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Anjali Kshirsagar Director* Center for Modeling and Simulation Savitribai Phule Pune University

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Savitribai Phule Pune University installs Fujitsu HPC platform based on PRIMERGY servers with DDN storage, enabling it to analyze data much faster.

At a glance

Country: India Industry: Education Founded: 1949 Website: unipune.ac.in



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Challenge

Savitribai Phule Pune University (formerly University of Pune), was reliant on shared access to a HPC cluster, which limited the research it could undertake. It wanted to implement a dedicated in-house HPC platform to enable nano-material and other leadingedge materials research.

Solution

The university selected a Fujitsu HPC environment built on FUJITSU Server PRIMERGY RX and CX, using Intel[®] Xeon[®] processors, with DDN storage. The cluster installation, management monitoring, and job scheduling process were simplified with HCS and FUJITSU Software Gateway.

Benefit

- Research tasks now completed in days rather than weeks
- Ten-fold increase in system sizes that can be handled
- Enables Savitribai Phule Pune University to attract new students and solve critical research problems
- Outstanding reliability has seen only one failure despite running 24/7





Customer

Savitribai Phule Pune University (formerly University of Pune), considered one of the premier universities in India, is positioned in the north-western part of Pune city, occupying an area of approximately 411 acres. Established in 1949, it houses 46 academic departments and is popularly known as the 'Oxford of the East', with 307 recognized institutes and 705 affiliated colleges offering graduate and under-graduate courses. The Center for Modeling and Simulation was established in 2003 to promote, support, and facilitate academic and research activities related to modeling and simulation.

Products and Services

- FUJITSU Software HPC Cluster Suite Advanced, including FUJITSU Software Gateway
- FUJITSU Server PRIMERGY RX2540 rack systems
- FUJITSU Server CX400 Scale-out systems
- DDN Storage



Building a dedicated HPC platform

The Center for Modeling and Simulation benefits from the on-going, active, and enthusiastic participation of experts from industry and academics specializing in high-performance computing (HPC) and the modeling of complex systems and materials. Previously, the Center relied upon shared access to advanced cluster computing, however, this was proving insufficient for its needs. It wanted to find a dedicated HPC solution that would deliver the requisite processing power at an affordable cost.

"We had access to a shared pool of two clusters with 250 nodes, but were limited in terms of compute power," explains Anjali Kshirsagar, Director, Center for Modeling and Simulation, Savitribai Phule Pune University. "Our aim was to enable super-advanced research into subjects such as nano-material modeling. I applied for and received a grant from the Indian government, which gave us the means to go to market."

The university worked with Intel Corporation to benchmark HPC solutions, focusing on performance and local systems integration capability. Applications, including Gromacs, VASP, Car–Parrinello molecular dynamics (CPMD), Quantum ESPRESSO (QE), WIEN2K, QuantumWise Nanolab with ATK, were among software road-tested.

"Ultimately, it came down to cost and Fujitsu was less expensive while also providing a more comprehensive design and build process," adds Kshirsagar. "It also gave us the scalability to meet our growing compute requirements. It was simply the best possible technical and commercial solution."

Custom-built, best-in-class

The university worked closely with Fujitsu to design, configure, and build the new FUJITSU Software HPC Cluster Suite Advanced with FUJITSU Software Gateway. The result is built on Fujitsu PRIMERGY RX2540 and CX400 servers, combined with storage from DataDirect Networks (DDN). FUJITSU Server PRIMERGY CX Scale-out systems are the ideal basis for cloud, hyper-converged, and HPC solutions. They provide massive computing power for virtualized environments and complex calculations, as well as consolidation and high-availability scenarios.

FUJITSU Server PRIMERGY RX rack systems are versatile rack-optimized servers providing best-in-class performance and energy efficiency. They deliver more than 20 years of development and production knowhow, resulting in an extremely low failure rate and leading to continuous operations and outstanding hardware availability. Together, the RX and CX servers deliver 66 teraflops using Intel[®] Xeon[®] E5-2695 processors.

"We sent two scientists to Fujitsu in Augsburg, Germany, and one person from Fujitsu in Delhi was working so that they could input into the build process and benchmark our applications in the lab," says Kshirsagar. "This collaborative approach from the outset ensured that the hardware would be configured to our exact specifications."

With the equipment built, it was shipped to the university for installation, a process which took just four weeks. Thanks to the help of the local Fujitsu engineering team and the automated installation and cluster management tools included in the FUJITSU Software HPC Cluster Suite (HCS), end-users can now quickly and efficiently use the cluster resources through the integrated FUJITSU Software Gateway web portal.

This integrated offering for a complete HPC solution is globally known as FUJITSU Integrated System PRIMEFLEX for HPC, and it enables users to better manage their jobs, monitor research progress and review their simulation results.

Ten-fold increase in analysis

"We can conduct research which we simply couldn't do before, such as building two-dimensional structures like graphene sheets and their functionalization, as well as modeling electron transport across semiconductor-metal nanojunctions," comments Kshirsagar. "Previously, we could only focus on 200 atoms – this is now 2,000 atoms, a ten-fold improvement on the detail we can exploit."

Moreover, the university has been impressed with the reliability of Fujitsu's hardware – in the year since its installation there has only been one failure, despite the fact that the HPC platform runs 24/7. It's also scalable, although VASP scaling capabilities limit the number of cores the university can use.

"The system is very stable, and we are delighted with the performance," remarks Kshirsagar. "Tasks that previously would have taken weeks can now be done in days, so we can bring new solutions to market much faster."

The result is that Savitribai Phule Pune University can offer world-class HPC facilities and remain competitive, while also addressing some of the most pressing issues facing India and the wider world. Climate modeling, nanotech, quantum chemistry, solar cells, and bio-informatics are some of the ground-breaking areas students can delve into.

"We are the only Indian, state-level university to have a dedicated HPC platform, which helps us attract students and produce better research for the benefit of us all," concludes Kshirsagar. "We can also easily enhance compute power and extend the HPC capability to other university departments. I am confident that in future Fujitsu will extend their full technical support to Savitribai Phule Pune University."

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