The Scuola Normale Superiore Success Story

THE SCUOLA NORMALE: PBS PROFESSIONAL DRIVES COMPUTATIONAL SCIENCE

The Palazzo della Carovana is a palace in Knights' Square, Pisa, Italy, presently housing the Scuola Normale Superiore di Pisa.

Customer Profile

Formally founded on October 18, 1810 by a Napoleonic decree, the Scuola Normale Superiore (SNS) is a public institution of university education at the forefront of global research. Students are selected only on the basis of merit, lessons are held in seminar form, and an intimate link connects education and research. Student life is deeply integrated with the university experience, and significant space is devoted to international exchanges according to the best models of higher instruction in Europe.

SNS research activities are traditionally divided into two primary areas: Arts and Sciences. Graduates include scientists, politicians and intellectuals, many of whom have made remarkable achievements in their fields.

The Mission: Converting IT Innovation into Opportunities in Computational Science

The SNS Faculty of Science hosts several internationally recognized research groups in Biology, Chemistry, Physics and Mathematics, which are involved in theoretical and applied research in nearly every scientific field, but also operate at a truly interdisciplinary level between art and technology. In this context, with the goal of supporting state-of-the-art research investigations with a strong theoretical/computational background—especially in the fields of material science, emerging nanotechnologies and cultural heritage—SNS has recently established a center dedicated to high-performance computing (HPC) and cutting-edge visualization and virtual reality techniques: DREAMSLab, directed by Professore Vincenzo Barone.

The core scientific investigations at DREAMSLab are devoted to computational chemistry applications; this work was rewarded with an ERC-funded project titled "Development of a Research Environment for Advanced Modelling of Soft Matter" and includes advanced code-development activities in collaboration with Gaussian, Inc., one of the leading global players in the field.

Within DREAMsLab, the "DreamsHPC cluster" represents the reference platform to run processor-intensive numerical simulations with large data sets, which requires parallel efficiency, scalability and fast memory access. This is provided via a private network combining low-latency, high-bandwidth Infiniband switches with a homogeneous HNAS uplink servicing clients at 20 Gb/s over a Fiber Channel back-storage working at 8x8 Gb/s.

The core of the DreamsHPC computational facility is a Dell cluster with over 2600 cores monitored in real time. The computing nodes are divided into families based on their CPUs, ranging from Xeon

THE SCUOLA NORMALE: PBS PROFESSIONAL DRIVES COMPUTATIONAL SCIENCE

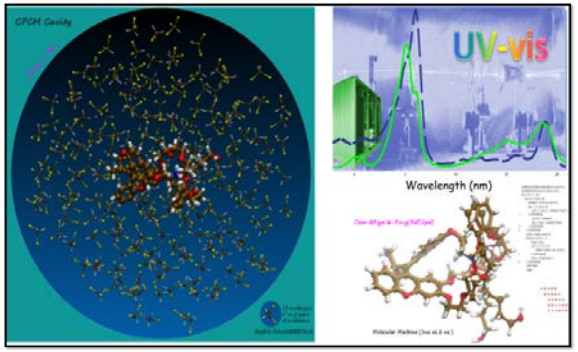
E5500 series cores up to the latest Xeon and AMD Opteron processors, as well as hardware capabilities which allow users to effectively tackle the variety of tasks required by the ensemble of projects carried out within DREAMSLab. The storage capabilities are entirely dedicated to simulation data with 60 TB of space automatically mirrored over a pool of two 30 TB hard-disks. In this environment, a portion of the cluster is used for pilot implementations and applications of novel IT developments to computational science.

Towards a More Realistic Modeling of the Nanoworld

Given the complexity of the simulations running on the DreamsHPC cluster, it was necessary to carefully plan the software layer to be deployed on the infrastructure. The key requirements were overall ease of management of the already-present heterogeneous hardware, as well as significant simplification for the addition of new computing nodes in the existing structure and the distribution of computational programs on the nodes. The goal was maximized user productivity by offering transparent access to computing nodes and increasing HPC resource availability.

"We're always looking for technology solutions allowing us to obtain a better description of complex molecular and supra-molecular systems to simulate their working mechanisms under natural conditions," said Prof. Barone. "This research is in line with The Nobel Prize in Chemistry 2013 awarded 'for the development of multi-scale models for complex chemical systems' and we aim toward the simulation and the efficient description of physical-chemical processes involving complex molecular systems. The goal is the definition of calibrated computational protocols for real-size non-periodic systems over length-scales of tens of nanometers, capturing molecular motions and supra-molecular interactions over several time scales. To this aim, we have to deal with and combine several atomistic levels of theory, ranging from empirical force field–based molecular dynamics simulations to full quantum mechanical calculations, and coupled to phenomenological (continuum, stochastic) descriptions.

Prof. Barone explains: "The novelty and cutting-edge character of the project lies precisely in the definition of original, reliable, flexible and user-friendly computational codes for describing with increasing accuracy and effectiveness complex systems of current interest in biological and/or technological processes, and requires dedicated technology solutions. We are talking about highly detailed numerical experiments of great interest to the scientific community; this is extremely challenging as they involve a large number of interacting and flexible molecules, which have to be treated at a reasonable level of theory in order to obtain the right responses at the state-of-the-art."



A schematic view of a complex simulation scenario. With PBS Professional the Scuola Normale Superiore has improved its computational efficiency (with an almost 50% higher cluster utilization and remarkably reduced waiting times in average when normalized over single user for computing results) without changing the underlying hardware forming the HPC simulative environment.

"From a scientific point of view, focused models in which different parts of the system are described at different levels of sophistication (depending on their role in the overall process) are the key ingredients for reaching this goal. From a technological point of view, flexible highly parallel architectures are

mandatory together with robust, user-friendly management tools," added Prof. Barone.

Hardware/Software Adaptive Templates

The DreamsHPC cluster installed software and tools comprise a mix of advanced C and FORTRAN compilers, Fast-Fourier and Mathematical libraries optimized for both Intel and AMD architectures, and a wide range of parallel software packages distributed under open-source and proprietary licenses, as well as in-house written codes using either MPI or OpenMP paradigms. The DreamsHPC cluster also supports computations using a mixed CPUs/GPUs hardware scheme.

For the HPC workload management, SNS chose Altair's PBS Professional, an industry-leading product with thousands of users and support in 20 countries worldwide.

Why PBS Professional?

In the SNS site, there are nearly 150 computing nodes divided in different families depending on own hardware. As a consequence, PBS Professional needs to allocate the available computational power in a self-consistent way by means of a queue-label for each node-family. The similar products available from the open-source community were not as efficient, flexible and robust.

"PBS Professional perfectly matches the solution we were searching for our HPC environment," said Professor Barone. "Among commercial schedulers PBS is the best choice for complex HPC workload management, and open source tools really can't compare to the reliability and support that Altair PBS Professional provides."

Thanks to PBS Professional, the HPC users at SNS now have dynamically (and mutually exclusive if necessary) balanced access to the available computational resources to run their jobs in up to a month of wall-clock time. Moreover, the management of the submitted computational instances is completely transparent to the user; this is important because typically users want to follow the status of their simulations without losing time interacting with the OS environment.

According to the DreamsHPC technical staff: "The clarity of Altair's documentation and support greatly simplifies the work of our HPC administrators, who can easily pinpoint the necessary information to intervene quickly and efficiently on the cluster."

Among the common tasks to be carried out on the HPC infrastructure are: installation of license tokens; configuration of both the PBS Server and the daemons executed on the nodes; creation of the desired computational slots hosting simulations; and realization of a well-defined and optimized hardware/software resource.

"Altair's strong expertise in cluster management and configuration, together with its responsiveness, provide valuable help for us to quickly address the various challenges we face. For example, questions concerning the optimal parameters for queues (related to the remarks of SNS reference users about cluster configuration) were rapidly solved by Altair's technical support. A dedicated PBS Works Product Specialist suggested the right course of action, and his prompt reply allowed a quick solution of the problem and a very rapid release of the overall computational resource, taking into account specific requirements," explained the DreamsHPC staff.

The Scuola Normale Superiore Success Story

THE SCUOLA NORMALE: PBS PROFESSIONAL DRIVES COMPUTATIONAL SCIENCE

Benefits: Higher Cluster Utilization Rate and Availability

As a result of the PBS Professional installation, SNS has seen the following benefits:

- The HPC cluster has significantly increased its occupation rate, with a 50% higher cluster utilization over the previous configurations
- PBS Professional has also improved the computational balance over the HPC cluster, avoiding potential conflicts among simulations that require a different ratio between computational intensity and memory bandwidth.
- Overall, in view of the global usage of DreamsHPC resources since their availability to users, the Scuola Normale Superiore has been able to optimize the returns on its HPC investments by employing PBS Professional, which allows users to increase cluster utilization while maximizing the performance of the entire infrastructure.

Future Projects

Given the gains already achieved, the Scuola Normale Superiore is currently extending the HPC facility with the short-term aim of doubling the computational power both in terms of the number of cores and memory allocation. For this reason, SNS has already planned to test additional Altair features and products designed to manage complex computational schemes with hybrid CPUs and GPUs/coprocessors (such as Intel® Xeon Phi™).

Another project already on the way will address the potentialities of combining PBS Professional with Altair's PBS Analytics to support data-driven analysis and making real-time decisions.

For More Information

- To learn more about the DreamsLab and DreamsHPC cluster at the Scuola Normale Superiore, visit: http://dreams.sns.it/
- To learn more about Altair's PBS Professional cluster workload manager, visit: http://www.pbsworks.com/