



**Barcelona
Supercomputing
Center**
Centro Nacional de Supercomputación

SUMMARY 2020

Who we are



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-1 members of the European PRACE (Partnership for Advanced Computing in Europe) research infrastructure. We manage the Spanish Supercomputing Network (RES), a Singular Scientific and Technical Infrastructure (ICTS) 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 more than 700, thanks to the continuous commitment of our trustees and our ability to raise competitive funds from companies and 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



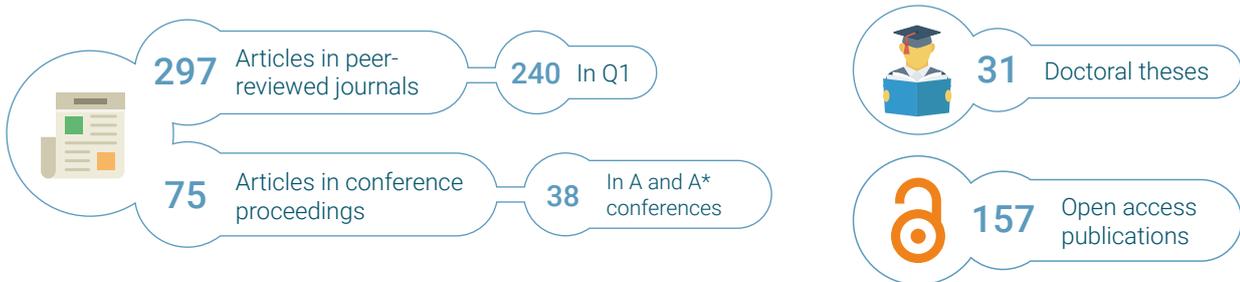
Knowledge transfer (education, tech transfer and public engagement)

BSC is a public consortium made up of:



BSC in numbers

RESEARCH



TECHNOLOGY TRANSFER

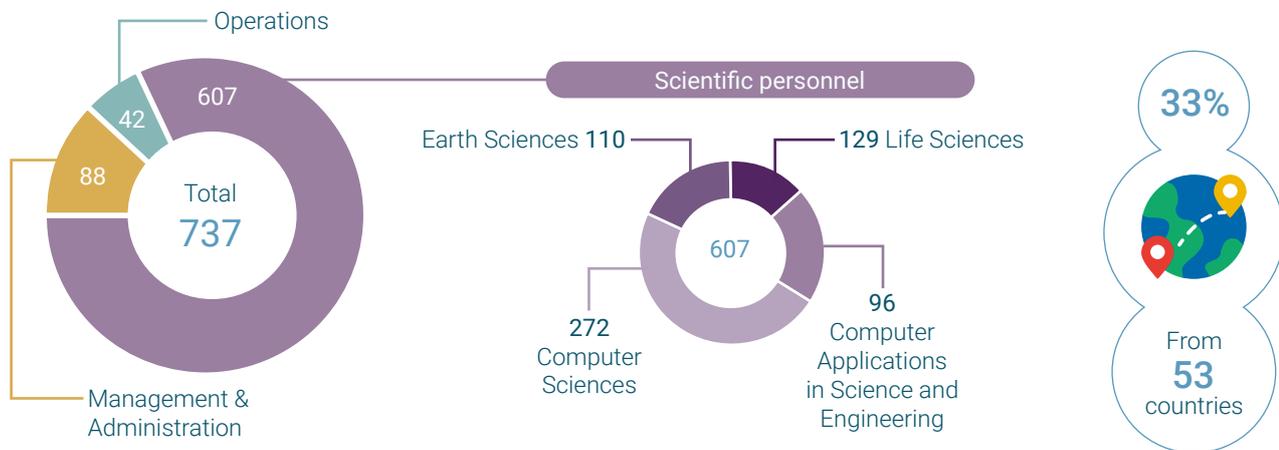


SUPERCOMPUTING



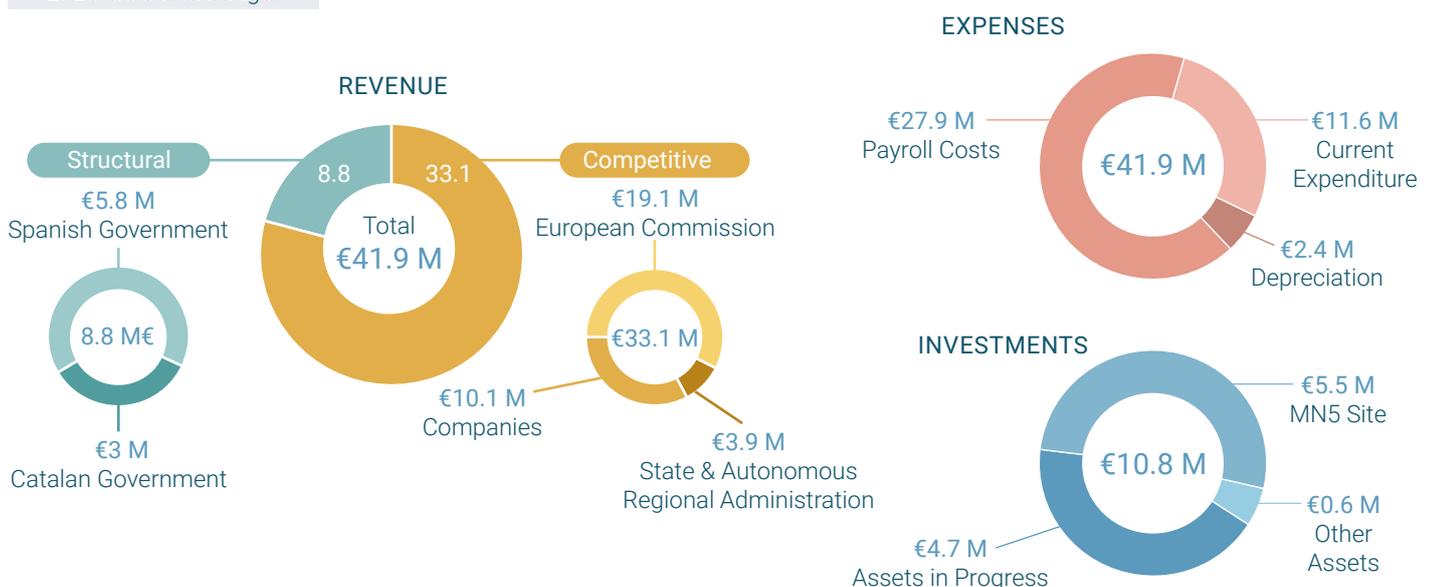
PEOPLE

Data as of December 31, 2020



RESOURCES

2020 executed budget



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

Revenue and expenses according to finance criteria. Investments according to budgetary criteria.

Where we are, where we are going



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

2020 was undoubtedly the most intense year in our recent history at an institutional level and, especially, at a personal level for each and every one of us at BSC. The COVID-19 pandemic brought about many changes in very little time, which we had to react to like everyone else: without knowing exactly what would happen or what tools we had.

COVID-19 took centre stage in our country too. On the one hand, because in March we switched to carrying out practically all of our work far from the physical workplace. Seminars, talks and virtual meetings became the new normal; but we should not forget the people who physically held the fort to ensure that our infrastructures would continue to work normally.



And, on the other hand, because the pandemic also involved new directions and opportunities for some groups. In collaboration with the public authorities and the main hospitals in our country, we contributed to developing knowledge and tools that are helping control the pandemic, to study the spread of the virus, to the search for new vaccines and the use of artificial intelligence to predict the disease's course.

All this was possible thanks to the titanic effort made by BSC's entire team to do the same good work as always under complex circumstances. So the words we repeated the most in 2020 were definitely "thank you": thank you for your work, effort, and commitment.

This enormous effort explains how, in spite of the circumstances, the results and figures for 2020 have been spectacular. We have continued to grow with more than 700 people from over 50 different countries. For the first time, our annual budget for work performed exceeded 40 million euros and this difficult year has brought about a new leap in scientific productivity.

Some figures and achievements deserve special mention. For example, we are still the third Spanish institution in being awarded competitive funds as part of the European Horizon 2020 programme, and the first among Catalan institutions. We have exceeded the figure of 100 million euros awarded through this program due, among other things, to our great involvement in European HPC centres of excellence and projects related to the European Processor Initiative.

We are also continuing to collaborate with many companies, renewing agreements with old travel companions such as Repsol, IBM and Lenovo and we have signed new agreements, as in the case of Grífols, Decathlon, Suez and Huawei. To these new collaborations, we must add the new spin-offs created, raising the number of companies set up through BSC to 10.

In terms of infrastructure, MareNostrum 4 continued to work uninterruptedly, offering its services to the European research community through both PRACE and RES. We started operation of the latest MareNostrum 4 clusters and new data infrastructure, Ágora, which will continue to grow in the coming years. Our corporate building is now ready for more than 500 employees to work there. We have also started work on the site that will house the future MareNostrum 5. We are pressing ahead with the procedures so it can arrive in Barcelona in 2021.

The pandemic obviously also affected physical tours of the chapel, but we made a virtue of necessity and digitized them: it is now possible to visit the chapel and MareNostrum 4 online, which has enabled us to continue tours and the technological training of thousands of primary school students.

Many other things also took place: from the first steps to access the new NextGenEU funds, through numerous institutional visits adapted to the public health safety standards, to our contribution to the Spanish candidacy for the new ECMWF headquarters, which we unfortunately just missed out on.

However, there is one fact that stands out above all the others for its future impact: the three institutions that govern us (Spanish government, Catalan government and UPC) signed a historic agreement guaranteeing structural funding for BSC for an entire decade until 2029. This agreement gives us unprecedented stability, which will help us a great deal in ensuring our future objectives are achieved. Once again, we must say “thank you” to our patron institutions.

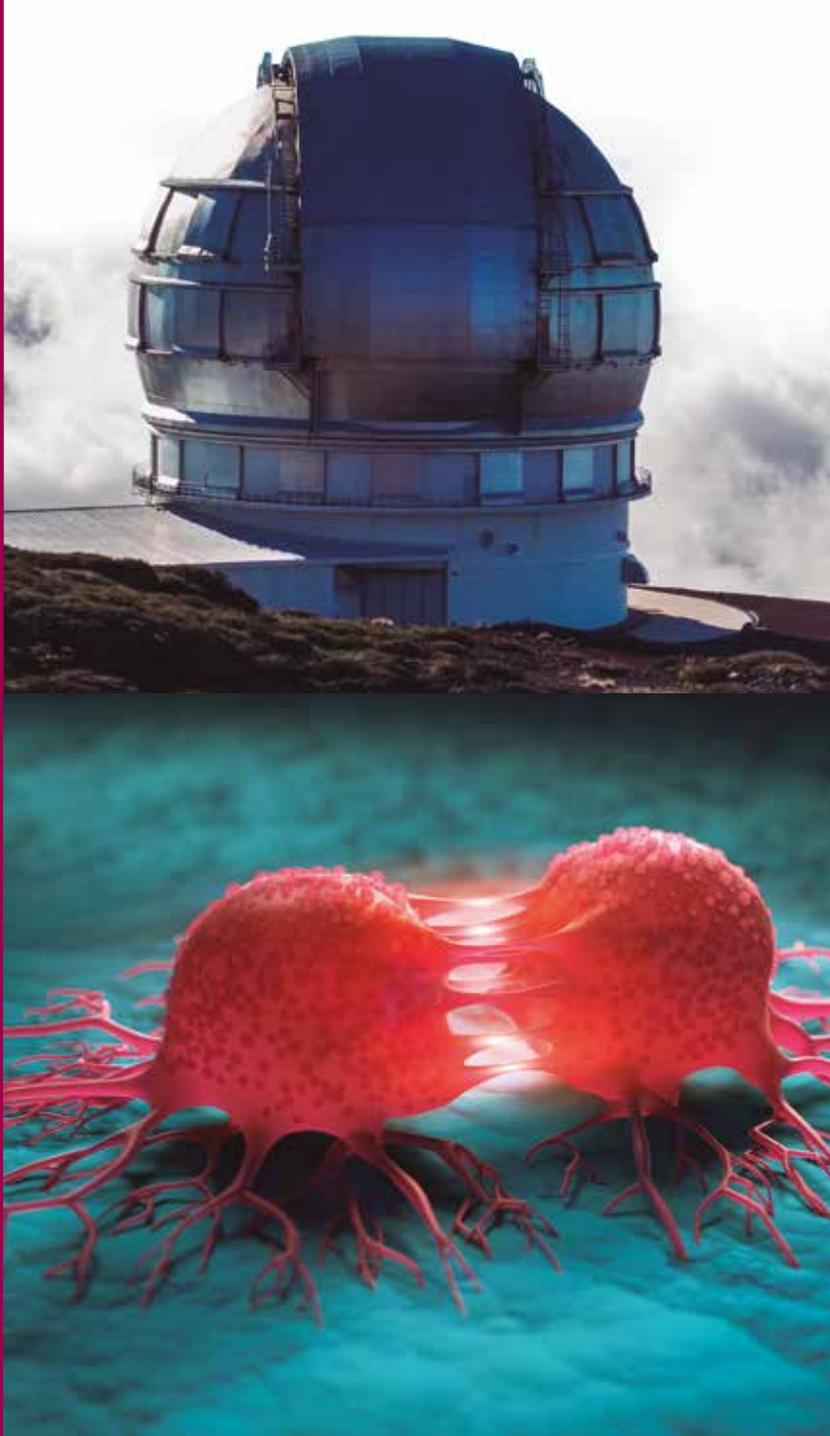
2020 was thus a very complicated year but, thanks to the great effort made by everyone, we have overcome it and achieved extremely good results. The successes should be a new stimulus to tackle the coming years with more strength than ever before and achieve the missions that our patrons have entrusted us with. Thank you and congratulations, everyone!



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 kind 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 behavior of the object of 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 suffering and perform experiments that could not be done in the real world, because they would be too expensive, too dangerous or simply impossible to carry out.

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 demonstrated 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 is a great accelerator for science and engineering and is used and considered increasingly essential in the majority of scientific disciplines.

MareNostrum versus the pandemic

In 2020 the MareNostrum 4 supercomputer contributed to speeding up research to combat COVID-19.

BSC's Operations Department provided support for internal and external researchers, who used more than 39.5 million computation hours for research related to COVID-19.

The majority of the research was related to the virus's biology, its mechanisms of infection and its interaction with drugs that might be used. However, it also hosted work related to the spread of the disease by aerosols, propagation of the pandemic in Spain and Europe, evaluation of protection mechanisms and prediction of the disease's evolution in patients with medical images.



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 share 80% of its calculation capacity. This is assigned through open application processes in which researchers present their proposals, which are then assessed by expert scientific committees in the different disciplines. The remaining 20% of the supercomputer's capacity is assigned to BSC.



MareNostrum 4 has a maximum power of 13.9 petaflops or, in other words, 13,900 trillion operations per second.

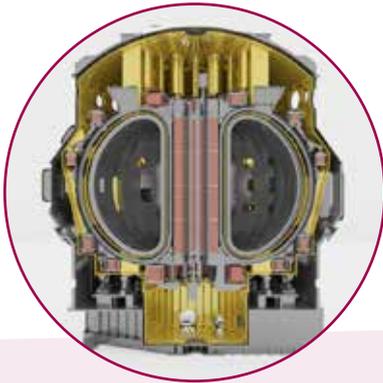


MareNostrum 4 is co-financed by the Intelligent Growth Operating Programme 2014-2020 of the European Regional Development Fund (ERDF)



Research with MareNostrum 4

MareNostrum 4 provided 1.18 million processor hours in 2020. 80% of these were used by researchers who gained access to the supercomputer through the European PRACE (Partnership for Advanced Computing in Europe) infrastructure network or the Spanish Supercomputing Network (RES). The computation hours assigned to PRACE and RES are valued at 8.5 million euros. Here are some examples of projects that used the supercomputer.



UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH

Shimpei Futatani

JOREK; Non-Linear MHD simulations of tokamak plasmas for validation and implications for JT-60SA and ITER



Philipp Schlatter

TBLFST - Transition in boundary layers with free-stream turbulence



Barcelona Supercomputing Center Centro Nacional de Supercomputación

Víctor Guallar

In silico toxicology prediction for compounds binding to the SARS-CoV-2 protease

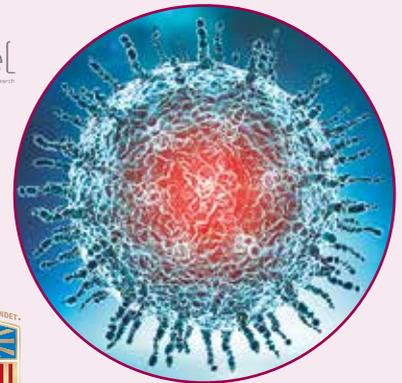
Modesto Orozco

Exploring COVID-19 Infectious Mechanisms and Host Selection Process



Iñaki Tuñón

MultiScale Simulations of the Activity of 3CL Protease of SARS-CoV-2



F. Javier Luque

Searching for small compounds as stabilizers of the inactive spike protein in SARS-COV-2



UNIVERSITAT ROVIRA I VIRGILI

Alexandre Fabregat Tomás

Turbulent dispersion and surface deposition of pathogen-laden droplets in enclosed rooms



Universitat de les Illes Balears

Carlos Palenzuela

LESBNS - Large-Eddy-Simulations of magnetized binary neutron star mergers



Xavier Luri

Gaia: Fourth Data Reduction Cycle (DRC-04) and Early Data Release 3 publication (EDR3)



Maria Ramos
Biodegrading plastics



Roberto Verzicco
TORNADO - Rotating double diffusive and Rayleigh-Bénard convection



Roberto San José
Modelling International Initiative



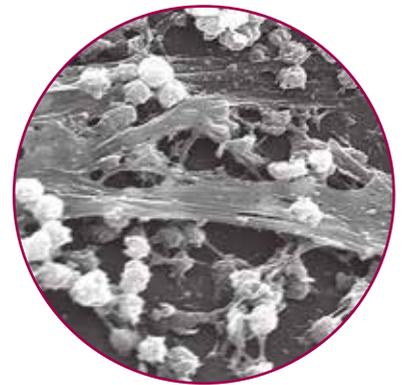
UNIVERSIDAD DE MÁLAGA

Jorge Macías Sánchez
Development of the HPC aspects of a Probabilistic Tsunami Forecast tool for the Mediterranean Sea. A pilot set up.

Chantal Valeriani
Adhesion and Cohesiveness of biofilm to surfaces from in silico studies



Carme Rovira
Engineering glycosidase enzymes for phosphorylation reactions



Carmen Domene
Characterisation of the affinity of broadly neutralizing anti-HIV antibodies for the membrane interface



Agora, BSC's new data infrastructure

We have started installing a new infrastructure to store data, which will have a final capacity of 165 petabytes (165 million gigabytes). This infrastructure will host data of interest to researchers and public research centres from various scientific disciplines.

The new facility is called Agora. BSC staff chose this name through a vote, after more than 300 proposals were received in a call put out on social networks.



The year that COVID-19 locked us down



#BSCatHome

The COVID-19 pandemic and social distancing measures did not prevent BSC from continuing to perform its research activity, in spite of the entire staff having to work from home for several months. Our activity was able to be maintained due to the effort made by the researchers and the rest of the centre's workers to keep up the pace while teleworking. Here is an example of their efforts, for which we thank everyone.



Pedro Gómez

His dining room was turned into a workshop

One of the departments that faced the greatest challenges was Operations, which had to meet the staff's needs in new working conditions. Pedro Gómez, the coordinator of the Helpdesk service, can now look back, more relaxed, at the disruption during the first few months: "It was the worst time because Operations, not just the Helpdesk service, had to adapt everything so that people could work from home, starting with a VPN, which was in the testing stage and had to provide a service to more than 700 users from one day to the next. Luckily, everything worked, but during the first few weeks we had to work twelve to fourteen hours a day, including Saturdays and Sundays."

"During the first few days, we focused on setting up everyone's equipment, implementing new software, using Zoom to communicate, creating manuals, providing user support ... It was then time to deliver equipment to the new staff. In spite of the situation, there were 185 of them from March to December 2020. "During the first few months, the work system consisted of me going to BSC, filling my car with equipment, taking it home and preparing it there to send it anywhere in the world. It was chaos in my house: the dining room was turned into an equipment storeroom because we reserved the office for my wife to work in. Couriers kept ringing the doorbell and my two-year-old son was wandering around all over the place." Meanwhile, the rest of the Helpdesk team, who were also home, answered the tickets and provided support for all kind of requests. "It was either that or close," he recalled, and all hands had to be on deck.

"The news and the stress kept increasing rapidly"

"On Monday, March 9, we drafted an internal e-mail about measures to prevent contagion and we never expected that we would all be working from home by Friday. The news and the stress kept increasing so rapidly that it was hard to manage," explained Octavi Monfort, the health and safety manager at BSC. "Normally, when we write e-mails to the entire staff, from the time someone drafts it to when it is finally sent, it goes through various consultations and revisions, but this time it had to be quick. They were days of great tension and stress. We received an avalanche of questions and we could not reply to some of them for weeks, even though we were working twelve- or thirteen-hour shifts."

During the months of full lockdown ("the worst"), they had to keep up to date with the vast amount of information about how COVID-19 spreads and the measures the public authorities were taking. "Initially, it was not even clear that 100% teleworking would be allowed," Monfort explained. "At the beginning, there were people who needed to come in to pick up materials or equipment. Later on, we started to find that some people were finding it very tough to work from home and we decided to make some exceptions." These were very specific cases, such as people who lived in a shared apartment and had to work from their bed because they did not have a desk in their room." From the end of May, when restricted access to the facilities was allowed, this had to be coordinated. Travel justifications had to be sent in case the police asked for them and anti-contagion measures had to be coordinated with the cleaning company and other subcontractors. "From that moment on, the priority was to avoid contagion within BSC," he explained, and the stress did not end until the teams were able to regulate their presence in the facilities again.

Octavi Monfort





Mervi Mantsinen

“I feel like I am more connected to the group than I was before”

In spite of how complicated the situation was, Mervi Mantsinen, the leader of the Fusion group, thinks that the pandemic brought some positive things. “I think I am now more connected to the group than before,” she explained. “Working from home forced us to get better organized. It was not easy. I made a great effort to try to provide emotional support for everyone. I said we were not only working from home but also in a pandemic and that we had to take care of ourselves and give ourselves flexibility. Sometimes, people with children sent us messages in the early hours of the morning!”, she commented. “Another positive aspect was that we no longer had to constantly travel. And we managed to make everything work well, save time and expand the possibilities for collaboration and visibility,” Mervi said.

Her overall assessment is positive: “I think we have done well as a group.” There were major challenges, such as performing experiments online and bringing in nine new researchers. “Our experience has shown that people are committed and that we can give them more flexibility in the future”, she explained. She does not want to travel so much anymore. “Except to Finland. I have not seen my family for a year. That is the greatest personal sacrifice and it is very tough.”



Alfonso Valencia

“We have made progress with biomedicine and data, but we do not know how to replace informal communication”

“One great advantage has been not travelling because it wastes a great deal of time. When you are not travelling, you get much more done.” This is one positive aspect of the pandemic according to Alfonso Valencia, the director of the Life Sciences Department at the BSC. Even more important is the boost to the field of data and biomedicine. “Coronavirus has refloat topics that were always very difficult, such as access to hospital or genome data. Collaborations have accelerated and they are a prototype of what should be done with other diseases. In this sector everyone thinks that we cannot go back to how things were before.”

However, regarding decreased travel, he said, “There is a part of scientific diplomacy (informal contacts, speaking about things that were not the purpose of the meeting, etc.) that we do not know how to replace.” Something similar applies at laboratory level. “In the future, teleworking will become a major part of what makes a position attractive,” he predicted and this “raises problems, such as how to organize work, groups and new staff ... It is impossible to reproduce contact within the laboratory and we will definitely lose out in terms of creativity. Master’s degree and PhD students bear the brunt of it. Those are periods in which you discover how the scientific environment works and learn to solve the problems that arise. Doing this from home is sometimes impossible and on other occasions frustrating,” he commented.

Giulia Carella



“We arrived in Barcelona and everything was closed”

This physicist with a PhD in applied statistics is one of the 185 people who joined BSC from March to December 2020. Giulia remembers that moving in the middle of the pandemic was not easy, nor was beginning her mission to build, together with another recently arrived colleague, a line of research on artificial intelligence for the entire Department of Earth Sciences, without knowing anyone in person. “Our mission requires us to know very well who does what and how we can help them,” she explained. COVID-19 also made it harder for her to settle in the city: “We arrived and everything was closed,” she said.



Vladimir Dimic

He defended his doctoral thesis from home

“It was nothing like I had imagined. No public presentation, no buffet, no celebration with friends. I defended my thesis online from my home in Serbia. Luckily, I was with my girlfriend and parents, and was able to share it with them.” Vladimir is grateful for the help provided by the researchers, who were always available for questions, and technical support from BSC. “It was actually easy because I already knew everyone and I knew how to ask for help for anything I needed. But if the pandemic had come at the beginning of my doctorate, it would have been very complicated,” he said.

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 2020.



Cost-aware prediction of uncorrected DRAM errors in the field

The authors present and evaluate a method to protect uncorrected DRAM errors that cause node failure. The method reduces lost compute time by up to 57% for a mixed real HPC workload, a net saving of 21,000 node-hours per year. Six machine learning approaches are compared and a trained random forests classifier is used and assessed with error logs from more than two years of MareNostrum 3 production. [Isaac Boixaderas](#), [Darko Zivanovic](#), [Sergi Moré](#), [Javier Bartolomé](#), [David Vicente](#), [Marc Casas](#), [Paul M. Carpenter](#), [Petar Radojković](#), [Eduard Ayguadé](#). Proceedings of the International Conference for HPC, Networking, Storage, and Analysis (SC). November 2020.

Improving predication efficiency through compaction/restoration of SIMD instructions

Most modern processors, including SIMD extensions, rely on predication to support divergence control, which reduces system efficiency as vector length increases. The article proposes a novel approach to improve execution efficiency in predicated SIMD instructions with efficiency improvements of up to 25% and reductions in dynamic energy consumption of up to 43%. [Adrián Barredo](#), [Juan M. Cebrián](#), [Miquel Moretó](#), [Marc Casas](#), [Mateo Valero](#). IEEE International Symposium on High Performance Computer Architecture (HPCA) 2020: 717-728.



Figure 2. CR basic functionality.

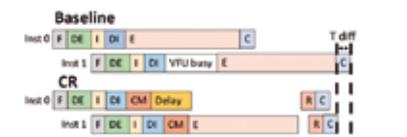
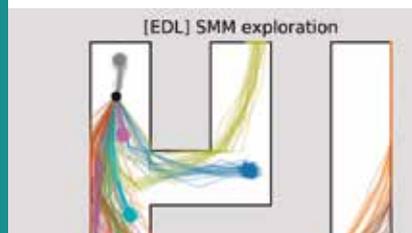


Figure 3. Baseline/CR time diagram. Fetch (F), Decode (DE), Issue (I), Dispatch (DI), Execute (E), Commit (C), Compact (CM), Restore (R).

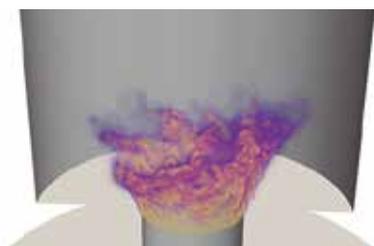


Explore, discover and learn: Unsupervised discovery of state-covering skills

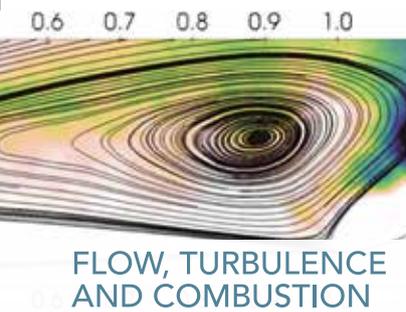
The aim of reinforcement learning is to train agents to take optimal decisions, which is generally achieved through interaction with simulated environments. The scalability of these approaches tends to be limited by our ability to define reward functions that assess competence in each task of interest. The work explores unsupervised methods to discover useful skills without human supervision. [V́ctor Campos](#), [Alexander Trott](#), [Caiming Xiong](#), [Richard Socher](#), [Xavier Giró-i Nieto](#) and [Jordi Torres](#). 37th International Conference on Machine Learning. 2020.

Numerical characterization of a premixed hydrogen flame under conditions close to flashback

A numerical study of a technically premixed swirling combustor with central air injection at conditions close to flashback using large-eddy simulation with flamelet modelling. This burner has the characteristics of showing flashback at low equivalence ratios, so numerical simulations are set to identify the mechanisms behind the flashback formation. [Daniel Mira](#), [Oriol Lehmkuhl](#), [Ambrus Both et al.](#) Flow Turbulence Combust. 104, 479–507. January 2020.



FLOW, TURBULENCE AND COMBUSTION



Effects of the actuation on the boundary layer of an airfoil at Reynolds number $Re = 60000$

Synthetic jets are an active flow control technique to manipulate the flow field in wall-bounded and free-shear flows. This article focuses on the role of the periodic actuation mechanisms on the boundary layer of an SD7003 airfoil at $Re = U_{\infty}c / \nu = 6 \times 10^4$. Here, Reynolds number is defined in terms of the free-stream velocity U_{∞} and the airfoil chord. [C. Ivette Rodríguez](#), [Oriol Lehmkuhl](#) and [Ricard Borrell](#). *Flow Turbulence Combust* 105. 2020.

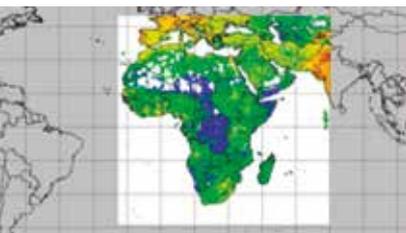
FLOW, TURBULENCE AND COMBUSTION

Making seasonal outlooks of Arctic sea ice and Atlantic hurricanes valuable - not just skillful

The study presents two international cooperative platforms that provide large sets of predictions of hurricanes and seasonal sea ice. These platforms have been designed so that user oriented weather services can integrate forecasting these phenomena into their operational context. [Louis-Philippe Caron](#), [François Massonnet](#), [Philip J. Klotzbach](#), [Tom J. Philip](#) and [Julienne Stroeve](#). *Bulletin of the American Meteorological Society*. January 2020.



AMS
American Meteorological Society



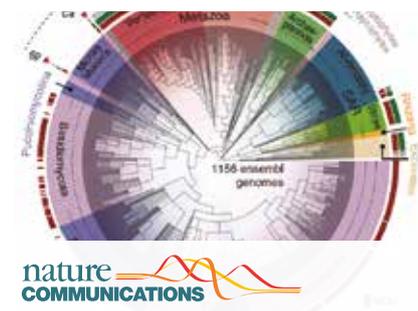
Geoscientific Model Development

HERMESv3, a stand-alone multi-scale atmospheric emission-modelling framework – Part 2: The bottom-up module

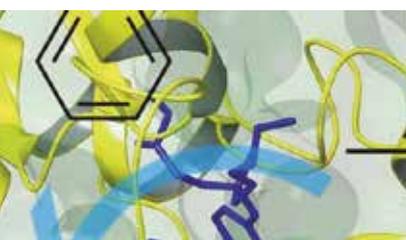
Presentation of the bottom-up module of the High-Elective Resolution Modelling Emission System version 3 (HERMESv3), which estimates anthropogenic emissions at high spatial (e.g. road link level) and temporal (hourly) resolution using state-of-the-art calculation methods that combine local activity and emission factors along with meteorological data. [Marc Guevara](#), [Carles Tena](#), [Manuel Porquet](#), [Oriol Jorba](#) and [Carlos Pérez García-Pando](#). *Geoscientific Model Development*. March 2020.

Discovery of EMRE in fungi resolves the true evolutionary history of the mitochondrial calcium uniporter

Computational analysis of the complete genome of more than a thousand organisms reveals that the transporter that regulates calcium levels in cells was duplicated around a billion years ago and that the fungal models currently used to study mitochondrial regulation of calcium are inadequate. [Alexandros A Pittis](#), [Valerie Goh](#), [Alberto Cebrián-Serrano](#), [Jennifer Wettmarshausen](#), [Fabiana Perocchi](#) and [Toni Gabaldón](#). *Nature Communications*. August 2020.



nature COMMUNICATIONS



nature catalysis

Genetically engineered proteins with two active sites for enhanced biocatalysis and synergistic chemo- and biocatalysis

This study analyzes proteins with two active sites of biological and/or abiological origin, with enzyme engineering methods. The approach increases the catalytic properties, such as enzyme efficiency, substrate scope, stereoselectivity and optimal temperature window, of an esterase containing two biological sites. [Sandra Alonso](#), [Gerard Santiago](#), [Isabel Cea-Rama](#), [Julia Sanz-Aparicio](#), [Víctor Guallar](#), [Manuel Ferrer et al.](#) *Nature Catalysis*. 2020.

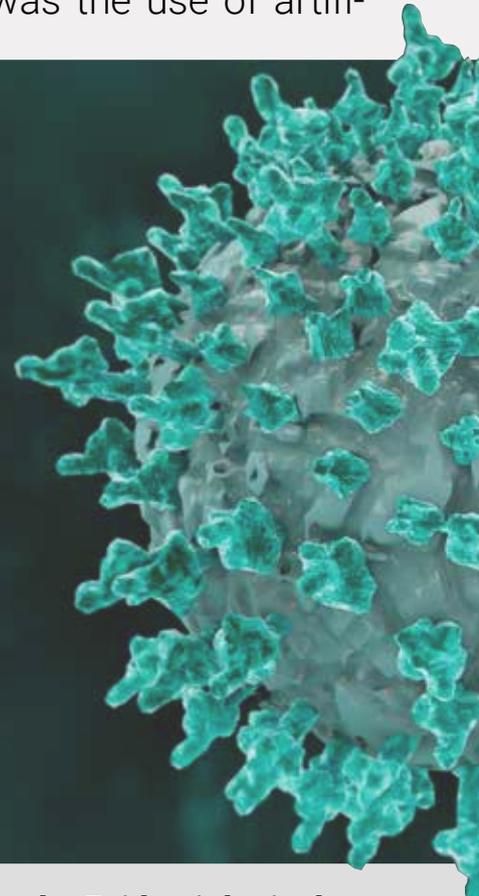
Applied Research & Innovation

In 2020, BSC threw itself into research to counter the coronavirus pandemic and, as befits the centre's multidisciplinary nature, it did so on various fronts. From the biomedical perspective, the genome of the virus and its mutations were investigated, and we participated in various collective projects searching for vaccines and treatments. Another major work area was the use of arti-

Hospital Clínic and BSC use artificial intelligence to predict the progress of COVID-19 patients

They create an AI model based on information from more than three thousand clinical reports produced by Hospital Clínic during the acute stage of the pandemic.

Hospital Clínic in Barcelona, Hospital 12 de octubre in Madrid, Hospital Virgen del Rocío in Sevilla and BSC are working together to create an artificial intelligence (AI)-based model that will help medical teams predict the progress of COVID-19 patients and help hospital managers to plan their internal organization for the various waves of the pandemic. The project is part of the Secretariat of State for Digitization and Artificial Intelligence's Plan to Promote Language Technologies and is open to collaboration with more hospitals.



Tool to visualize the relationship between public mobility and the risk of the pandemic spreading

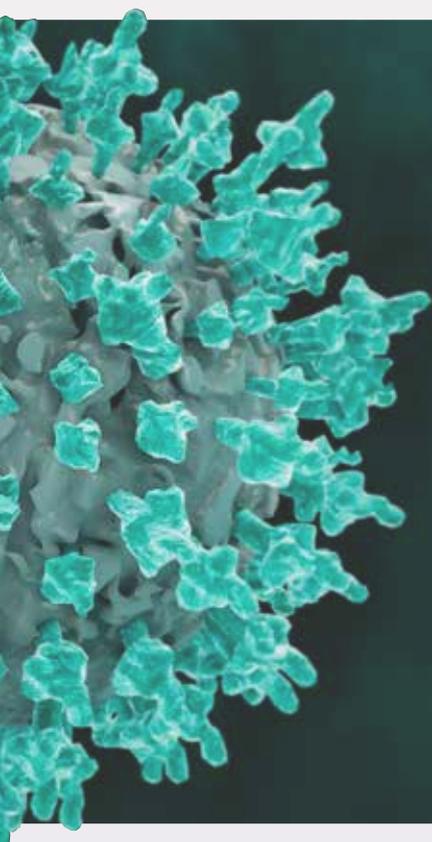
BSC has provided public authorities, researchers and the public with a geographical information tool that makes it possible to view the risk of COVID-19 spreading associated with population mobility. The COVID-19 Flow-Maps platform integrates COVID-19 case data from the public authorities (Ministry of Health and the regional health ministries of Castile and León, Catalonia, Madrid, Navarre and the Basque Country) and public mobility data from the Ministry of Transport, Mobility and the Urban Agenda. All of these data are georeferenced, which makes it possible to show them on a map and facilitate their integration, analysis and interpretation.

BSC participates in the Epidemiological Observatory of Catalonia, based on big data and AI techniques

The aim of the observatory, which is part of the Catalan Government's Catalonia.AI strategy, is to produce a new collection of innovative epidemiological models for public institutions to aid prevention, early detection and mitigation of the spread of epidemics. BSC will collaborate through both research and provision of computational infrastructure, alongside medical and health institutions, technological research centres, cell phone operators and Mobile World Capital Barcelona.



cial intelligence, big data and natural language processing to create predictive models of patient progress and hospital occupancy, and to analyze data concerning the spread of the pandemic and its impact on society. The impact of mobility restrictions on air quality in Spain and Europe was also studied.



Bioinformatics in the search for vaccines and drugs

BSC has taken part in several projects aimed at finding COVID-19 vaccines and treatments through genomic and molecular research and bioinformatic simulations, which seek to computationally reproduce the various ways of attacking the virus.

A major EXSCALATE4CoV (E4C) project, financed by the European Commission as part of the H2020 programme, has placed the emphasis on basic and applied research. The research performed by the BSC consortium, IrsiCaixa and CreSa-IRTA, in collaboration with Grífols, focused its efforts on finding immunological therapies. In addition, the SARA - A ISCIII project, in collaboration with the Advanced Chemistry Institute of Catalonia and Nostrum Biodiscovery, financed by the Carlos III Health Institute's COVID-19 fund, focused on research into antivirals to inhibit coronavirus SAR-V2, which causes COVID-19, and subsequent coronaviruses.

Bioinformatic simulations use supercomputers' computing capacity to reproduce the interactions that take place in living beings at molecular level, which are a key factor in speeding up the discovery of new treatments.

COVID-19 disease map, a platform to combine and order scientific information about the virus

BSC researchers, together with researchers from 25 countries, participated in the COVID-19 disease map. This repository brings together and organizes knowledge generated about the virus's molecular map and mechanisms of interaction between the SARS-CoV-2 virus and the host, guided by contributions from experts in the field and based on published papers. These maps are fundamental to produce computer simulations of the virus's behavior at molecular level and contribute to the search for vaccines and treatments against the disease it causes.

BSC researchers study mobility in Spain during the COVID-19 pandemic using data from Facebook and Google apps

This work demonstrated how the correct use of data from large social platforms can provide a detailed interpretation of mobility and be a useful tool to assess the measures taken and contribute to improving the response to future crises. The data used were from tracking apps—Facebook (Facebook Data for Good Program) and Google (Google Mobility Assessment)—installed by users on their cell phones with explicit prior consent to record their location. These data were used to analyze mobility patterns in Spanish regions during the first lockdown.



COVID-19 Disease Map

Applied Research & Innovation

The EC approves two new centres of excellence for High-Performance Computing applications led by BSC



The European Commission has announced the creation of six new Centres of Excellence (CoEs) for High-Performance Computing (HPC) applications and BSC will lead two of them, with an overall budget of 10 million euros, and will participate in a third.

The new centres led by BSC are the Centre of Excellence in Combustion (CoEC) and PerMedCoE, a centre of excellence in personalized medicine. BSC will also participate in the newly created NOMAD2, which will search for new materials, and AISEE, focused on AI and Simulation-Based Engineering at Exascale.

This decision consolidates BSC's presence in the centres of excellence for HPC applications promoted by the European Commission, since out of a total of 15 centres, it leads four and participates in a total of 12. The other centres coordinated by BSC are ChEESE, for solid earth simulations, and PoP, for code optimization and efficiency. It is also participating in Bioexcel2, CompBioMed, EoCoE, Esiwace2, Excellerat and Max.



BSC and Intel enable inference from large homomorphically encrypted neural networks

BSC and Intel are developing Homomorphic Encryption, which for the first time has enabled inference from homomorphically encrypted production-size neural networks, thanks to Intel PMem technology. The advantage of this encryption is that it does not need to be decrypted to operate, which guarantees privacy in unsafe environments (such as the cloud). Up until now, there had only been tests on small-scale networks.

BSC develops open source hardware platforms for critical systems

BSC researchers are developing open source hardware platforms for critical systems, as part of the SELENE project. Some HPC commercial platforms offer the computation performance required by autonomous systems in fields such as the motor industry, space, avionics, robotics and industrial automation, but their use is traditionally considered outside the scope of the industry due to difficulties with the certification process.



MareNostrum processes large quantities of texts to create Catalan and Spanish language models

BSC is collaborating with the public authorities to generate Catalan and Spanish language models. These models are fundamental to integrate linguistic knowledge into digital environments based on artificial intelligence.

The MareNostrum supercomputer has already processed large quantities of texts in Catalan and Spanish. These data, which will be increased as new contributions are added, will be used to build a corpus to train neural networks and generate models capable of reproducing the use of both languages, including slang and geographical variants.

The creation of these models is being carried out with funding from the Spanish Secretariat of State for Digitization and Artificial Intelligence and the Catalan Department of Digital Policies.



BSC and SUEZ collaborate on a project to apply big data technologies to the water cycle

BSC and SUEZ in Spain have signed an agreement to exploit the use of reinforcement learning in efficient management of drinking water networks. BSC will contribute its knowledge of computing technologies, high-performance algorithms, AI, visualization and big data, and SUEZ will provide its expert knowledge in operating supply networks. Deep reinforcement learning (or Deep RL) is a novel AI technique that uses neural networks and reinforcement learning techniques to train software agents to take decisions autonomously.

Progress in the project for smart management of visitors to FC Barcelona's facilities

BSC and FC Barcelona have completed the first phase of the IoTwins project, an innovative system that uses the Internet of Things and artificial intelligence to analyze and predict people's movement inside and outside of the club's facilities and that, once developed, will make it possible to improve management related to visitor mobility and the offer of services. The IoTwins project consists of modelling movements of people through the club's facilities by collecting anonymous data and creating a computer simulation that reproduces the crowd's usual movements.



Applied Research & Innovation

A scientific team tracks deserts to decipher dust and its effects on the climate



Researchers from various institutions led by BSC are carrying out expeditions to deserts around the world to collect various data that should make it possible to understand and quantify the global composition of mineral dust and analyze its effects on the climate. These campaigns, which are part of the FRAGMENT project, are important because we don't currently have a full understanding of the physical processes of dust emissions and need experimental data to answer key scientific questions and assess theories and models, such as those executed at MareNostrum. The campaigns were brought to a halt by the pandemic and will restart in 2021.

The Copernicus Atmospheric Surveillance Service uses AI techniques developed at BSC to calculate the reduction in emissions during the pandemic



BSC has developed AI-based techniques to calculate the reduction in pollutant emissions attributable to restrictions connected with the COVID-19 pandemic. The Copernicus Atmospheric Surveillance Service has used these techniques to calculate the reduction in emissions at European level. The collaboration was entered into through an agreement with the European Centre for Medium-Range Weather Forecasts (ECMWF). The study resulting from this collaboration provides a daily breakdown of emissions by sector and area, as well as information about contributions at country level and the different of pollutants.

The paradox of Anak Krakatau, the Indonesian volcano that froze the atmosphere, is unlocked

Volcanic activity that occurs in tropical moist atmospheres can promote deep convection (heat transfer) and trigger volcanic thunderstorms. A simulation carried out at BSC shows how these phenomena can last continuously for more than a day.



Photographs used with permission of the copyright owner, Dicky Adam Sidiq / Kumparan

DST: the tool for predicting renewable energy sources

BSC coordinates the S2S4E Decision Support Tool (DST), which can show, for the first time, both sub-seasonal and seasonal forecasts of rain, solar radiation, temperature, and wind adapted for the renewable energy sector.



BSC's cutting-edge technologies have enabled the creation of ten new companies in five years

The research and technology generated at BSC has led to the creation of ten pioneering companies in the last five years. These spin-offs offer advanced services in fields as diverse as biomedicine, aerospace safety and the motor industry, as well as quantum computing.

 **93**
Jobs

 **23**
Technologies transferred

 **€3.5M**
Capital raised

ELEM Created with UPC, it is a biomedical software company to create virtual human beings. With technology based on Alya (code developed at BSC), they replicate organs and physiological systems to test and improve medical devices and drug efficiency.

 **EAS** Created with UPC, it provides commercial solutions capable of offering monitoring, optimization and analysis of HPC centres from the viewpoint of consumption and energy efficiency.

FrontWave Imaging Created with Imperial College London (ICL). It develops and markets advanced imaging techniques to diagnose breast tissue to improve the detection and diagnosis of breast cancer.

 **MASPA TECHNOLOGIES** It offers tools for the analysis of temporal behavior and security of multicore processors for critical systems such as aviation and the motor industry.

 **MITIGA SOLUTIONS** Created with UPC. It is based on SORT-ATM, software for air traffic management during emergency situations involving atmospheric natural hazards, especially volcanic eruptions.

 **NBYCOMP** Nearby Computing It was created with UPC, Nearby-Sensors and Cellnex Telecom. It provides advanced orchestration technologies and network process automation for edge computing, with applications for IoT and 5G.

 **NEXTMOL** It develops tools for atomistic simulation and data analysis to identify the best candidate molecules to meet the desired properties and accelerate the design of new chemical products.

 **NBD** INOSTRUM BIODISCOVERY A biotech company that uses simulations and artificial intelligence to speed up drug discovery. Created with IRB Barcelona, ICREA, CIC-UB, Fundació Bosch i Gimpera and Fundación Botín.

 **beast** It offers a platform for big data analysis with Data Leverage, providing great insights while accessing only the minimum quantity of raw data.

 **ILMANJARO** QUANTUM TECH Created with UB and IFAE. Its mission is to build a unique, first-to-market, coherent quantum annealing computer and offers quantum algorithms for application in companies in various sectors.

Meet us in person



Online activities for people of all ages

We never let people down who want to know more about us. Although 2020 was the year when in-person visits had to be cancelled, it was also the year that we made all kinds of online activities available.

We go into classrooms to explain what a supercomputer is



Primary school classes no longer have to travel to BSC to enjoy the interesting and fun activities in the “We are young women researchers” programme. The games in this successful programme, which invites 6,000 pupils every year to visit the supercomputer, can now be played in their classrooms. All of the games designed to introduce young school students to the world of supercomputers and computational thinking are available on our website: www.bsc.es/alaula. If you are a teacher, you can ask one of our outreach teachers to go to your school to guide the activity, if you prefer.



You can now go on a virtual tour of the MareNostrum supercomputer



You can now visit the MareNostrum supercomputer from home or anywhere in the world. There is a link on our website to access the interesting virtual tour, which is full of information about what supercomputers are, how they work and what we use them for at BSC. If you would like a guided tour, we also offer online talks for audiences of all ages, given by the centre’s tour manager. You can find links to the virtual tours and the form to request a guided tour on our website: www.bsc.es/visits.

Online course on machine learning and artificial intelligence

“AI & Predictive Analytics in Data-Centre Environments” is a course designed to teach IT students, professionals and researchers in all fields that work with data protection and analysis algorithms about the use of artificial intelligence. The course is divided into three main parts: performance in data processing centres, machine learning and distributed data processing technologies. It has been created by Josep Lluís Berral, BSC researcher, with funding from Intel, and is intended for both students and researchers with some knowledge of the topic and those who want to start finding out about it.

You can find it at <http://dcai.bsc.es>.

BSC gratefully acknowledges the support of:



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BSC is a public consortium made up of:

