Case study

Université Paul Sabatier saves space and energy with HP Moonshot

Researchers explore the future of complex quantum chemistry in a green micro-supercomputer environment

Industry
Academic research

Objective
Run highly complex quantum Monte Carlo simulations on low-energy consumption compute infrastructure that provides results comparable to traditional high-performance computing infrastructure

Approach
Deploy HP Moonshot System with HP ProLiant m350 Servers

IT matters
- Produced twice as many gigaFLOPS per watt as traditional servers
- Delivered desired results in 4.3U compared to 17.2U of traditional servers
- Completed 7,200 quantum Monte Carlo blocks 17.2 times faster than traditional servers

Business matters
- Reduced data center space and energy costs
- Gained new perspectives on how to run quantum Monte Carlo simulations
- Set the stage for bring highly energy-efficient software code into the commercial marketplace

"We need to achieve as many gigaFLOPS as possible while using very little power. With HP Moonshot we get twice as many gigaFLOPS per watt as traditional servers. HP Moonshot has opened up a whole new perspective on how we run our quantum Monte Carlo simulations."

– Anthony Scemama, Research Engineer and HPC Scientist, Centre National de la Recherche Scientifique

The world-renowned research organization at Université Paul Sabatier needed an energy-efficient supercomputing environment to run highly complex quantum Monte Carlo simulations. By running their software code on the HP Moonshot System, university researchers could produce twice as many gigaFLOPS per watt as traditional Dell rack servers. HP Moonshot also produced desired Monte Carlo results in five times less space than required by the Dell servers. Providing an ideal balance of performance and efficiency, HP Moonshot met the university's objectives to save energy and money.

Named for the 1912 Nobel prize-winning chemist, Paul Sabatier, Université Paul Sabatier Toulouse III (UPS) has its roots in one of the oldest universities of Europe—Université de Toulouse, founded in 1229. While steeped in ancient tradition, the modern UPS is world-renowned for its diverse array of programs in the sciences, health, technology, athletics, and engineering. It is also one of France's preeminent research institutions, engaged in publicly funded advanced research largely performed in partnership with major scientific organizations.

One such organization is the Centre National de la Recherche Scientifique (CNRS), or national center for scientific research. CNRS is the largest governmental research organization in France and the largest fundamental science agency in Europe. Working in collaboration with CNRS, the university conducts advanced laboratory research in quantum chemistry. Deep in UPS labs, researchers test new theories in hopes of discovering scientific insights that could ultimately be applied in the real world, such as life-saving developments in the pharmaceutical industry.

As part of its quantum chemistry research, UPS uses a non-traditional method for computing the electronic structure of molecules with quantum Monte Carlo (QMC) simulations, using "random walks" to solve the Schrödinger equation (a differential equation applied to very large dimensional spaces) rather than a traditional analytical approach. While not new, the random walks method was rarely used until recent years when massively parallel high-performance computing (HPC) systems made it more feasible. Now, more and more researchers are using the random walks method because it produces more accurate results than traditional methods.

Each QMC simulation involves billions of Monte Carlo steps, and can require thousands of computing nodes to handle such CPU-intensive floating-point calculations. Standard x86 servers not only take up a lot of physical space, they also consume enormous amounts of power. Therefore, researchers at UPS turned to a much more energy-efficient computing architecture: HP Moonshot System.

Anthony Scemama, a research engineer and HPC scientist with CNRS, is working under the direction of Dr. Michel Caffarel who is leading the university's quantum Monte Carlo project now running on HP Moonshot. "We wanted to find a way to run these computationally intensive calculations using as little energy as possible," Scemama explains. "So we engaged a team of computer scientists to run benchmarks to optimize the green efficiency of our software code running on HP Moonshot. "

Supercomputing in a fraction of the space

UPS deployed HP Moonshot with 45 HP ProLiant m350 servers running Ubuntu Linux in the HP Moonshot 1500 Chassis. With eight cores per server, the ProLiant m350 is the densest CPU core count available in a Moonshot System, enabling UPS to run a very large number of low-frequency CPUs in a fraction of the space compared to traditional servers.

"We need to achieve as many gigaFLOPS as possible while using very little power," says Scemama. "With HP Moonshot we get twice as many gigaFLOPS per watt as traditional servers. And with Moonshot's dense scale-out architecture we have no problem running hundreds of nodes. It's like having a micro-supercomputer where we can develop and test

Customer at a glance

Hardware
- HP Moonshot System
  - HP ProLiant m350 Servers
  - HP Moonshot 1500 Chassis

Software
- Ubuntu Linux
- Quantum Monte Carlo simulations

Our partners support

the distributed parallelism of our software code without taking up a huge amount of space."

In UPS's benchmark tests, a single 4.3U HP Moonshot System produced total gigaFLOPS equivalent to 17.2U of Dell PowerEdge R620 rack servers. The Dell servers would also required 2.4 times more power to get the same output as HP Moonshot. What's more, when idle the HP Moonshot System consumed 0.8 watts per core compared to 5.25 watts per core for the Dell servers.

"The power savings from HP Moonshot is enormous," Scemama remarks. "That not only meets our objectives to be more green but also reduces our energy costs dramatically."

The right balance of performance and efficiency

HP Moonshot also provides UPS with optimal performance for its quantum Monte Carlo project. While it's easy to expect a faster CPU to run calculations faster, some very complex software code can execute only so quickly. In fact because CPU speeds have increased so dramatically, it has become more and more difficult for certain code to approach the theoretical performance peaks on today's high-performance processors.

Due to the unique characteristics of UPS's algorithms, they perform much better when spread across large numbers of compute nodes that deliver sufficient but not excessive speed. The university's benchmark tests proved this point.

A Dell PowerEdge R620 with the Intel Xeon Processor E5-2670 and 16 cores completed 7,200 quantum Monte Carlo blocks in 13,216.0 seconds. By comparison, the HP Moonshot System based on the Intel® Atom™ Processor C2730 with 1,440 total cores completed the same workload in 768.12 seconds—17.2 times faster.

"HP Moonshot provides the right balance of performance and efficiency, enabling our researchers to run their quantum Monte Carlo simulations with the desired speed and the least amount of energy consumption," notes Scemama. "Based on our studies HP Moonshot's CPUs, which are low-frequency and not highly vectorized, prove to be very performance-efficient for the types of calculations we perform."

He concludes, "HP Moonshot has opened up a whole new perspective on how we run our quantum Monte Carlo simulations, and that's exactly what we were looking for. Using the insights we gained from these initial studies we'll now see how our other software code performs on HP Moonshot. By proving HP Moonshot here in the lab, we hope to bring highly energy-efficient software code into the commercial marketplace to help businesses more green and cost-effective."

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