Case study

Build a World-Class Energy Research Institute

Dalian Institute of Chemical Physics (DICP) builds a "catalysis and dynamics computing system" platform with HP High Performance Computing cluster solution

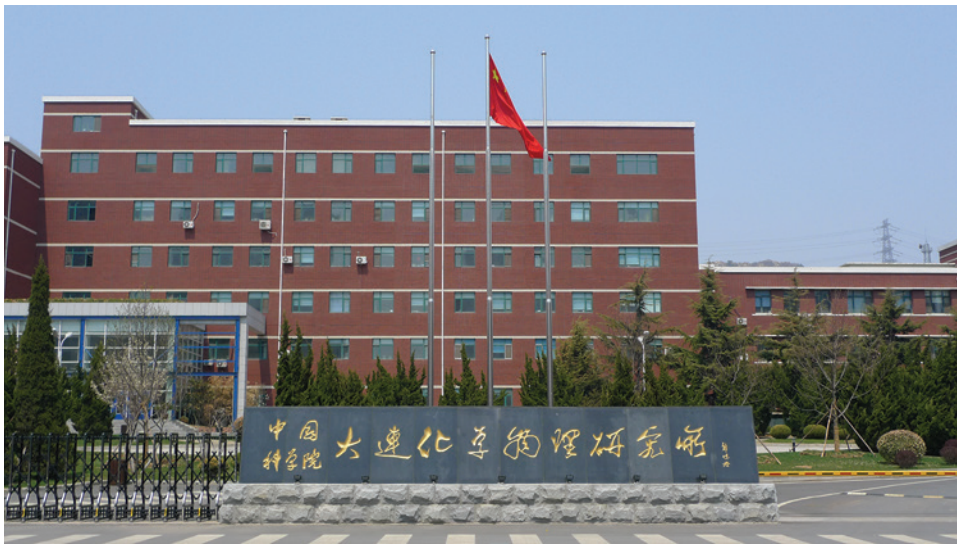
Industry
Research institute

Objective
In order to ensure the smooth development of scientific research and orderly advancement of the research projects in State Key Laboratories, DICP has decided to build a "catalysis and dynamics computing system" platform to help achieve its strategic objectives and tasks with theoretical computing. The "catalysis and dynamics computing system" platform requirements include: high floating-point computing performance, scalability, price performance, energy conservation, and other features.

Approach
Build the "catalysis and dynamics computing system" platform as an HP High Performance Computing cluster solution to provide IT support for DICP in its scientific research. The HPC cluster will include such products as HP ProLiant DL360p Gen8 Server, HP ProLiant SL210t Gen8 Server, HP SL2500 Scalable Systems, HP P2000 G3 MSA Array Systems, and HP InfiniBand switches as along with HP iLO management engine and HP Insight Cluster Management Utility (CMU) for monitoring and management.

IT matters
- A "catalysis and dynamics computing system" platform that delivers high floating-point computing performance, scalability, price performance, and energy efficiency
- High performance rack and scalable HP ProLiant servers that provide a 100% investment protection for the computing service platform
- Significantly reduced operating costs and total cost of ownership for DICP's theoretical computing platform for chemistry

Business matters
- Increases the compute capacity and speed for high-density large-scale quantum chemistry such as heterogeneous catalysis, homogeneous catalysis, activity and selectivity of photocatalytic reactions, chemical reaction dynamics
- Aids in the advancement of research projects by State Key Laboratories by providing superior theoretical computing infrastructure for chemistry at DICP
- Provides a substantial HPC cluster platform for theoretical computing that will further DICP's research and cultivation of research talent



"We based our choice of HP primarily on its overall strength. HP outshined any other IT rival in meeting every criteria of the DICP proposal for a "catalysis and dynamics computing system" platform. DICP finds HP's strength convincing and trustworthy."

– Dai Dongxu, Assistant Director of DICP's State Key Laboratory of Molecular Reaction Dynamics

Dalian Institute of Chemical Physics (hereinafter referred to as DICP) is an integrated research institute that focuses on both basic and applied research, combined applied research and technical information transfer, as well as task-driven research talent development. Formerly known as Dalian University Research Institute, it was established in March 1949 and renamed Dalian Institute of Chemical Physics (DICP) affiliated with the Chinese Academy of Sciences in 1970. Its disciplines include catalytic chemistry, engineering chemistry, laser chemistry, molecular reaction dynamics, modern analytical chemistry, and biotechnology. The State Key Laboratory of Catalysis and the State Key Laboratory of Molecular Reaction Dynamics at DICP were recognized twice consecutively as "outstanding" in 2009 and 2014 in the assessment of China's State Key Laboratories.

HP ProLiant DL360p Server

Challenge

The mission of DICP is to meet China's strategic needs by focusing on both basic and applied research with the Dalian National laboratory of Clean Energy by supplying research platforms that consistently provide significant creative theoretical and technical results in the fields of optimized petrochemical resource use, high-efficiency chemical energy conversion, clean energy and renewable energy, and insure the orderly implementation of its State Key Laboratory research projects.

To enhance its capabilities, DICP decided to build a "catalysis and dynamics computing system" platform. The platform will help DICP accomplish its strategic growth objectives and tasks with a basic chemistry platform for theoretical computing. To this end, DICP engaged with a professional tendering company and set up an expert group to conduct strict appraisals of IT vendors and their solutions in accordance with DICP's detailed bid requirements in terms of the price, technology, configuration, and services.

The total solution must provide high performance and reliability that both meet current needs and support future growth.

- DICP's "catalysis and dynamics computing system" platform will be used for the research of heterogeneous catalysis, homogeneous catalysis, activity and selectivity of photocatalytic reactions, and chemical reaction dynamics that span multiple space and time scales with static and dynamic catalysis reaction dynamics involving a variety of inorganic, organic, and composite materials. All of these subjects entail intensive large-scale scientific computing; therefore, the new solution and its computing server products must be able to provide high performance, powerful computing, and effectively expand and improve to suit DICP's current and future needs.

The selected solution and IT infrastructure products must offer outstanding price performance and energy efficiency.

- Price performance is one of the most vital criteria for DICP. As a key institute affiliated with the Chinese Academy of Sciences, DICP is always very careful to select purchases that will further research achievement and help cultivate the largest number of sophisticated staff and research talents. To ensure this, the new computing server products must deliver high levels of performance for their cost. In addition, as an authoritative institute in energy research in China that is committed to research in new energy sources and renewable resources, DICP purchases nothing but green products to save cost and fulfill its social responsibilities.

The system must eliminate complex operations management so DICP can focus on scientific research by providing easy-to-manage system software and professional, comprehensive technical services.

- DICP has a large number of experts in scientific research. When completed, the "catalysis and dynamics computing system" platform will be managed by DICP's Public Support Platform Equipment Management Committee, the State Key Laboratory of Molecular Reaction Dynamics and the Theoretical Computing Center. The ability of the system to remove the complexity of routine IT operation and management so these institutions can invest more time and energy in scientific research has become an important purchase criteria for DICP. Therefore, DICP requires the computing server vendor to provide full technical support, and comprehensive services for pre-planning, medium-term implementation, ongoing maintenance and support, while integrating the supporting management software to reduce management workload.

Solution

After a rigorous bid evaluation by the expert group, DICP chose HP's high-performance computing cluster solution, which was a set of loosely coupled computing nodes consisting of multiple servers (nodes). Designed to solve complex scientific or numerical calculation problems, this solution provides users with high-performance computing, network request-response or professional applications and other services. The details about server products and software are as follows:

Servers

The HP High Performance Computing cluster solution includes two HP ProLiant DL360p Gen8 Servers, HP ProLiant SL2500 Scalable Systems with 108 HP ProLiant SL210t Gen8 Servers contained in 27 HP ProLiant SL2500 shared infrastructure chassis. The two HP ProLiant DL360p Gen8 Servers are respectively configured with two Intel® Xeon™ E5-2620v2 processors, two 16GB DDR3 1600MHz RDIMM low-voltage memories, and two 600GB 15k rpm hard drives for management, login, job scheduling, and I/O nodes. This compact model provides more powerful performance, efficiency, storage capacity, and reliability. Its enterprise-class design, high reliability , and good scalability ensure durable services in the

HP ProLiant SL210t Gen8 Server

DICP environment that is demanding for both performance and reliability. Each of the 108 HP ProLiant SL210t Gen8 Servers is configured with two Intel Xeon E5-2650v2 processors, four 16GB DDR3 1866MHz RDIMM memories, a 600GB 15k rpm hard drive, and a storage controller HP Smart Array P222 (with 512MB FBWC cache for persistent data protection).

These servers, installed in the 27 HP ProLiant SL2500 chassis, constitute the computing nodes in the HPC cluster. They have all the outstanding characteristics of enterprise-class servers, and are specifically optimized for efficiency, density, and flexibility. This is the best choice for users who have mainstream or high-performance computing tasks but limited space in computer rooms. In addition, the new generation of iLO4 technology in the HP iLO management engine provides four major innovations, enabling virtual media, remote console, virtual KVM, and other advanced features. Its unique functional configuration integrates all system software and drivers on the main board, allowing installation and deployment without the requirement for CD-ROM start-up, and online updates may be implemented at any time at no additional costs.

The HP ProLiant server family is a standardized solution featuring three major advantages:

1) Powerful. It provides dual channel quick connection that boosts performance by up to 80%;

2) Stable and reliable. It provides superior reliability, availability, and serviceability (RAS) with support of advanced ECC, data mirroring, and online backup;

3) Easy to use and manage. Its high degree of standardization and modular design enable easy expansion/upgrade and protect 100% of existing investments.

Storage and Switches

The HPC solution for DICP includes the HP P2000 G3 MSA Array Systems storage configured with dual active controllers (each has 4GB cache and two 8Gb Fibre Channel host ports), 25 4TB 7.2K rpm 3.5" hard disks, and standard management tools, snapshot and volume replication function, and the high-bandwidth low-latency HP InfiniBand switches designed for the parallel cluster computing systems that are demanding for data exchange between networks.

Management Tools and Software

The HPC solution provides HP iLO management engine and HP Insight Cluster Management Utility (CMU), in addition to the cost-effective IT infrastructure products. HP iLO management engine features proprietary technologies including HP intelligent supply, HP agentless management, HP active health system, and HP Insight remote support. Besides faster deployment and more effective management, it also includes an active health monitoring system with continuous diagnostic and analysis. HP CMU provides tools independent of Linux, MPI or other software components. The HP CMU allows the user to manage a single node or multiple nodes in the cluster, and add or delete nodes in the cluster. Furthermore, CMU is the only management tool proven to be able to efficiently manage 1,000s of compute nodes with a comprehensive set of monitoring features.

Benefits

Thanks to policy support and the great efforts and meticulous work of its researchers over the past decades, DICP has achieved remarkable results: 770 achievements in scientific research as of 2013. DICP has received more than 230 provincial and ministerial awards, including 86 national awards and 73 first prizes at the Chinese Academy of Sciences, at the provincial and ministerial levels. A total of over 14,200 papers have been published. DICP also has 526 ongoing research projects. Regarding applied research, the world's first MTO plant (methanol-to-olefins) with methanol purchased outside as raw material was put into commercial operation; the demonstration project of the world's largest energy storage system with vanadium redox battery was successfully completed and accepted; the fuel cells played an important role in the disaster relief after the Lushan earthquake; the technology of ultra-deep catalytic and adsorptive desulfurization of gasoline on a fixed bed has passed appraisal.

In talent cultivation, 17 DICP scientists have been elected to the Chinese Academy of Sciences and the Chinese Academy of Engineering, three elected Fellow of Academy of Sciences for the Developing World, one elected to the European Academy of Humanities and Natural Sciences, and 20 are the winners of the National Outstanding Youth Fund. By the end of 2013, DICP had 103 doctoral advisors, 161 graduate advisors, and 798 graduates (including 531 doctoral and 267 master's students). DICP had produced 1,973 graduate degree holders, including 1,215 doctorate holders. DICP also has a mobile postdoctoral station with 104 postdoctoral students.

Customer at a glance

Hardware

- HP ProLiant DL360p Gen8 Server
- HP ProLiant SL2500 Scalable Systems with HP ProLiant SL210t Gen8 Servers
- HP SL2500 chassis
- HP P2000 G3 MSA Array Systems
- HP InfiniBand switches

Software

- HP Insight Cluster Management Utility (CMU)
- HP Integrated Lights-Out (iLO)

As a technology leader in high-performance scientific computing clusters, HP provides a series of cluster solutions that are most powerful and at the same time easy to manage. They integrate the industry's best application software, high-speed internal interconnection, industry-standard computer platforms, cluster technology experts, and professional and comprehensive technical support and services, providing the user with high-performance cluster systems which are cost effective, scalable, and expandable.

As DICP puts the "catalysis and dynamics computing system" platform into use, HP's High Performance Computing cluster system will, at the basic hardware level for theoretical chemistry computing, help DICP achieve its strategic objective to leverage comprehensive disciplinary strengths, promote technology integration and innovation, focus on research for sustainable energy, boost the optimization of resources and the environment, and coordinate the development of biotechnology and advanced materials, play an irreplaceable role in the national economy and national security, and build a world-class research institute. This system will also promote the interaction and integration of various disciplines within the institute to make DICP an important base for nurturing research talent.

"HP's high-performance computing cluster solution is very advanced and complete. It provides not only basic products that are highly reliable, scalable, cost-effective, energy-saving, and environment-friendly, but also services that are very professional and comprehensive. The management tools and software effectively help reduce our IT operations and management workload, so that we can focus more on research. Our overall experience of the platform so far is very good!" said Dai Dongxu, assistant director and doctoral advisor of DICP State Key Laboratory of Molecular Reaction Dynamics, and also the project owner of the Catalysis and Dynamics Computing System, when talking about the user experience.

"HP is an outstanding supplier of high-performance computing servers. The "catalysis and dynamics computing system" platform that HP built for us features both high performance and cost-effectiveness. It significantly improves our high-performance computing and provides support for the future development of DICP's theoretical chemistry with its high scalability."

— Dai Dongxu, Assistant Director of DICP's State Key Laboratory of Molecular Reaction Dynamics

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