Academic Research | India

Expanding access to HPC to advance research

Birla Institute of Technology and Science, Pilani

To give researchers access to the compute resources they need to further their cutting-edge work, BITS Pilani built a central HPC platform based on Lenovo ThinkSystem SR665 V3 and SR645 V3 servers, powered by AMD EPYC™ 9004 Series processors.

1 Customer background

Who is BITS Pilani?

The Birla Institute of Technology and Science, Pilani (BITS Pilani) is consistently ranked among the top universities in India. It provides high-quality technical education to students from all over India admitted on the basis of merit. Established in its present form in 1964, BITS Pilani is a globally recognized center of academic and research excellence, and home to a diverse community of more than 17,000 undergraduate and postgraduate students.

BITS Pilani
Pilani | Dubai | Goa | Hyderabad

2 The challenge

BITS Pilani’s mission is to advance knowledge and educate students in science, technology, and other areas of scholarship that will best serve India and the world today. Its research facilities cover a wide range of areas, including biotechnology, chemistry, data science, energy and environmental studies, materials science, mechanical engineering, and physics. This research requires specialized laboratories, high-precision equipment, and high-performance computing (HPC) resources.

2 The challenge

Previously, research groups at BITS Pilani were responsible for acquiring their own compute resources with their own funding. “Research groups would typically procure one or two standalone servers to run their workloads, which only a handful of people had access to,” says Virendra S Shekhawat, Unit Chief, IT Services Unit, BITS Pilani. “Usually, due to budget constraints, these were not high-end servers, so they didn’t really meet researchers’ compute requirements. This forced many groups to use costly third-party cloud services for some jobs, and slowed down research for those whose budget didn’t stretch to the cloud.”

Determined to give all researchers access to the compute resources they need, BITS Pilani set out to build a central HPC platform.

“We made the decision to establish a central HPC facility open to all. To meet the technical requirements of all the different research groups and support emerging AI and ML workloads, we needed a state-of-the-art system.”

Virendra S Shekhawat

Unit Chief, IT Services Unit, BITS Pilani

3 The solution

HPC for all

Working with Harsys Technology and Lenovo, BITS Pilani deployed a cluster based on nine Lenovo ThinkSystem SR665 V3 and ThinkSystem SR645 V3 servers, powered by AMD EPYC™ 9004 Series processors to replace the existing HPC systems. In total, the new cluster boasts 1,100 AMD EPYC processor cores, delivering exceptionally high performance for demanding research workloads.

In recognition of the growing demand for AI-enabled HPC workloads, the cluster also includes two Lenovo ThinkSystem SR665 V3 servers with NVIDIA L40S GPUs to support AI and ML workloads, as well as a Lenovo ThinkSystem SR665 V3 management node with 100 TB usual storage capacity integrated.

Hardware

Lenovo ThinkSystem SR665 V3 Rack Server
Lenovo ThinkSystem SR645 V3 Rack Server
AMD EPYC™ 9004 Series processors
NVIDIA L40S GPUs

Software

Rocky Linux
xCAT/confluent
HPC Libraries
OpenPBS

HARSYS TECHNOLOGY

“We were impressed by the high memory bandwidth and capacity of the AMD EPYC processor cores. Powered by AMD EPYC processors, our Lenovo ThinkSystem servers are optimized to handle very demanding scientific research and AI workloads.”

Virendra S Shekhawat

Unit Chief, IT Services Unit, BITS Pilani

4 The results

With the Lenovo cluster now operational, faculty from across BITS Pilani have been given access to powerful HPC resources to support their work. The institute plans to expand access to undergraduates and postgraduates in due course.

“We’re currently fine-tuning the system based on faculty utilization and their feedback,” explains Shekhawat. “We currently have around 100 active users from almost every department running diverse workloads—from molecular orbital theory to atomic interaction research.”

- Expands access to HPC resources
- Boosts computational power available
- Helps academics advance their research

4 The results

Shekhawat continues: “The response has been extremely positive so far. Previously, research groups could not do certain experiments because of the limitations of their standalone servers. Thanks to our new Lenovo and AMD infrastructure, researchers can analyze larger and more complex datasets than was previously possible.”

Offering a total peak performance of 100 TFLOPS on CPU and 5.8 PFLOPS on GPU, the Lenovo cluster will empower BITS Pilani academics to advance their work and transform their ideas into impactful solutions for a better tomorrow.

4 The results

Examples of cutting-edge research running on the Lenovo cluster include:

Electronic structure computation

Researchers are working on electronic structure computation of molecules which includes computational study of bonding-patterns, energies, energy-gaps, spectroscopic parameters, properties, thermochemistry, etc. This is especially challenging in the ‘strongly degenerate regime,’ where multiple electronic states have nearly the same energy. This complexity requires the use of high-accuracy methods like equation-of-motion coupled-cluster (EOM-CC), a sophisticated quantum chemistry technique which is computationally challenging and demands not only high-end facilities to cater the massively-parallel algorithms but also requires high memory and storage.

Strong-field interactions

In addition to their work on molecular electronic structure, the group also studies how atoms behave when they interact with strong electromagnetic fields, like those from a powerful laser. This area is known as strong-field interaction. For these simulations, they use the Lenovo cluster’s GPU nodes, which are highly efficient at performing the parallel computations required for such simulations.

4 The results

Vision-Language Navigation

Meanwhile, a computer science research group is using the Lenovo cluster to train and run complex AI models for Vision-Language Navigation (VLN). VLN agents must process vast amounts of data from two different modalities—visual information (images, videos) and natural language instructions—in real time to make navigation decisions. The Lenovo HPC system, powered by AMD EPYC processors, provides the necessary high-speed storage and data transfer capabilities to feed this data to the compute nodes without creating a data bottleneck.

“Going forward, research groups don’t need to worry about procuring and maintaining their own servers. They now have access to a state-of-the-art central HPC platform, managed and maintained by the IT Services Unit. This means that they can focus their time and energy on what’s most important: their research.”

Virendra S Shekhawat

Unit Chief, IT Services Unit, BITS Pilani

Why Lenovo and AMD?

For BITS Pilani, Lenovo's deep technical expertise set it apart from other vendors at the pre-RFP stage. "Lenovo's advice and guidance helped us make an informed decision on which solution was the best fit for our needs," recalls Shekhawat.

The institute's chosen Lenovo ThinkSystem SR665 V3 and SR645 V3 configuration featuring 1,100 AMD EPYC™ 9004 Series processor cores offer high performance at a competitive price point. "The AMD EPYC processors offered higher per-core performance than other CPU architectures we evaluated," explains Shekhawat. "The Lenovo team helped us ensure we got the best performance for our budget."

How can universities help researchers advance their work?

By providing access to a central HPC facility based on Lenovo and AMD technology, BITS Pilani is helping academics further their research.

Explore Lenovo HPC Solutions