

# EUSJA

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## Learning Supercomputer

BY VIOLA EGIKOVA – 1. JUNE 2014

POSTED IN: BLOG, NEWS, STUDY TRIPS



By Bartolomeo Buscema,

science journalist, ITALY (UGIS)

Last May EUSJA along with the European network **CommHERE** organized a study trip to Barcelona to visit some research facilities that join forces on many common projects to understand the complexity of life – from the genome to the cell to a whole organism, and the mechanisms that underlie genetic diseases. The genomic research and imaging technologies produce increasingly immense amounts of electronic data that need to be processed, learned and stored. The **Barcelona Supercomputing Centre** is a right place to help solve this challenge and avoid its limitations. Italian member of EUSJA shares his impressions with his colleagues.

The Barcelona Supercomputer Center (BSC), constituted in April 2005, represents the National Supercomputing Facility in Spain. It manages MareNostrum, one of the most powerful supercomputers in Europe, located at the Torre Girona chapel in Barcelona.

The mission of the BSC is aimed to develop and manage information technology in order to improve scientific progress in several areas such as Computer Sciences, Life Sciences, Earth Sciences and Computational Applications in Science and Engineering. All the above research activities are complementary to each other and very tightly related.

From the foundation of the Centre it has been handled around 3000 external research projects. The Centre also collaborates with IT industries such as IBM, Intel, Microsoft.

Many activities are carried out at the Centre. In this report I would like to give a general overview of the Life Science department where researcher work in different aspects of computational biology, ranging from bioinformatics for genomics to computational biochemistry, with the main target to gain a deep insight into the origin, evolution and function of living organisms using theory and computation. The research lines ranging from molecular modeling and bioinformatics, computational genomics, electronic and atomic protein modeling, protein interactions and docking. As far the last line researchers aim to develop and optimize computational algorithms for characterizing and understanding protein-protein association, which is one of the most important challenges in Structural Biology. We asked some general and specific questions to [Juan Fernandez-Recio](#), Research Director of Protein Interactions and Docking department, to better understand the activities of the BarcelonaSupercomputerCenter.

**Q: What are the main projects you are involved?**

BSC has a wide variety of projects, from the study of climate's change to the development of software for wind

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farms or oil companies, and also many projects related to the development of new hardware and software for supercomputers.

In the Life Sciences area, where I work, we work on genomics and on molecular simulations. My group is mostly focused on the development of computer tools for the prediction of the structure of proteins and the complexes they form. We have modeled the structure of different cases of biomedical interest, and we currently plan to identify inhibitors of xCT, in search of new therapeutics for cancer.

**Q: What is the main activity at the center ?**

We are the national supercomputing centre in Spain. We specialise in high performance computing (HPC) and our mission is two-fold: to provide infrastructure and supercomputing services to European scientists, and to generate knowledge and technology to transfer to business and society.

We are a Severo Ochoa Center of Excellence and a hosting member of the European research infrastructure PRACE (Partnership for Advanced Computing in Europe). We also manage the Spanish Supercomputing Network (RES). Through these programs, many research groups at national and European level are using our supercomputing facilities for a large variety of scientific and engineering projects.

As a research centre we have almost 300 experts and R&D professionals organized into four main research areas: computer sciences, life sciences, earth sciences and computer applications in science and engineering.

These scientists conduct their own research and take part in other centers' projects, facilitating the use of HPC through their experience in developing applications suitable for this kind of computing. Nowadays HPC specialists are an essential link for scientific projects in all manner of specialities.

**Q: What is the calculation capacity of the Center ?**

MareNostrum, the centre's emblem, is one of the most powerful supercomputers in Europe. Currently, MareNostrum has a capacity of 1.100 Petaflop/s (1,100 trillion operations per second), what puts Spain and the BSC-CNS in the leading group of the European supercomputing infrastructure PRACE (Partnership for Advanced Computing in Europe). MareNostrum has 48,896 processors, which are distributed in 6.112 Intel SandyBridge chips of 2.6GHz, each of which has 8 cores and 3,056 nodes, and 84 MIC chips. To have an estimation of this capacity that can be understood in human practical terms, we could say that it is equivalent to around 50,000 home computers, but the capabilities for high-performance computing is actually much larger than putting together all the computers. Its main memory is almost of 100 TB, has a high-performance file system of 2 petabytes and it is connected to Big Data infrastructures, with a combined total capacity of 14 petabytes. The entire system is connected to major universities and research centers in Europe through optical fiber. This facilitates the transfer of data to researchers who need to use our infrastructures.

TAGS: [eusja](#), [science](#), [science journalists](#), [study trip](#)



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# EUSJA News

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Letter from Barbie Drifilina, EUSJA president

## Time to stand up proudly for our profession

Just like wine vintages there are good and not so good years. I don't think 2013 was a particularly fine one – maybe it was because it was an odd number. However, ever the optimist, I am sure 2014 is going to run much more smoothly.



Barbie Drifilina at the European Health Forum Gastei EHFG 2013 (photo by Wolfgang C. Goede)

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But turmoil there was in 2013 in the world of science journalism. Jobs lost; television stations closed down without notice; respected science correspondents told their contracts were not being renewed and invoice payments were delayed to the point where we all ought to set ourselves up as charity. It is not all doom and gloom, however. EUSJA has fared quite well, thanks to the efforts of the board. We, mainly due to the hard work by MarekŁan Sołtys, have enough funding to offer several paid jobs to EUSJA members. The applications are in for the first three and job offers will either be out or finalized as I write. A further six posts are currently being prepared for offer to our membership.

We also have had two session proposals approved and accepted. For the first time EUSJA will be taking part in the International Public Communication of Science and Technology Conference taking place in Salvador, Brazil in May.

And we have a good slot at ESCF in Copenhagen. Wolfgang Goede has

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**ON EMBARGOES AND MANIPULATION**

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