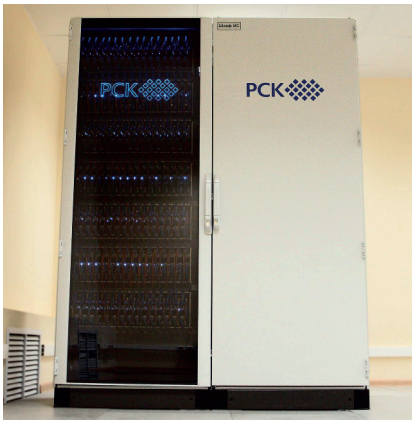
CASE STUDY
Intel® Xeon® Processor E5-2690
High-Performance Computing

Cracking molecular codes with high-performance computing

Intel® technology supports ground-breaking bioinformatic and pharmaceutical research while helping slash energy requirements

Moscow Institute of Physics and Technology (MIPT) was created in 1946 by leading Soviet scientists and the national government as an advanced educational and research institution specializing in physics. MIPT has eight departments and currently hosts about 3,600 students. As part of its commitment to ongoing innovation and excellence in high-performance computing (HPC), it has implemented a new cluster powered by the Intel® Xeon® processor E5-2690. It has since seen total cost of ownership (TCO) drop by 60 percent while computing performance has doubled. Since the first pilot system was implemented, computing performance has seen a 33-fold increase.



МФТИ
SAPERE AUDE

"We can now calculate the molecular dynamics trajectories in bacterial membranes containing more than 50,000 atoms within one week. This is much faster than has ever been possible before, and means that we are now closer to developing antibiotics that are not susceptible to bacterial resistance."

Professor Roman Yefremov,
Biochemistry Institute,
Russian Academy of Sciences

CHALLENGES

- **Support complex research:** Provide scientists with HPC tools they need to carry out complicated and in-depth calculations and simulations
- **Lead with innovation:** Demonstrate commitment to using the latest technologies to maintain reputation for scientific excellence

SOLUTIONS

- **Tailored platform:** The combination of the RSC miniDC* HPC solution with Intel Xeon processor E5 family computing power creates the ideal research foundation
- **Proven performance:** Computing performance with latest version of the new platform has increased by a factor of at least 33

IMPACT

- **Energy savings:** More energy-efficient direct liquid cooling and more efficient processors mean power consumption has dropped, cutting TCO by 60 percent
- **Effective computing:** New cluster achieves more than 90 percent in LINPACK benchmark
- **Greater performance:** Computing performance has doubled in 2012, to 83.14 teraflops

Life-changing research

As one of the leading research centers in Russia, MIPT plays a significant role in supporting the local scientific community. It operates an open laboratory for biomedicine, pharmacology and small-scale structures, called I-SCALARE (Intel Super Computer Applications Laboratory for Advanced Research). This was created by a Russian government grant to MIPT, for use by researchers from surrounding universities and institutions.

Most of the research carried out using the HPC cluster focuses on elements of bioinformatics and pharmaceutical modeling. The calculations and simulations explore complex processes such as the impact of viruses on cell membranes. Interest and investment in these fields are growing steadily, meaning there is an ever-increasing demand for the resources I-SCALARE offers – not simply in terms of supporting more users but also to run more complicated processes.

For the team running the cluster at I-SCALARE, this means they must keep on top of the latest computing technologies to ensure their cluster can deliver the high performance its users need, while minimizing the typically high energy costs charged in the Moscow area.

When looking for a suitable new computing platform, the team has three top priorities: efficiency of space and energy, high computing performance, and low TCO.

HPC center doubles performance and cuts TCO by 60 percent with Intel Xeon processor E5-2690 and direct liquid cooling

Lessons learned

Where potentially ground-breaking scientific and medical discoveries are at stake, the tools that make them happen are critical. By using the combination of RSC Group's miniDC and energy-efficient direct liquid cooling expertise, along with the HPC-ready Intel Xeon processor E5-2690, MIPT has created an ideal foundation for such discoveries.

A platform optimized for HPC

As part of its ongoing assessment of the technologies it uses, MIPT evaluates new offerings regularly to maximize its IT investments. Having run a series of benchmarks to assess the performance of key applications and processes on a variety of platforms, it identified the RSC miniDC energy-efficient all-in-one solution for HPC environments, powered by the Intel Xeon processor E5-2690.

This innovative platform is built on RSC Tornado* architecture and based on the Intel Xeon processor E5 family with direct liquid cooling. It is a high-density architecture characterized by high energy efficiency with scalable performance and reliability.

RSC miniDC includes all the subsystems required by a modern data center, including a powerful server farm based on the Intel® Server Board S2600JF family, communication networks, data storage systems as well as power supply, cooling and fire-fighting subsystems.

Intel® Turbo Boost Technology 2.0, a feature of the Intel Xeon processor E5 family, is always on thanks to direct liquid cooling that provides a clock speed gain of up to 400 MHz to optimize the handling of peak workloads and the distribution of power consumption among processor cores. For example, if all computing tasks are processed by a single core, then the processor can increase its performance by redirecting power from an unused core to an active one.

MIPT enlisted solution provider RSC Group (www.rscgroup.ru), the developer of RSC miniDC, to design, build and implement the solution within its I-SCALARE environment, including a powerful, energy-efficient mini-data center with 224 servers, communication networks, data storage and power supply. It was also tailored to enable advanced liquid cooling.

Originally deployed using the Intel® Xeon® processor 5600 series to provide the computing power, subsequent upgrade stages ensured that the final cluster benefitted from the latest Intel Xeon processor and a corresponding 33 times increase in performance over the first pilot model.

More research, more efficiently

Since implementing the new cluster at I-SCALARE, the team has seen significant improvements in the platform. Records have been broken in energy efficiency, since the power used for cooling is now firmly under six percent of the data center's total energy bill (power usage effectiveness of 1.06). Computing effectiveness has also broken new ground, with the cluster achieving more than 90 percent in the LINPACK benchmark.

Thanks to the lower power consumption enabled by direct liquid cooling and boosted floating point computer power, I-SCALARE has found the TCO of the cluster is 60 percent lower than with the previous HPC platform. Meanwhile, computing performance has doubled to 83.14 teraflops.

The numbers are borne out by the enhanced experience that the researchers and students are now enjoying when they use the cluster. Professor Roman Yefremov of the Biochemistry Institute of the Russian Academy of Science (RAS), for example, uses the platform to research the construction of a new class of antimicrobial compounds based on natural antibiotics. "We can now calculate the molecular dynamics trajectories in bacterial membranes containing more than 50,000 atoms, within one week. This is much faster than has ever been possible before, and means that we are now closer to developing antibiotics that are not susceptible to bacterial resistance."

Find the solution that is right for your organization. Contact your Intel representative, visit Business Success Stories for IT Managers, or explore the Intel IT Center.

0912/JNW/RLC/XX/PDF 328033-001EN