HPC system startup manual (version 1.80)

| Issue | Date | Change | Modified | Notes |
|-------|------------|---|----------|-------|
| | | | pages | |
| 1 | 12/1/2012 | New document | | |
| 2 | 10/22/2013 | Added the information of supported OS | P2 | |
| 3 | 10/22/2013 | Changed the example 1 for data | P2 | |
| | | download | | |
| 4 | 3/4/2014 | Added the chapter of Torque/Maui | P2 | |
| | | batch job system | | |
| 5 | 3/4/2014 | Changed text font | | |
| 6 | 10/2/2014 | Changed the example 1 for data | P2 | |
| | | download | | |
| 7 | 5/26/2015 | Changed the example 4 for browse | P4 | |
| | | SACLA Database | | |
| 8 | 10/16/2015 | Changed the section 5 for Data | P3 | |
| | | handling in SACLA HPC system | | |
| 9 | 9/1/2016 | Replacement SACLA HPC system | | |
| 10 | 9/8/2020 | Changed the section 3 for the host name | P2 | |
| | | specified in the ssh command. | | |
| 11 | 9/1/2021 | Changed the section 1 for the | P1 | |
| | | Obverview. | | |
| 12 | 2/28/2022 | Changed the section 6 for the Installed | P3, P4 | |
| | | software List and how to use. | | |

Document change log

1 **Overview**

The high performance computing (HPC) system in the SACLA facility consists of 60 compute nodes, with two 24-core processors per node, for a total of 2880cores. The theoretical peak compute performance is 138.2 TFLOPS. The system supports a 2PB shared storage system, managed by the Lustre file system. Nodes are interconnected with Infiniband with a 100 Gbps bandwidth. This manual introduces the startup from account creation to the launch of software installed in the SACLA HPC system.

2 Account creation

After your experiment proposal accepted, a responsible researcher of the SACLA is assigned to your proposal. Contact him by e-mail and request the use of the SACLA HPC system. He will create your account and give the username and password. Note that "/home" directory is limited by quota to 100 GB per user. When you are going to use more storage area for a large amount of experimental data and the result data of the analysis, "work" directory can be used. Please talk with your contact researcher for the use of "/work" directory.

3 How to login SACLA HPC system

The access of the SACLA HPC system is limited to be within SPring-8 local network. First of all, you have to connect your computer to the SPring-8 local network by using VPN service. After that, you can login the HPC server through SSH protocol.

[step 1. Connect the SPring-8 network with VPN service.]

- Access the web page: <u>https://hpc.spring8.or.jp</u> with a web browser.
- Login the web page of VPN installation service. (Enter your username and password given in Sec. 2)
- Download and install VPN connection software into your computer. Supported OS for VPN service is as follows.

[Windows]

Windows 11

Microsoft-supported versions of Windows 11 and 10 for ARM64-based PCs

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Windows 10 x64(64-bit)
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Windows 8.1 x86(32-bit) and x64(64-bit)

[Mac]

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macOS 12, 11.x (64-bit), 10.15(64-bit), and 10.14(64-bit)
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[Linux]

Red Hat 8.3 and 7.9 (64-bit)

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Ubuntu 20.04 (LTS) and 18.04 (LTS)(both 64-bit)
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SUSE (SLES) 15.3 and 12.5

[step 2. Login SACLA HPC system.]

• Type "ssh -X [username]@xhpcfep.hpc.spring8.or.jp". The username is given in Sec.2.

• Enter your password given in Sec.2.

4 Batch job system

The queuing system on SACLA HPC system is PBS. You need three main commands to use this system: qstat, qsub, and qdel.

[qstat]

"qstat" display status of PBS batch jobs, queues, or servers.

[qsub]

"qsub" submits a job. In its simple form you would run "qsub *myscript*", where *myscript* is a shell script that runs your job. For those who don't want to write scripts, you can do an interactive qsub with the -I option. You can also use -X option for enabling X11 forwarding (e.g. "qsub -I - X").

[qdel]

"qdel job_number" deletes your job.

5 Data handling in SACLA HPC system

Access the web page: http://xhpcfep.hpc.spring8.or.jp/#SaclaSoftware via VPN service.

6 Installed software List and how to use

The available software is listed below.

[FireFox]

- Login the SACLA HPC system as stated in Sec. 3.
- Type "qsub -I -X" in the terminal window.
- Type "firefox" in the terminal window.

[Evince]

- Login the SACLA HPC system as stated in Sec. 3.
- Type "qsub -I -X" in the terminal window.
- Type "evince" in the terminal window.

[Hdfview]

- Login the SACLA HPC system as stated in Sec. 3.
- Type "qsub -I -X" in the terminal window.
- Type "module load hdfview"
- Type "HDFView" in the terminal window.

[ImageJ]

- Login the SACLA HPC system as stated in Sec. 3.
- Type "qsub -I -X" in the terminal window.
- Type "module load ImageJ"
- Type "ImageJ" in the terminal window.