Super Fast Molecular Simulator

Fujitsu PRIMEQUEST

Fujitsu PRIMEQUEST has scalar-parallel architecture, providing the total performance of 4096 GFLOPS by 10 nodes. Each node consists of 64 Cores (32 dual-core CPUs) and 256 GB of shared memory. The nodes are connected with the fiber inter-connect, and any pair of nodes can thereby communicate at the bandwidth of 160 Gbps using the message-passing library (MPI). The system is also equipped with a RAID disk device about 24 TB for temporal storage. This server is mainly used for large-scale molecular dynamics and Monte Carlo calculations, including application to biomolecules.
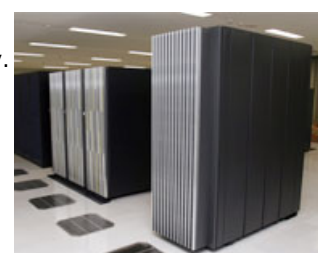
SGI Altix4700

SGI Altix4700 is a super-parallel computer with the peak performance of 4096 GFLOPS. This system consists of two node; one has 512 Cores (256 dual-core CPUs) with 6 TB shared memory, and the other 128 Cores (64 CPUs) with 2 TB, where the extensive shared memory is logically provided by the cc-NUMA architecture. As a peripheral configuration, the system has also a high-performance RAID disk device with the total effective amount of about 114 TB and with the I/O speed of 40Gbps. This I/O speed of the disk is nearly equivalent to that of the memory transfer. This system is particularly suitable to large and accurate calculations of electronic states and other purposes which require huge memory and/or disk space.

High performance molecular simulator

Hitachi SR16000

Hitachi SR16000 has a scalar-parallel architecture with shared memory, providing you the performance up to 5414 GFLOPS using 288 Cores. 1 node has 32 Cores and 2250 GB memory. Peripheral configuration the system has about 21 TB RAID disk device which provides you a huge amount of storage.

Front-end server

The front-end server of RCCS consists of 2 nodes of Hitachi EP8500/550Q. The front-end machines are open to the RCCS users via ssh or other protocols for interactive use. The job-queuing system (JQS) for the batch uses of other system is also controlled by the front-end server.

File Server

The file server consists of 2 sets of Hitachi EP8500/550Q(16CPU model) with 120 TB RAID disk device and backup disk device. The disk device is NFS mounted by other system, and is used as the home directories of the RCCS users.