

HOKUSAI BigWaterfall System

1.1 System Overview

The HOKUSAI BigWaterfall system consists of the following key components:

- Massively Parallel Computers (BWMPC)
- Application Computing Server with Large memory(GWACSL)
- Front end servers that provide the users with the application interface for the system
- Two types of storages with different purposes, one of which is the Online Storage and the other of which is the Hierarchical Storage

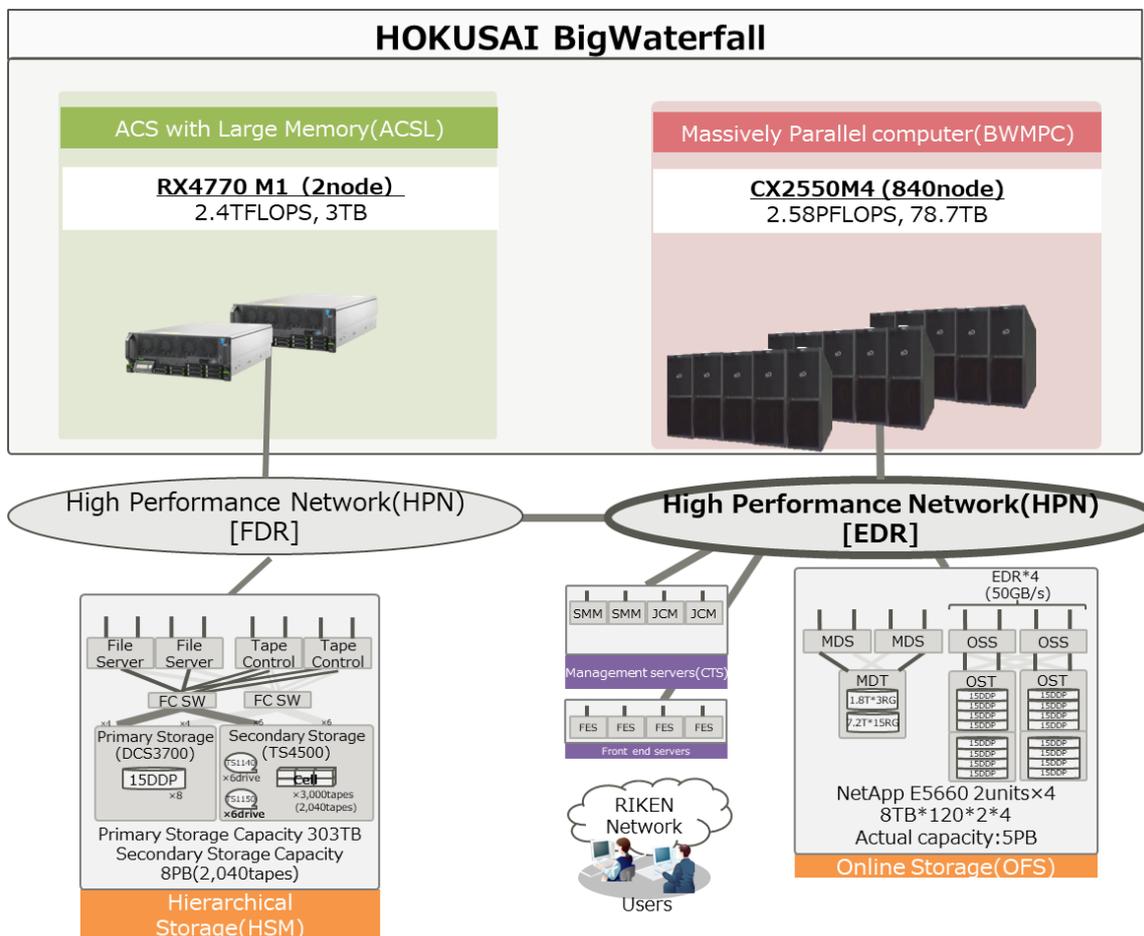


Figure 0-1 System diagram

The Massively Parallel Computer (BWMPC) comprises 840 nodes of CX2550 M4. Each node provides a theoretical peak performance of 3.07 TFLOPS and a memory capacity of 96 GB. The InfiniBand EDR of 12.6 GB/s is used to connect each node to enable high performance communication and file sharing.

The ACS with Large memory (GWACSL) comprises two nodes of PRIMERGY RX4770 M1. Each node provides a theoretical peak performance of 1.2 TFLOPS and a memory capacity of 1.5 TB. The InfiniBand FDR of 6.8 GB/s is used to connect each node to enable high performance communication and file sharing.

The storage environment consists of the Online Storage (OFS) and the Hierarchical Storage (HSM).

The Online Storage (OFS) is a high bandwidth online file system used for the users' home directories, the shared directories for projects and so on, and can be accessed from the Massively Parallel Computers, the Application Computing Servers with Large memory, and the front end servers. The total capacity is 5 PB.

The Hierarchical Storage (HSM) consists of the primary storage (cache disks) of 300 TB and the secondary storage (tape library devices) of 7.9 PB (uncompressed) and is the file system used to store large volumes of data files that should be retained for a long term. The users can read or write data to the tapes without manipulating the tape library devices.

You can access the HOKUSAI BigWaterfall system using ssh/scp for login/file transfer, or using HTTPS for the User Portal. On the front end servers, you can mainly do the following:

- create and edit programs
- compile and link programs
- manage batch jobs and launch interactive jobs
- tune and debug programs

1.2 Hardware Overview

1.2.1 Massively Parallel Computer (BWMPC)

- Computing performance
 - CPU: Intel Xeon Gold 6148 (2.4GHz) 840 units (1,680 CPUs, 33,600 cores)
 - Theoretical peak performance: 2.58 PFLOPS (2.4 GHz x 32 floating-point operations x 20 cores x 1,680 CPUs)
- Memory
 - Memory capacity: 78.7 TB (96 GB x 840 units)
 - Memory bandwidth: 255GB/s/CPU
 - Memory bandwidth/FLOP: 0.08Byte/FLOP
- Local disk
 - Disk capacity: 100.8TB (120GB x 30 units)
- Interconnect
 - InfiniBand EDR
 - Theoretical link throughput: 12.6 GB/s x 2 (bidirectional)

1.2.2 Application Computing Server with Large Memory (GWACSL)

- Computing performance
 - CPU: Intel Xeon E7-4880v2 (2.50 GHz) 2units (8 CPUs, 120 cores)
 - Theoretical peak performance: 2.4 TFLOPS (2.5 GHz x 8 floating-point operations x 15 cores x 8 CPUs)
- Memory
 - Memory capacity: 3 TB (1.5TB x 2 units)
 - Memory bandwidth: 42.7 GB/s/CPU
 - Memory bandwidth/FLOP: 0.14 Byte/FLOP
- Local disk
 - Disk capacity: 3.6 TB ((300 GB x 2 + 1.2 TB) x 2 units)
- Interconnect
 - FDR InfiniBand
 - Theoretical link throughput: 6.8 GB/s x 2 paths x 2 (bidirectional)

1.3 Software Overview

The softwares available on the HOKUSAI BigWaterfall system are listed as follows:

Table 0-1 Software overview

Category	Massively Parallel Computer (BWMPC)	Application Computing Server with Large Memory(ACS)	Front End Servers
OS	Red Hat Enterprise Linux 7 (x 56nodes) CentOS7(x 784nodes) (Linux kernel version 3.10)	Red Hat Enterprise Linux 7 (Linux kernel version 3.10)	Red Hat Enterprise Linux 7 (Linux kernel version 3.10)
Compiler	Intel Parallel Studio XE Cluster Edition Intel C/C++ and Fortran compiler Intel TBB Intel Distribution for Python		
Library	IntelParallel Studio XE Cluster Edition Intel MKL Intel MPI Library Intel IPP Intel DAAL		
Tool	Intel Parallel Studio XE Cluster Edition Intel VTune Amplifier XE Intel Advisor Intel Inspector Intel Trace Analyzer & Collector		
Application	Gaussian(Only supported Red Hat Enterprise Linux 7(x 56nodes), ADF, AMBER,Q-Chem,GAMESS, GROMACS, NAMD, ROOT	Gaussian, ADF, AMBER, ANSYS, GAMESS, GROMACS, NAMD, ROOT	GaussView, ANSYS(preppost) VMD, ROOT