Academic Research | Germany

Boosting HPC performance and efficiency for innovative research

Zuse Institute Berlin

To gain new AI capabilities and expand its high-performance computing resources, Zuse Institute Berlin deployed three new highly energy-efficient clusters with Lenovo and pro-com DATENSYSTEME GmbH, and the latest innovative water-cooled cluster is powered by AMD EPYC™ 9004 Series processors.

1 Customer background

Who is Zuse Institute Berlin?

Zuse Institute Berlin (ZIB) is an interdisciplinary research institute for applied mathematics and data-intensive high-performance computing (HPC) with strong connections to the leading universities in Berlin, Germany. ZIB is also one of nine centers in the NHR Alliance for National High Performance Computing in the country. The institute facilitates research by running advanced modelling, simulation and optimization workloads. Through its MODAL research campus, a public-private partnership connecting businesses to cutting-edge research, ZIB supports over 30 industrial partners in growth areas such as green energy, mobility, healthcare, and nano sciences.

ZIB
ZUSE INSTITUTE BERLIN

2 The challenge

As a research organization, ZIB has a long history in optimizing applied mathematics and numerical challenges with high-performance computers. The institute's compute power is regularly used by researchers in life sciences to perform molecular simulations to better understand complex biological processes. Additionally, ZIB helps to advance foundational research in chemistry, material science, and earth-system science.

As more algorithms benefit from running on GPUs, ZIB wanted to expand its supercomputing cluster capabilities with the latest GPU technologies. At the same time, the institute needed to adapt to a change in its funding cycles, moving away from large multi-year investments to more granular annual planning.

2 The challenge

Dr. Thomas Steinke, Head of Supercomputing at ZIB, says: “Our goal was to find the most cost and energy efficient solution that would enable us to flexibly add new capacities to our HPC environment in a way that aligns with continuous, annual budget plans.”

“Leading researchers rely on us to run a very wide variety of **supercomputing workloads**, from traditional physics-based simulations to evaluating cutting-edge photonic and quantum technologies, as well as leveraging artificial intelligence methods and algorithms. Performing research in HPC-related topics ourselves, we wanted to gain access to a **diverse set of technologies** to be able to **continue developing tools and services for the scientific community** across specific vendors and implementations to support openness and freedom of choice.”

Dr. Thomas Steinke

Head of Supercomputing, Zuse Institute Berlin

3 The solution

Maximizing efficiency with warm water cooling

After detailed evaluation, Zuse Institute Berlin selected pro-com DATENSYSTEME GmbH, Lenovo and AMD to deliver new supercomputing cluster capacities.

With cost-efficiency being the top priority, the Lenovo Neptune® direct water cooling platform delivered the required energy efficiency to manage operating costs. By choosing Lenovo, ZIB also benefits from a modular cooling solution that it can easily use across different systems and architectures.

Hardware

Lenovo ThinkSystem SD665 V3
Neptune® DWC Server with AMD EPYC™ 9004 Series processors
Lenovo ThinkSystem DW612S
Lenovo ThinkSystem SR645 V3
Lenovo Neptune® Liquid Cooling

Software

Lenovo Energy Aware Runtime (EAR)

Services

pro-com DATENSYSTEME GmbH

“The modularity and options of Lenovo solutions powered by AMD EPYC™ processors offer us **performance and flexibility**, while delivering **highly efficient heat management** based on the unique Lenovo Neptune direct water cooling platform.”

Dr. Thomas Steinke

Head of Supercomputing, Zuse Institute Berlin

3 The solution

Gaining new capabilities for AI workloads and research

Working with Lenovo and pro-com DATENSYSTEME GmbH, ZIB deployed 168 Lenovo ThinkSystem SD665 V3 Neptune® DWC servers powered by AMD EPYC™ 9004 Series processors based on the Lenovo Neptune® direct water cooling. Each AMD EPYC processor includes 96 “Zen 4” cores with exceptional memory bandwidth and capacity, helping ZIB to maximize performance while managing the system footprint.

The latest-generation Lenovo Neptune® direct water cooling platform was a key decision-factor for the institute. The water cooling design circulates water through all high-heat-producing components separately. This approach together with the use of high quality materials such as copper and dedicated cold plates increases overall efficiency, reducing energy consumption and, crucially, operating costs.

3 The solution

Unique heat management with direct water cooling

To support next-generation AI workloads, 42 additional Lenovo ThinkSystem servers are configured with GPU accelerators and high-performance networking. To analyze which workloads might perform best on which GPU architectures, support portability, and optimize open-source tools and configurations across different GPUs, ZIB implemented an additional small eight-node cluster using more Lenovo ThinkSystem servers, creating a high-performance, high-density solution that allows ZIB to conduct important machine learning research.

The Lenovo water cooling solution, in combination with 100% renewable energy from the local electricity provider, supports ZIB's long-term strategy to further improve sustainability and ultimately achieve a highly regarded ecolabel certification.

To provide access, management and infrastructure services for its high-performance cluster, ZIB deployed Lenovo ThinkSystem SR645 V3 servers.

“Driven by increasing energy costs, our number one priority is always **compute efficiency**. Lenovo and pro-com DATENSYSTEME GmbH designed and implemented a solution powered by AMD EPYC™ processors that **leverages Lenovo Neptune direct warm water cooling to achieve an impressively high heat absorption in water of 98%**. That’s higher than any other system we evaluated, and it keeps our cooling costs down. As a side effect, this also **boosts our overall sustainability**, and the **outstanding performance density** means that we still have enough space available for future extensions as new budget becomes available.”

Dr. Thomas Steinke

Head of Supercomputing, Zuse Institute Berlin

4 The results

Today, ZIB runs over 120,000 CPU cores and more than 50 GPU nodes, achieving a peak performance of 9 PFLOPS. Thanks to this new, highly efficient set of clusters, ZIB can gradually retire older, less efficient nodes without tangible impact on the capacity it can provide to users for vital scientific research.

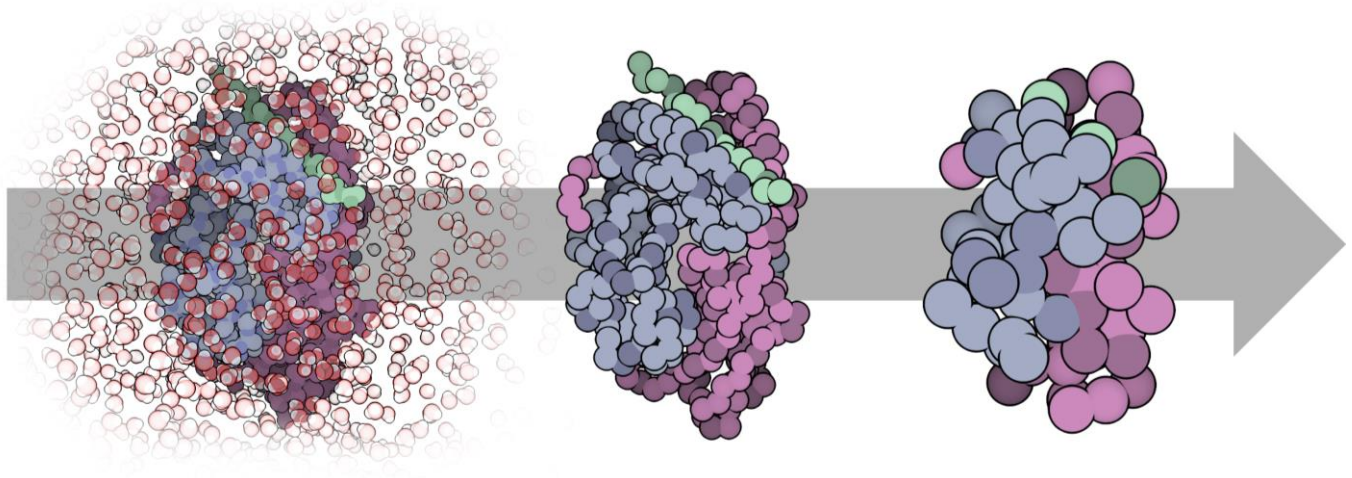
By using the optimized Lenovo Neptune® direct water cooling platform across its clusters, ZIB streamlined systems management and maintenance with a central coolant distribution unit (CDU) to simplify heat management in its data center.

- 98% heat transfer using water cooling
- Lower operating costs thanks to high energy efficiency
- >120,000 cores and >50 GPU nodes deliver 9 PFLOPS

4 The results

Providing the foundation for life-changing insights

The new Lenovo HPC resources at ZIB have already achieved a high level of user acceptance. For example, one team from the field of life sciences uses neural networks, artificial intelligence and machine learning algorithms to train neural network force-fields to enable realistic coarse-grained simulations of large biomolecules to better understand dynamic behavior and interactions of proteins. This research aims at gaining new insights into slow biological processes, with a view to eventually help develop more effective health treatments, without the need for running traditionally expensive molecular-dynamics simulations.



4 The results

As a next step on its efficiency journey, ZIB is currently installing the Lenovo Energy Aware Runtime (EAR), a software solution that helps optimize and tune the sustainability of supercomputers using application power monitoring.

“We really enjoy working with Lenovo and pro-com DATENSYSTEME GmbH. The new HPC systems powered by AMD EPYC™ processors are running smoothly, and **our users are very happy with the performance and reliability**. Based on our positive experience, the IT and data service department is considering solutions with direct water cooling technology for our general IT infrastructure where performance density is also constantly increasing, creating new challenges for data center heat management.”

Dr. Thomas Steinke

Head of Supercomputing, Zuse Institute Berlin

Why Lenovo and AMD?

ZIB was impressed by the comprehensive and professional presales consulting and support provided by Lenovo and pro-com DATENSYSTEME GmbH. By relying on standardized building blocks, the solution architecture is simple, and the clusters can be expanded with new capabilities easily as and when additional budget becomes available.

Powered by AMD EPYC™ 9004 Series processors, the Lenovo ThinkSystem SD665 V3 Neptune® DWC servers offer the ideal combination of performance and energy efficiency.

“It is always very rewarding to work with a team of experts with deep knowledge of the industry and HPC requirements,” recalls Steinke.

“With our **specialized expertise in HPC systems**, we helped ZIB achieve its objectives with a cost-efficient and extensible solution. By using creative approaches to connecting and integrating different systems, architectures, environments, and networking technologies, we enabled a gradual upgrade and expansion of the supercomputing environment with a seamless migration path for ZIB and its users. As a result, **ZIB and its users benefit from easy access to data and systems across all its HPC clusters**, covering the existing solution that is now being gradually retired and the new Lenovo servers.”

pro-com DATENSYSTEME

Oliver Kill

CEO, pro-com DATENSYSTEME GmbH

How can supercomputers be efficient and flexible?

Working with Lenovo, Zuse Institute Berlin deployed cluster nodes based on the Lenovo Neptune® direct water cooling platform, powered by AMD EPYC™ processors.

Explore Lenovo Neptune® Solutions