RESEARCH NEWS

20 million supercomputing hours for science

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A total of 20 million supercomputing hours have been allocated to the Spanish Supercomputing Network (known as Red Española de Supercomputación or RES).

Some 87 research projects will be executed in the following four months using the supercomputing hours.

Last year the Spanish National Network was established with the aim of sharing the supercomputing experience and resources for Spanish scientists. Every four months the Access Committee, formed by 44 external scientists, evaluate individually each received project to be executed in the following seven nodes included in the RES network: the Barcelona Supercomputing Center (BSC) with MareNostrum; the Politechnical University of Madrid, with Magerit; the Instituto de Astrofísica de Canarias (IAC) with LaPalma; the Cantabria University, with Altamira; the Malaga Universty, with Picasso, the University of Valencia, with Tirant; and Zaragoza University, with CaesarAugusta. These 87 scientist projects are divided into the four scientific areas: astronomy, space and earth sciences; biomedicine and health sciences; physics and engineering; and chemistry and material science and technology.

‘The RES network is a powerful platform at the service of the Spanish scientific community. I hope that these 87 scientific projects selected by the Access Committee can improve their results especially thanks to the RES calculation capacity,’ said Francesc Subirada, associate director of BSC, coordinator of the RES network.

Two examples of scientific projects included in the computing hours allocated to the RES network are the cosmological project called GHALO, done by a group of the University of Valencia, and another one focused on quantum simulation of biological processes that contribute to form or break chemical bonds, leaded by a research group of the University of Barcelona.

The first project, done by a team leaded by the principal researcher Vicent Quilis of the University of Valencia , studies about the formation and evolution of a halo of dark material similar to the Milky Way through a computational simulation of 3.000 millions of particles.

The second project, headed by Professor Carme Rovira from the University of Barcelona, studies a multi-functional enzyme that activates isoniazid (INH), a drug used to treat tuberculosis. This project aims to intend to model the KatG enzyme mechanism and find the most likely binding site for the INH drug in order to understand the mechanism of drug activation. In this sense, this research project pretends to design new drugs as well as variables of the enzyme.

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