

Secrets of the universe

French organization builds one of the world's most powerful supercomputers using the Intel® Xeon® processor E5-2680

Grand Equipement National pour le Calcul Intensif (GENCI) is a government-owned organization in charge of coordinating high-performance computing (HPC) for France's research institutes. It was created in 2007 to ensure France is at the international forefront of scientific research. GENCI is charged by the Ministry for Higher Education and Research with implementing and ensuring the coordination of the French national HPC centres by providing funding, assuming ownership and promoting the use of HPC in fundamental and industrial research. GENCI is also the French representative of the Partnership of Advanced Computing in Europe (PRACE) and, as such, also has responsibility for driving HPC across Europe. With these objectives in mind, GENCI asked system integrator Bull to develop an HPC computing cluster based among others on the Intel® Xeon® processor E5-2680. The cluster consists of 92,000 cores installed and operated at the Très Grand Centre de calcul du CEA (TGCC) close to Paris.





"The Intel® Xeon® processor E5-2680 ensures European scientists have one of the most powerful HPC platforms possible so they can address some of the most pressing issues facing our world today."

> Stephane Requena CTO GENCI

CHALLENGES

- Platform for discovery. GENCI wanted to build a powerful HPC platform to help scientists across Europe address challenging problems and advance scientific research
- Ambitious reach. Much of this scientific research requires enormous processing power for example, to understand the evolution of the universe by simulating the distribution of dark matter throughout the full universe from the moment of the big bang

SOLUTIONS

- New technology. GENCI explored the benefits of the Intel Xeon processor E5-2680, which
 includes features designed to increase memory bandwidth and help double floating point
 performance compared to previous generation Intel Xeon processors
- Benchmarking software. It benchmarked the Intel Xeon processor E5-2680 using up to 12 real-life applications from various scientific domains. On some of them, like Monte Carlo computational algorithms, it achieved a 40 percent efficiency improvement and three time peak performance improvement compared to previous generation Intel Xeon processors

IMPACT

- **Powerful processing muscle.** GENCI built a supercomputer consisting of 92,000 Intel Xeon processor E5-2680 cores with a potential petaflop rating of over 2 petaflop peaks
- **New order of simulations.** The cluster is so powerful that it allows GENCI and affiliate organizations to carry out simulations that have never previously been possible due to practical time constraints and accuracy

Future developments

GENCI was formed by the French government to enable scientists and academic institutes to compete in HPC research with their peers in United States, Japan and China. Some of the organizations that use GENCI's HPC facilities are world renowned such as the Observatoire de Paris and the University of Toulouse, which have both used HPC to make significant contributions to astronomical and medical research.

GENCI is also the French representative of the PRACE research infrastructure, a pan-European organization with 21 member states dedicated to enhancing European competitiveness and scientific discovery through HPC. France (through GENCI) is one of the four country members (along with Germany, Italy and Spain) committed to hosting a petaflopic supercomputer.

Fighting disease

PRACE members acknowledged the need to further high-impact European scientific discovery, engineering research and development across all disciplines to enhance European competitiveness for the benefit of society.

These included, for example, gaining a greater understanding of precisely how Alzheimer's disease develops in the brain, addressing chemical problems that need highly accurate computer models, and simulating the evolution of the complete universe and the distribution of dark matter.



Ninety-two thousand cores of the most advanced processing power available

Consequently, each of the four PRACE hosting members contributed over EUR 100 million [USD 132 million] towards HPC clusters capable of driving performance of more than one petaflop of computing. One petaflop provides one quadrillion floating point operations per second (FLOPS).

Stephane Requena, CTO of GENCI, said: "Every scientific domain needs HPC. Since GENCI's founding, we have endeavored to provide our scientists with the best HPC platforms possible. Given the nature of some of the challenges that face society today, we wanted to deploy a new HPC cluster to accelerate scientific research in areas that are important for society."

Landmark technology

The Intel Xeon processor E5 family is the world's first server processor to support full integration of the PCI Express* 3.0 specification. This can double interconnect bandwidth compared to previous generations of Intel Xeon processors while enabling lower power and higher-density server implementations.

Early performance benchmarks revealed that the Intel Xeon processor E5-2680 delivers up to 2.1 times more performance in raw FLOPS as measured by LINPACK* and up to 70 percent more performance using real HPC workloads compared to the previous generation of Intel® Xeon® processors 5600 series.¹

GENCI benchmarked the Intel Xeon processor E5-2680 using a set of more than 12 different scientific applications including QMC=Chem, a code developed by M. Caffarel (University of Toulouse) based on Quantum Monte Carlo computational algorithms. Monte Carlo methods applied to quantum chemistry are deemed important because they simulate polypeptide growth. Understanding how polypeptides develop in the brain is critical to a comprehensive understanding of Alzheimer's disease. Gaining this insight is one of GENCI's aims in making a new HPC cluster available.

As a result, developers of the QMC=Chem code worked with the Exascale Computing



Research Center (ECR Lab), GENCI, and Intel engineers to co-design a new version of the code specifically to benchmark the performance of the Intel Xeon processor E5-2680.

CURIE

Stephane Requena says: "Monte Carlo is a very useful tool for simulating systems or modeling phenomena with significant uncertainty in inputs, such as in chemistry. However, that said, it can be time-consuming and inefficient. In fact, 15 percent peak performance efficiency is actually the norm when running a typical scientific application on a regular HPC system.

By running a fine-tuned version of the Monte Carlo code on a system powered by the Intel Xeon processor E5-2680, we achieved an efficiency rating of up to 40 percent and the quality and accuracy of the results validated the interest of such Monte Carlo methods for electronic structure in chemistry.¹

Following these results, GENCI tasked HPC system integrator Bull with building and developing an HPC cluster built on the Intel Xeon processor E5-2680. This new cluster consists of 5,040 two-socket Bull B510* blade servers, a total of 10,080 processors and 80,640 cores. The cluster is called CURIE*, after Pierre and Marie Curie, renowned physicists and chemists famous for their pioneering research on ra-

famous for their pioneering research on radioactivity. With CURIE, GENCI has reached a peak computing power of 2 petaflops and expects more to come. CURIE IS installed and operated by CEA teams at TGCC, close to Paris.

Top ranking

CURIE is meeting the expectations of both GENCI and PRACE and the organizations are preparing to use the cluster to launch some of the most ambitious HPC simulations ever attempted.

For example, the aim of one simulation is to establish how dark matter has been distributed across the universe from the moment of the big bang until today. Carried out by the Observatoire de Paris, the simulation will incorporate three models of dark matter distribution. It's an enormous simulation that

Spotlight on GENCI

GENCI is owned 49 percent by the French State represented by the Ministry for Higher Education and Research. A further 20 percent is owned by the Alternative Energies and Atomic Energy Commission (CEA), 20 percent by the National Centre for Scientific Research (CNRS), 10 percent by the French universities represented by Conférence des Présidents d'Universités and 1 percent by INRIA, a public research body dedicated to computational science. GENCI is also co-ordinating the major supercomputing equipment for French national HPC civil center by providing financing and assuming ownership. Within this context, it makes these facilities accessible to all interested scientific communities, academic or industrial, national, European or international.

requires the clusters' full complement of 92,000 cores and will use 300 terabytes of distributed memory and generate over 1.5 petabytes of data. This project is a world first in terms of its scope and ambition, and could not be achieved on any other platform within a reasonable length of time.

Other simulations are equally ambitious and include; optimization of the combustion engine, performing fusion simulations for the design of ITER, a project that aims to demonstrate that fusion is an energy source of the future, climate modeling based on multi-resolution (regional and global) coupled models (ocean and atmosphere) to assess the development of cyclones in the Indian Ocean, as well as the growth of polypeptides within the context of Alzheimer's disease.

Similarly, these simulations could not be practically carried out on other platforms. It is only the processing muscle of the Intel Xeon processor E5-2680 and the balanced architecture of the system that enables GENCI to carry out and support these simulations. Stephane Requena said: "The Intel Xeon processor E5-2680 ensures our scientists have one of the most powerful HPC platforms possible so they can address some of the most pressing issues facing our world today."

More information available at www.genci.fr and www.prace-ri.eu

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