Infinite performance

University of Coimbra evaluates performance and scalability benefits of the latest Intel® technology

Since 1290, the University of Coimbra has been one of Portugal's leading higher education institutions. Its 24,500 students are supported by eight faculties, with study subjects ranging from art to engineering. The university is also the founding member of the Coimbra Group of European research universities. Wanting to provide some of the best possible research tools to students and industry research projects, the university tested the new Intel® Xeon® processor E5-2680 with Intel® True Scale Fabric based on InfiniBand® to underpin and connect its server cluster and key applications.

CHALLENGES

• Strong tools. Equip researcher with some of the best resources to conduct complex computational simulations
• Performance testing. Evaluate core applications’ performance and scalability when running on the latest Intel® technology

SOLUTIONS

• Processing power. Servers tested were powered by Intel Xeon processors E5-2680
• Inter-connectivity. Server nodes are connected using Intel True Scale Fabric based on a quad data rate (QDR) InfiniBand network

TECHNOLOGY RESULTS

• Execution speed. Chroma* and Hybrid Monte Carlo* (HMC*) applications were sped up almost 16-fold when using 16 nodes connected by InfiniBand
• More capacity. Intel True Scale Fabric based on QDR-80 doubles the node bandwidth capacity and increases message passing interface rate by a factor of seven1

BUSINESS VALUE

• Growth potential. Core applications can run more simulations and support more users when running on a compute cluster with more nodes that is supported by Intel True Scale Fabric based on QDR-80
• Higher quality. Scientists can generate higher standards of research to drive the university’s competitiveness and good reputation

Striving for excellence

As a leader in scientific research in Portugal, the University of Coimbra values its computing resources very highly. Paulo Silva, a post-doctoral fellow at the university’s Center for Computational Physics, explains: “Computer simulations provide a new way of conducting scientific research, enabling us to understand many phenomena that would be very difficult or impossible to study through traditional experimentation or where our knowledge of the underlying theory is incomplete.” Across the university, but especially in Silva’s department, many scientists rely on these computational simulations to conduct their work. “High-performance computing (HPC) is therefore very important for maintaining our high standards of excellence and competitiveness in these fields of research,” adds Silva.

Committed to staying abreast of the latest and most compelling HPC solutions, the university chose to work with Intel to carry out a series of evaluations. The goal was to test the performance on Intel technology (including the Intel Xeon processor E5 family and Intel True Scale Fabric based on InfiniBand) of the university’s core quantum chromodynamics (QCD) applications. The applications to be tested were Chroma, HMC and Landau*. Although Landau is an application developed by Silva, these are all based on the Chroma library developed by the United States Quantum Chromodynamics (USQCD) organization. This body is a collaboration of scientists developing and using large-scale computers for calculations in lattice QCD, which help them understand the results of particle and nuclear physics experiments around QCD, the theory of quarks and gluons.

Paulo Silva, Post-Doctoral Fellow, University of Coimbra
Leading research center demonstrates the combined benefits of Intel technology and InfiniBand for HPC

Performance plus connectivity
For the testing with Chroma and HMC, Coimbra University used an infrastructure based at the Intel lab in Swindon, UK. It was composed of a cluster of 16 nodes with Intel Xeon processors E5-2680 and Intel True Scale Fabric based on a QDR InfiniBand network. A slightly different set-up was needed for Landau. Typical InfiniBand solutions use only one InfiniBand card (HCA) per node. In dual-socket architectures, only one socket with its integrated PCIe bus has direct access to the HCA. The other socket, though, needs to transit the processor socket-to-socket bus, since it does not have direct access to the first socket's PCIe bus and its attached InfiniBand adapter. This can have a significant impact on the message passing interface (MPI) rate and latency performance of a compute cluster, and can thereby seriously impact the performance of some applications, such as Landau. Consequently, Landau tested a version of the Intel True Scale Fabric in QDR-80 mode, which uses a dual-rail InfiniBand implementation.

Compelling results
During testing, Coimbra University found that the time required to execute the Chroma and HMC applications was reduced more than 15.7-fold when going from one node to 16 nodes, showing that the QDR Intel True Scale Fabric offered an almost direct scalability for these applications. This combination of scalability and performance was a key feature of the combination of the Intel True Scale Fabric with Intel Xeon processor-based technology. The communication patterns of Chroma and HMC showed a need for extensive small MPI message throughput and collective performance, both of which benefit from Intel True Scale Fabric.

The Landau application proved to be more communication-intensive, especially in terms of MPI message rate size. In such cases, the team at Coimbra University found that having a single InfiniBand card on the node may limit its scalability. However, as soon as it tested the application on Intel True Scale Fabric in QDR-80 mode, the results showed again a direct link between node availability and application performance.

Intel True Scale Fabric in QDR-80 mode, uses two cards per node in a dual rail mode configuration. Each Intel True Scale Fabric adapter is connected to the PCIe bus associated with each processor socket. This implementation has two main benefits. First, it doubles the bandwidth capacity of a node when compared to a single-rail QDR solution. It also gives both processor sockets direct access to their attached HCA, improving by up to seven times the MPI performance of the nodes, based on the tests and simulations run by the University of Coimbra. For this reason, the testing of the Landau application using Intel True Scale Fabric in QDR-80 mode showed that it offered a performance improvement of as much as 40 percent at 16 nodes.

Coimbra University tested the Landau application in a reduced bandwidth configuration of 20Gbps. This testing showed that the application was not bandwidth sensitive. The key factor determining performance was the MPI message rate, which is one of the main improvements offered by Intel True Scale Fabric in QDR-80 mode.

Research improvements
"For these QCD applications, Intel True Scale Fabric offers an effective way to scale up the capacity of the applications, enabling us to benefit from the performance of the Intel Xeon processor E5-2680," Silva observes. "In very particular cases, the application needs high-message-rate performance in order to scale, for which using a single InfiniBand card can be a limiting factor. In such cases, Intel has developed Intel True Scale Fabric in QDR-80 mode, which enables the performance of applications to be scaled up with additional nodes in the compute cluster."

He also adds: "For large parallel computer simulations, a good interconnecting network is critical for the scalability of the applications we use. Without the Intel True Scale Fabric version of InfiniBand, the use of a large number of cores would not have the same benefit for the performance of our applications."

"A new cluster with powerful processors like the Intel Xeon processors E5-2680, connected by an InfiniBand network, would allow our computational scientists to boost the quality of their work," he concludes. The university hopes to implement such a solution soon, with a view to creating a high-quality computing cluster that would enable it to take part in the Europe-wide PRACE* HPC grid, as well as benefitting its own researchers.

Lessons learned
Coimbra University needs to provide its researchers with the optimum tools to carry out competitive research. In-depth testing showed the university that while strong performance is critical, its impact can be further enhanced by adding scalable interconnectivity through InfiniBand technology.

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