

An Italian Job – Ensuring the SNS HPC Environment Runs Effortlessly

CASE STUDY



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— Giordano Mancini
PhD, Scuola Normale Superiore

The Computational Chemistry Research Group is part of Scuola Normale Superiore and is led by Professor Vincenzo Barone. It comprises a team of 30 researchers, graduate students, post-docs and staff. The group develops, validates and applies methods based on quantum mechanics and statistical thermodynamics to the study of complex systems of interest in fields such as life sciences and materials, astrophysics and molecular astrochemistry, meta-materials and devices with low environmental impact with particular reference to renewable energy sources.

The HPC environment that runs the Computational Chemistry Research Group’s projects is complex, with over 100 servers and multiple architectures. However, a team of three people manage it; taking care of installation, management and maintenance.

Back in 2012, the IT team took the decision to implement Bright as the de facto infrastructure management platform. As an academic institution, the team needed a solution that was up, running and self-sufficient in no time, to allow the rest of the group to concentrate on their research. Today, the HPC architecture is run on a single cluster, named Avogadro, which is based on Linux and uses Bright technology for cluster management and monitoring.

Since then, the group’s HPC environment has doubled in size. This in turn spurred a growth in HPC tools, resources and complexity which was easily absorbed by Bright. The power of Bright was also tested when the Research Group moved from one physical location to another. During the move the Avogadro cluster had to be turned off and completely disassembled before being moved and reassembled in the new datacentre. Once the head nodes were back up, Bright rebooted all other elements of the new HPC environment in a matter of hours.

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The Research Group works proactively, so the HPC environment needs to be dynamic; often researchers develop their own software and sets of calculations that run for many days and cannot be stopped. Everything is managed in house using Bright technology; from cooling to power; from infrastructure to security; from systems management and software to the helpdesk.

The Computational Chemistry Research Group places high demands on the Avogadro cluster, particularly in terms of stability and uptime. Bright enables the IT team to automate management and monitoring tasks, ensuring that the cluster is as easy to use - and as reliable - as possible. The researchers are able to queue up their jobs, and keep track of the progress being made on their computations, from Bright’s easy to use interface.

“Managing a cluster using Bright is so easy. We can process changes, upgrades, and security updates in minutes. Our researchers are able to run their projects themselves; Bright empowers everyone to be more efficient and more successful.”

