Trial Operation Briefing of HOKUSAI BigWaterfall2(HBW2)

Information Systems Division

RIKEN Information R&D and Strategy Headquarters

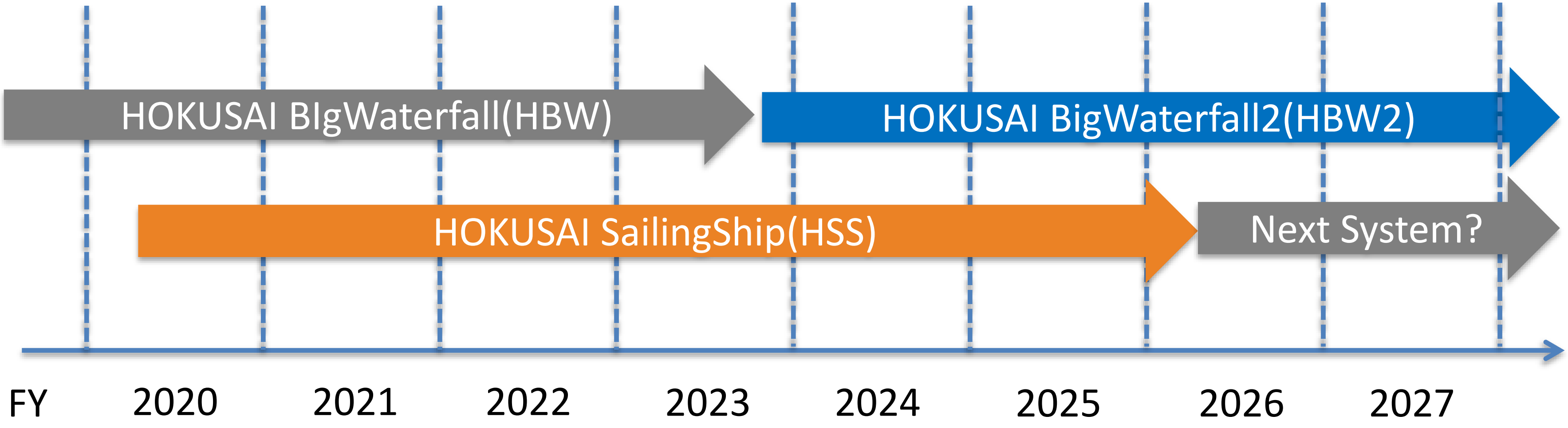
Today's Overview

- Overview of HBW2 System
- HBW2 Resource Provision to HPCI
- Operation Policy of HBW2 System
  - Trial operation, regular operation, usage fee
- How to use HBW2 Trial Operation
  - User Registration and Project Submission at HBW2 Portal
  - Job execution on HBW2 login node

OVERVIEW OF HBW2 SYSTEM

Operation schedule of the Shared Use Computers HOKUSAI

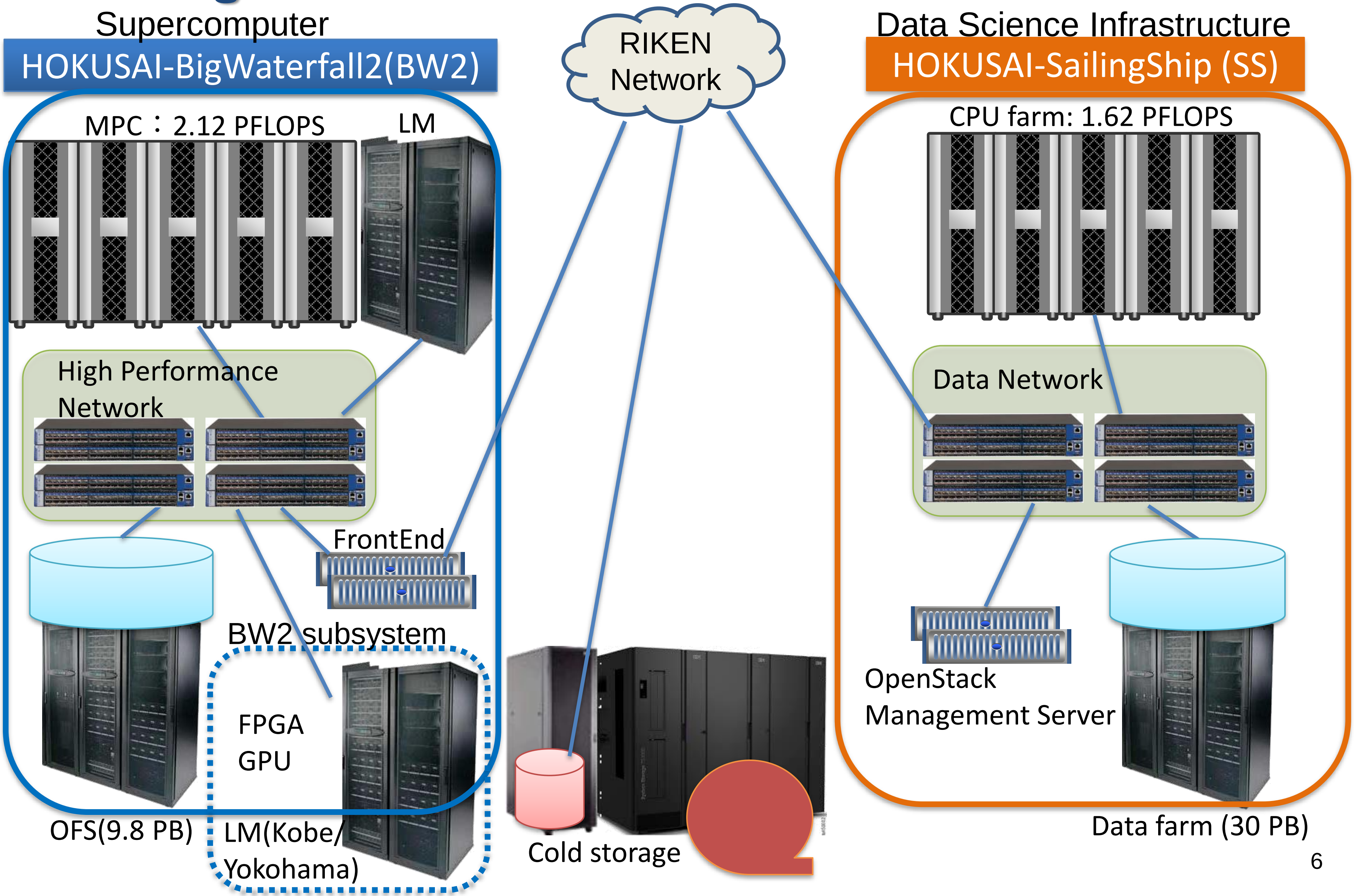
- Supercomputer
  - October 2017 – November 2023: HOKUSAI BigWaterfall(HBW)
    - Half of MPC ended operation at the end of July 2023
  - December 2023 – November 2029: HOKUSAI BigWaterfall2 (HBW2)
    - Test operation until the end of March 2024
- Data Science Infrastructure
  - June 2020 – May 2026: HOKUSAI SailingShip(HSS)


HOKUSAI BIgWaterfall(HBW)
HOKUSAI BigWaterfall2(HBW2)
HOKUSAI SailingShip(HSS)
Next System?
FY
2020
2021
2022
2023
2024
2025
2026
2027

End of HBW and Start of BW2

- The end of HBW operation
  - Until 9:00 a.m. on November 27
  - Application for usage fee and additional computing time
    - Until November 7
  - Accepting period of Usage Report
    - Until 5:00 p.m. on November 28
    - Check box for continuation request is invalid
- Start of BW2 trial operation
  - From 1:00 p.m. on December 4
    - Applications for use will also be accepted on the HBW2 portal at the same time
    - Trial operation will continue until the end of March 2024
    - Regular operation will start in April 2024
  - HBW2 Trial Operation Briefing
    - From 10:00 a.m. on November 22

Image of HOKUSAI after introduction of HBW2



Supercomputer

HOKUSAI-BigWaterfall2(BW2)

MPC：2.12 PFLOPS

LM

High Performance Network

FrontEnd

OFS(9.8 PB)

BW2 subsystem

FPGA
GPU

LM(Kobe/Yokohama)

RIKEN Network

Cold storage

Data Science Infrastructure

HOKUSAI-SailingShip (SS)

CPU farm: 1.62 PFLOPS

Data Network

OpenStack
Management Server

Data farm (30 PB)

HBW2 System

- MPC
  - Total theoretical FP(64bit) computing performance: 2.12 PFLOPS
- Node perfomance
  - Theoretical FP(64bit) computing performance: 6.8 TFLOPS
    - Intel Xeon next-generation CPU(1.9 GHz, 56 cores) x 2
  - Memory
    - HBM2e: 128 GiB、3260 GB/s
- High Speed Network (HPN)
  - Infiniband NDR: 50 GB/s
    - Quarter of full bisection between nodes including MPC
    - Full bisection otherwise
- Shared Storage
  - Lustre file system: 9.8 PB、400 GB/s
- Large Memory Server (LMC)
  - 2 nodes, 3 TiB/node

Comparison of HBW and HBW2

	HBW	HBW2
FLOPS	2.5 P	2.12 P
Total core number	33,600	34,944
Node number	840	312
Memory	96 GiB、255 GB/s	128 GiB、3260 GB/s
LMC	2ノード、1.5 TiB/ノード	2ノード、3 TiB/ノード
Communication performance	IB EDR (12.5 GB/s)	IB NDR (50 GB/s)
Shared storage	5 PB	9.8 PB
Job execution by containers	None	Singularity

HBW subsystem is being procured separately

- Wako: GPU servers, FPGA servers
    - 4 GPU servers：H100 x 4
    - 2 FPGA servers：IA-840F x 2
- Kobe/Yokohama: Large memory servers
    - 1 node each: 8 TiB
- Scheduled to start operation in April 2024

HBW2 RESOURCE PROVISION TO HPCI

About HPCI

◎High-Performance Computing Infrastructure (HPCI)

- A shared computational environment that connects major supercomputers as well as storages of universities and research institutions in Japan via high speed networks
- HPCI realizes the scientific and technological computing environment where a wide range of users in Japan can access national HPC resources efficiently
- HPCI resources are available to researchers who apply for access to the HPCI management organization and have their proposals reviewed and approved.

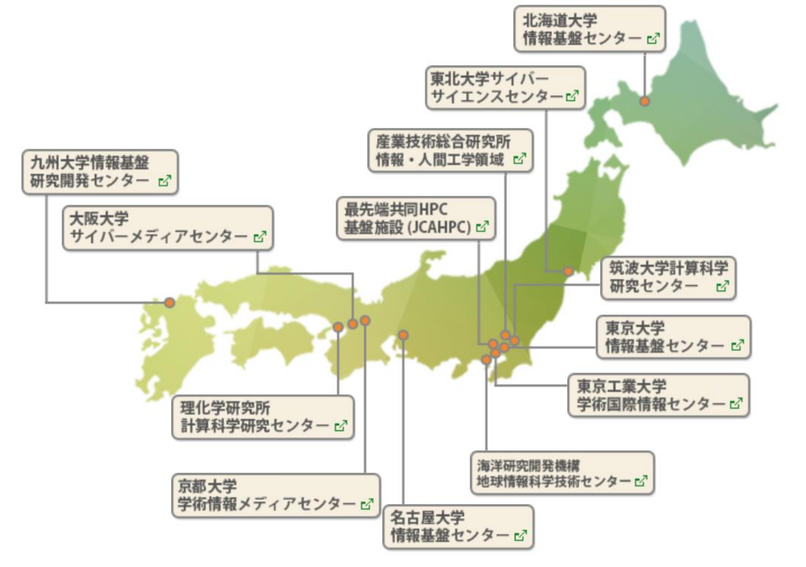
◎HPCI Computing resources

◆Tier 1

・Fugaku

◆Tier 2

・Computing resources of universities and research institutes nationwide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情報基盤センター
東北大学サイバー
サイエンスセンター
産業技術総合研究所
情報・人間工学領域
九州大学情報基盤
研究開発センター
大阪大学
サイバーメディアセンター
最先端共同HPC
基盤施設 (JCAHPC)
筑波大学計算科学
研究センター
東京大学
情報基盤センター
東京工業大学
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海洋研究開発機構
地球情報科学技術センター
京都大学
学術情報メディアセンター
名古屋大学
情報基盤センター

図1：HPCIシステムを構成する計算機資源を提供するシステム構成機関 (2021年度)

https://www.hpci-office.jp/より

Providing HBW2 resources to HPCI

President Gonokami presented the following policy for the start of procurement of HBW2.

- Actively participate in HPCI and promote its use.
- Provide HBW2 resources to the HPCI system.
- While implementing these measures, RIKEN should consider what its computational resources should be in the future.。

Even as we move forward with the TRIP initiative, we aim to diversify the computational resources available to RIKEN researchers and to collaborate with a variety of researchers, with the following objectives

- Enable HPCI computational resources to be considered as a choice of computational resources.
- Not only to use them unilaterally, but also to be actively involved in HPCI, including providing resources.

Implementation measures

1. Proving HBW2 resource to HPCI
    - Provide HBW2 as an HPCI resource from the FY2024 application period.
        - Closed for FY2024.
2. Support for use of Fugaku's paid use
    - Full subsidy for usage fees for paid proposals at Fugaku (closed)

OPERATION POLICY OF HBW2 SYSTEM

HBW Trial Operation

- Trial operation will be conducted from December 2023 to March 2024.
  - Usage application for the trial operation is separate from that for HBW.
    - Usage report for HBW will be received from mid-October to early November.
  - No usage report and usage fee for trial operation
- Classification of project
  1. (Internal RIKEN) project
     - **Each proposal can use 5% of the total computing resources of MPC**
     - If computing time is used up, low-priority execution is possible
     - Large memory servers can be added up to 20%
- Storage (same as in regular operation)
  - Home (/home) area is 4TB per account
  - Data (/data) area is allocated on a project basis
- Data transfer from HBW
  - HBW data (home and data area) is being backed up on HSS
  - Users should move data from HSS to HBW2 by themselves during the trial operation period using scp, etc.

HBW2 Regular Operation

- Regular operation will be start from April 2024
- Classification of project
  1. (Internal RIKEN) project
     - **Each project can use 1% of all computing resources of MPC free of charge**
     - Additional computing time can be added for a fee
     - If computing time is used up, low-priority execution is possible
     - Large memory/GPU/FPGA servers can be added up to 20%
  2. HPCI project
     - **Plans to provide about 50% of computing time to HPCI**
       - Each project is up to 10%
     - Users can apply for HPCI projects and use HBW2 if they are accepted
       - No user burden for usage fee (paid by HPCI to RIKEN)

Small-scale users (less than 1%) will still be able to use the system
Above mid-scale users (more than 1%) can use HPCI project, paid use or execution with low priority.

HBW2 Usage Fee

- From April 2024 when HBW2 main operation starts
  - No change in HSS

- HBW2 computing resources are **720 core hours for 300 JPY.**
  - For internal RIKEN project, 1% of all computing resources and low priority use are free of charge.
  - For HPCI proposals, no burden on the user.
  - Example: 403,200 JPY for 1 additional node (112 cores) for 1 year (approx. 970,000 core hours)
    - 112 cores x 24 hours x 360days / 720 core-hours x 300 JPY = 403,200 JPY
- HBW data area is **180 JPY for 1 TB for 1 month**
  - Home area per account (4 TB) is free of charge.
  - Example: 10TB of data area for 1 year is 21,600 JPY
    - 10 TB x 12 months x 180 JPY = 21,600 JPY

*Usage fees are set so that usage fees cover about 25% of the total annual payment.
The total annual payment for HBW2 is about 300 million JPY
- Hardware leasing, maintenance and support, etc.
- Excluding location and electricity cost

HBW2 User Management

- HBW2 portal user
  - Created when you log in to the HBW2 Portal for the first time
  - Required to use HBW2 Portal and become an project member
- HBW2 account
  - Created when joining a project
  - Linux account required to use computing resources and storage
- HPCI related
  - HPCI ID: Required for HPCI project applications
  - HPCI account: For logging in to the HPCI support system, etc.
    - Created after the HPCI project is accepted
  - Local account: Account for each computing resource
    - HBW2 account for HBW2

HBW2 Portal

- HBW2 portal
  - Integrating HBW's Online Application System and HPC Portal
  - Users can now check usage status as well as submit projects
  - RIKEN researchers log in with Shibboleth authentication
- Functions of the HBW2 portal
  - Various information
    - Notices, user guide, system status
  - User Management
    - HBW2 portal user registration
    - ssh public key registration for HBW2 account
  - Project Management
    - New project submission
    - Various submissions
      - Change project information
      - Change project member
      - Purchase of core time/storage
    - Submission of Usage Report
    - Apply to use the next year's project

HOW TO USE HBW2 TRIAL OPERATION

Procedures for using HBW2 Trial Operation

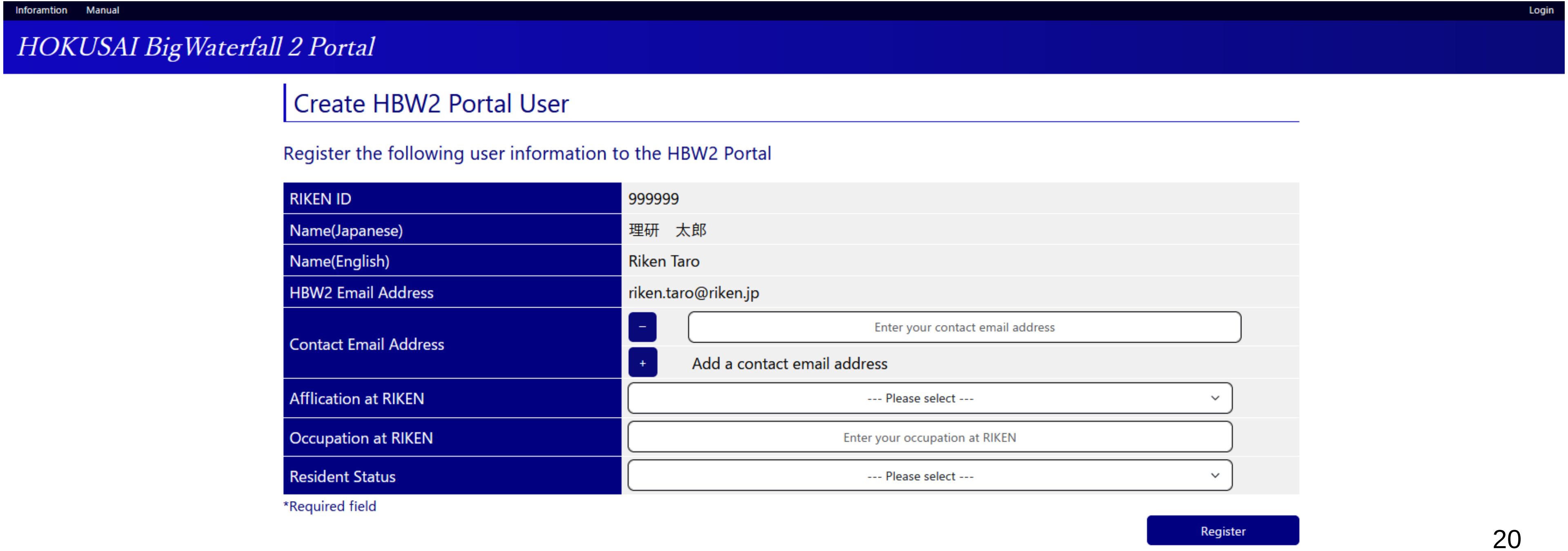
1. Preparation for use on the HBW2 portal
   1. All project members create users on the HBW2 portal
   2. New project submission in HBW2 portal
      - The Usage Policy and the Operational Procedures will be updated by the start of regular operation.
      - Security export control review for non-residents, etc.
        - In preparation, so review at a later date
        - Assumed to be added to the form at the time of admission to RIKEN
      - If all is well, register the project and HBW2 accounts
   3. Each proposal member registers their public key for ssh
2. Job execution on HBW2 login node
   1. Log in to the HBW2 login node via ssh
   2. Compile the software, configure the environment, and execute the job
      - HBW2 introduces slurm as a job manager
      - Singularity jobs can also be executed

Please understand that trial includes HBW2 portal and other operations.

Creating a user on the HBW2 Portal

- User created at first login to HBW2 portal
  - RIKEN researchers log in with Shibboleth authentication
  - After filling in the required fields, click "Register" to complete user creation
    - HBW2 email address is automatically obtained upon Shibboleth authentication
    - Contact email address is the email address you would like to add for contact purposes

The screen is under development.



Create HBW2 Portal User

Register the following user information to the HBW2 Portal

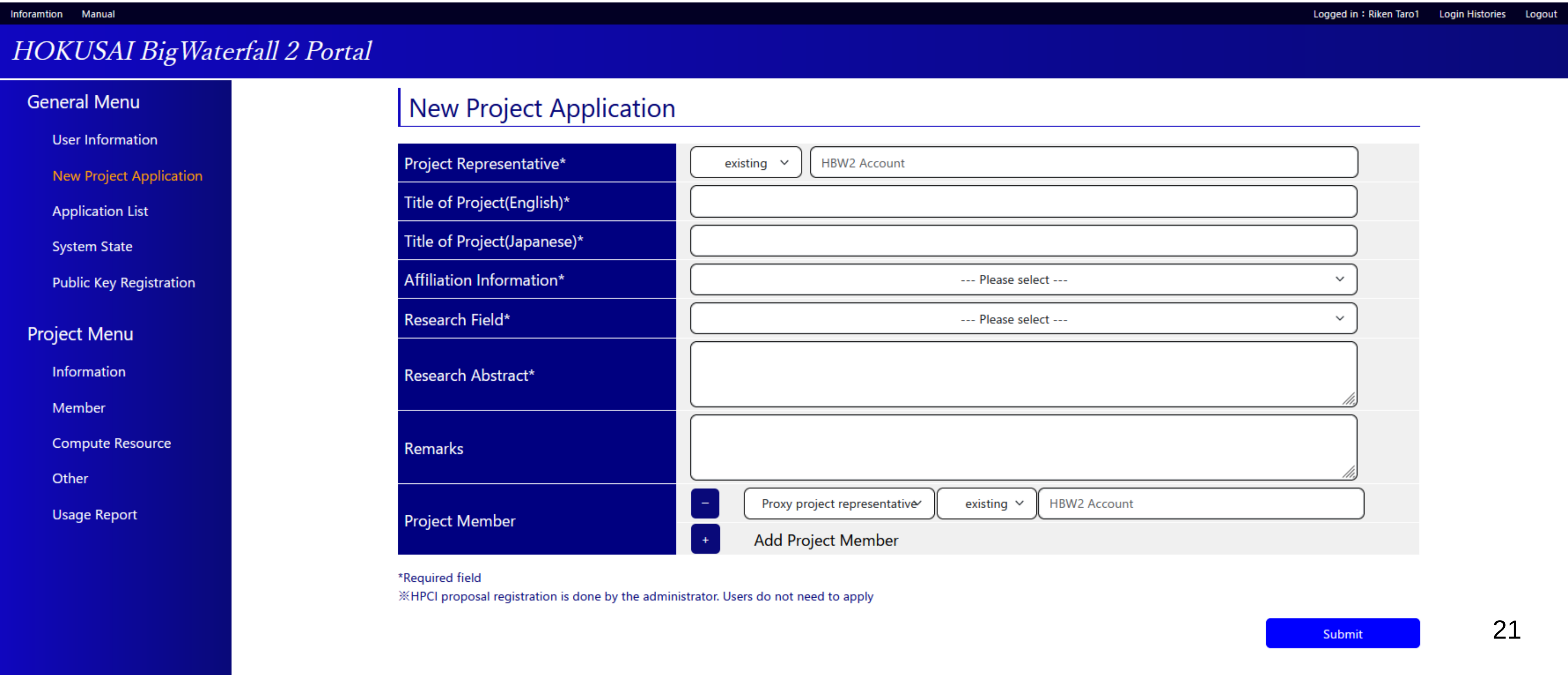
RIKEN ID	999999
Name(Japanese)	理研　太郎
Name(English)	Riken Taro
HBW2 Email Address	riken.taro@riken.jp
Contact Email Address	− Enter your contact email address + Add a contact email address
Affilication at RIKEN	--- Please select ---
Occupation at RIKEN	Enter your occupation at RIKEN
Resident Status	--- Please select ---

*Required field

New Project Application in the HBW2 Portal

- Submit a new project from the HBW2 Portal New Project Application Menu
  - Project members are created as HBW2 Portal users in advance
    - Project members can be added at a later date
  - After entering the required information, click "Submit" to complete the application
    - HBW users must also select a new HBW2 account

The screen is under development


Inforamtion
Manual
Logged in：Riken Taro1
Login Histories
Logout
HOKUSAI BigWaterfall 2 Portal
General Menu
User Information
New Project Application
Application List
System State
Public Key Registration
Project Menu
Information
Member
Compute Resource
Other
Usage Report

New Project Application

Project Representative*	existing ⌄ HBW2 Account
Title of Project(English)*	
Title of Project(Japanese)*	
Affiliation Information*	--- Please select --- ⌄
Research Field*	--- Please select --- ⌄
Research Abstract*	
Remarks	
Project Member	− Proxy project representative ⌄ existing ⌄ HBW2 Account + Add Project Member

*Required field
※HPCI proposal registration is done by the administrator. Users do not need to apply

How to transfer HBW data

- Data transfer from HBW to HBW2
  - HBW data (home area and data area) is being backed up to HSS
  - Users move data from HSS to HBW2 by themselves during the trial operation (by scp, etc.)
  - When transferring the data, set read-only access to the data on HSS
- How to transfer HBW home area (/home)
  - When creating a new HBW2 account, enter the same account name as the HBW account
    - If you are not the same person as your HBW account, you cannot use the same account name.
    - If you change the account name from the HBW account name and want to take over the HBW account, write that in the remarks column.
- How to transfer HBW data area (/data)
  - When applying for an HBW2 Trial Proposal, enter the name of the HBW project you wish to transfer in the remarks column
    - If the representative of the HBW2 project is different from the representative of the HBW project, we will check with the representative of the HBW project

Note: Please follow the instructions on the HBW2 portal
as the data transfer method may change slightly.

Job execution environment in HBW2

- Job management on HBW2
  - HBW2 introduces slurm as a job manager
  - Singularity jobs can also be executed
- Prepare Singularity image
  - Distributed Singularity image
  - Convert docker image to Singularity image
  - Create Singularity image by yourself
- Applications prepared by HBW2
  - Gaussian, GAMESS
  - Gromacs, AMBER, NAMD, VMD
- Hyperthreading of computation nodes
  - Basically, as in HBW, hyperthreading is turned off
  - Hyperthreading on some nodes for testing