

PBS Professional Manages Workload for Czech National Supercomputing Center



IT4Innovations
national
supercomputing
center

Key Highlights

Industry

Government and Research

Challenge

Support the needs of a massive supercomputing system with a large, diverse user base

Altair Solution

PBS Professional, PBS Analytics

Benefits

- Implementation speed and simplicity
- Ease of user adoption
- High functional performance

Customer Profile

The National Supercomputing Center IT4Innovations is a research institute at the VŠB - Technical University of Ostrava (VŠB-TUO) in the Czech Republic, funded by the EU Operational Programme Research and Development for Innovation. The hundreds of researchers who utilize this Center come from leading institutes across the Czech Republic. Since 2011 IT4Innovations has been part of the prestigious European network of PRACE supercomputing centers and thus provides resources to other European researchers as well.

The Challenge: Meeting the Computing Needs of a Large, Diverse User Base

As part of the IT4I National Supercomputing Center, a unique supercomputer is being built to support the leading-edge computational research that will be performed by the Center's users. The supercomputer is being built in two parts: a cluster called Anselm which has been

in operation since June 2013, and another larger cluster which, when put into operation in early 2015, is expected to be one of the 100 most powerful supercomputers in the world. Already the Anselm system is the largest cluster in the Czech Republic and is part of PRACE as a DECI TIER-1 system. Visit www.it4i.cz/hardware/en for details about these systems.

There are six research directions at the IT4I National Supercomputing Center dealing with a wide variety of computational problems (including real time traffic analysis/management, flood modeling/predictions, air pollution modeling/preventions, molecular dynamics simulations, modeling of new materials etc.) using methods including computational fluid dynamics (CFD) and finite element analysis/finite element method (FEA/FEM).

Given the wide variety of users and applications, IT4I realized they needed a reliable, high-performing workload

Czech National Supercomputing Center

Success Story

“PBS Professional offers fast, easy implementation so our users could get up and running quickly, and it provides the robust commercial functionality we need in a scheduler. In addition, Altair offers the high quality support a facility like ours needs to rely on.”

Branislav Jansík,

Director of Supercomputing Services at IT4I

management product for the Supercomputing Center’s users. In the procurement procedure, IT4I demanded an advanced job scheduler and resource manager along with advanced tools for utilization analysis. Products satisfying these requirements were bundled within the offer made by Bull, the hardware supplier.

Criteria to be met in the procurement for the workload manager included: High-efficiency and utilization of compute resources; Robust batch and interactive runs of jobs; Support for scheduling of nodes with GPU/co-processor cards; Support for job dependencies and job arrays; Fault tolerant, high availability operation; Static and dynamic resource availability for scheduling and job execution, including external dynamic resources like software licenses; Resource reservation support; Backfilling; User notification of job lifecycle events; Limits/quotas on users/groups and resources; High quality, well documented API for common languages like C and Python; and many more specific technical requirements.

“Of course we needed a high-quality scheduler – all supercomputing centers need this to ensure the highest levels of resource utilization which is a key to successful center,” said Martin Palkovič, director of the Center. “When

you are putting this much time, resource and energy into building a supercomputing system to support the needs of hundreds of users, you have to make sure the workload management system will be reliable and deliver the performance you need.”

The Solution: Altair’s PBS Professional for Consistent Performance and Reliability

The experts at Bull evaluated many commercial and open source products before deciding to recommend Altair’s PBS Professional® as the workload manager to fulfill the tight requirements for the scheduler in this procurement.

“PBS Professional is an excellent choice for high-quality workload management at scale,” said Olivier David, ISV Alliances Director at Bull. “We have tightly integrated PBS Professional with our bullx supercomputer suite; coupled with our optimized bullxMPI, it guarantees the efficient use of user applications on the bullx supercomputer. Bull and Altair both have a long history of delivering award-winning solutions for the HPC market, and this joint solution provides our customers with a high standard of performance and robustness, including for very large configurations.”

The decision was confirmed by the director of Supercomputing Services at IT4I Branislav Jansík, who said: “There are a number of options out there, but PBS Professional provides one of the most advanced and mature solutions and we are happy that Bull in its offer decided to select this scheduler.”

Jansík adds: “We were already familiar with PBS Professional as a job scheduler for our HPC clusters at the University. Still, with the magnitude of the system we are operating now, we wanted to start fresh and give the vendors the possibility to provide a new system with the best scheduler they could imagine. I am glad PBS still came out on top.”

The experts at IT4Innovations Supercomputing Services department used their previous experience with PBS Professional to define the functional criteria for the new desired scheduler. “PBS Professional sets a high standard for functionality,” explains Branislav Jansík, “and any scheduler we chose would have to perform at least as well.”

In the end, the vendor decision to use PBS Professional came down to ease of implementation and use. “PBS Professional is easy to install and use, and it meets all of our functional requirements,” said Branislav

Project Summary

The IT4I National Supercomputing Center uses PBS Professional to manage its new Bull supercomputer being shared by over 200 planned users. PBS Professional's ease of implementation and use, along with the product's reliability, were cited as key differentiators. The Center is also using PBS Analytics and plans to investigate more products as cluster usage grows.

At right: *The Cluster at IT4I National Supercomputing Center*



Jansík. "Now our users have a workload management system they can rely on, and we are poised for growth with a system that will scale with us."

All researchers at the Center are now using PBS Professional to allocate and utilize the computational resources of the Anselm supercomputer, an x86 cluster delivered by Bull with Rpeak approx. 94 TFLOP/s.

PBS Professional was delivered pre-installed by Bull, so users at the Center could get up and running quickly. IT4I was able to easily customize the product to their needs by analyzing user and operational needs, then implementing customizations during initial stages of the project.

"With PBS Professional we can quickly create plugins and prologue/epilogue scripts to secure optimal resource usage, enhance security to our specifications, and keep the compute nodes in a clean and consistent state after job usage," said Filip Staněk, deputy director of IT4I Supercomputing Services and one of its senior administrators. "We have highly complex customization needs to satisfy our user base, and PBS Professional made this easy." The IT4I National Supercomputing Center

has also implemented PBS Analytics, which came pre-installed with the solution, for user analytics and reporting.

"To know exactly how much the users and projects are consuming from their allocations and to bill them accordingly is important for every supercomputing center. The advanced analysis and reporting offered by PBS Analytics allows us to better understand utilization details and project future load," said Martin Palkovič.

The Results: Supercomputing Delivered – Fast and Easy

According to IT4I National Supercomputing Center administrators, the biggest value of choosing PBS Professional is the quick and easy adoption and usage.

"It was a simple matter to get familiar with PBS Professional and get our users up and running," said Filip Staněk. "We know with Altair we have access to the first-class support which is a differentiator for PBS Professional over open source alternatives like SLURM or Torque."

Currently, over 100 active users at the IT4I National Supercomputing Center users are using PBS Professional as the only way

to allocate and use the computational resources in the cluster. On the Anselm cluster, new applications are being installed on a daily basis, and the Center plans to evaluate other Altair technologies as part of their preparation for future expansion.

Most applications being run by PBS Professional are codes developed by users or open source software such as OpenFOAM, ParaView, and Octave. However, commercial software such as ANSYS, EnSight, LS-DYNA, MATLAB and COMSOL are already present. In addition, the Center plans to implement VASP, Wien2K and others.

"We are confident PBS Professional is the right solution for our supercomputing system," said the Center's director Martin Palkovič.

"PBS Professional is an excellent choice for high-quality workload management at scale."

Olivier David,
ISV Alliances Director, Bull

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About Altair

Altair empowers client innovation and decision-making through technology that optimizes the analysis, management and visualization of business and engineering information. Privately held with more than 1,800 employees, Altair has offices throughout North America, South America, Europe and Asia/Pacific. With a 27-year-plus track record for high-end software and consulting services for engineering, computing and enterprise analytics, Altair consistently delivers a competitive advantage to customers in a broad range of industries. Altair has more than 3,000 corporate clients representing the automotive, aerospace, government and defense, and consumer products verticals. Altair also has a growing client presence in the electronics, architecture engineering and construction, and energy markets.

About PBS Works

PBS Works™, Altair's suite of on-demand cloud computing technologies, allows enterprises to maximize ROI on existing infrastructure assets. PBS Works is the most widely implemented software environment for managing grid, cloud, and cluster computing resources worldwide. The suite's flagship product, PBS Professional®, allows enterprises to easily share distributed computing resources across geographic boundaries. With additional tools for portal-based submission, analytics, and data management, the PBS Works suite is a comprehensive solution for optimizing HPC environments. Leveraging a revolutionary "pay-for-use" unit-based business model, PBS Works delivers increased value and flexibility over conventional software-licensing models.

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