

AMD ROME CALCULATION NODES FOR COMPUTER CHEMISTRY

In early July 2020, SIE installed new nodes for the cluster of Computational Chemistry at the University of Barcelona. Saying supply had been won in a contest of almost 360,000 euros.

Through 26 SIE Ladon nodes, based on Gigabyte platforms and AMD Rome processors, a total of 1,664 cores are offered to the customer to 2.9 Ghz and 26 TB of RAM for scientific calculation. The nodes are integrated through a 10G network, connected to fiber with the outside and a gigabit network for IPMI communications, through switches DLINK, which allows remote control of machines with KVM over LAN and via the free GSM application (Gigabyte Server Management).

The Institute of Computational Chemistry is specialized in various fields of theoretical and computational chemistry. The activity of research conducted at the IQTCUB covers the development of methods and computational tools, the application of various techniques of electronic structures and simulation to problems in the science of materials, the study of reactivity and reaction dynamics in chemical reactions, as well as biological systems and soft matter.

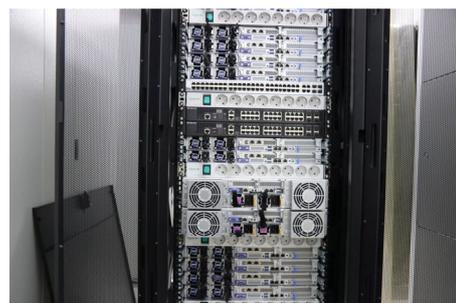


Photo of the University of Barcelona.

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According to the administrator Jordi Inglés, the center works with the HPC system more than 100 researchers with a power of global calculation of almost 4000 cores and 37TB of RAM memory. Now adding the new SIE cluster we have increased considerably the computing power of the center.

The institute is currently expanding thanks to the award-winning María de Maeztu award, opening the institute to various fields of research from molecular dynamics, artificial intelligence, machine learning, design and printing of molecular structures in 3D and applications designed in virtual environments so that users researchers manage and interact in a 3D environment with glasses virtual reality Oculus..



Photos of the expansion of the University of Barcelona cluster.