CASE STUDY

High Performance Computing

Intel® Omni-Path Architecture, Intel® Xeon® Processor, and Intel® Xeon Phi™ Processor Enable Faster, Higher Quality Research at University of the Free State

South Africa's oldest higher educational institution takes a significant departure to Intel® Architecture for its HPC resources

"The speedup is simply phenomenal. It has allowed me to investigate more possibilities within my current research timeframe."

–UFS Researcher

The new fifth-generation cluster at University of the Free State enables faster, higher quality research.

- 16 nodes of Intel® Xeon® Processor E5-2697A v4 plus eight nodes of Intel® Xeon Phi™ Processor 7250
- Intel® Omni-Path Architecture adapters and switches
- Supermicro SYS-F628R3-RC1BPT+ storage units with Intel Xeon Processor E5-2640 v4, Seagate 1TB (for OS) and 24 TB (for users), and Intel SSD DC P3600 NVMe
- Accelerates complex molecular dynamics simulation 2.7X

Executive Summary

The University of the Free State (UFS) was running on borrowed time with their existing High Performance Computing (HPC) clusters. The oldest system was seven years old. Besides exhibiting problems because of their age, they were affecting the quality of research their users could achieve and slowing down results. Their new system, built on Intel® Xeon® Processor E5-2697A, Intel® Xeon Phi™ Processor 7250, and Intel® Omni-Path Architecture, has enabled results from detailed simulations not possible just five years ago.

Challenge

University of the Free State (UFS) is one of the oldest institutions of higher education in South Africa. It opened its doors in 1904, and it has grown to more than 37,851 students, spread across seven faculties over three campuses. The university has two campuses in Bloemfontein and one in Qwaqwa.

UFS installed its latest cluster four years ago. Like that cluster's predecessor installed in 2010, it was based on AMD* processors, NVIDIA* GPUs, and InfiniBand* Architecture interconnect.

"Our users come from diverse backgrounds, from various fields of science," stated Albert van Eck, Director of the High Performance Computing Unit at the University of the Free State. "Convenience, speed, and reliability are the most important aspects to them. They need to be able to efficiently use the system independently, and, of course, the results need to be accurate and in a timely manner."

Time-to-solution on the existing systems was slowing down the results researchers needed to achieve. "The speed had become inefficient," added van Eck.

With these clusters, besides impacting the quality of research, the costs of maintenance and repair were increasingly affecting their IT budget. "The old systems were procured in 2010 and 2012," commented van Eck. "They were no longer optimal, and they started to have failures. The storage also started to become a restraining factor to our researchers; we had limited storage for user data and backups."

Solution

UFS' Fifth-generation HPC system is a significant departure from their previous systems, including different CPU vendors, fabric technologies, and supporting software for optimizing the codes their researchers run. In the older clusters, besides AMD processors and InfiniBand* Architecture, they used open source compilers to build their codes.

The new system, assembled by Supermicro, is built on Intel® Scalable System Framework (Intel® SSF) with a theoretical maximum of about 100 teraFLOPS. It's the first Intel SSF and Intel OPA installation in South Africa. It comprises 16 nodes of dual-socket servers with 16-core Intel Xeon Processor E5-2697A v4, 512 GB of DDR4 memory, and interconnected by Intel OPA. Complementing the Intel Xeon processors are eight nodes of Intel Xeon Phi Processor 7250 with 68 cores each, 192 GB of memory, and interconnected with Intel OPA. Additionally, UFS chose Intel® Parallel Studio XE for their software optimization tools.

"Due to the fact that our old system was an AMD-based system with InfiniBand interconnect, we had to really make sure that the effort of moving over to a different configuration would be worth it," described van Eck. "Our design of the new system had to implement a high throughput interconnect with low latency due to the distributed jobs that our users run. The CPU core count per node also had to be high enough, because some of our users have software that is restricted to single-node execution. Lastly, the design had to have higher memory per node, because we also have users that need more memory and fewer CPUs per job."

According to van Eck, researchers employ about 390 software packages. They all had to be recompiled to optimize them for the new hardware. That meant running all packages and libraries through Intel Parallel Studio XE to optimize them for both the Intel Xeon processors and Intel Xeon Phi processors to get the best performance out of each package. That was a significant investment.

To expand storage capacity, UFS upgraded their storage system with 24 TB of hard drives and two Intel® SSD Data Center P3600 Series NVMe drives (400 GB), running on a dual-socket server powered by Intel Xeon Processor E5-2640 v4.

Result

"Compared to the previous systems, the new Intel Xeon processor cluster is over 4X faster than the oldest AMD cluster," stated van Eck. These were measured using BOINC, purely for comparison of instruction throughput.

According to a UFS researcher in computational structural bioinformatics, "my research involves running long time-scale Molecular Dynamics (MD) simulations of large protein—nucleic acid—complexes using GROMACS. Due to the size of the systems I investigate (~800,000 atoms), I have occupied the user space at the scaling limit for the last half-decade. With the current hardware available, I can investigate ~800,000 atom systems, which was not possible 5 years ago. With a previous generation HPC setup, simulating a system for 600 ns took approximately 3-4 months. With the new Intel Xeon Phi platform, I performed the same simulation in roughly 1.5 months. The speedup is simply phenomenal. It has allowed me to investigate more possibilities within my current research timeframe."

The new system also introduces researchers and developers to the capabilities of multiple Intel components—Intel Xeon processors, Intel Xeon Phi processors, and Intel OPA—in an infrastructure they've not seen before. And, it introduces UFS programmers to the benefit of using Intel® Compilers to optimize codes for Intel® Architecture (IA).

Solution Summary

To advance its research capabilities and modernize it HPC resources, UFS made a dramatic change from its previous cluster architecture to an Intel-based infrastructure built on Intel Xeon processors, Intel Xeon Phi processors, and Intel OPA. The results have allowed researcher to improve the quality of their findings and return solutions much faster.

Where to Get More Information

Learn more about University of the Free State at https://www.ufs.ac.za/.

Learn more about Intel Omni-Path Architecture at https://www.intel.com/omnipath.

Solution Ingredients

- 16 nodes of Intel Xeon Processor E5-2697A v4 (Supermicro servers)
- Eight nodes of Intel Xeon Phi Processor 7250 (Supermicro servers)
- Intel Omni-Path Architecture 100 Series Host Fabric Adapters
- Supermicro* SSH-C48Q switch using Intel OPA
- Supermicro SYS-F628R3-RC1BPT+ storage units with Intel Xeon Processor E5-2640 v4, Seagate 1TB (for OS) and 24 TB (for users), and Intel SSD DC P3600 NVMe