

Science Department at Ivy League University Innovates IT Architecture

Harvard University's Chemistry and Chemical Biology Department Selects Cisco's InfiniBand and MDS SAN solutions for High-Performance Computing

EXECUTIVE SUMMARY

HARVARD UNIVERSITY (CHEMISTRY AND CHEMICAL BIOLOGY DEPARTMENT)

- **Industry:** Education
- **Location:** Cambridge, MA

BUSINESS CHALLENGE

- Create a high-performance server fabric with shared pools of I/O and storage resources offering high throughput support for research cluster computing
- Support the use of advanced computational methods for undergraduate and graduate-level chemistry courses.
- Provide a cost-effective way to maximize price-performance based on dollar investment, and provide compatibility for scientific computing applications.

NETWORK SOLUTION

- Build a unified HPC fabric with Cisco® Catalyst®, Cisco InfiniBand, and Cisco MDS Multilayer SAN Switches to support cluster computing, shared storage, and highly available access to a centralized resource that can offer a deeper understanding of chemistry "research in the large."

BUSINESS RESULTS

- Higher performance than general proprietary system with significant capacity for growth
- Acceleration that keeps up with the pace of research
- HPC solution meets current needs and serves as a template for future computing.

Business Challenge

Harvard's Chemistry and Chemical Biology Department is the center of research for chemistry and chemical biology in the university's Faculty of Arts and Sciences and has an extensive, high-performance computing infrastructure to support teaching and research. The department's IT environment is a heterogeneous mix of vendor products and technologies, and much of the infrastructure is Cisco-based, including the high-performance computing (HPC) fabric.

The software applications that the department utilizes for coursework include Q-Chem and WebMO. Q-Chem is a comprehensive molecular modeling software application for quantum chemistry that incorporates many semi-empirical and ab-initio calculation techniques for molecular orbitals and associated properties. WebMO is a computational chemistry package that features a variety of powerful enhancements that are suitable for serious education, commercial, and research-level users.

The computational methods used in chemistry can vary as they relate to the department's IT resources. Processes such as molecular orbital calculations

using ab-initio methods are typically CPU-intensive calculations that often use large amounts of storage, whereas molecular dynamics simulations often push the limits of cluster interconnectivity and system memory. To host these applications, a new cluster was built around this HPC fabric designed to handle classes with 20-50 students and one or two faculty at a time. The computing equipment is used for both research and teaching, and all students involved in faculty-sponsored independent research projects have access to the instrumentation.

According to Dr. Gerald Lotto, Assistant Director of Information Technology for the Department of Chemistry and Chemical Biology and manager for the project, problems experienced by the department prior to the implementation of this cluster included professors having to schedule access and timing, often months in advance, in order to support course work and research. When trying to use shared cluster resources for teaching; often many students would be accessing the

system at the same time to meet class assignment deadlines. As a result, the business challenge was threefold:

1. Create a high-performance server fabric with shared pools of I/O and storage resources offering high throughput support for research cluster computing.
2. Support the use of advanced computational methods for undergraduate and graduate-level chemistry courses.
3. Provide a cost-effective way to maximize price-performance based on dollar investment, and provide compatibility for scientific computing applications.

Network Solution

Dr. Lotto met with Cisco and IBM engineers and tested high performance shared disk filesystem designs that took advantage of the Cisco Infiniband fabric. Dr. Lotto's research ultimately resulted in the Chemistry and Chemical Biology department's decision to design and implement this cluster around a unified HPC fabric with Cisco Catalyst, Cisco InfiniBand, and Cisco MDS Multilayer SAN Switches to support cluster computing, shared storage, and highly available access to a centralized resource that could offer a deeper understanding of chemistry "research in the large."

Business Results

Cluster performance has improved with Cisco SFS 3012 InfiniBand Multifabric Server Switches and MDS 92161 Multilayer SAN Switches, and the new cluster solution can handle the students' and teachers' load (cluster performances are as much as 50 percent faster than a fibre channel architecture).

The new infrastructure is suited to the computational workload demands of the department, and the bandwidth and capacity challenges previously experienced are virtually nonexistent since upgrading the file system.

PRODUCT LIST

CISCO APPLICATION AND STORAGE NETWORKING SERVICES:

- Cisco SFS 3012 InfiniBand Multifabric Server Switches
- Cisco MDS 9216i Multilayer SAN Switches

InfiniBand has provided numerous configuration possibilities. The new infrastructure will help the chemistry department leverage an under-subscribed fabric for multiple purposes or multiple silos, and the department anticipates leveraging the HPC fabric in more enterprise uses.

For More Information

To find out more about Cisco InfiniBand and Cisco MDS Multilayer Switches solutions, please visit <http://www.cisco.com>.



Americas Headquarters
Cisco Systems, Inc.
170 West Tasman Drive
San Jose, CA 95134-1706
USA www.cisco.com
Tel: 408 526-4000
800 553-NETS (6387)
Fax: 408 527-0883

Asia Pacific Headquarters
Cisco Systems, Inc.
168 Robinson Road
#28-01 Capital Tower
Singapore 068912
www.cisco.com
Tel: +65 6317 7777
Fax: +65 6317 7799

Europe Headquarters
Cisco Systems International BV
Haarlerbergpark
Haarlerbergweg 13-19
1101 CH Amsterdam
The Netherlands
www-europe.cisco.com
Tel: +31 0 800 020 0791
Fax: +31 0 20 357 1100

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