

Weizmann Institute Chemistry Faculty Switches to PBS Professional



Customer Profile

The Weizmann Institute of Science is one of the world's leading multidisciplinary research institutions. Hundreds of scientists, laboratory technicians and research students embark daily on fascinating journeys into the unknown, seeking to improve our understanding of nature and our place within it.

Groundbreaking medical and technological applications that have emerged from basic research conducted by Weizmann Institute scientists include: amniocentesis, a prenatal diagnostic test; sophisticated laser systems for high-precision diamond cutting; living polymerization, one of the most fundamental techniques of the modern polymer industry; and ribosome structure analysis, for which the Institute's Professor Ada Yonath was awarded a Nobel Prize in Chemistry.

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

The high-performance computing (HPC) facility at the Weizmann Institute's Chemistry Faculty enables scientists to perform cutting edge research in a variety of fields, including quantum mechanics, protein folding, DNA recognition, turbulence physics, climate modeling, and much more.

The HPC cluster serves hundreds of Chemistry Faculty members, with 20-30 users from various departments active on the cluster at any given time. The cluster currently consists of 1242 cores, and the Institute is in the process of adding HP SL 230s gen 8 machines to increase the core count to 3096.

Key Highlights

Industry

Government and Research

Challenge

Deliver consistently high cluster performance while balancing complex requirements

Altair Solution

PBS Professional for reliable workload management

Benefits

- Higher cluster utilization rates
- Improved user productivity
- Better services and support

Weizmann Institute Success Story

“PBS Professional is the best workload management solution for our needs. It offers the most robust and flexible management of our diverse user policies and requirements, and it’s simple to install and use. In addition, Altair’s expertise and dedication to implementation success is unbeatable.”

Dr. Mark Vilensky,

Scientific computing manager, Chemical Physics department, Weizmann Institute

The installed software includes a mix of advanced C and FORTRAN compilers, mathematical libraries, and a variety of free, academic, commercial and homegrown dedicated software tools. Workload types vary widely: structural biology calculations performed with Gaussian; quasi-classical molecular dynamics using homemade software; atmospheric dynamics analysis using Geophysical Fluid Dynamics Laboratory’s Flexible Modeling System (FMS); and more. In addition, different teams have different priorities and needs, for which usage policies must be developed and enforced.

In short, the computing environment comprises a complex system of users, resources, requirements and policies that need to be carefully managed.

“We needed a reliable workload management product that could deal with our situation: heavy demand from diverse users for limited resources,” says Dr. Mark Vilensky, scientific computing manager at the Chemical Physics department in the Weizmann Institute. “A job scheduler alone is just a tool that queues jobs for submission – it doesn’t necessarily include the intelligence to manage a full landscape of users, all with different priorities and computing requirements.”

Thus, the Weizmann Institute’s Chemistry Faculty sought a workload management software vendor that could provide:

- Consistently high performance
- Support for complexity in user priorities and profiles
- A proactive, collaborative approach to solution delivery
- Reliable user support

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

The manager of the HPC facility investigated several workload management software alternatives to replace their previous solution, Moab from Adaptive Computing, before selecting Altair’s PBS Professional®. Among the decision factors were PBS Professional’s flexibility in handling complex requirements and the company’s first-rate level of service and support.

“It was a clear choice to go with PBS Professional,” says Vilensky. “Altair’s outstanding approach to customer service was an important factor. The collaborative relationship Altair has built with our Institute and their ability to understand and fulfill our requirements was unmatched.”

PBS Professional was easily able to handle the complex user policies in place at the Institute, where both hard and soft limits need to be managed. For example, the cluster might have 1242 CPUs available – a hard limit – but User X might have permission to access only 100 of these while other priority users are in line. That’s a soft limit that needs to be implemented through robust policies which a workload management system must comprehend and apply.

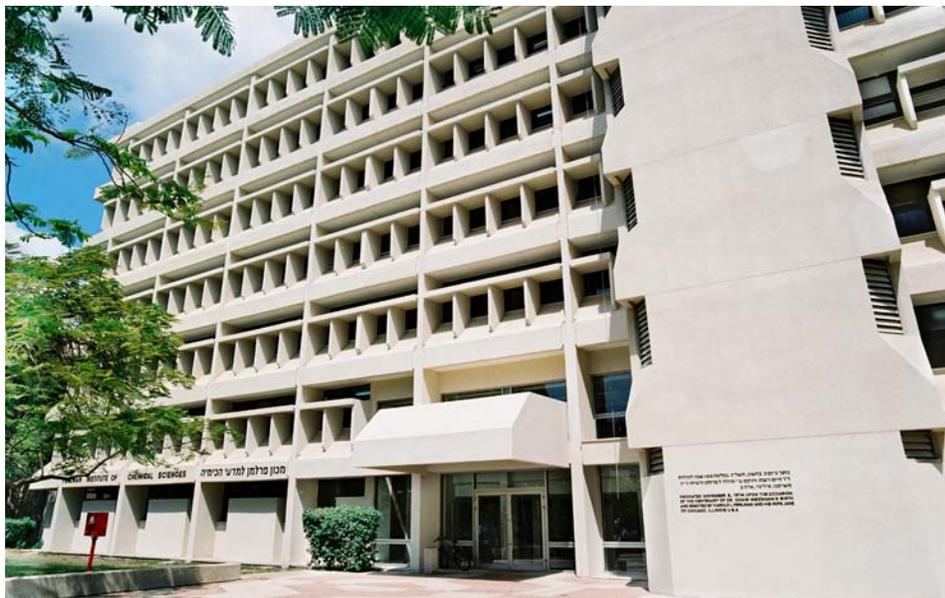
“PBS Professional manages user priorities and hard and soft limits very well, so we get much better cluster utilization,” says Vilensky. “Also, PBS Professional’s plugins made it possible to set up our policies in a fast and accurate way.”

PBS Professional installation was a very smooth process, taking about 30 minutes. In addition, Altair’s support expert was able to translate policies used with the previous scheduler directly into PBS Professional in less than a week, greatly simplifying the transition process.

“It was no problem to switch to PBS Professional,” says Vilensky. “Anyone can supply transition tools, but there is no recipe to build complex policies since every site is

Project Summary

The Weizmann Institute replaced Moab with PBS Professional to manage a 3,096-core HP cluster shared among hundreds of users. The transition process was easy, thanks to Altair's excellent customer services and support. Now, the Institute enjoys higher cluster usage rates and greater productivity from their award-winning scientists.



The Perlman Chemical Sciences Building at the Weizmann Institute of Science

different. Setting policies was complicated before, but Altair made it easy. Their support personnel are excellent – they just do the work, and you're up and running."

The Result: Improved Usability and Productivity

As a result of the PBS Professional implementation, the Weizmann Institute's Chemistry Faculty users have benefited from:

- 30% higher cluster utilization rates
- Reduced wait times for computing results
- More consistent product performance
- Improved user productivity via greater resource availability
- Improved user experience thanks to a reliable support team

"Before, we'd sometimes have hundreds of CPUs idle yet a queue of several hundred jobs," says Vilensky. "Now, we're filling up the cluster while reducing wait time on the queue. It's a double benefit of increased cluster utilization plus improved user productivity."

"The improvement in the current scheduler is significant," says Asaf Azuri, a Ph.D. student user in Weizmann's Chemistry Faculty. "It multiplies the number of jobs I can run by a factor of 4 to 6, and I have to wait just a few days instead of a few weeks for the computation to be finished. In addition, I can submit many more jobs than before. For instance, I can now submit a full calculation with about 3000 jobs while in the former scheduler I had to divide it into several parts. It makes the work much more pleasant and in a sense I feel that the new scheduler works for me."

In addition, Altair has been instrumental in ensuring the system load is well managed. The PBS Professional support engineer provided a custom extension that deletes or resubmits suspended jobs based on certain user choices. "The ability to customize and extend the capabilities of the product with the assistance of Altair's excellent services is something you can't find everywhere," says Vilensky. The Weizmann Institute is now investigating

additional Altair features and products from the PBS Works suite. They are also currently expanding the cluster from 1242 cores to 3096 cores, all of which will be managed by PBS Professional.

Says Vilensky: "We've now found the right solution in PBS Professional."

"With PBS Professional, we've maximized the availability of resources for our users. This means our scientists are able to be more productive and dedicate more of their valuable time to the groundbreaking research they are here to do."

Dr. Mark Vilensky,
Scientific computing manager, Chemical Physics department, Weizmann Institute

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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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