of Earth-abundant heterogeneous (electro)-catalysts

Karolina Zofia Milowska
Combining low-dimensional carbon structures with organic-inorganic hybrid perovskites for sustainable energy generation

Maria Gonçalves
Significance of mineral dust composition towards aerosol radiative forcing in Earth System Models

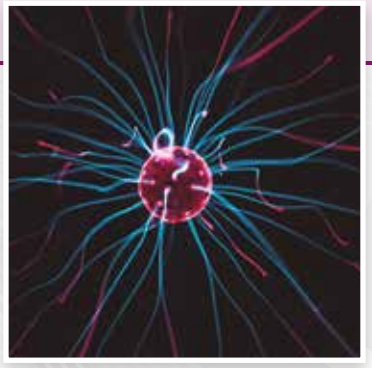
Manuel Ruiz Villarreal
Biophysical Model Datasets for Simulations of the Iberian Atlantic Ecosystem (PENDECO)

Carme Rovira
Computer simulation of disease-related carbohydrate-active enzymes

Iñaki Tuñón
Impact of Mutations on the Inhibition of SARS-CoV-2 Main Protease with Paxlovid

Rebeca García-Fandino
A database of innate immune system peptides and their cell membrane interactions

Cecilia Hognon
Design of new therapeutic and diagnostic strategies to fight COVID-19



Alicia Palacios Cañas
Free electron lasers applications for ultrafast molecular physics

Universidad Autónoma de Madrid

Nicolas Noirayn
Control of Combustion Instabilities Using Non-Equilibrium Plasma in Sequential Combustors

ETH zürich

Riccardo Broglia
Large Eddy Simulation of a Tip-Loaded Propeller (LESTLP)

Consiglio Nazionale delle Ricerche

Igor Abrikosov
Large-scale defect characterization and design for quantum technologies

LINKÖPING UNIVERSITY

Daniel Nóbrega Siverio
Coronal Bright Points on the Sun: a study from the photosphere to the corona

Universitat de les Illes Balears

Carlos Palenzuela
Magnetic field amplification and neutrino transport in the 100 ms after a binary neutron star merger

Providing a service for researchers all around Europe

The MareNostrum 4 supercomputer is available to researchers all around Europe. The Spanish Supercomputing Network (RES) and the European PRACE network allocate 80% of its computing capacity. This is assigned through open application processes in which researchers present their proposals, which are then assessed by scientific committees that are experts in the different scientific disciplines. The remaining 20% of the supercomputer's capacity is assigned to BSC research.

MareNostrum 4 has a maximum capacity of **13.9 PetaFlop/s** or, in other words, **13,900 trillion operations per second**

MareNostrum 4 is co-financed by the Intelligent Growth Operation Program 2014-2020 of the European Regional Development Fund (ERDF)

Unión Europea
Fondo Europeo de Desarrollo Regional "Una manera de hacer Europa"

Gobierno de España · Ministerio de Economía y Competitividad

Research **acknowledgements**

Mateo Valero is awarded an honorary doctorate by Universidad Cristóbal Colón in Mexico

Mateo Valero, the director of Barcelona Supercomputing Center (BSC), has been awarded an honorary doctorate in engineering and architecture by Universidad Cristóbal Colón in the city of Veracruz, Mexico. This is the first honorary doctorate awarded by this institution, which is inaugurating this new award by granting it to BSC's director.

The university gave this award to Mateo Valero "in recognition of his extraordinary contribution to the field of computing and his outstanding commitment to using information technologies for the service, development and wellbeing of society".

Leonidas Kosmidis receives the HiPEAC Tech Transfer Award 2021

Leonidas Kosmidis, a senior researcher at Barcelona Supercomputing Center (BSC), has won a HiPEAC tech transfer award for the second time. His winning technology, "GPU4S Bench: An open GPU benchmarking suite for space on-board processing," provides a resource to help evaluate the suitability of new high-performance devices such as graphics processing units (GPUs) for processing tasks normally found in space applications.

Antonio J. Peña is awarded an ERC Consolidator Grant for the "HomE" project

The European Research Council (ERC) has awarded an ERC Consolidator Grant to Barcelona Supercomputing Center (BSC) senior researcher Antonio J. Peña, the leader of the Accelerators and Communications for HPC team. Peña is the principal investigator in the ERC-awarded proposal, HomE (Enabling Homomorphic Encryption of Deep Neural Network Models and Datasets in Production Environments), which aims to enable the feasibility of privacy-preserving machine learning in untrusted environments, such as cloud services.

Forbes magazine recognizes Àtia Cortés as one of the 40 leading futurists in Spain

The researcher of the Social Link Analytics group of the life sciences department Àtia Cortés was designated by Forbes Spain magazine as one of the 40 best futurists in our country.

This list recognizes the 40 Spanish professionals who are dedicated to analyzing future scenarios, more or less distant, to prepare companies for the challenges they may face. International referents of prospective based in Spain or who maintain strong ties with our country have also been taken into account.

Francisco Cazorla and his team receive the "Best paper award" at the ECRTS conference

The CAOS (Operating System / Computer Architecture Interface) research group, led by Francisco Cazorla, received the "Best paper award" for their publication "Using Markov's inequality with power-of-k function for probabilistic WCET estimation" at the Euromicro Conference on Real-Time Systems (ECRTS).

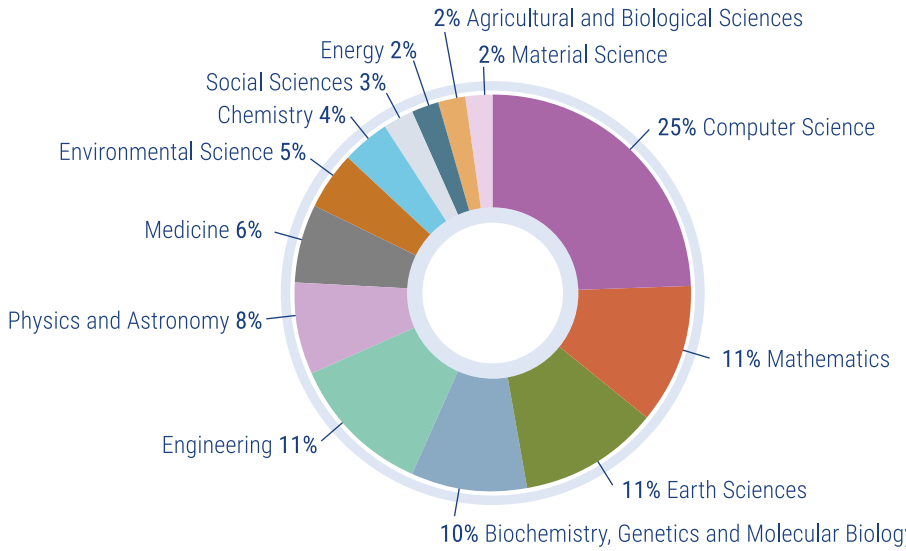
Scientific **impact**

One of the BSC's mechanisms to ensure the exploitation of the centre's scientific production is by publishing the main research results in the most appropriate media and channels for each of them, including works derived from doctoral theses. This section shows the multidisciplinary nature of the BSC research through the top journals where BSC researchers publish their results and their scientific domains, as well as the evolution of the scientific production of the centre in the last five years.

Top 10 journals with BSC publications in 2022

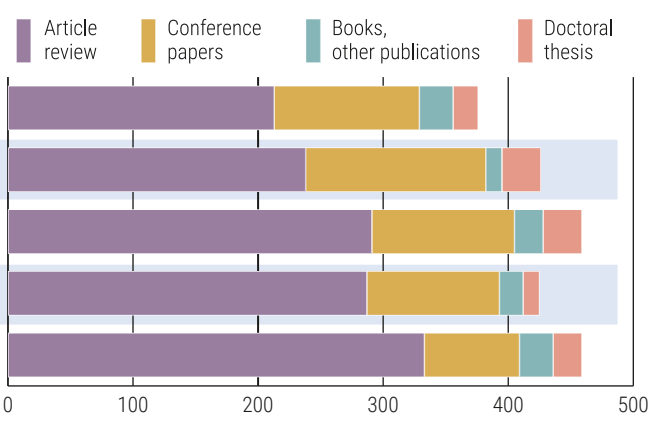
IEEE Conferences	33
Bulletin of the American Meteorological Society	12
Climate Dynamics	12
Nature Communications	12
Lecture Notes in Computer Science	10
Geoscientific Model Development	9
Atmospheric Chemistry and Physics	7
Nuclear Fusion	6
Nucleic Acids Research	5
Science of the Total Environment	5

Multidisciplinarity



Scientific output 2018 - 2022

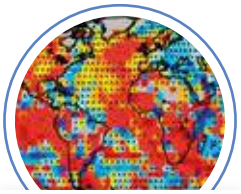
Year	Articles & review	Conference papers	Books, other publications	Doctoral Thesis
2018	213	116	27	20
2019	238	144	13	31
2020	291	114	23	31
2021	287	106	19	13
2022	333	76	27	23



Featured **publications**

The multidisciplinary nature of BSC can be seen in the wide range of fields in which researchers publish scientific articles.

Below is a selection of the most notable publications in 2022.



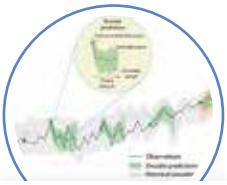
Earth System Dynamics

Constraining low-frequency variability in climate projections to predict climate on decadal to multi-decadal timescales – a poor man's initialized prediction system

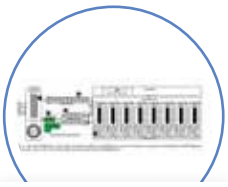
This paper introduces a new method to reduce the uncertainty from internal climate variability in estimates of near-term climate change in the next 20 years. This method was newly developed within the Climate Variability and Change Group at BSC, and the method was shown to improve the accuracy of near-term climate change predictions in many regions of the world. Mahmood, R., M. G. Donat, P. Ortega, F.J. Doblas-Reyes, C. Delgado-Torres, M. Samsó and P.-A. Bretonnière (2022). Earth System Dynamics, 13, 1437–1450. October 2022.

How decadal predictions entered the climate services arena: an example from the agriculture sector

Pioneering the application of the knowledge coproduction process to make actionable the latest climate sciences achievements on decadal timescale, this study is an excellent example of the potential of the interdisciplinary collaboration at the BSC's Earth Sciences Department. Solaraju-Murali, B., Bojovic, D., Gonzalez-Reviriego, N., Nicodemou, A., Terrado, M., Caron, L. P., & Doblas-Reyes, F. J. (2022). Climate Services, 27, 100303. August 2022.



Climate Services



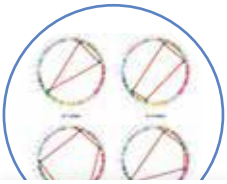
IEEE International Symposium

Adaptable Register File Organization for Vector Processors

This paper presents Adaptable Vector Architecture (AVA), a vector architecture designed for short vectors (MVL=16 elements) but with the functionality of reconfiguring the MVL, thereby allowing to exploit the benefits of having a longer vector of up to 128 elements microarchitecture when abundant DLP is present. AVA yields a 2X speedup over the default configuration for short vectors and shows competitive performance when compared to a design for long vectors while saving 50% of area. Cristóbal Ramírez Lazo, Enrico Reggiani, Carlos Rojas Morales, Roger Figueras Bagué, Luis A. Villa Vargas, Marco Antonio Ramírez Salinas, Mateo Valero Cortés, Osman Sabri Unsal, Adrián Cristal. IEEE International Symposium on High-Performance Computer Architecture (HPCA), pp. 786-799, May 2022.

Clustering and graph mining techniques for classification of complex structural variations in cancer genomes

We present a new statistical approach to analyze SVs patterns from 2,392 tumor samples from the Pan-Cancer Analysis of Whole Genomes (PCAWG) Consortium and identify significant recurrence, which can inform relevant mechanisms involved in the biology of tumors. The method is based on recursive KDE clustering of 152,926 SVs, randomization methods, graph mining techniques and statistical measures. The proposed methodology was able not only to identify complex patterns across different cancer types but also to prove them as not random occurrences. Gonzalo Gomez-Sanchez, Luisa Delgado-Serrano, David Carrera, David Torrents & Josep Ll. Berral. Scientific Reports, Nature, vol. 12, no. 3244. February 2022.

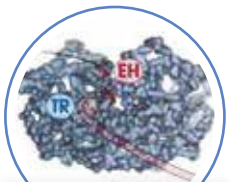


Scientific Reports

PerSVade: personalized structural variant detection in any species of interest

Genome Biology

Structural variants (SVs) underlie genomic variation but are often overlooked due to difficult detection from short reads. Most algorithms have been tested on humans, and it remains unclear how applicable they are in other organisms. To solve this, we develop perSVade (personalized structural variation detection), a sample-tailored pipeline that provides optimally called SVs and their inferred accuracy, as well as small and copy number variants. PerSVade increases SV calling accuracy on a benchmark of six eukaryotes. Miquel Àngel Schikora-Tamarit, Toni Gabaldón. Genome Biology. 2022 August 16. (doi:10.1186/s13059-022-02737-4).

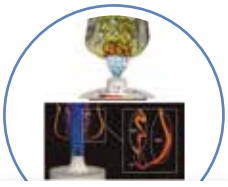


Angewandte Chemie

A Plurizyme with Transaminase and Hydrolase Activity Catalyzes Cascade Reactions

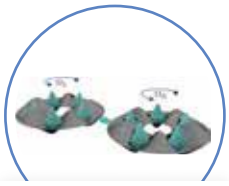
Engineering dual-function single polypeptide catalysts with two abiotic or biotic catalytic entities (or combinations of both) supporting cascade reactions is becoming an important area of enzyme engineering and catalysis. Herein we present the development of a PluriZyme, TR2E2, with efficient native transaminase (kcat: 69.49±1.77 min−1) and artificial esterase (kcat: 3908±0.41 min−1) activities integrated into a single scaffold, and evaluate its utility in a cascade reaction. TR2E2 (pHopt: 8.0–9.5; Topt: 60–65 °C) efficiently converts methyl 3-oxo-4-(2,4,5-trifluorophenyl) butanoate into 3-(R)-amino-4-(2,4,5-trifluorophenyl) butanoic acid, a crucial intermediate for the synthesis of antidiabetic drugs. Sergi Roda, Laura Fernandez-Lopez, Marius Benedens, Dr. Alexander Bollinger, Dr. Stephan Thies, Dr. Julia Schumacher, Dr. Cristina Coscolín, Dr. Masoud Kazemi, Dr. Gerard Santiago, Dr. Christoph G. W. Gertzen, Jose L. Gonzalez-Alfonso, Prof. Francisco J. Plou, Prof. Karl-Erich Jaeger, Prof. Sander H. J. Smits, Prof. Manuel Ferrer, Prof. Víctor Guallar. Angewandte Chemie (International ed. in English). 2022 September 12 (doi: 10.1002/anie.202207344).

Analysis of local extinction of a n-heptane spray flame using large-eddy simulation with tabulated chemistry



Combustion and Flame

The next-generation of propulsion technologies for medium and long range airliners mainly rely on liquid-fueled combustion operated with sustainable aviation fuels (SAF). In such systems, spray combustion plays a major role in the efficiency and pollutant control from the aeroengine, but the charactarization of this process remains challenging for both experimental diagnostics and numerical simulations. In this paper, we develop an efficient methodology to perform high-fidelity simulations of spray flames and we apply it to the study of local extinction in an aeronautical combustor. Comparisons of the simulations results with experimental data show excellent agreement demonstrating the validity of the proposed methodology, and detailed analysis of the results are used to obtain further understanding on the interactions between droplet evaporation, turbulence, and combustion. J Benajes, JM García-Oliver, JM Pastor, I Olmeda, A Both, D Mira. Combustion and Flame. Volume 235, January 2022, 111730.



Physical Review Research

Coherent phase slips in coupled matter-wave circuits

We simulate an atomtronic device to transfer and entangle states of different angular momentum in an ultracold gas by harnessing coherent phase slips. The device consists of a condensate gas confined in optical traps in the shape of two sided lattice rings, and where by switching on and off the tunneling between the rings, current in one ring is transferred to the other while maintaining the density in each ring constant. Axel Pérez-Obiol, Juan Polo, Luigi Amico. Physical Review Research 4, L022038, May 2022.

Research & Innovation

BSC and Lenovo form a partnership to advance supercomputing technology

Lenovo will invest $7 million over three years—the largest sum the company invests in research in Spain—to advance precision medicine through the use of supercomputing, the design and development of European open-source chips (RISC-V), and the creation of more supercomputers and energy-sustainable data centres. This collaboration is the result of six years of joint work by BSC and Lenovo.

In this context, the BSC team led by researcher Miquel Moretó will study genomic analysis algorithms to design new accelerators that will be integrated into the HPC platforms of the future. These will improve the efficiency of these highly-sophisticated analyses. Moreover, through joint research, BSC and Lenovo will seek to build more energy-efficient, sustainable and cost-effective supercomputers and data centres. The group coordinated by researcher Julita Corbalán will lead this challenge at BSC.

Danlaw, a world leader in automotive and connected cars electronics, acquires the Maspatechnologies SL spin-off

Danlaw Inc., a leading global provider of electronic solutions for the automotive and aerospace industries, has acquired Maspatechnologies SL, a BSC spin-off. Maspatechnologies is now part of the Rapita Systems group, owned by Danlaw. It will operate as Rapita Systems SL from its offices in Barcelona.

The acquisition expands multicore verification expertise within the Rapita Systems group and provides the industry with a comprehensive solution for analyzing and certifying the next generation of integrated multicore avionics and automotive systems.

Maspatechnologies develops software technology to verify and certify the timing behavior of applications on multicore processors used in safety-critical embedded systems.

Key role for BSC in EU's bid to fight climate change: a virtual replica of Earth

BSC is participating in the development of the so-called digital Earth twins, as part of the European Union's Destination Earth (DestinE) initiative. The aim is to create, with high precision, a virtual replica of the Earth system to predict the effects of and build resilience to climate change. With a total budget of around €4.5 million, BSC is one of the European institutions with the largest contribution in this first round and one of the few participating in both twins.

DestinE is an ambitious initiative that combines the green transition driven by the EU and the Digital Europe Program in an effort to find solutions to the climate change crisis.

The initiative has an initial investment of €150 million from the Digital Europe Program until mid-2024. It is being implemented by three organizations: the European Centre for Medium-Range Weather Forecasts (ECMWF), the European Space Agency (ESA) and the European Organization for the Exploitation of Meteorological Satellites (EUMETSAT).

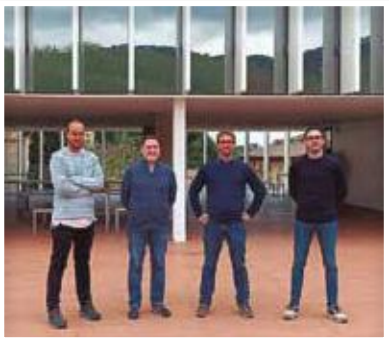
It will be carried out over a 7 to 10-year period, after which a complete digital replica of the Earth will have been created through the convergence of the digital twins developed. This reproduction will make it possible to monitor and predict the state of our planet's health, taking into account the effects of climate change and the evolution of natural systems such as the oceans, atmosphere and forests. It will also provide stakeholders with an assessment of the effectiveness and impact of public policies on the environment.

The Lancet Countdown in Europe shows the impact of climate change on public health

The Lancet Countdown in Europe 2022 report on Health and Climate Change highlights an alarming increase in health-related hazards, vulnerabilities, exposures and impacts of climate change across Europe. The paper puts on the table the urgent need for ambitious mitigation targets to restrict the global temperature rise to less than 1.5°C above pre-industrial times, as well as effective adaptation strategies to build resilience to the growing health threats of climate change.

The Lancet Countdown in Europe (LCDE), the European Regional Centre of The Lancet Countdown, is led by BSC and co-directed by the Barcelona Institute for Global Health (ISGlobal), a centre supported by "Fundación la Caixa". The initiative is a collaboration between 44 leading researchers, which was set up to look at the relationship between health and climate change in Europe, and shape a robust, evidence-based response that can protect human health in Europe and beyond.

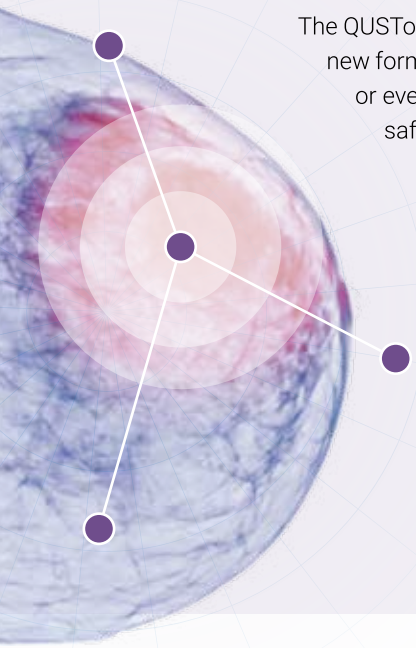
A BSC study establishes a methodology to mitigate energy crises in Europe through climate predictions



A new study by BSC scientists led by Francisco Doblas, head of the Department of Earth Sciences, and Llorenç Lledó, a researcher in the same department, has shown for the first time how changes in planetary-scale atmospheric circulation patterns—known as teleconnections—affect renewable energy generation in different European countries.

According to the study's authors, the results are of particular relevance to the future of electricity systems in Europe, as they propose a method for forecasting variations in renewable energy generation months in advance through climate predictions. These forecasts can be of great use to electrical grid operators in scheduling alternative energy sources; to distributors in estimating electricity prices; and to governments in preventing energy price shocks.

BSC coordinates a project to use supercomputing to detect breast cancer more effectively



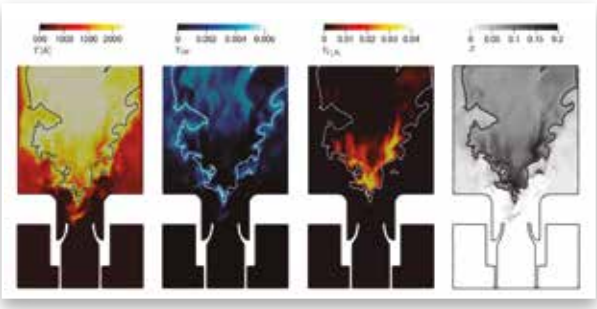
The QUSTom (Quantitative Ultrasound Stochastic Tomography) project, coordinated by BSC, seeks to introduce a new form of medical imaging based, for the first time, on ultrasound and supercomputing. This will supplement or even replace current techniques using X-rays such as mammograms. This technology will be completely safe for patients since it does not use any kind of radiation. It also provides superior image quality and enables better monitoring of tumors, among other advantages.

The algorithms to be developed for medical imaging will provide two kinds of images simultaneously: the image of the patient's tissue, and the image of its associated uncertainty. This shows, pixel by pixel, how reliable the information is. The project also incorporates concepts such as multimodality imaging and real 3D imaging, which is an unprecedented combination in ultrasound breast imaging.

The project has five other partners in addition to BSC: Karlsruher Institut für Technologie, Vall d'Hebron Research Institute - VHIR, Arctur and FrontWave Imaging, a BSC and Imperial College London spin-off, which is aligned with this project's objectives, in addition to Imperial College London itself as an associate partner. Physicists, engineers, data exploitation experts and radiologists will thus work together to develop the next generation of radiation-free, precise and scalable diagnostic tools for breast cancer.

The ESTiMatE project provides insight into soot formation in aircraft engines

The ESTiMatE project has developed a set of advanced techniques to better understand the soot formation process in aircraft engines, three years after its began. The researchers have focused on developing advanced soot models based on fundamental principles that can be integrated into Computational Fluid Dynamics (CFD) codes.

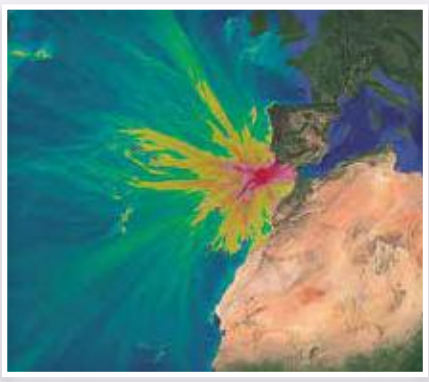


The main effort was invested in the appropriate description of the chemical kinetics of PAHs (polycyclic aromatic hydrocarbons), such as benzene, naphthalene and pyrene, etc. PAHs play a key role in soot nucleation. Reliable chemical models are thus needed to correctly represent this initial process. To do this, flames were measured over a wide range of conditions, and large databases with detailed information on thermodynamic states were generated.

The ChEESE project creates exascale technologies to mitigate potential geohazards

After three and a half years of research, the Center of Excellence for Exascale in Solid Earth (ChEESE), financed with European funds, has succeeded in developing geohazard mitigation simulation codes and applications that can be used to support public and private sectors in decision-making related to earthquakes, volcanoes and tsunamis.

The potential services developed by ChEESE have been tested in high-performance computing facilities such as MareNostrum 4 and SuperMUC-NG at Leibniz Supercomputing Centre (Germany). The services include: using urgent supercomputing to create seismic motion maps, performing fast and robust tsunami simulations, and assessing the seismic hazard based on physics with state-of-the-art multiphysics seismic simulation software, among others.



BSC coordinates a project to create a European digital environment to speed up cancer research

Together with ELIXIR, BSC is coordinating the EOSC4Cancer project, a European digital ecosystem of shared data to accelerate cancer research. The initiative, funded with nearly €8 million by the European Union (EU), will enable secure, federated access to various types of cancer data across European borders, with the aim of processing and reusing information from cancer research across the EU.

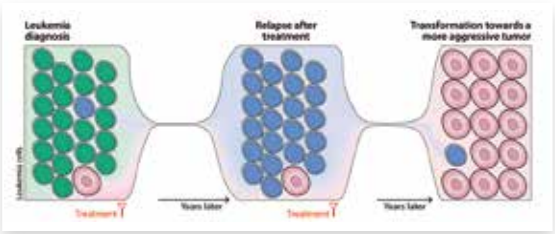
The project, a key part of Horizon Europe's European Mission on Cancer, brings together a consortium of 29 organizations from 13 countries coordinated by BSC. These include cancer research centres, scientific infrastructures, leading research groups, hospitals and supercomputing centres.

The purpose of EOSC4Cancer is to aid cross-country interoperability of genomic, imaging, medical, clinical, environmental and socioeconomic data through appropriate analysis environments, including machine learning and artificial intelligence.

Through five use cases, EOSC4Cancer covers the entire cancer patient journey, from prevention through diagnosis to treatment. Each step leaves a data trail, which is systematically organized into relevant and useful information for translational research, medical practice and health outcomes.

EOSC4Cancer will be carried out until 2025 within the framework of the European Open Science Cloud (EOSC) ecosystem and the European Health Data Space (EHDS).

BSC participates in a study that changes the current view of the evolution of leukemia



Researchers from BSC have taken part in a study coordinated by IDIBAPS-Clínic Barcelona-UB to identify the mechanisms that determine the evolution of leukemia, relapses after treatment and its transformation into a very aggressive lymphoma in the final stage in some patients.

The study, published in the journal Nature Medicine, and funded with a grant of one million euros by the CaixaResearch call for health research, shows that the cells that cause a relapse after treatment and that will lead to leukemia becoming a very aggressive tumor can already be detected in a tiny amounts at the onset of the disease, many years before these complications manifest clinically. Romina Royo, BSC researcher, was one of the co-lead authors of the study, which was coordinated by Elías Campo, director of IDIBAPS and a professor at the Faculty of Medicine and Health Sciences at UB.

AINA seeks millions of voices and MarIA receives the Archiletras Award

Under the slogan 'Our language is your voice', the Catalan Government launched a campaign to record voices to generate the first corpus or "dictionary" of Catalan voices. The campaign is part of the AINA project to make technology understand and speak Catalan.

Meanwhile, the MarIA project, the language model system created at BSC, which is based on the web archives of the National Library of Spain (BNE) and funded within the framework of the Language Technology Plan of the Secretariat of State for Digitalization and Artificial Intelligence (SEDIA), was awarded the Innovation Prize at the first edition of the Archiletras Language Awards.

The annual Archiletras Awards recognize outstanding action in the promotion, support, research and development of the Spanish language or any of the other languages in contact with Spanish in any of its territorial areas.

In November 2022, the Spanish government approved a grant of €3 million for the AINA project. It will also receive €12 million from the Catalan Government by 2026. The Spanish government's investment in both AINA and MarIA are part of the Recovery Plan's Strategic Project for Economic Recovery and Transformation (PERTE) in the New Language Economy.

Meet us in person

BSC brings together the alliance of Spanish centres of excellence in research to discuss major challenges in science

100xScience.6: "Science for the future. Building a fairer and more sustainable horizon", a meeting jointly organized by BSC with the Severo Ochoa and María de Maeztu Alliance (SOMMa), brought together more than 200 attendees at the Royal Palace of Pedralbes in Barcelona to analyze major challenges facing science today, such as climate change and superbug resistance.

The director of BSC, Mateo Valero; María Blasco, the president of SOMMa and the director of Centro Nacional de Investigaciones Oncológicas (CNIO), and Raquel Yotti, the Secretary General of Research at the Ministry of Science and Innovation, opened the meeting. Janet Kelso, a researcher at the Max Planck Institute for Evolutionary Anthropology (Germany), gave the keynote talk at the event about the latest technological advances that have made it possible to recover and sequence DNA from bones and other remains found in archaeological digs, and reconstruct the genomes of several Neanderthals.

This year's meeting was structured into four roundtables dealing with different topics with great impact on our society: artificial intelligence and digitalization, major health challenges, the climate emergency and sustainable development, and basic research, as the foundation of great discoveries.

Record number of visits to MareNostrum

The year 2022 closed with the highest number of visitors to the MareNostrum supercomputer. In total, there were 18,730 people who physically visited the centre and more than 2,600 who visited our facilities remotely.

Of the total number of visitors, more than 6,000 were third and fourth grade students from Catalan schools who participated in the "We Are Young Women Researchers" programme. This programme aims to bring technology closer to the youngest students, with special emphasis on the role of women.

SC22 Dallas, TX | hpc accelerates

ISC High Performance

BSC returns to the ISC and SC congresses for first time since the pandemic

After two years of forced absence due to the COVID-19 pandemic, Barcelona Supercomputing Center (BSC) once again physically attended the ISC and SC 2022 supercomputing congresses, which took place in Hamburg (Germany) and Dallas (USA), respectively.

BSC's new corporate building, as well as the MareNostrum 5 supercomputer, which will be operational in 2023, were the two backbones of the centre's stands at both supercomputing congresses.

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

BSC gratefully acknowledges the support of:

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UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

Plaça Eusebi Güell, 1-3
08034 Barcelona (Spain)
info@bsc.es
www.bsc.es

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