

Institute for Protein Research at Osaka University

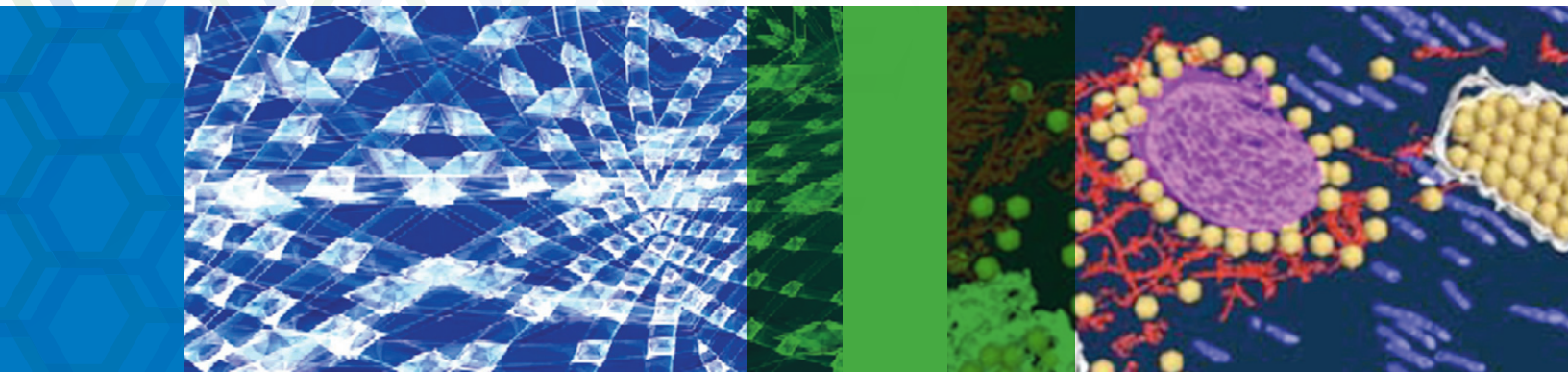
SGI UV 100 and SGI InfiniteStorage 4100
Provide Best Price/Performance

Key Facts

Organization:
Institute for
Protein Research,
Osaka University

Location:
Osaka, Japan

Application:
Life Sciences



Osaka University had been active in the study of proteins and enzymes since its establishment in 1931. It had been a longstanding desire of University experts to promote this feature of the university's activities by establishing a research institute that specialized in protein science. In 1955, a plan was submitted to the ministry of education, science, and culture, and thus formally funded on April 1, 1958 as the Institute of Protein Research (IPR) at Osaka University.

Since then, IPR has developed significantly in terms of its scientific organization. IPR consist of more than 300 people, including faculty members, technicians, undergraduate, graduate students, post-doctoral fellows, and administration. In early 2011, IPR purchased a new technical computing infrastructure from SGI which consisted of an SGI UV 100 coherent shared memory computer and an SGI InfiniteStorage 4100.

The New SGI Platform

The installation includes:

- SGI UV 100 with 48 Intel® Xeon® X7542 6 core processors, total 288 cores
- 1.5TB memory
- SUSE® Linux® Enterprise Server 11
- SGI ProPack 7
- SGI InfiniteStorage 4100 with 100TB of RAID

IPR considered other vendors that provide similar products, such as Dell and IBM, but IPR reports that the SGI solution provided the best price/performance ratio.

SGI Server and Storage Combination Ideal

SGI UV is the leading scalable shared memory architecture in the industry today. Providing compelling advantages in performance and economy by leveraging SGI technology to new levels of scalability and price performance, SGI provisions UV with off-the-shelf hardware and standard off-the-shelf software. The SGI UV scalable coherent shared memory system addresses a broad range of the most demanding data-intensive applications.

SGI InfiniteStorage 4100 (IS4100) brings high performance and capability to a wide range of requirements, giving customers the peace of mind that their data is available and protected. It combines the performance of the next generation 8Gb/s FibreChannel host interface with a proven modular architecture that allows customers to start small and grow over time.

Equally adept at supporting high IOP requirements such as databases and OLTP, and bandwidth-intensive applications such as high performance computing, IS4100 is well suited for the diverse demands and mixed workloads of the challenging environments SGI customers demand. With exceptional per drive performance, configuration efficiency and enclosure-based FC/SATA drive intermixing, IS4100 assures lower drive and enclosure requirements. Seamless on-line scalability addresses growth as requirements change.

Professor Atsushi Nakagawa, of the Laboratory of Supermolecular Crystallography states, “We use our SGI UV for foreground and background jobs without needing any batch queuing system, and the IS4100 is our file server. This combination allows us to perform huge jobs with limited electricity, as the system is very energy-efficient.”

System Used for Both In-House and Commercial Applications

“On the platform, we use in-house applications as well as free applications for protein structure analysis, X ray crystallography, nuclear magnetic resonance (NMR, a useful tool for the analyses of protein structures and dynamics with atomic resolutions), and molecular dynamics,” says Nakagawa.

He continues, “The new system can perform huge computations, giving very valuable results for our scientific research. We used an SGI Altix® 3700 before, but the current system offers huge improvements in performance, as well as better compatibility with other smaller systems in our institute. This advantage reduces our manpower.”

Further, Nakagawa states, “SGI UV provides good price/performance for huge jobs that require large memory without a lot of effort. And SGI professionals support us so much that we did not need to place a lot of effort on installation or customization.”

“We can run both huge memory-dependent jobs and CPU-dependent jobs without any difficulties. SGI UV combines reliability and high-performance computing with easy use, while SGI IS4100 provides reliable file storage,” Nakagawa concludes.

Chemistry Research a Major Use¹

Professor Toshimichi Fujiwara, of the Laboratory of Molecular Biophysics, commented, “UV is used for molecular dynamics calculation and NMR data analysis through NMR spectra simulation. In the area of molecular dynamics calculation, Charmm and Amber are the primary applications used. Most notably, using Replica Exchange Molecular Dynamics Simulation for Implicit Membrane, we have successfully conducted structural analysis of 300 residues of dimerised membrane-spanning protein, tens of residues of peripheral membrane peptide, and transmembrane peptide through molecular dynamics calculation taking NMR constraints into consideration.”

He continues, “In the area of spectra simulation, we’ve successfully conducted structural analysis of main chain structure from MNR chemical shift. We used internally developed programs in Fortran using both the replica-exchange and fragment-assembly methods for this analysis.”

“These research results have only been achieved using UV with tens of computing cores, allowing us to simulate tens of residues of protein and peptides,” Fujiwara concludes.

About IPR

Conceptualized in 1931, The Institute for Protein Research (IPR) was founded formally on April 1, 1958, as a part of Osaka University. Now, The IPR comprises four divisions with 12 laboratories and an attached research center with six laboratories, serving as a joint-use facility for scientists working in the fields of protein and related sciences.

Please visit www.protein.osaka-u.ac.jp/index_e.php

¹ Keisuke Ikeda, Tomoshi Kameda, Erisa Harada, Hideo Akutsu and Toshimichi Fujiwara, “Combined use of replica-exchange molecular dynamics and magic-angle-spinning solid-state NMR spectral simulations for determining the structure and orientation of membrane-bound peptide,” J. Phys. Chem. B, 115, 9327-9336 (2011). <http://pubs.acs.org/doi/abs/10.1021/jp205290t>

