News

BSC develops new bioinformatics tool against HIV
The method represents a step towards personalised medicine, in which treatment is determined following genetic analysis of the cause of the disease in each patient.
More information on page 3

García-Pando returns to BSC thanks to an AXA chair
Carlos Pérez García-Pando returns to the BSC to hold the AXA chair on Dust Storms, financed by the AXA Foundation.
More information on page 3

Application of cognitive computing to financial innovation
CaixaBank and BSC have signed a collaboration agreement for joint research into advanced deep learning systems.
More information on page 4

Recognition for the director of BSC
In recent weeks, Mateo Valero has received recognitions from the University of Granada, the Festibity and the Catalan Government.
More information on page 4

Social simulation and 3D animation in Simulados
The film Simulados shows how a computer generated simulation recreates humanity’s struggle with climate changes and the importance of cultural interaction.
More information on page 4

Director’s View
It is a pleasure to be able to write this editorial for the BSC newsletter, and through it, address all the members of the centre. It is also a challenge, because I am writing this just a few weeks after joining the BSC.
More information on page 2

Events and Training

ISC High Performance
14 March 2016, Barcelona

PATC Course: Introduction to CUDA Programming
17 March 2016, Barcelona

More events on page 2

Inside BSC

BSC and IBM create Deep Learning Center
This year, BSC and IBM have renewed their research agreement and have created the IBM-BSC Deep Learning Center. The agreement will provide a framework to conduct joint research and development projects in the Deep Learning domain, an essential component of cognitive computing, with a focus on the development of new algorithms to improve and expand the cognitive capabilities of deep learning systems. The centre will also do research into flexible computing like data centric systems and applications.
More information on page 4

©BSC-CNS, 2016. Legal Notice c/Jordi Girona 31. 08034 Barcelona (Spain) Tel. (+34) 93 413 77 16 newsletter@bsc.es www.bsc.es
Director’s View

It is a pleasure to be able to write this editorial for the BSC newsletter, and through it, address all the members of the centre. It is also a challenge, because I am writing this just a few weeks after joining the BSC.

My previous connection with the BSC was through a shared area of knowledge -“machine learning” was one of the keywords of my doctoral thesis- and because for the last five years I was fortunate enough to be a member of the governing bodies of the centre, representing the Catalan Government.

The latter role has given me the chance to get to know the BSC really well: through long periodic meetings to review the performance of the centre, strategic discussions about European infrastructures, and brainstorming sessions on how to overcome administrative difficulties. All of this has provided me with a vision of the BSC where, if I had to choose just one keyword, it would be “strength”: Strong and solid leadership, a strong economic position as a result of the work well done in the past 11 years, and a clever technological roadmap, among others.

In the past five years, the BSC has also worked a small miracle. In a complex period for Spanish science, while the majority of the R&D system has experienced overwhelming difficulties, the BSC has been able to manage the situation and to continue with double-digit annual growth. Knowing, as I do, a great part of the scientific institutions of the country, I can assure you that this is a huge achievement.

Since my arrival at the centre I have been able to corroborate my initial ideas, and add two more: the high quality of a very committed group of professionals and the grand scale of the challenges (which are also opportunities) that we face in the immediate future. Not only the more visible challenges such as the procurement and installation of the MN4 or the continuation of our building, but others still to be clearly defined, where the keywords could be precision medicine, European HPC technology or cognitive computing.

The good work carried out through these difficult years should be an encouragement and a guide to meet these challenges, together with the professionalism and planning necessary for the current moment at the BSC: we are not just a great institution, we are already a large one.

Josep Maria Martorell, BSC Associate Director.

Calendar of Events and Training

- **Jun 19**: ISC High Performance
  - 19 June 2016, Frankfurt
- **Jul 4**: PATC Course: Introduction to CUDA Programming
  - 4 July 2016, Barcelona
- **Jul 4**: Integrative modelling of biomolecular interactions
  - 4 July 2016, Barcelona
- **Jul 11**: 7th PUMPS Summer School
  - 11 July 2016, Barcelona
- **Sep 20**: 10th RES Users’Conference & 5th HPC Advisory Council Spain Conference
  - 20 September 2016, Barcelona
- **Oct 25**: IOT Solutions World Congress
  - 25 October 2016, Barcelona
- **Nov 13**: SC 2016
  - 13 November 2016, Salt Lake City
BSC develops new bioinformatics tool against HIV

The effectiveness of antiretroviral drugs used to treat HIV is frequently affected by the virus’ ability to develop genetic mutations. BSC and IrsiCaixa have developed a bioinformatics method to predict the effect of each mutation on the resistance of the virus to such drugs.

An article published in the Journal of Chemical Information and Modeling explains how this method has effectively predicted the resistance of the virus with genetic mutations in the HIV-1 protease, a protein which is essential for the replication of the virus, to the drugs amprenavir and darunavir. The method could easily be applied to other drugs and proteins.

The BSC-IrsiCaixa method combines HIV DNA sequencing, identification of genetic mutations, computational protein modelling and the simulation of drugs binding with the proteins of the virus. The entire bioinformatics analysis can be performed in fewer than 24 hours on relatively small-scale computing equipment available to any laboratory. One of the main features of the system is the use of PELE, a piece of software developed at BSC to predict how drugs will interact with their targets, which has been shown to have competitive advantages over commercially available software.

Further information here

Carlos Pérez García-Pando returns to Barcelona thanks to an AXA chair

Doctor of Environmental Engineering, Carlos Pérez García-Pando, returns to the BSC to hold the AXA chair on Dust Storms, financed by the AXA Foundation. The researcher led the BSC research team on mineral dust from 2006 to 2009 and will join the centre full time again in October, as the leader of the group on atmospheric composition.

His research programme was selected for the section on environmental risks and will work on expanding knowledge on dust storms, and their effects on climate and society. The lecture series Understanding and predicting sand and dust storms to manage their impacts upon society and economy will study this extreme weather phenomenon, which entails serious damages to the health, environment and daily business and economic life in many countries, especially in North Africa and the Middle East.

This chair will be based at the BSC, whose facilities include the only regional centre of the World Meteorological Organisation devoted to warning, advice and assessment on dust storms. The financing for the chair is 1.5 million euros, distributed over 15 years.

Further information here (Spanish)
Application of cognitive computing to financial innovation

In May of this year, CaixaBank and the BSC signed a collaboration agreement for joint research into advanced deep learning systems, with applications in financial innovation and managing banking transactions. The financial organisation will study innovations that could contribute to customer service and optimise its operative efficiency using supercomputing.

The use of supercomputing will also be applied to analysing and evaluating technological evolution and future scenarios it could open up in the financial services arena. This collaboration will let the BSC open a new case study research project in the financial sector for optimising solutions in complex cognitive systems on high performance platforms.

Further information here

Recognition for the director of BSC

In recent weeks, Mateo Valero has received several recognitions. On 20 May, Valero was invested with a Doctor of Science, honoris causa from the University of Granada, along with singer Miguel Ríos.

Also in May, Festibity, the annual ICT party, granted an Honourable Mention for the year to Valero. In the awards ceremony, the vice-president of the Catalan government, Neus Munté, referred to him as 'one of the most influential European researchers in ICT and the first European to receive the greatest worldwide recognition in HPC, the Seymour Cray Award.'

Moreover, in April the Catalan Autonomous Government awarded him the Creu de Sant Jordi (the Cross of Saint George, one of the highest civil distinctions in Catalonia) ‘for his work in the field of computer architecture, for which he has received prestigious international awards.'

Social simulation and 3D animation in Simulados

How did humanity survive 10,000 years ago? Simulados, shows how a computer generated simulation recreates humanity’s struggle with climate changes and the importance of cultural interaction.

The BSC Visualisation Team produced the mini-documentary Simulados, whose protagonist is Unga, a hunter-gatherer who lived with his family in Gujarat (India) 10,000 years ago. The film mixes 3D animation and simulations excerpted from the research framed within the Simulpast project. By studying primitive societies, it aims to deepen knowledge of human behaviour by introducing artificial intelligence and supercomputing.

For Unga and his family, their resilience to the region’s extreme environmental variability is analysed, as well as their interaction with farmer-shepherd groups.

Further information here
BSC and IBM create Deep Learning Center to boost cognitive computing

In recent years we have seen the emergence of a new trend that is dramatically changing how the design of supercomputing systems and applications move forward: the emergence of data as the world’s newest, and arguably largest natural resource. Cognitive computing systems learn and interact naturally with people to extend what either humans or machines could do independently. **Cognitive computing is the simulation of human thought processes in a computerized model.** It involves self-learning systems that use data mining, pattern recognition and natural language processing to mimic the way the human brain works. Rather than being programmed to anticipate every possible answer or action needed to perform a function or set of tasks, cognitive computing systems are trained to sense, predict, infer and, in some ways, think. Cognitive systems will help human experts make better decisions by penetrating the complexity of Big Data.

This year, BSC and IBM have renewed their research agreement and have created the **IBM-BSC Deep Learning Center.** The agreement will provide a framework to conduct joint research and development projects in the Deep Learning domain, an essential component of cognitive computing, with a focus on the development of new algorithms to improve and expand the cognitive capabilities of deep learning systems. The centre will also do research into flexible computing architectures—which are fundamental for big data workloads—like data centric systems and applications.

The collaboration agreement’s goals revolve around enabling Cognitive Computing by focusing on greatly accelerating basic learning tasks that require Pattern Recognition and Machine Learning, with an emphasis on Deep Learning. The agreement will help BSC to evolve its scientific simulations in areas related with life and earth sciences, and engineering to adopt cognitive computing technologies in their applications and workflows, including cognitive IoT. One of the scientific areas that is considered strategic for both BSC and IBM is precision medicine.

The projects to be carried out in the framework of the agreement should plan for vertical integration and how to exploit the Cognitive applications in the marketplace, encouraging partnership with end-users of Cognitive applications in order to prove an impact in practice. The agreement also embraces education and deep learning skill-transfer to academia through various activities supported by scholarships and grants.

Authors:

- **Elisa Martin Garijo**
  Chief Technology IBM Spain, Distinguished Engineer & Member IBM Academy of Technology

- **Eduard Ayguadé**
  BSC Computer Sciences Associate Director, Full Professor at UPC’s Computer Architecture Department

Inside BSC

BSC Newcomers

We would like to welcome staff who have joined the centre over the last few months and we take this opportunity to inform you that we are distributing the Welcome Manual to all newcomers. The electronic version of the Welcome Manual is available for download on the intranet: https://intranet.bsc.es/en/node/2212

FELLOWSHIPS

JOSEP MARIA MARTORELL, Associate Director, Directors Dpt.

Josep Maria Martorell is the new BSC’s Associate Director. He has more than 12 years experience in Research Centres environment, in remarkable positions, as General Director of Research of the Catalan Government. Josep Maria graduated in Physics, holds a PhD in Computer Sciences by Ramon Llull University and several Postgraduate courses in Management (IESE and ESADE).
BSC hosts its 3rd Doctoral Symposium

Nearly 75 people participated in the third International BSC Doctoral Symposium hosted by BSC on 4-6 May. Six sessions of talks were organised, covering the following topics: postdoc research at BSC, algorithms, physics and data science algorithms, numerical methods and data science, life sciences, simulations and modelling, and performance. Twenty posters were exhibited and presented during four poster sessions that created lively discussion and gave the authors the opportunity to explain their research and results.

The keynote speaker, Francisco Doblas Reyes, gave a lecture titled ‘Big Data for the Study of Climate Change and Air Quality’. Doblas is the director of the earth sciences department at BSC and ICREA research professor at the Catalan Institute of Climate (IC3). The training courses, given by researchers from Computer Sciences Department, reviewed the fundamental algorithms and techniques for data and computationally intensive problems (Prof. Vassil Alexandrov, ICREA-BSC) and introduced scientific visualisation of data (Dr. Javier Espinosa), as well as providing opportunities to practice these concepts.

For further details, please visit the symposium website.

PhD BSC – La Caixa grants

On 18 May, the final phase of the candidate selection process took place for the 4th call for the International PHD Fellowship Programme BSC-la Caixa-Severo Ochoa.

The 10 finalists were invited to participate at a meeting to defend their candidatures before a selection board.

The two fellows who received the grants will be placed in the Computer Science Department, specifically in the Autonomic Systems and e-Business Platforms groups.

Further information here

Did you know...

Where you can find the new PhD regulations?

The new regulations of PhD students have been approved this year, you can find it in the intranet: intranet.bsc.es/en/node/2309

Job Vacancies

If you know someone who wants to join the BSC team, he/she can submit a CV to one of our current vacancies or fellowships' calls: www.bsc.es/vacancies-fellowships

For further information please contact Human Resources (rrhh@bsc.es)

BSC Annual Meeting 2016

On 10 June, BSC held its Annual Meeting. Providing an opportunity for BSC staff from different departments to get together, the event highlighted the strategic topics on which the centre is working.

Photos from the meeting can be viewed on the BSC Facebook page.