Unfolding protein mysteries with Intel® processor–based HPC

An HPC cluster with Intel processors helps University of Michigan Medical School researchers uncoil the secrets of protein folding.

Researchers at the University of Michigan Medical School are working to understand how problems with protein folding in human cells might contribute to devastating neurodegenerative illnesses, including Alzheimer’s disease. To conduct the protein structure prediction that is critical for their work, researchers needed a new high-performance computing (HPC) cluster. The cluster had to provide outstanding performance while fitting into a shared data center with limited power and real estate. By selecting HP servers based on the Intel® Xeon® processor 5500 series, researchers gained the compute power, energy efficiency, and density they need for their groundbreaking work.

CHALLENGES
- **Optimize price-performance.** Adopt a processing architecture that can deliver the raw compute power for running thousands of jobs per day at a price point that would allow deployment of a massive cluster.
- **Minimize power and real estate.** Fit thousands of processing cores into a shared data center with limited available rack space and power.

SOLUTION
- **HP servers with Intel® Xeon® processors.** The IT group built a 268-node cluster with HP ProLiant* DL1000 series servers based on the Intel Xeon processor 5500 series.

IMPACT
- **Outstanding price-performance.** The Intel Xeon processor 5500 series delivers approximately 23 percent better performance than previous-generation processors at a competitive price, enabling the medical school to build a cluster that runs 2,000 jobs around the clock.
- **High density.** With 32 cores in each 2U enclosure, the new Intel® processor–based servers enable the IT group to fit 2,144 cores into 20 percent less space than with other servers.
- **Reduced power consumption.** The Intel processor–based servers deliver the required performance within existing power limitations.
- **Better science.** By running thousands of jobs around the clock, the cluster helps researchers fine-tune protein structure predictions, producing better results in less time than before.

“Compared with the previous-generation Intel® processor, the Intel® Xeon® processor 5500 series delivers approximately 23 percent better performance for this code. As a result, researchers can run more jobs per day.”

—Traci Ruthkoski
HPC Team Lead
University of Michigan Medical School

To support the work of a prominent researcher, the University of Michigan Medical School needed to build a new HPC cluster for protein-folding research. “At a previous university, this researcher was using a relatively small cluster, which was shared with other labs,” says Traci Ruthkoski, HPC team lead for the University of Michigan Medical School. “We wanted to build a much larger, dedicated cluster that could provide a significant performance boost for this scientific work.”

In selecting hardware, the first challenge was to achieve the right price-performance ratio. “With this serial application, performance is primarily dependent on core count,” says Ruthkoski. “We needed a cluster with the largest number of cores possible for our budget.”
At the same time, the IT group had to fit the new cluster into a data center with limited available real estate and power. “Our computing resources are kept in the university’s primary data center, which is shared with other departments,” says Ruthkoski. “We needed a dense, energy-efficient infrastructure that would deliver exceptional performance without exceeding our allotted power and real estate.”

**Intel Xeon processors improve code performance by 23 percent**

After evaluating several servers and processing architectures, the IT group selected HP ProLiant DL1000 servers equipped with the Intel Xeon processor 5500 series. Each 2U server includes four nodes. The entire cluster comprises 268 nodes with a total of 2,144 cores.

The Intel Xeon processors help researchers achieve outstanding application performance. “We considered multi-core processors from other vendors, but for this lab’s code, it was clear that the Intel Xeon processor 5500 series delivered the best performance,” says Ruthkoski. “Compared with the previous-generation Intel processor, the Intel Xeon processor 5500 series delivers approximately 23 percent better performance for this code. As a result, researchers can run more jobs per day.”

Intel® Hyper-Threading Technology provides an additional performance boost while requiring only a fraction of the power that would be necessary to support additional processing cores. With Intel Hyper-Threading Technology, users can run up to 16 threads on each core for dual-socket, quad-core systems. “So far, we have seen an additional 10 percent performance boost by using Intel Hyper-Threading Technology,” says Ruthkoski. “Depending on the code, Intel Hyper-Threading Technology could deliver additional performance gains.”

**A dense infrastructure saves 20 percent of rack space**

The dense HP servers and multi-core Intel Xeon processors help the IT group fit tremendous computing power into a small space. “With a different server or another processing architecture, we might have needed 10 racks of space. Instead we use just eight,” says Ruthkoski. “That density is what enabled us to build such a large cluster within our existing data center real estate.”

The new processors are also helping control power consumption. “The Intel Xeon processor 5500 series contributed to a 30 percent reduction in the overall power consumption of our cluster,” says Ruthkoski. “We were able to get the entire cluster up and running without having to borrow power from other departments.”

**Cost savings facilitate new investments**

Because the Intel processor–based servers helped the medical school stay within budget, the IT group now can expand the use of HPC in the biological chemistry department. Administrators approved the construction of a smaller cluster based on the same hardware that will be used as a software development sandbox. “Developers previously not exposed to HPC systems will be able to optimize their code and see how it will perform in a true HPC environment,” says Ruthkoski.

**Faster results help improve research quality**

Researchers are capitalizing on the cluster’s performance to hone their work. “With Intel processor–based HP servers, researchers in this lab are able to run more jobs and get results faster than with previous departmental clusters,” says Ruthkoski. “As a result, they can experiment more and fine-tune their protein structure predictions. In the end, they should be able to produce better research, faster than before, and make important contributions to treatments for Alzheimer’s disease, mad cow disease, some forms of cancer, and more.”

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