

PBS Professional at The Scripps Research Institute: High-Performance Computing Workload Management Solution



Key Highlights

Industry

Life Sciences

Challenge

Fulfilling compute cycles for TSRI scientists.

Altair Solution

Provides a seamless interface to multiple platforms for TSRI scientists.

Benefits

- Does not require a lot of support (install and just runs), so it allows scientists be scientists

Customer Profile

The campus of The Scripps Research Institute (TSRI) overlooks the Pacific near San Diego. Its proximity to the famed (but unrelated) Scripps Oceanographic Institute occasionally causes confusion of identities. But TSRI is prestigious in a totally different way.

This is the world's largest private non-profit biomedical research facility, with more than a million square feet of laboratory space, a staff of 2,800, a faculty of 290, 800 post doctoral fellows, 164 graduate students, and at least 1500 technical & administrative support personnel. The talented TSRI staff generates constant high-performance computing workload managed by PBS Professional® on over a thousand CPUs.

TSRI's academic credentials are equally impressive. Faculty names include three Nobel laureates and numerous members of the National Academy of Sciences. TSRI is known worldwide for basic research in immunology, molecular biology, cell biology, chemistry, neurosciences, autoimmune diseases, cardiovascular disorders, and cancer. This work focuses on the structure and functions of biological molecules, in which TSRI is an acknowledged world leader.

Physically and professionally, TSRI is an attractive setting. In each campus building, offices and laboratories surround a central galleria that encourages interaction and synergy. This interdisciplinary approach stimulates innovation.

Scripps Success Story

“We use about 1,300 processors, all managed by PBS Professional. That’s one of the nice things about PBS Professional; it gives us a seamless, coherent interface to all three of the platforms we’re running.”

Bill Young,

Chief of Technical Computing / Associate Director of Research Computing, Scripps

Filling the Need for Compute Cycles

Most TSRI researchers work in one of the institute’s seven departments, which represent primary fields of study: Cell biology, chemistry, immunology, molecular biology, molecular and experimental medicine, neurobiology, and neuropharmacology. Others work in one of the other on-campus research organizations — The Skaggs Institute for Chemical Biology, the Harold L. Dorris Neurological Research Center, the Institute for Childhood and Neglected Diseases, or the Center for Integrative Molecular Biosciences.

Basic research at the molecular level is highly compute-intensive, and the Research Computing Department delivers the compute cycles needed by TSRI scientists.

The Department currently operates three HPC platforms: a 512-processor 32-bit Xeon cluster; a 128-CPU SGI Altix single-system-image system with 64-bit Itanium2 processors; and a new 64-bit cluster that provides 576 Xeon EMT processors.

“This is a shared resource that supports the computations of the Institute,” says Bill Young, Chief of Technical Computing and Associate Director of Research Computing.

“The work comes down to several broad categories in the life sciences, including classic theory and modeling, virtual chemistry, docking, proteomics, and molecular structure.”

PBS Professional: A Seamless Interface to Multiple Platforms

TSRI uses Altair’s PBS Professional

software to provide a consistent workload management infrastructure for its users across all three computing environments.

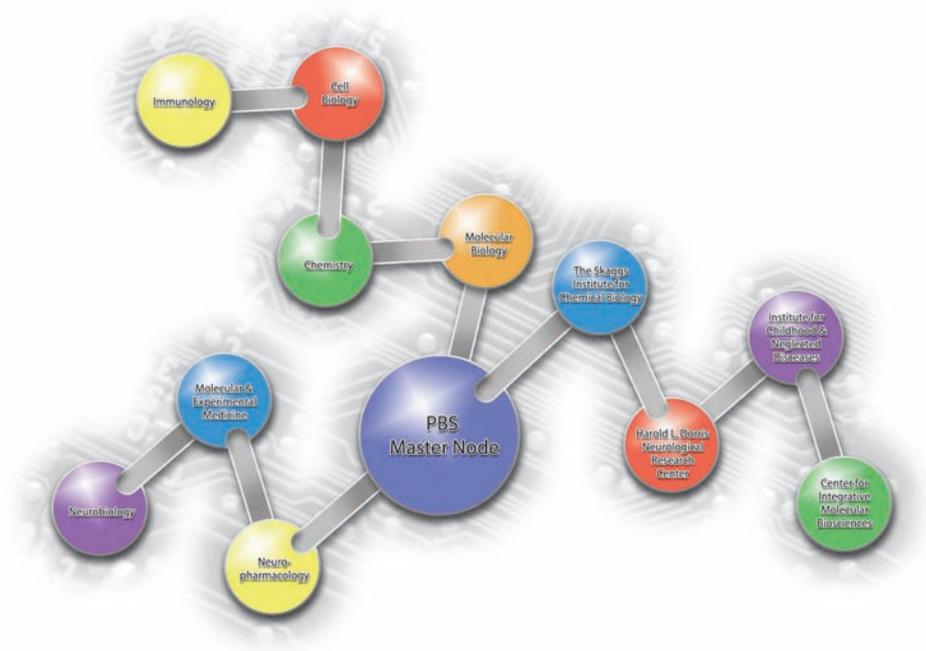
“All told, we use about 1,300 processors, all managed by PBS Professional,” says Young. “That’s one of the nice things about PBS Professional; it gives us a seamless, coherent interface to all three of the platforms we’re running.”

PBS Professional handles workload management for up to 500 account-holding users, of which 75-100 are most active. There are no off-campus users, and no external grid component; the Department’s mission is to support the needs of TSRI scientists. Having dedicated internal processing systems gives them control over priorities of use. This is important, because



An Interface to Multiple Platforms

PBS Professional handles workload management at the Scripps Research Institute of up to 500 account-holding users, of which 75-100 are most active.



every TSRI investigator is essentially an independent contractor responsible for securing grant dollars to support research projects. Funding, primarily from NSF and NIH, is used in part to support the TSRI infrastructure, including the Technical Computing Department, and has no provision for sharing resources with off-campus organizations. Researchers use a web page interface and PBS Professional to access a platform of choice based on their needs and the current level of utilization on each platform. “We’ve used PBS Professional for this purpose for years — ever since it was first available,” says Young. “It works well for us. It gives us a uniform interface to our clusters, and it’s a mature, stable product.

We deploy PBS Professional without extensive customizations; we use it basically

out of the box. Additionally, PBS Professional doesn’t require a lot of support; we install it and it pretty much just runs.”

Letting Scientists Do Science

“If you look at what we paid five years ago to get this much processing power, I think it’s pretty cheap and affordable today,” says Young. “And products like PBS Professional that are mature make that processing power really simple to use so our scientists don’t have to be computer scientists. They just want to get an answer out to help them move science forward. I think over the last couple of years we’ve really built up the infrastructure to facilitate that.”

TSRI scientists may not be computer scientists, but they have an impressive portfolio of scientific software development.

TSRI is home to primary authors of such well-known scientific codes as CHARMM and AMBER (molecular mechanics), SEQUEST (proteomics), and Autodock (protein-ligand docking). TSRI scientists run these and other codes such as Gaussian and BLAST on the Department’s clusters.

Although TSRI research is primarily aimed at the discovery of fundamental knowledge, it has significant ramifications for stroke and heart disease, cancer, neurological disorders, viral diseases, alcoholism and chemical dependency, diabetes, autoimmune diseases, and kidney dysfunction. The tools provided by the Technical Computing Department, including PBS Professional, ensure that this work will continue to move ahead.

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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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