Practice and Experience in JHPC-Quantum: HPC Oriented quantum-HPC integration

Miwako TSUJI

RIKEN Center for Computational Science (R-CCS)

Center for Computational Sciences (CCS) , University of Tsukuba

TQCI seminar 4th Dec. 2025

RIKEN Center for Computational Science (R-CCS) and supercomputer “Fugaku”

- 2010 July **RIKEN Advanced Institute for Computational Science (AICS)**
  - operate the **K** computer (京コンピュータ) as a shared facility
  - collaborate and integrate the fields of computational science and computer science
  - form an international research base for advanced scientific studies and technological breakthroughs
- 2018 April **RIKEN Center for Computational Science (R-CCS)**
- 2021 March **Public service of the supercomputer Fugaku has started**

Fugaku (富岳) : 432 racks, 158,976 general-purpose manycore CPUs

Fujitsu A64FX, 20MW power-consumption

Half exaflops in DP, 1 Exaflops in SP!

Ranking	Performance	2nd System Performance
TOP500	442.01 PFLOPS	148.6 PFLOPS (3.0)
HPGC	16.00 PFLOPS	2.9 PFLOPS (5.5)
HPL-AI	2.00 EFLOPS	0.55 EFLOPS (3.6)
Graph500	102.05 TTEPS	23.75 TTEPS (4.3)

Quantum-HPC Hybrid Platform Division @ R-CCS

The Division Founded on 1st Apr. 2023.

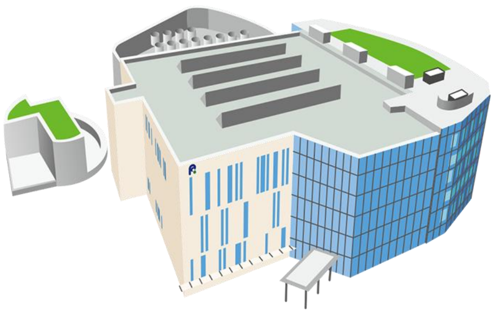
- a new computational infrastructure integrating quantum and supercomputing technologies to expand the computable domain.
- the software stacks for the platform and enhance its usability environment.

Director

Deputy Directors

- Research Teams
- Operations and Computer Technologies Division
- HPC and AI driven Drug Development Platform Division
- Quantum-HPC Hybrid Platform Division
- AI for Science Platform Division
- Office of the Center Director
  Office of the Fugaku Society 5.0 Initiative

Organization



Division Director

- Quantum-HPC Hybrid Software Environment Unit
- Quantum Computing Simulation Unit
- Quantum-HPC Hybrid Platform Operations Unit

Why Quantum-HPC !?

- Many problems can be solved using supercomputers (HPC), but problems requiring exponential execution time cannot be solved even with supercomputers.
  - Quantum simulation, optimization, graph problems, cryptanalysis, factorization ….
- When solving large and realistic scientific problems using a quantum computer, combining with HPC is required for preprocessing, postprocessing, etc.
  - In quantum many-body problems, the part that generates the model is well-suited to supercomputers and sufficiently fast. Considering realistic speed and scalability, replacing everything with a quantum computer is not practical.
  - In the future, when inputting quantum states at scales of hundreds or thousands of qubits, HPC will be necessary to prepare these states.
- Particularly in quantum chemistry and material science, combining quantum computer with existing quantum chemistry applications (approximate solution methods) on HPC is important.
  - Effective use of quantum computer involves first obtaining a “variational state approximately close to the true ground state” using HPC, then employing the quantum computer.
  - Similarly, for energy calculations on large molecules, it is necessary to identify the portions truly requiring quantum computer, and this requires HPC

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Quantum HPC related Projects in RIKEN R-CCS

TRIP3 (2024.04-

Expansion of Computationally Viable Region, Transformative Research Innovation Platforms of RIKEN Platforms,

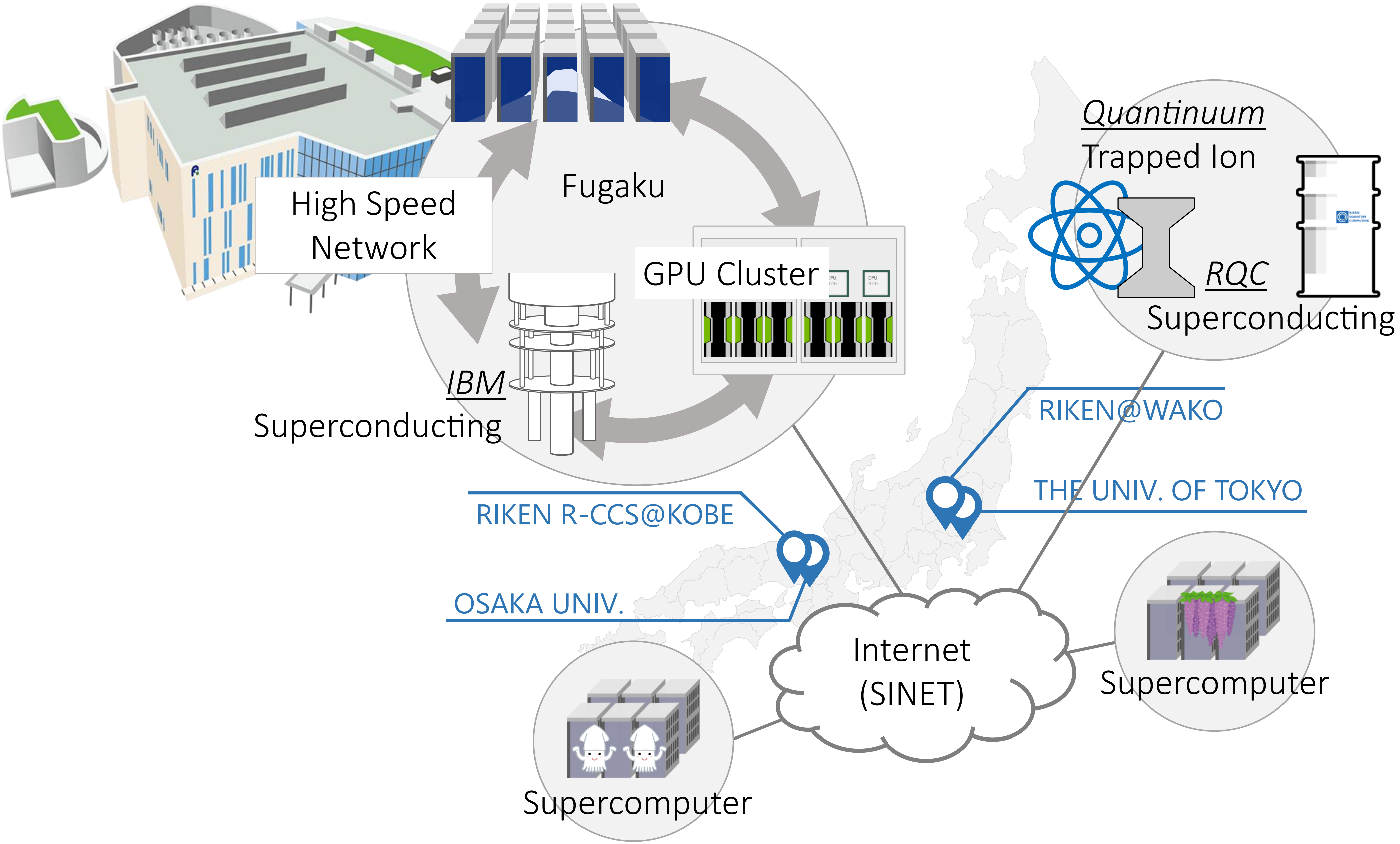
A cross-disciplinary project to establish connections among RIKEN’s cutting-edge research platforms such as *supercomputers*, *quantum computing*, large synchrotron radiation facilities, bioresource-projects.
R-CCS and Center for Quantum Computing (RQC) are tasked with “the value creation by quantum-HPC hybrid computing for Accelerating Research DX”.

JHPC-Quantum (2024.11-

Research and Development of Quantum-Supercomputers Hybrid Platform for Exploration of Uncharted Computable Capabilities

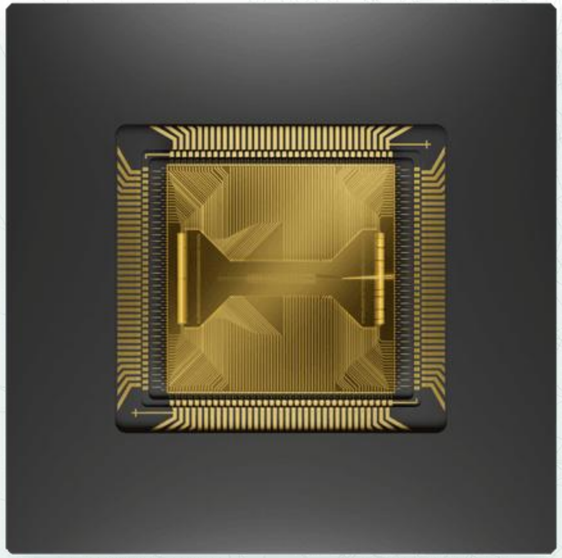
One of research projects in “Research and Development Project of the Enhanced Infrastructures for Post-5G Information and Communication Systems” in NEDO, an agency under the Ministry of Economy, Trade and Industry.
R-CCS, Softbank Corp., the university of Tokyo, and Osaka university
A platform that connects supercomputers and different types of quantum computers
to promote the early commercialization of quantum computers.

Overview (JHPC-Quantum & TRIP)



Recent Status of Quantum Systems

	IBM Kobe	Quantinuum 黎明 Reimei	RIKEN 叡 A
Name	Heron	System Model H1	A
Type	Superconductive	Trapped Ion	Superconductive
Qubit	156	20	64
Status	Running	Running	Running



Pictures
https://jp.newsroom.ibm.com/2023-12-05-IBM-Debuts-Next-Generation-Quantum-Processor-IBM-Quantum-System-Two,-Extends-Roadmap-to-Advance-Era-of-Quantum-Utility
https://www.quantinuum.com/products-solutions/quantinuum-systems/system-model-h1
https://www.riken.jp/medialibrary/riken/pr/news/2023/20231005_1_photo1.jpg

“A” RIKEN Superconductive Quantum Computer

- RIKEN Center for Quantum Computing
  - The successor of the *first* developed superconducting qubit
  - The cloud service started in Mar. 2023
  - 16 → 64 (now) → 144 qubits

    → 256 qubits (Fujitsu)

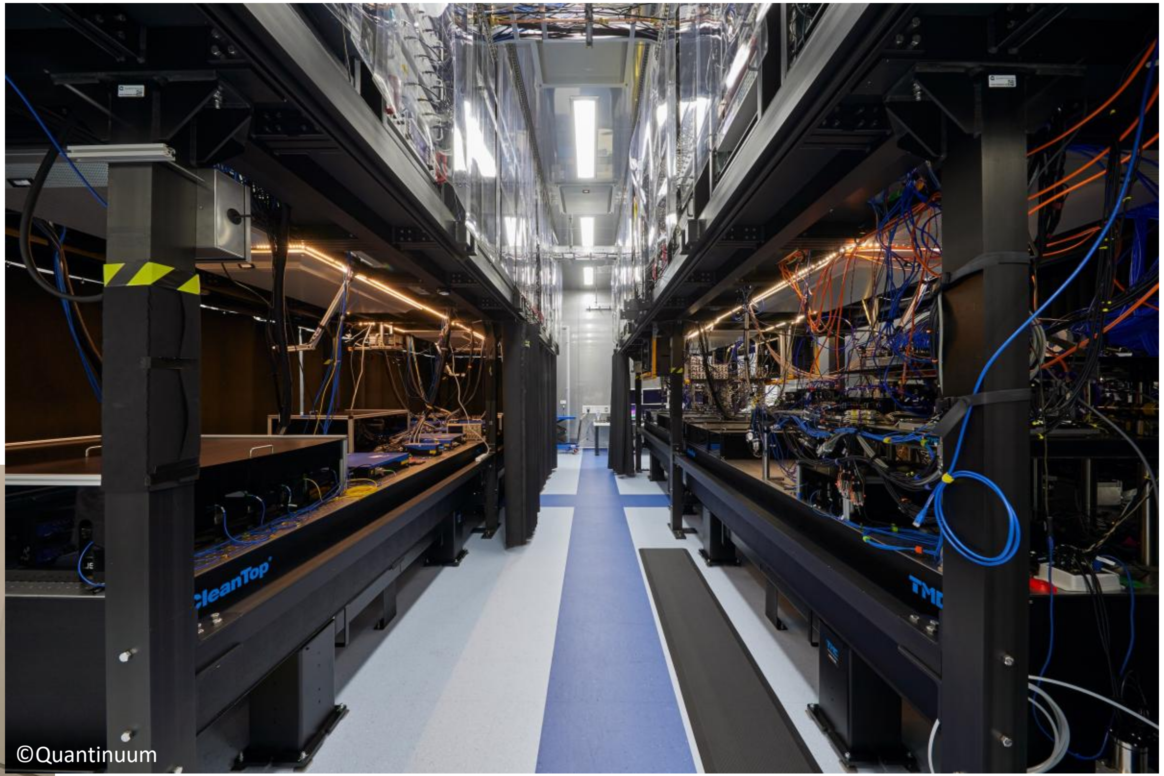
https://www.riken.jp/pr/news/2023/20231005_1/index.html

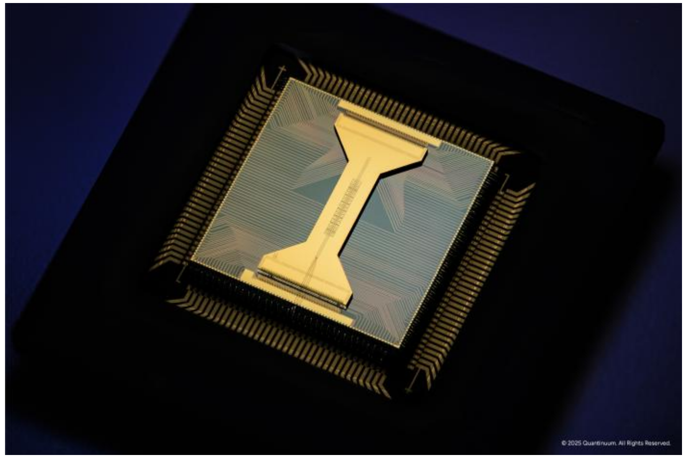
“Reimai” Quantinuum Trapped-Ion Quantum Computer

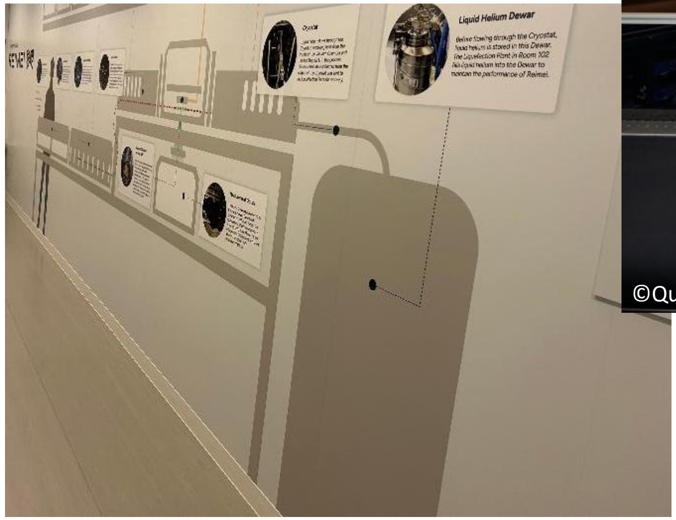
黎明

QUANTINUUM
REIMEI

Quantinuum Trapped-Ion Quantum Computer H1 (20 qubits) was installed in Wako Campus, Japan and is operated since Feb, 2025







IBM Superconductive Quantum Computer

- IBM Heron
  - 156-qubit

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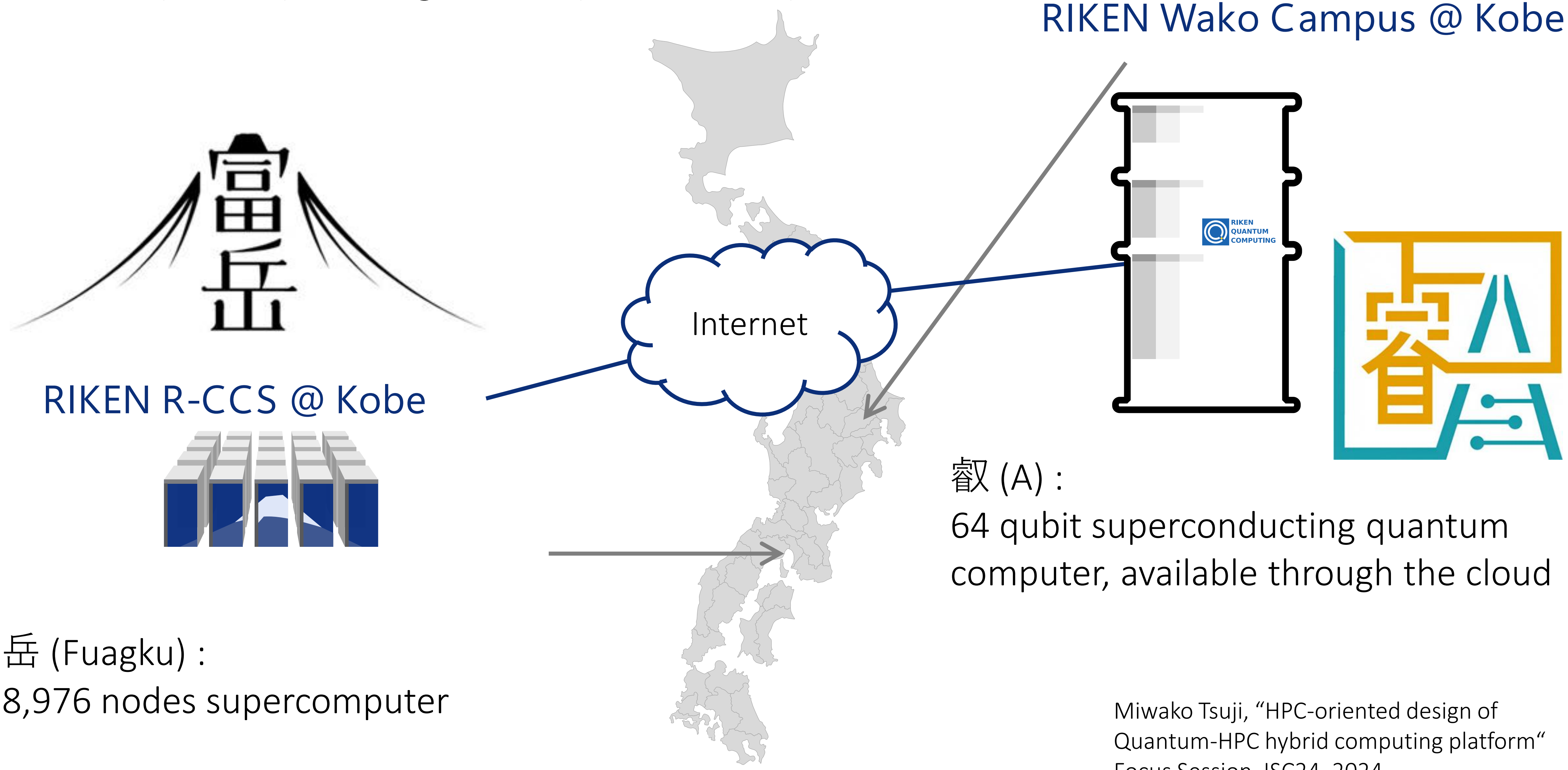
TRIP Proof of concept in 2023/2024 experiments and lessons learned

- Connect supercomputer **Fugaku** and quantum computer **A**



叡 (A) :
64 qubit superconducting quantum computer, available through the cloud

富岳 (Fuagku) :
158,976 nodes supercomputer

Miwako Tsuji, “HPC-oriented design of Quantum-HPC hybrid computing platform“ Focus Session, ISC24, 2024

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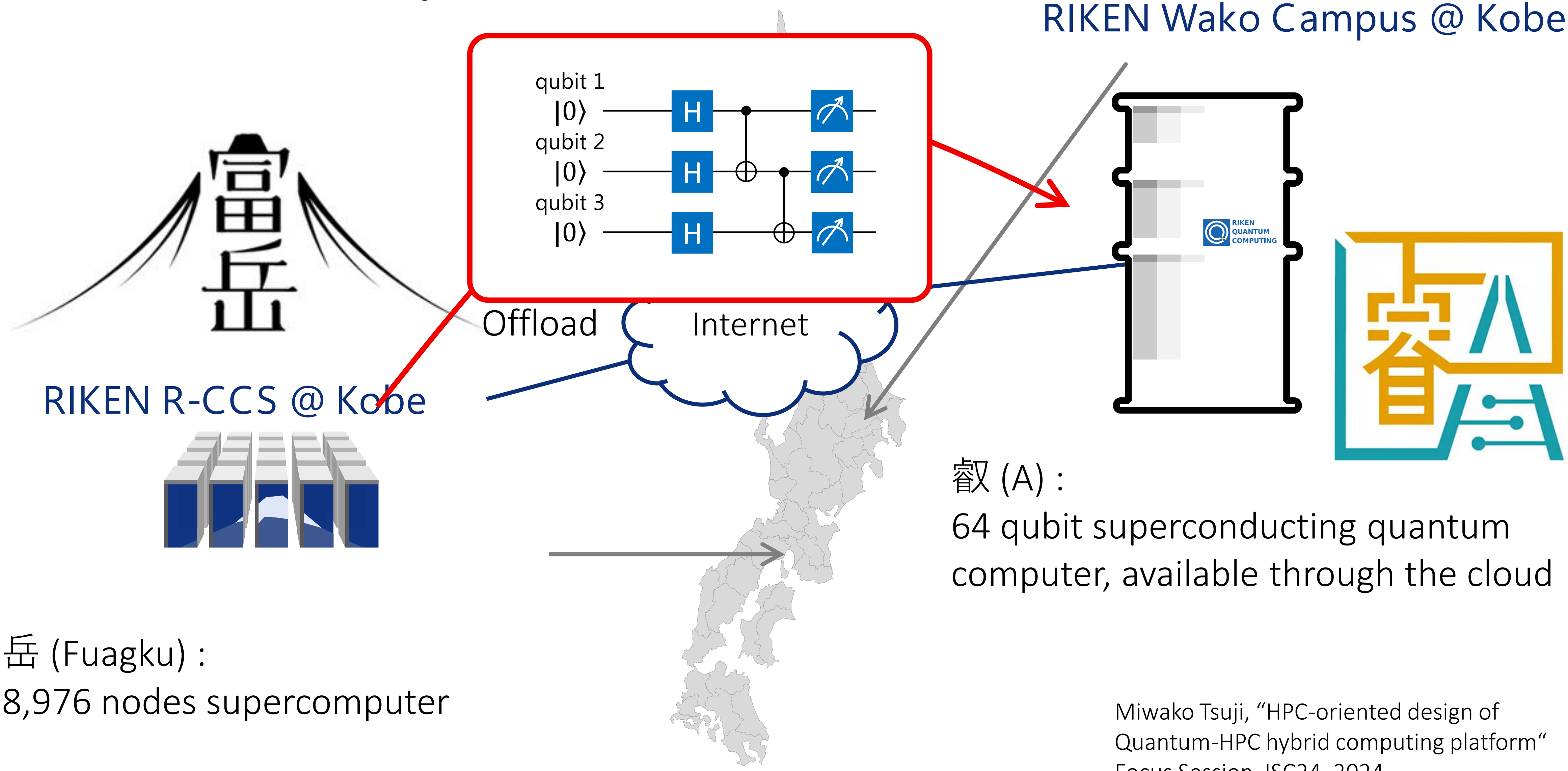

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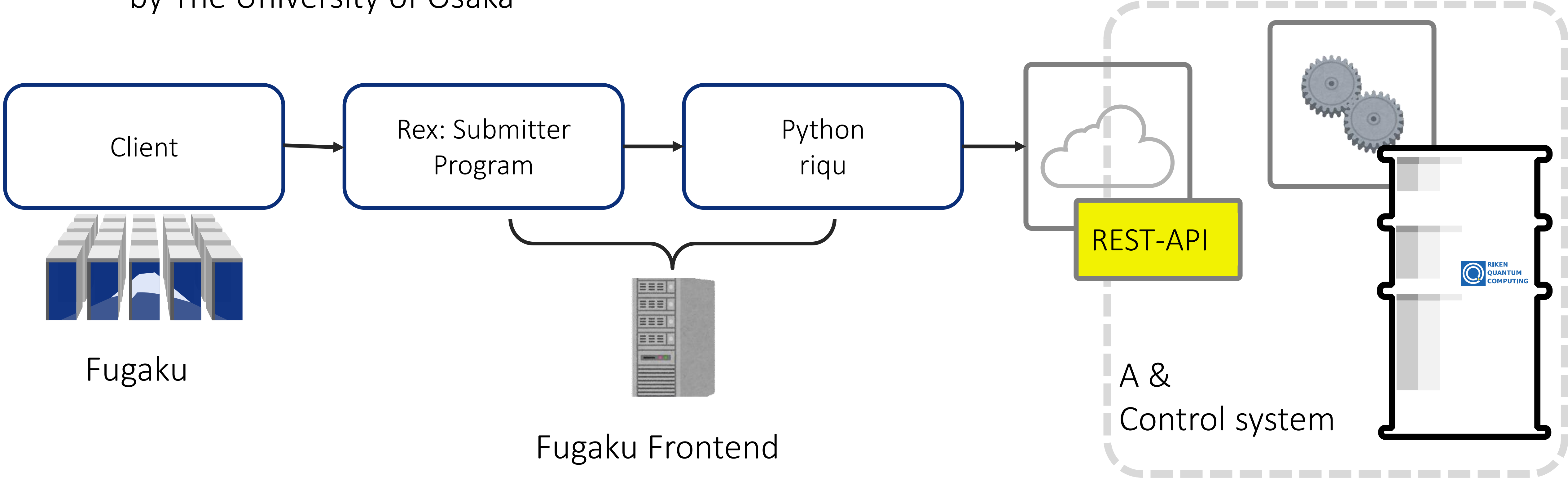
1st Experiment: RPC though a Python based library

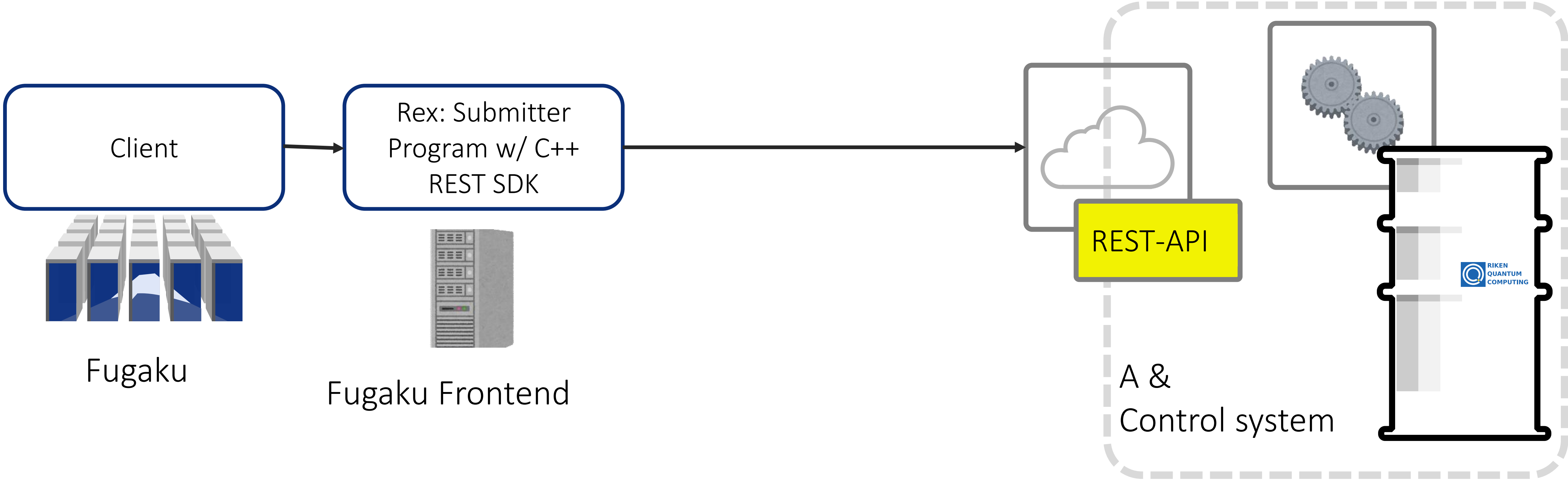
- A client program calls a remote submitter program
- The submitter program calls a Python library designed to use “A” through REST-API
- QURI Parts riqu: **R**EST **I**nterface for **Q**uantum **C**omputing
  - by The University of Osaka



Note: 4 of 64 qubit are available for us

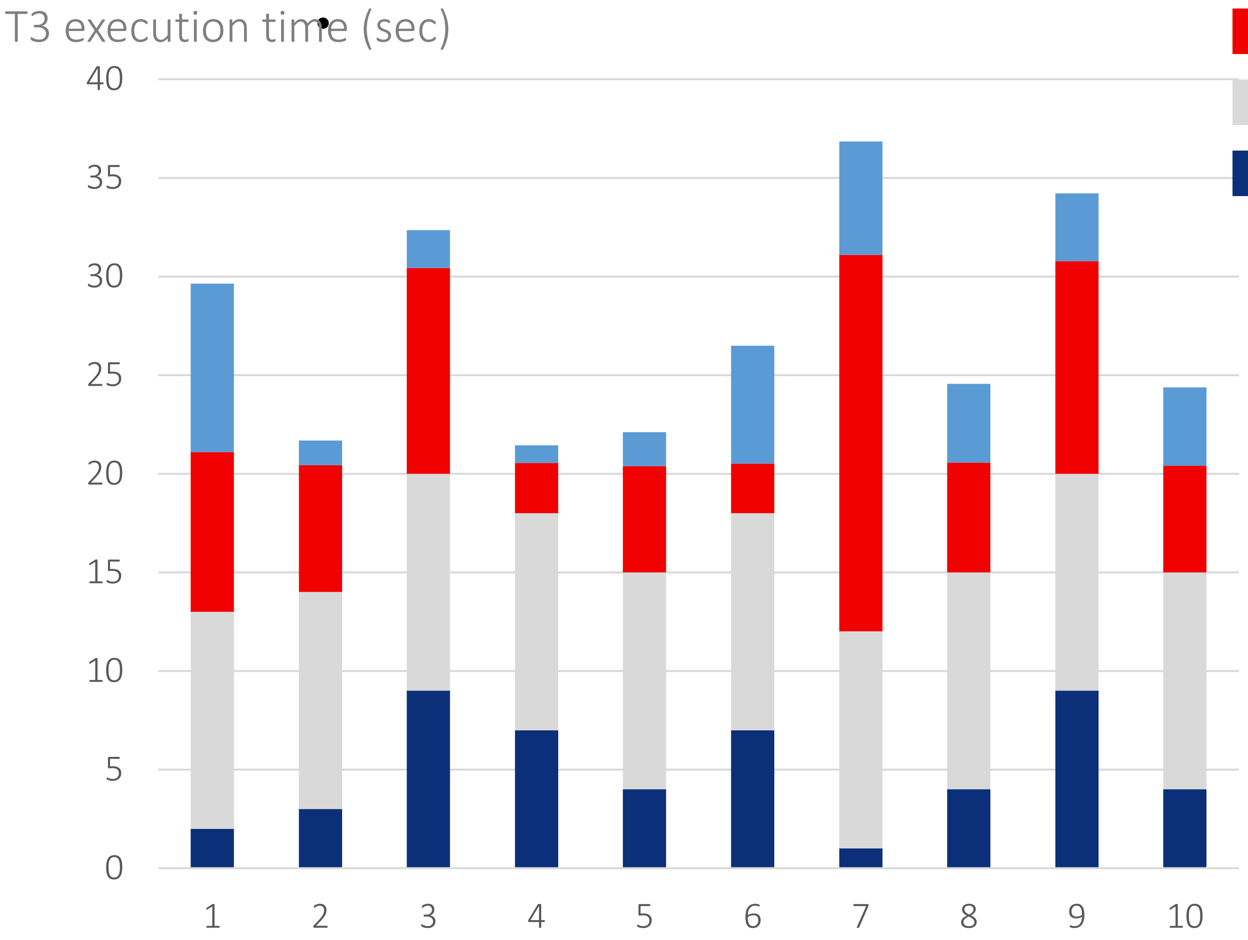
2nd Experiment: RPC though C++ based library

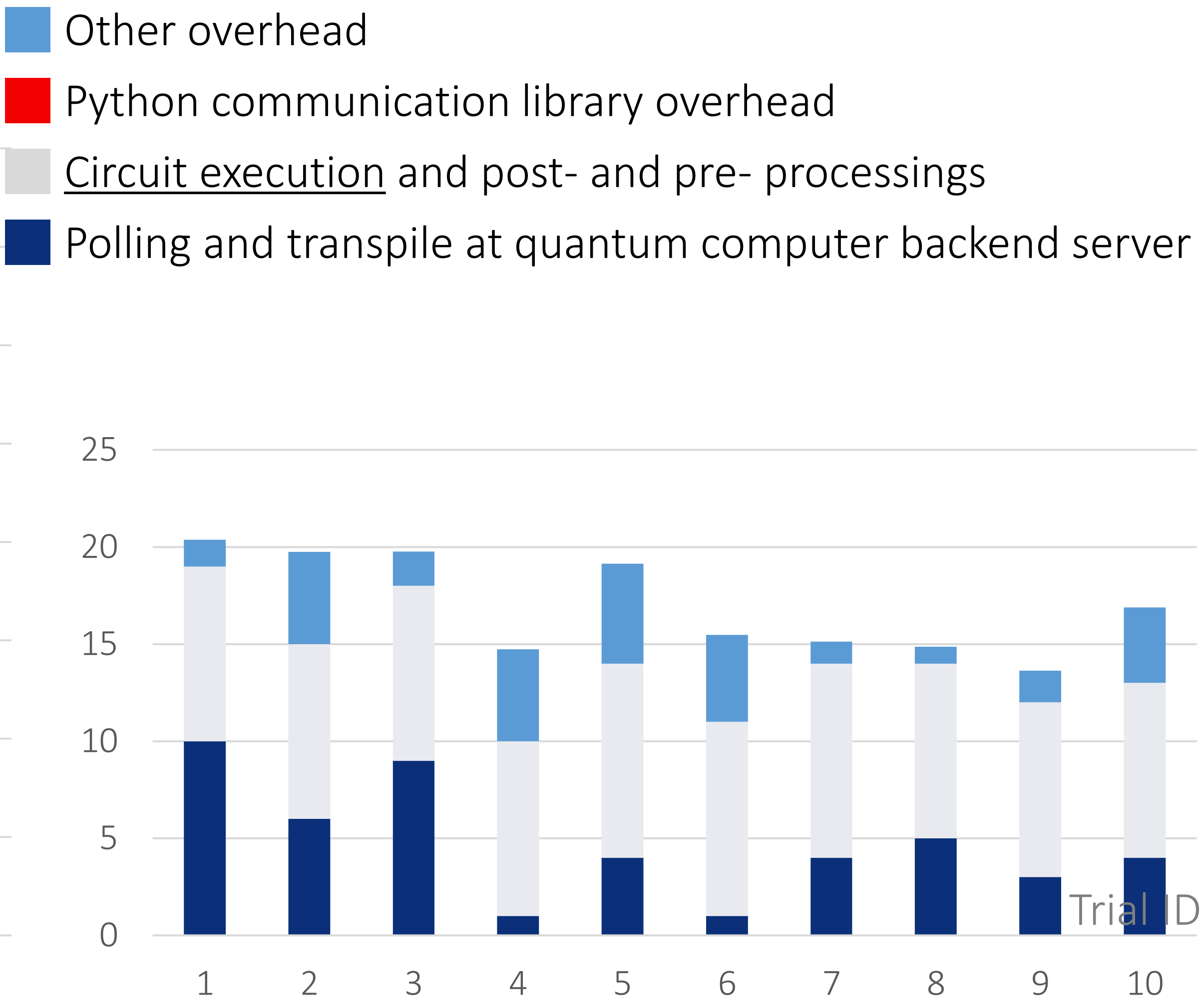
- The C++ REST SDK
  - https://github.com/microsoft/cpprestsdk



Result

- Quantum Circuit Encoding Workflow
- A simple step-by-step workflow
- Automatic quantum circuit encoding (AQCE) of a given arbitrary quantum state
  - Generate a circuit to make a gray scale image:
  - 4qubits, 4x4=16pixel





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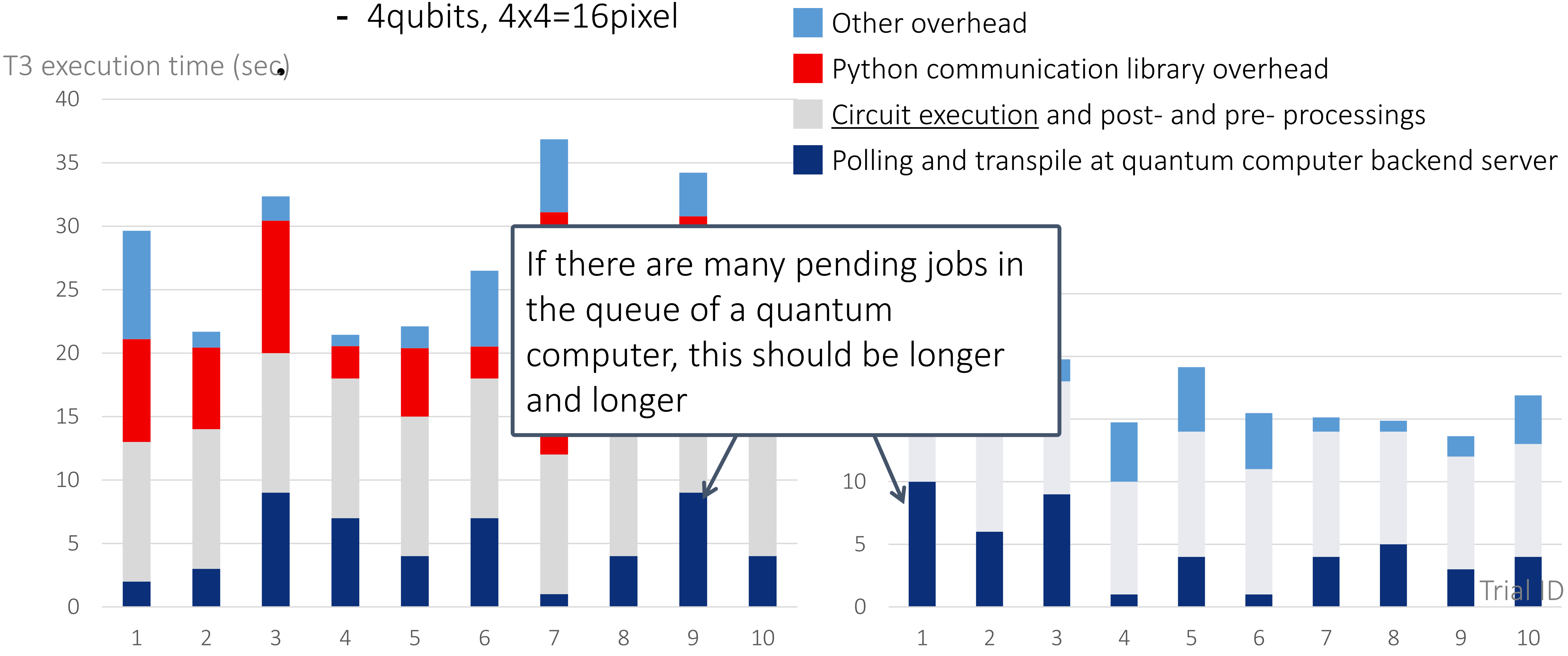

TRIP Proof of concept in 2023/2024 experiments and lessons learned

- We found our programming model cannot be used in our supercomputer system (esp "Fugaku")

- Coordinated scheduling with quantum computer and supercomputer is required.
- Execution of HPC programs running multiple nodes should not be idle as possible as it can.

- Major programming environments of quantum computer program development are Python-based frameworks.
    - Python is difficult to be combined with HPC programs such as MPI, multithreaded programs in C/C++ and Fortran.
    - Recently, some quantum computing programming frameworks in C/C++ are proposed

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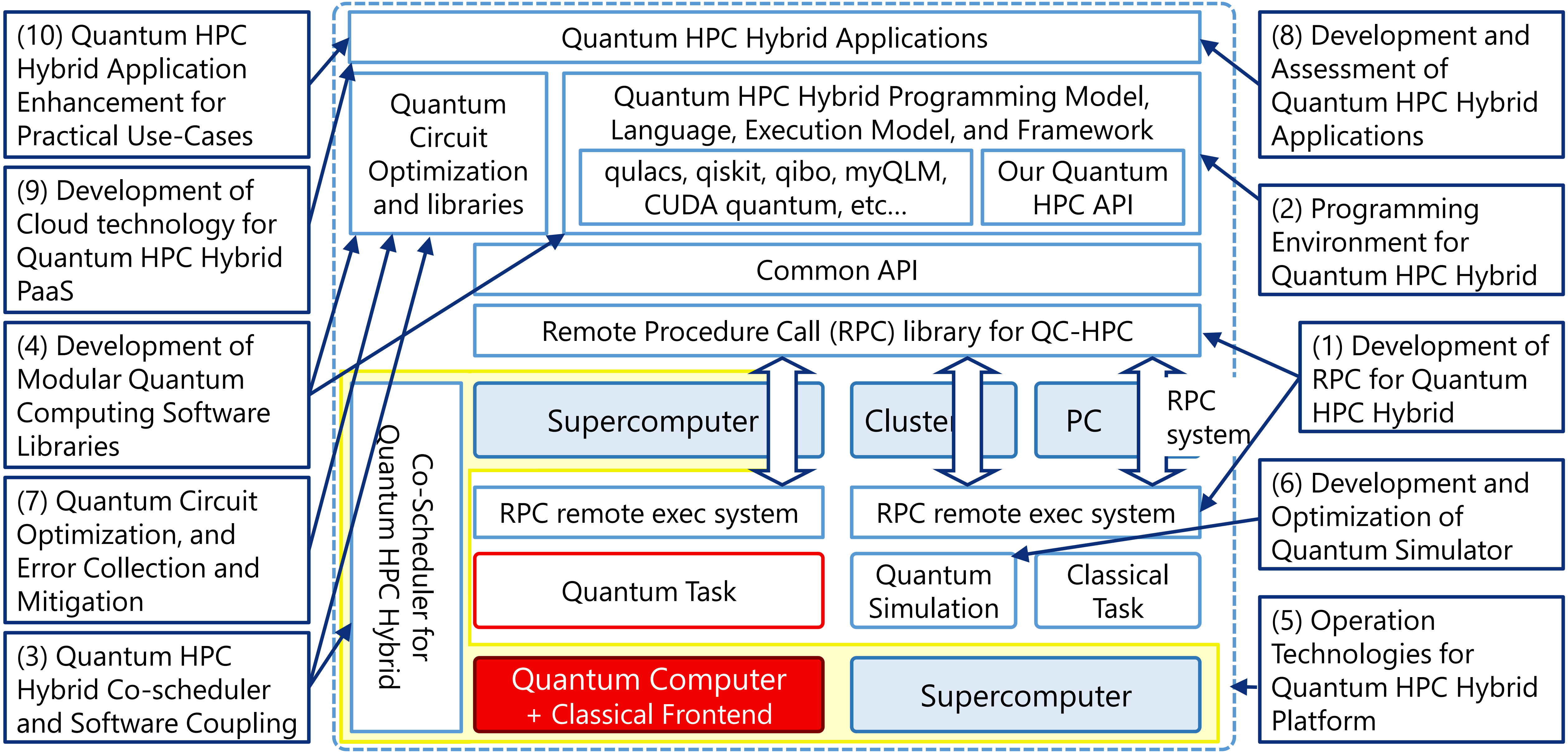
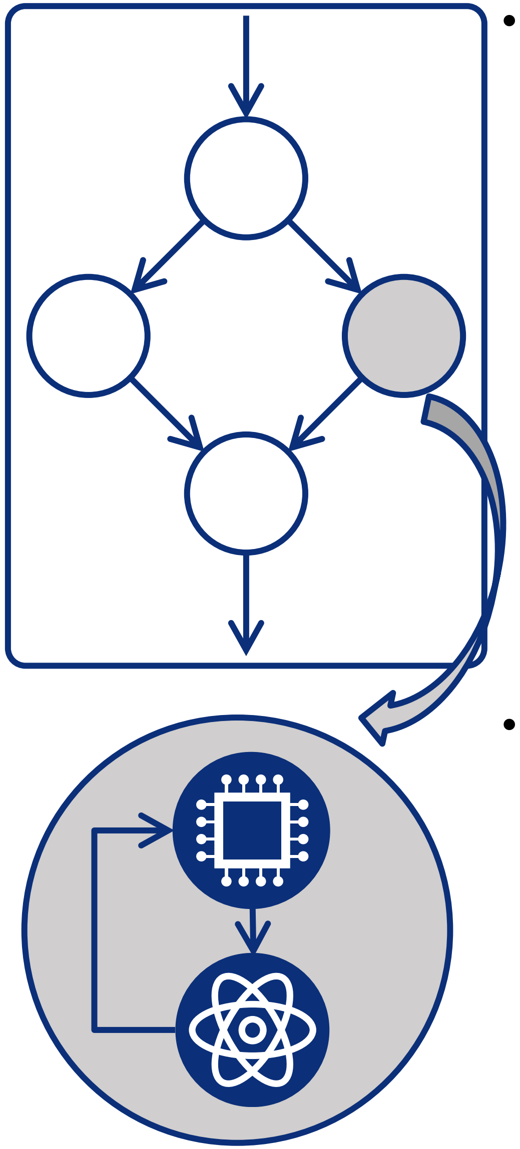
Research Items in JHPC-Quantum Project



Quantum HPC Middleware: Two Level Programming Model

- Workflow & Task based parallelism



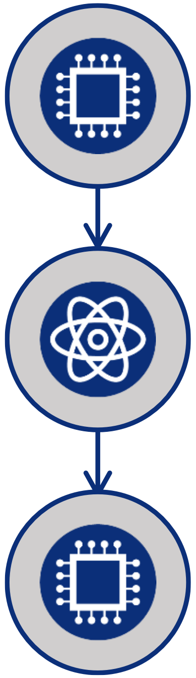
- Workflow
  - Tasks (different kernels) are managed by a workflow engine
  - The tasks are "**jobs**" in supercomputers and/or quantum computer
  - The workflow engine submit each of jobs in a certain order based on the descriptions about dependencies between jobs

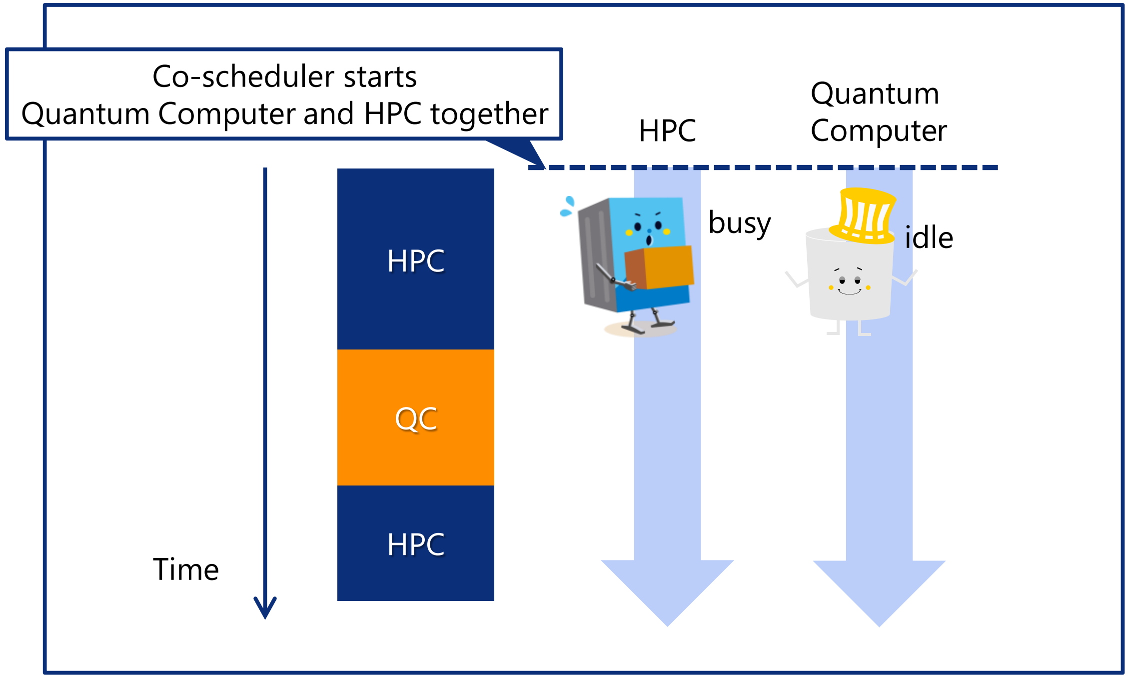
Simple HPC Job	Simple QC Job	HPC-QC Job
running a kernel only on HPC	offloads a quantum circuit to quantum computer	includes both of HPC and quantum kernels

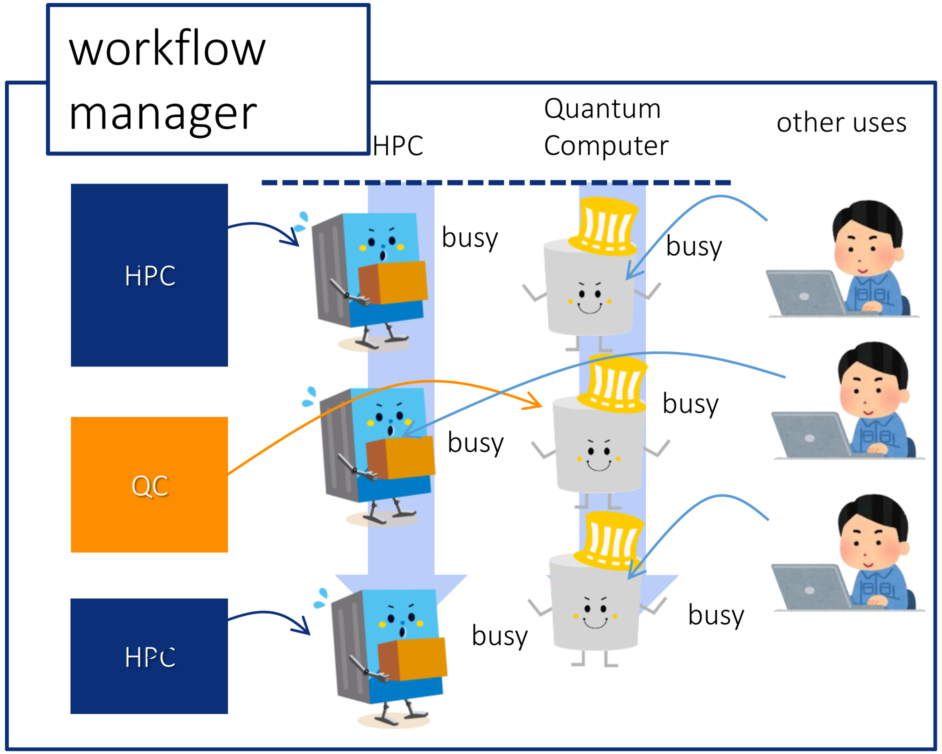
- Task based Parallelism in HPC-QC Jobs
  - offloads quantum kernel(s) to a quantum computer via remote procedure call (RPC)
  - A single HPC-QC job may offload multiple kernels
  - RPC is an asynchronous mechanism; Other classical kernels will be executed on CPU simultaneously

Why do we need the 1st Layer, Job-Scheduler Based Workflow?

- Avoid the waiting times in quantum computer and supercomputer
  - Uses separate quantum kernels and HPC kernels in their applications
  - Define the order of their execution
- Job-schedulers in both computers may arrange jobs to maximize the throughput in their systems.
- A job may have to wait the result from another job, but the waiting time does not consume any computational resource



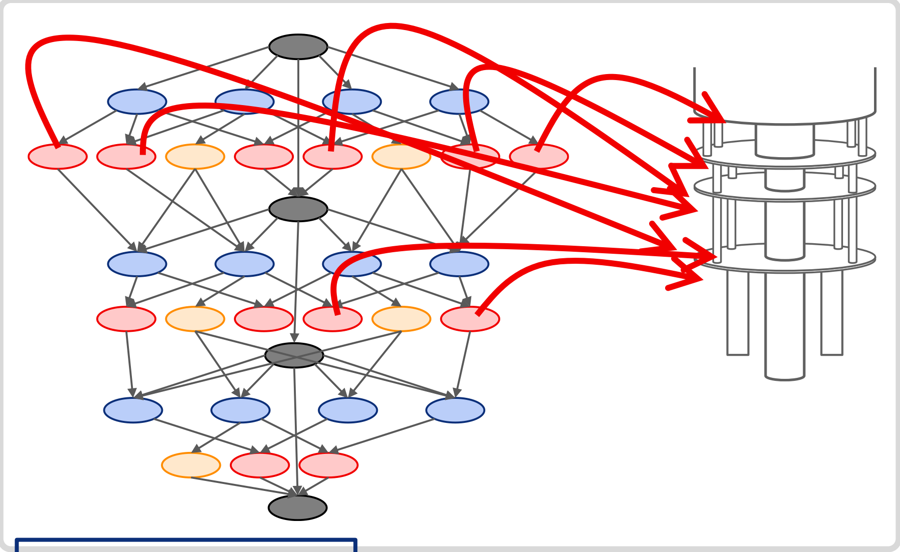


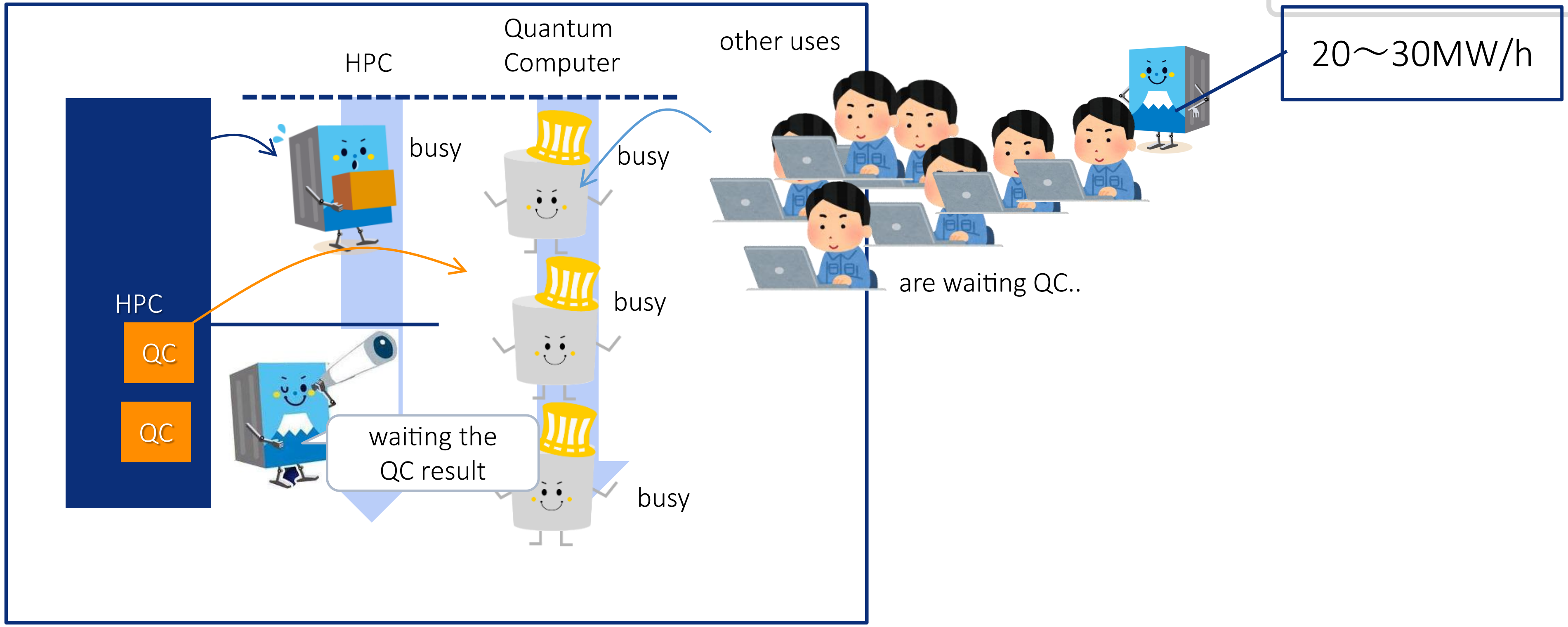


Why do we need 2nd Layer, task-based programming

- Tightly coupled quantum and HPC kernels in a single job
  - Difficult to separate quantum and HPC kernels completely
- Multiple quantum kernel calls from HPC in a short time (ex. VQE)
  - Difficult to wait each of the quantum circuit executions
- (Still) We must avoid the waiting time in HPC,

especially for large scale HPC jobs





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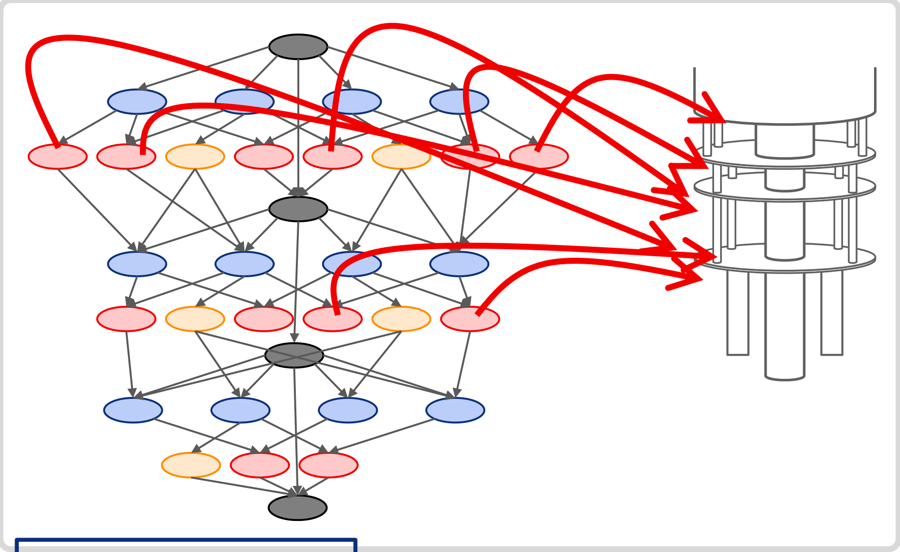
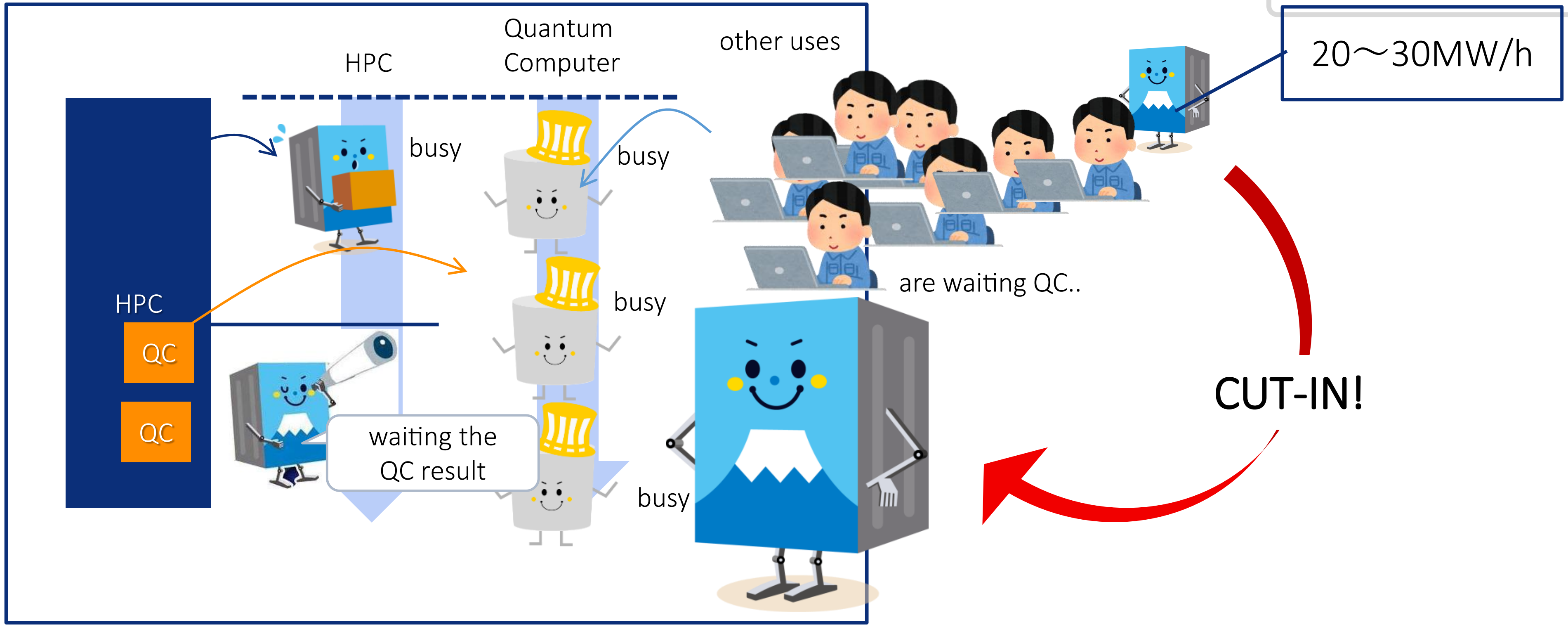
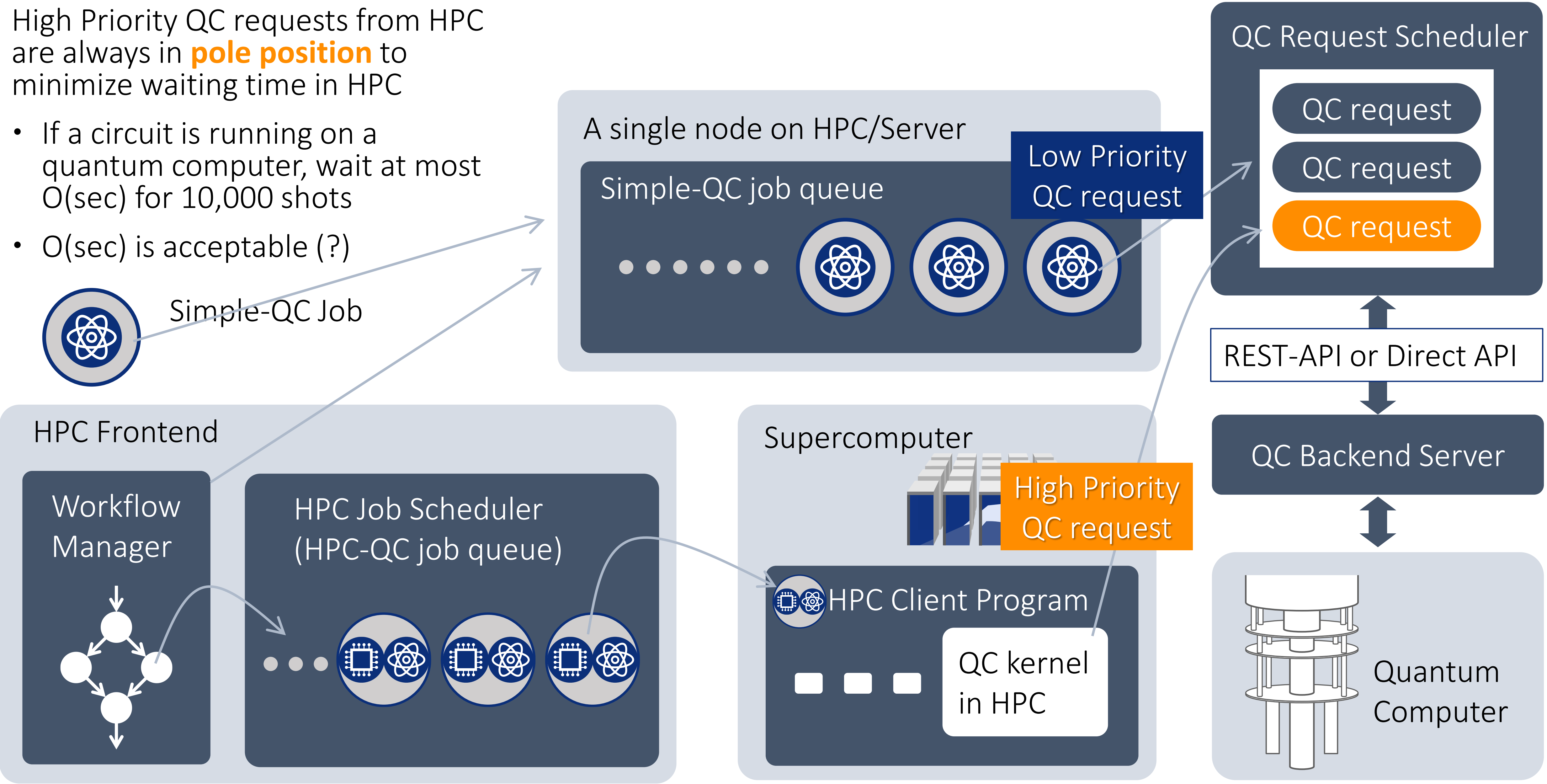




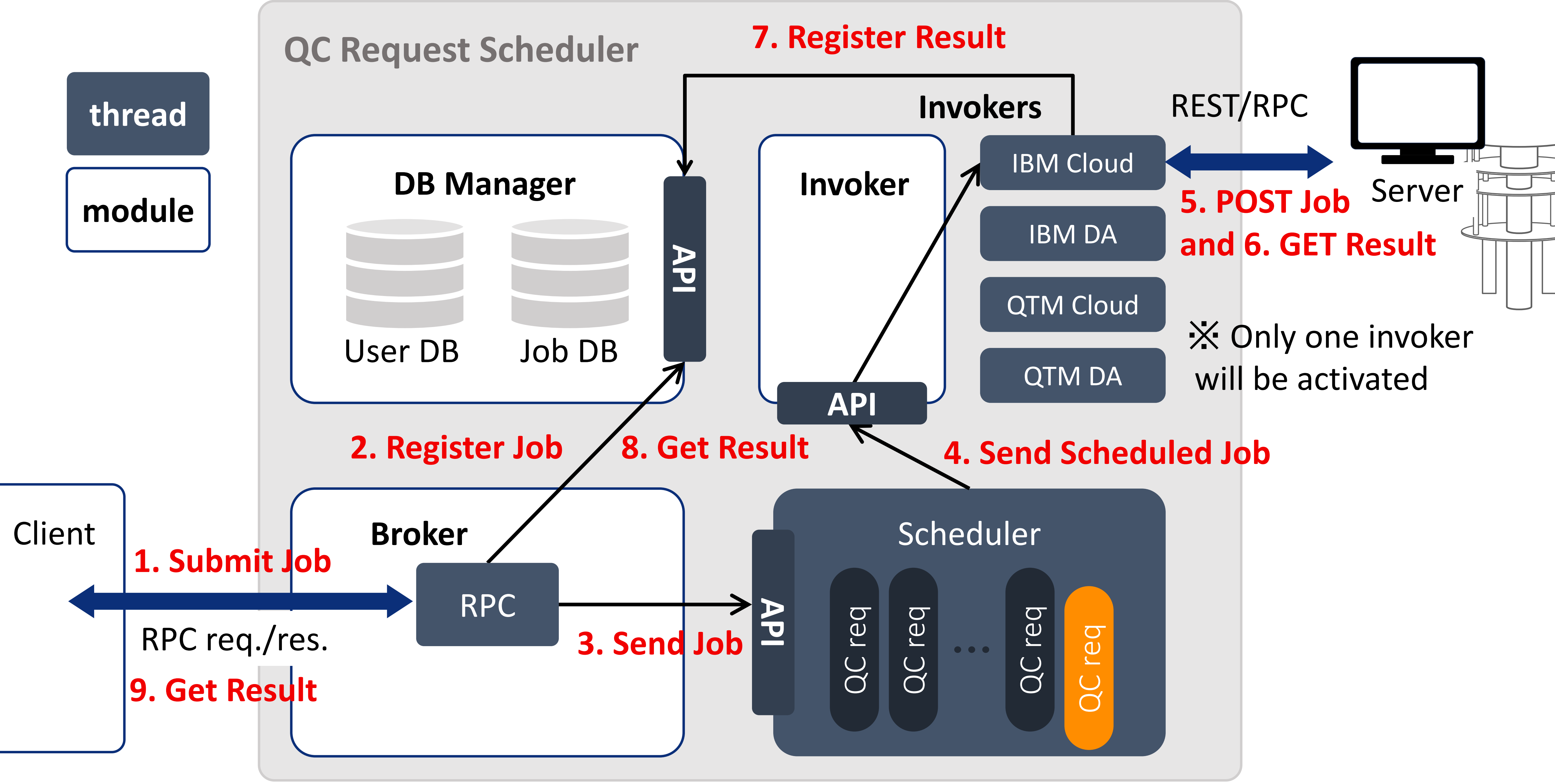
Execution Environment

High Priority QC requests from HPC are always in **pole position** to minimize waiting time in HPC

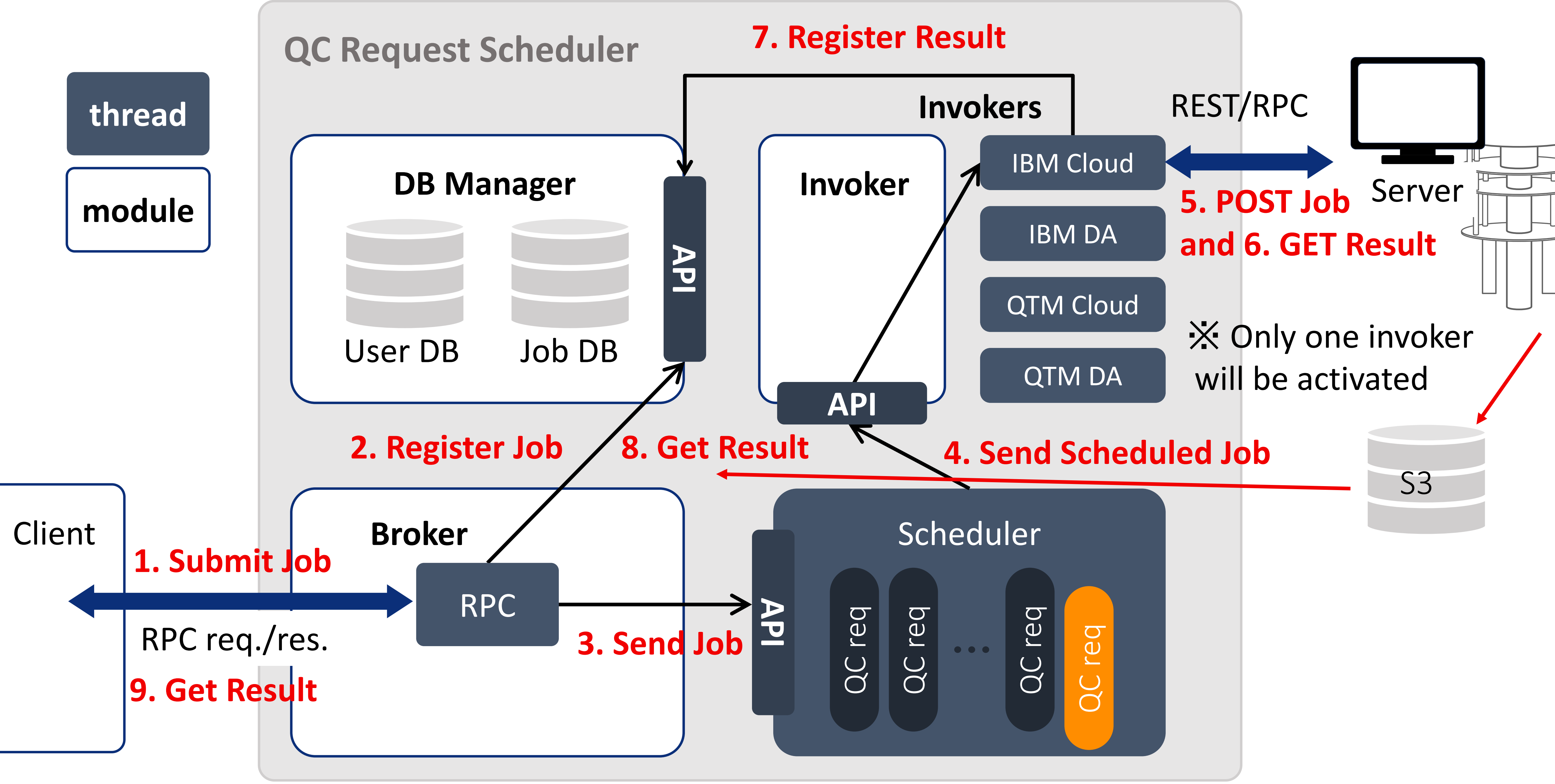
- If a circuit is running on a quantum computer, wait at most O(sec) for 10,000 shots
- O(sec) is acceptable (?)



SQC (Supercomputer Quantum computer Computation) Scheduler

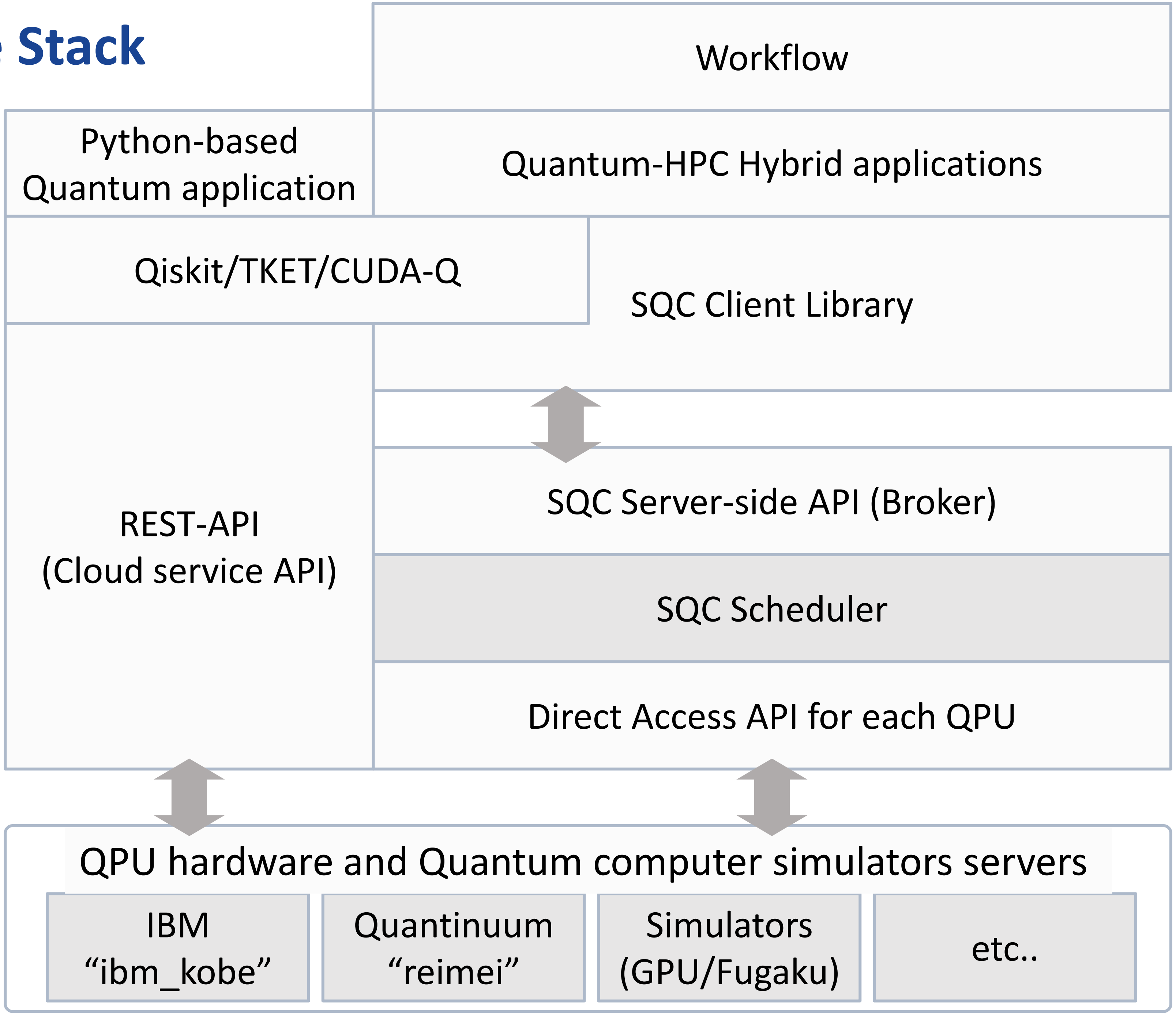


SQC Scheduler for IBM_Kobe



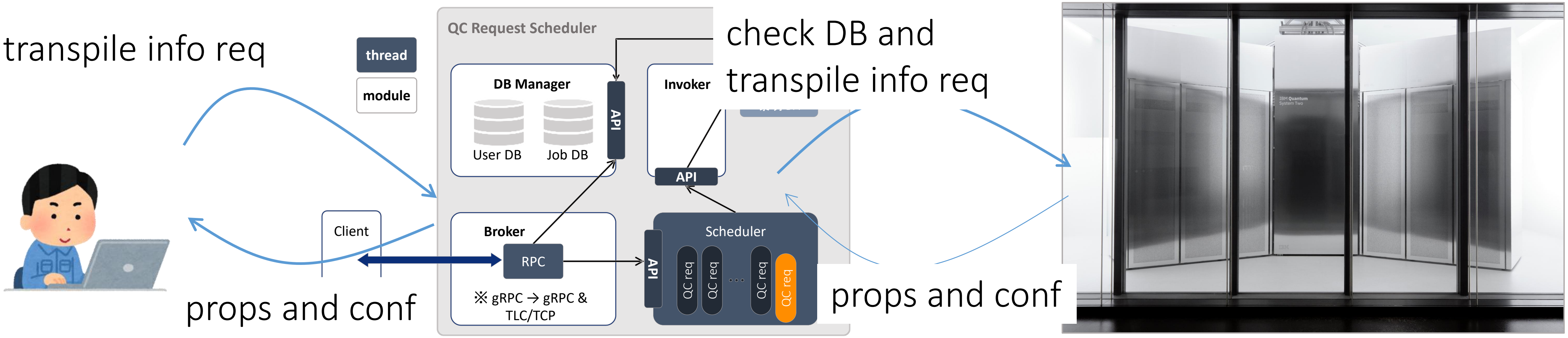
JHPC-Quantum Software Stack

- Two ways to access QC
  - Our SQC APIs and RPC. The RPC uses direct access APIs provided by QPU venders
  - REST-APIs through vender clouds
- Workflow tools
  - Tierkreis (Quantinuum), Prefect, Xcrypt
- QC software libraries
  - JHPC Quantum QC software lib
  - Qunasys QURI SDK
  - Error mitigation
  - Error suppression



Additional API for ibm_kobe, Transpile

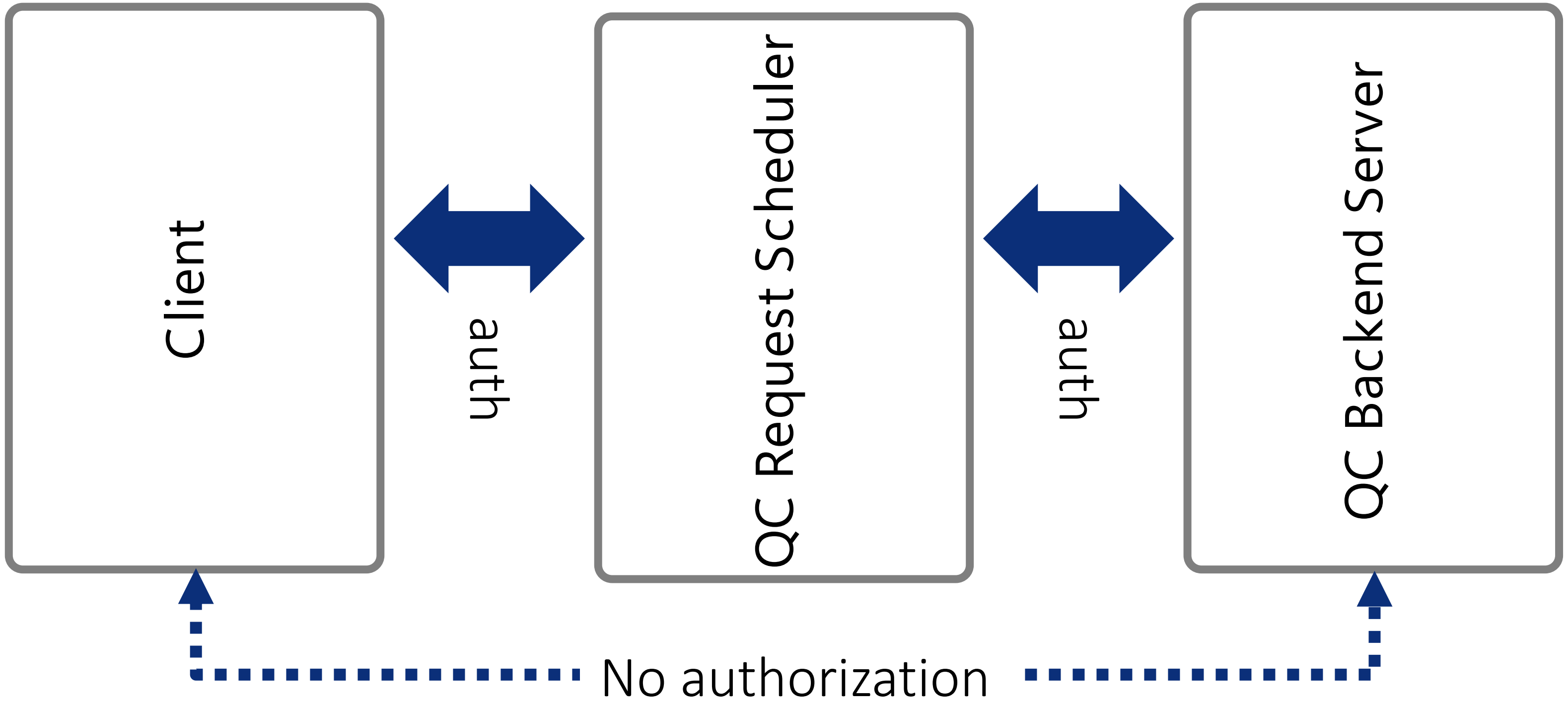
- `sqcIbmdTranspileInfo(circ, backend);`
  - User sends a request to SQC Request Scheduler to get backend property and configuration
  - results will be stored at `circ->backend_config_json` and `circ->backend_props_json`



- `sqcTranspile(circ, backend, topt);`
  - `SQC Library` transpiles a circuit by calling Qiskit python library internally
- `Users can provide the above QPU data to their own transpilers and tanspile circuits`

Authorization

- Client⇔SQC Scheduler
  - JSON Web Token (JWT) ＋TLS client certification
    - At the beginning of the session, JWT authentication is carried out over a TLS server-authenticated channel to guarantee communication confidentiality and integrity.
- SQC Scheduler ⇔ Backend Server for quantum computers
  - Authorization method specified by each quantum vendor
  - No authorization for end users



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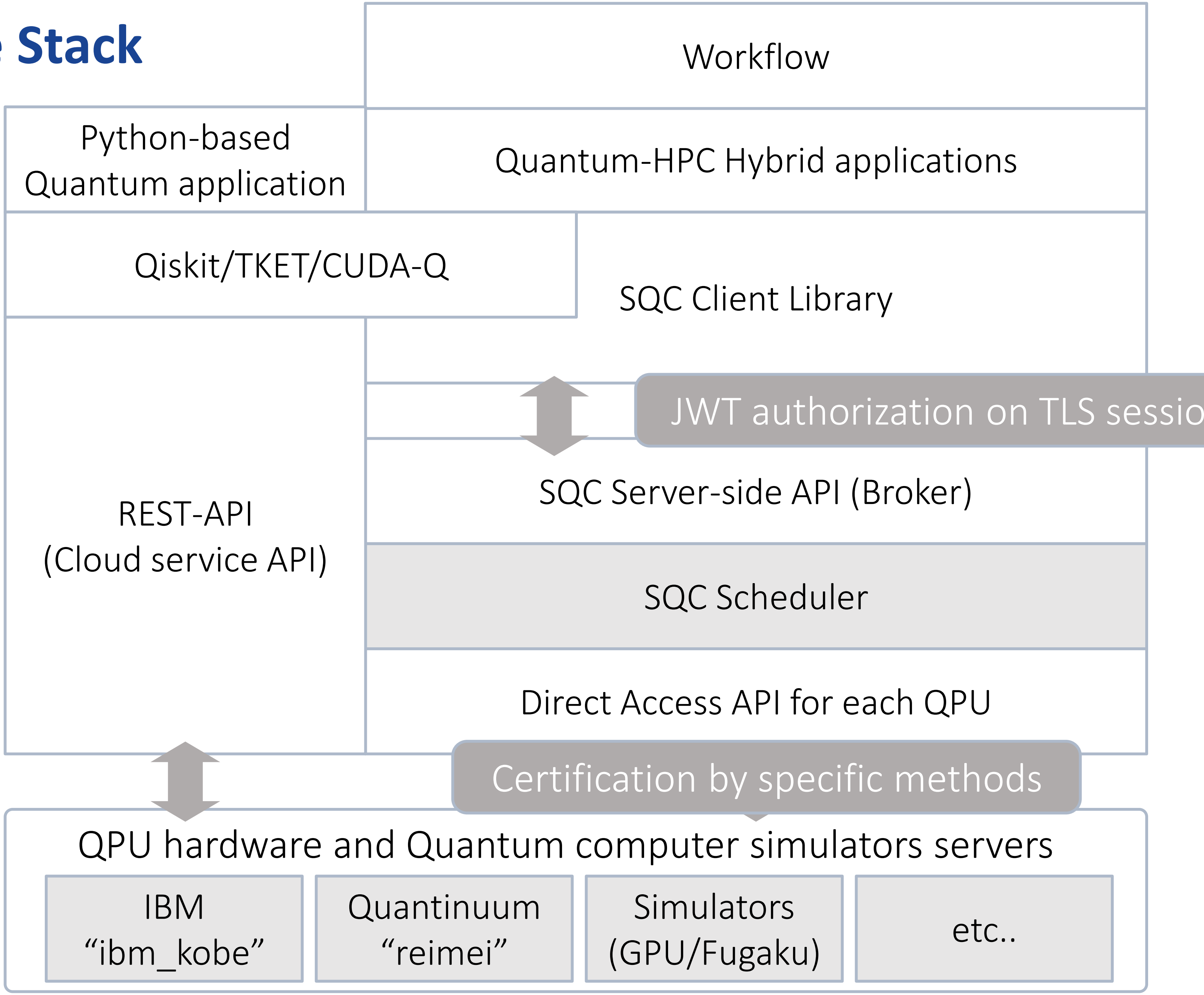
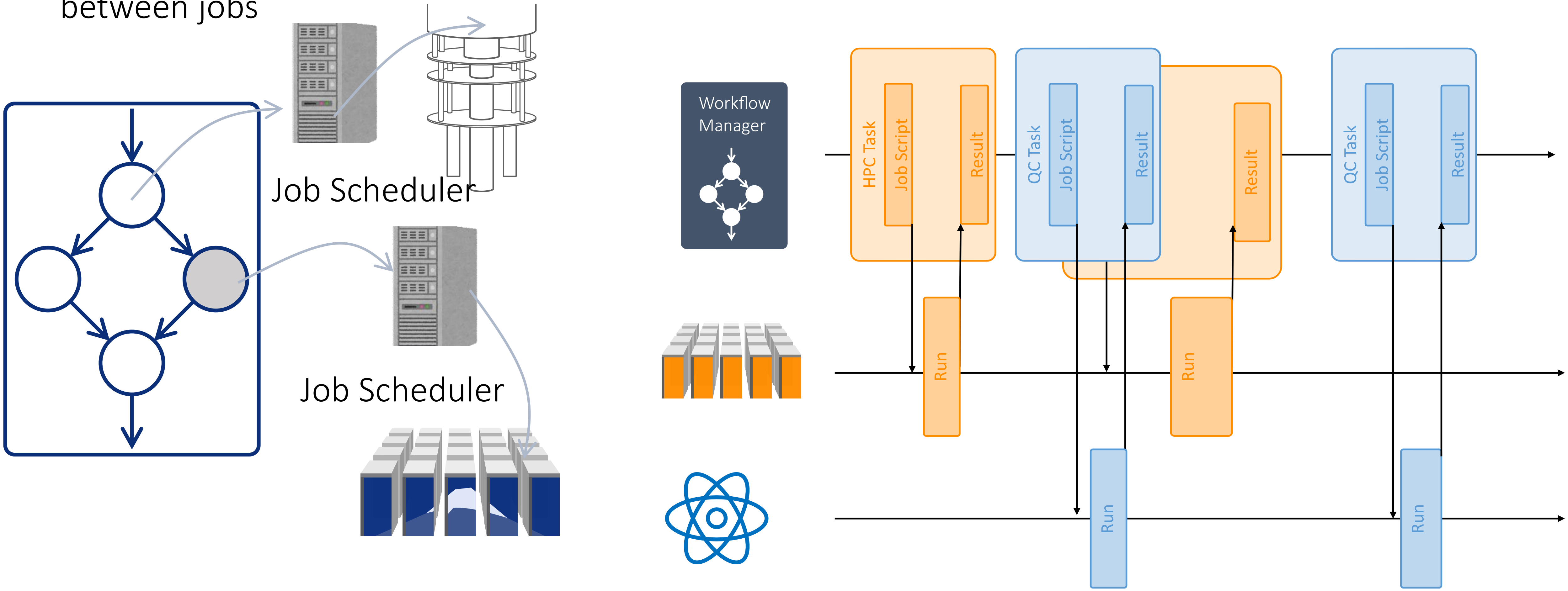


Quantum-HPC Workflow: Coarse Grained Task-based Programming

- Tasks are large, typically, whole programs, jobs in supercomputers or quantum computers
- A workflow manager will take care about the order of job submissions based on the dependency between jobs



Fine Grained Task based Programming: Example of C/C++ Program on SQC library

```c
#include<stdio.h>
...
#include"sqc_api.h"

int main(int argc, char **argv)
{
   const int nqubits = 10;
  sqcInitOptions        *iopt;
  iopt = sqcMallocInitOptions();
  sqcInitialize(iopt);

  sqcQC* circ;
  circ = sqcQuantumCircuit(nqubits);
  sqcHGate (circ, 1);
  sqcCXGate(circ, 0, 1);
  for(int i=0; i<nqubits; i++)
    sqcMeasure(circ, i, i, NULL);

  sqcBackend backend = SQC_RPC_SCHED_QC_TYPE_QTM_SIM_GRPC;
  sqcOut result;

  circ->qasm = (char *)malloc((circ->ngates)*128);
  int len = sqcConvQASMtoMemory(circ, backend,
                                     circ->qasm, len);
  if(len <= 0) { something;}
```

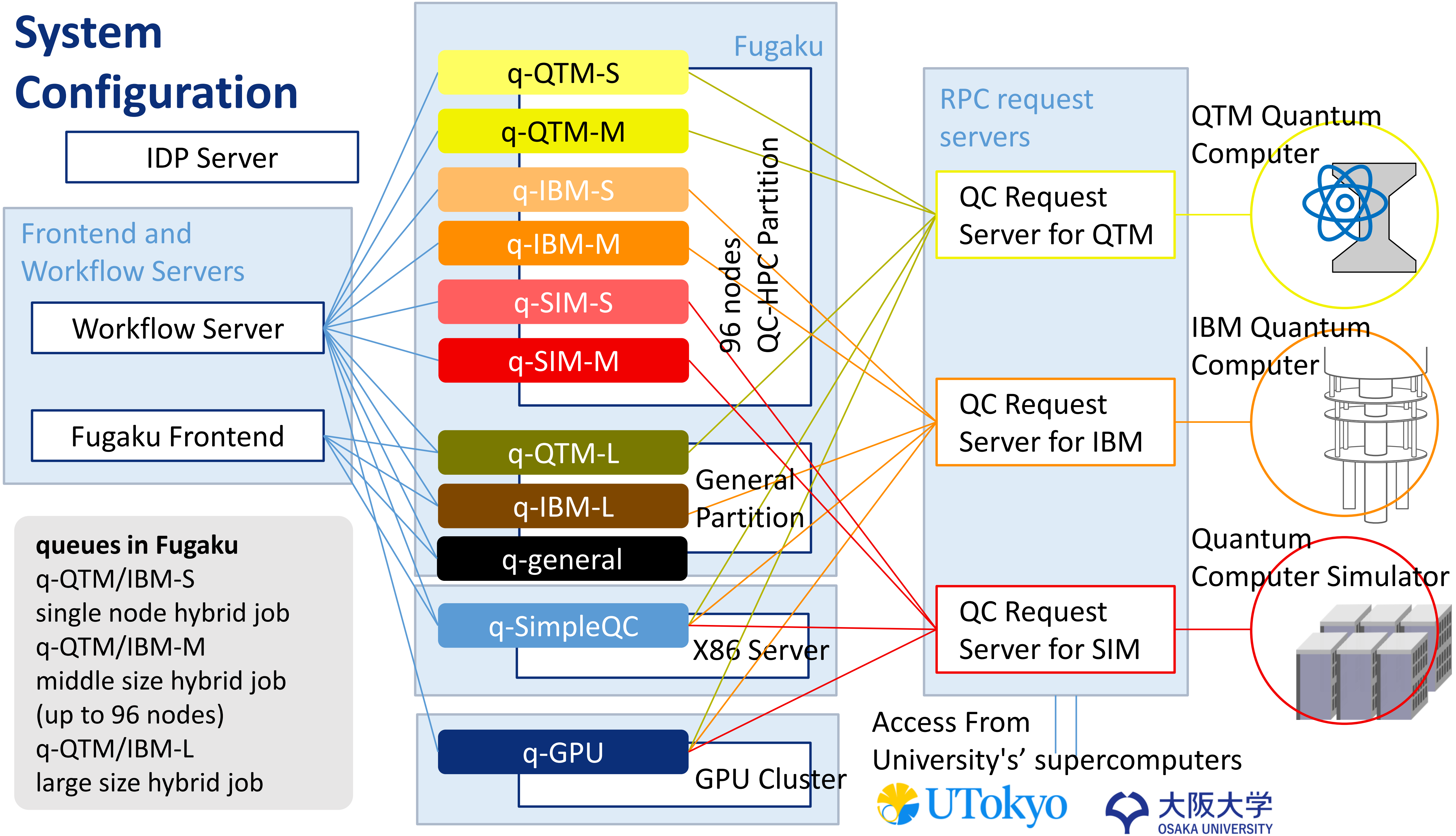
```c
 sqcTranspile(circ, backend, &ropt);

sqcRunOptions         ropt;
sqcInitializeRunOpt(&ropt);
ropt.nshots = 30;
ropt.qubits = nqubits;

int ret = sqcQCRun(circ, backend, ropt, &result);

sqcPrintQCResult(stdout, &result, ropt.outFormat);
sqcFreeOut(&result, ropt.outFormat);

sqcDestroyQuantumCircuit(circ);
sqcFinalize(iopt);
sqcFreeInitOptions(iopt);
  ....*
```

Example of Qiskit

```
from qiskit.transpiler.preset_passmanagers import
generate_preset_pass_manager
from qiskit_ibm_runtime.utils.backend_converter
import convert_to_target
from qiskit_ibm_runtime.models import
BackendProperties, BackendConfiguration
from qiskit.circuit import QuantumCircuit
from qiskit_sqc_runtime import SQCBackend,
SQCSamplerV2
from qiskit import qasm3

import json
import codecs

# Construct circuit
qc = QuantumCircuit(3, 3)
qc.h(0)
qc.cx(0, 1)
qc.cx(0, 2)
qc.measure(0,0)
qc.measure(1,1)
qc.measure(2,2)


# Get backend
backend = SQCBackend("ibm-dacc")
```

```
# Run quantum circuit
sampler = SQCSamplerV2(backend)
transpile_info = backend.transpile_info()

prop_json = json.loads(transpile_info[0])
backend_prop =
BackendProperties.from_dict(prop_json)
conf_json = json.loads(transpile_info[1])
backend_conf =
BackendConfiguration.from_dict(conf_json)

target = convert_to_target(backend_conf,
backend_prop)
pm = generate_preset_pass_manager(
  optimization_level=1,
  target=target,
)
isa_circuit = pm.run(qc)

job = sampler.run(isa_circuit, shots=10)

# Show result
result = job.result()
print(result)
print(job.status())
```

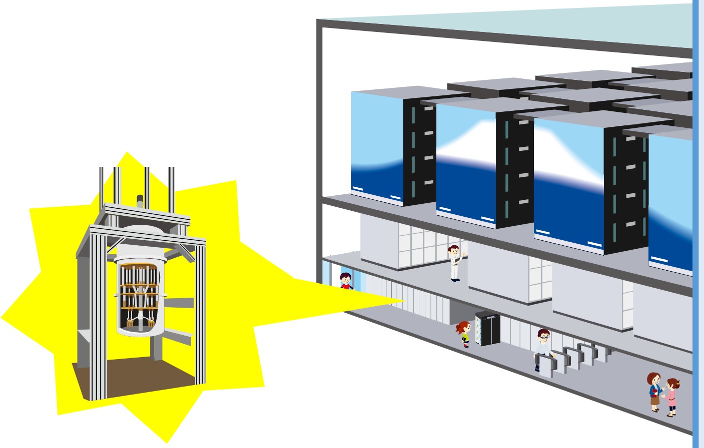
System Configuration

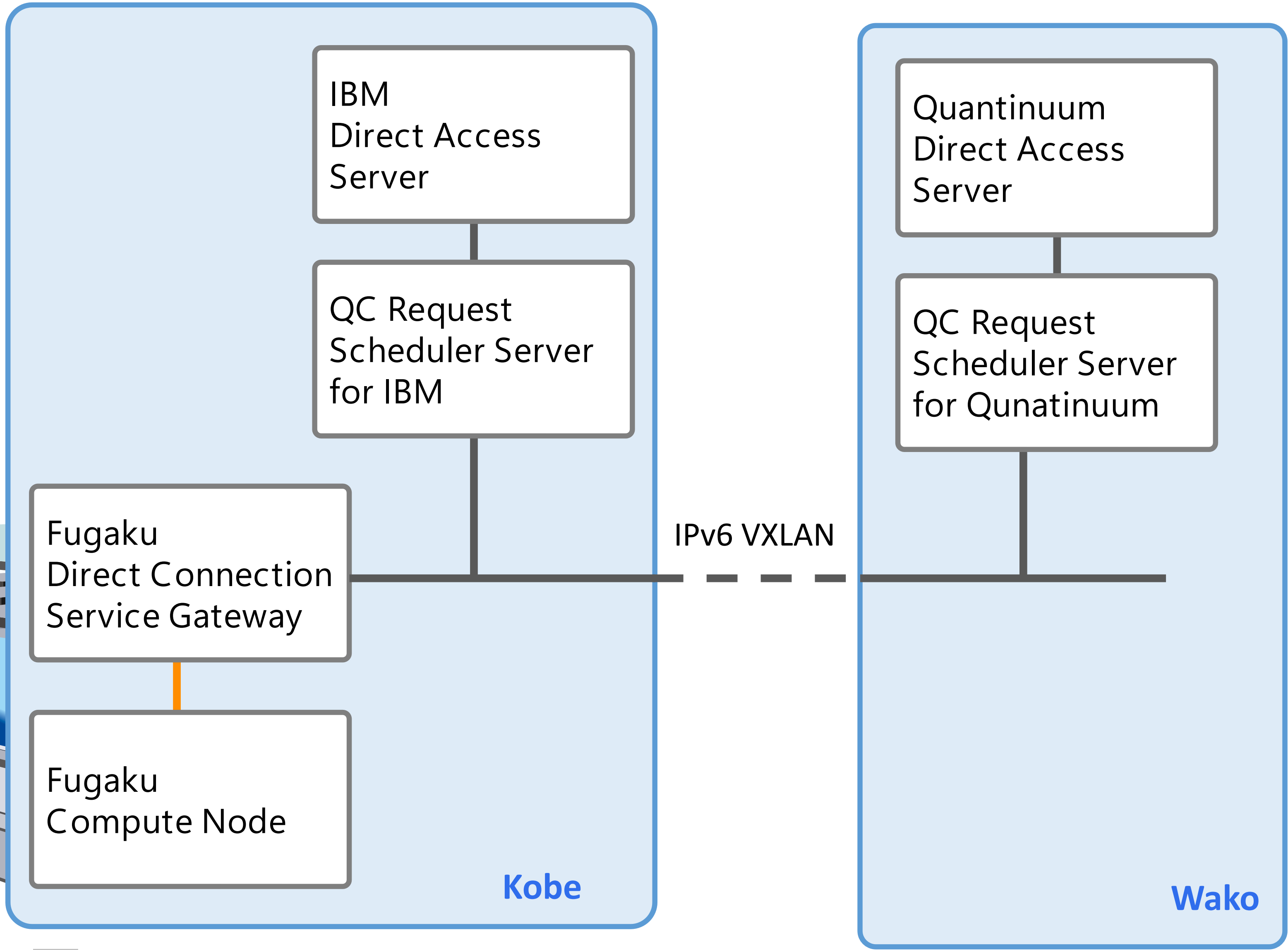


queues in Fugaku
q-QTM/IBM-S
single node hybrid job
q-QTM/IBM-M
middle size hybrid job
(up to 96 nodes)
q-QTM/IBM-L
large size hybrid job

QC Request Scheduler ⇔ Quantum Computer Backend Server

- Quantum Computer Backend Server
  - Cloud: Existing cloud-based service. Servers are in *somewhere in the world.*
  - **Direct Access**: Faster connection via direct local connection or virtual local connection. The server for IBM will be installed in Kobe, the server for Quantinuum is installed in Wako.



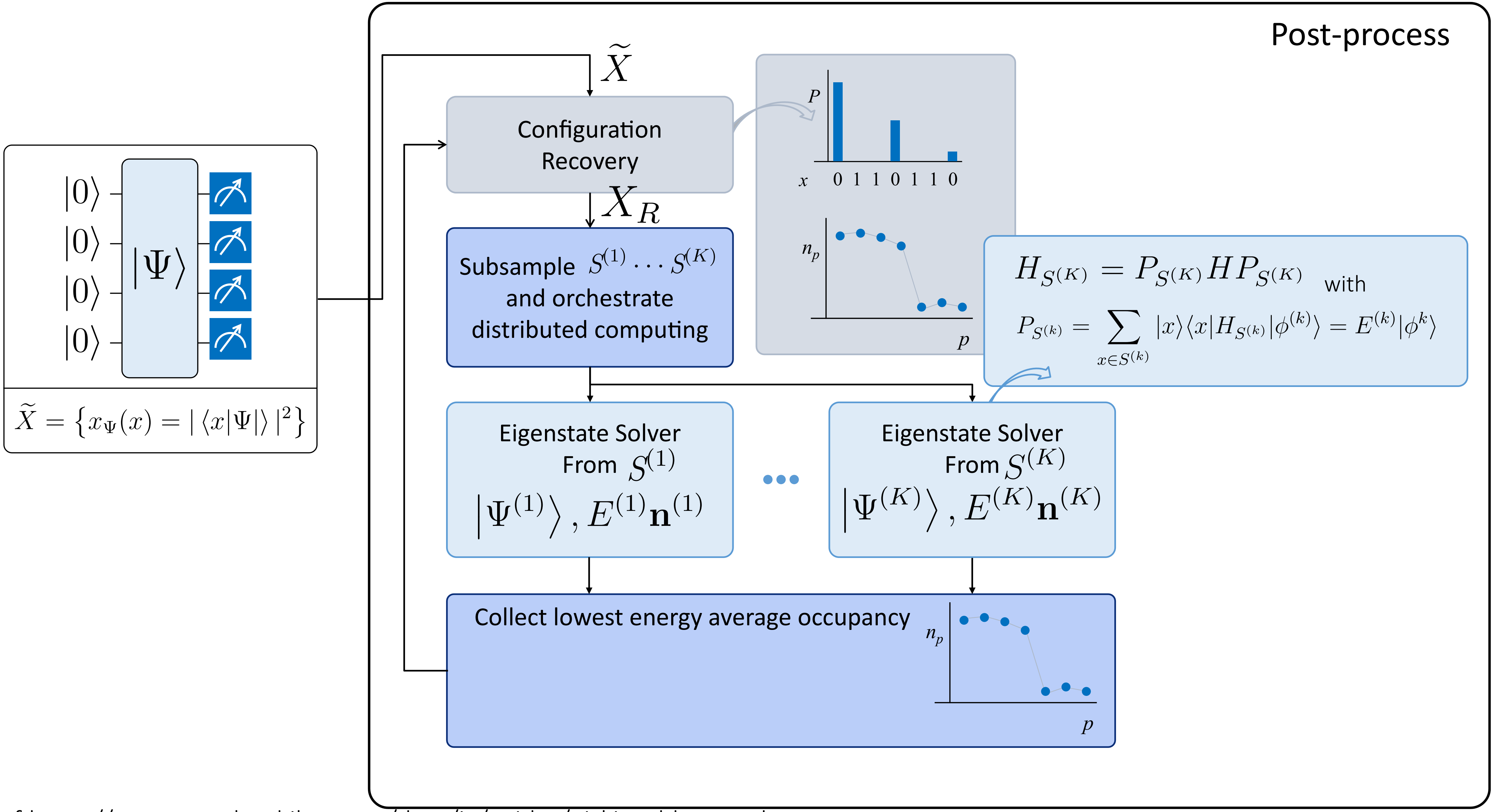


Quantum-HPC Hybrid Applications

- We are focusing on the following application areas for "Utility-Scale" Quantum-HPC hybrid computing
  - Quantum Chemistry
  - Quantum Machine Learning

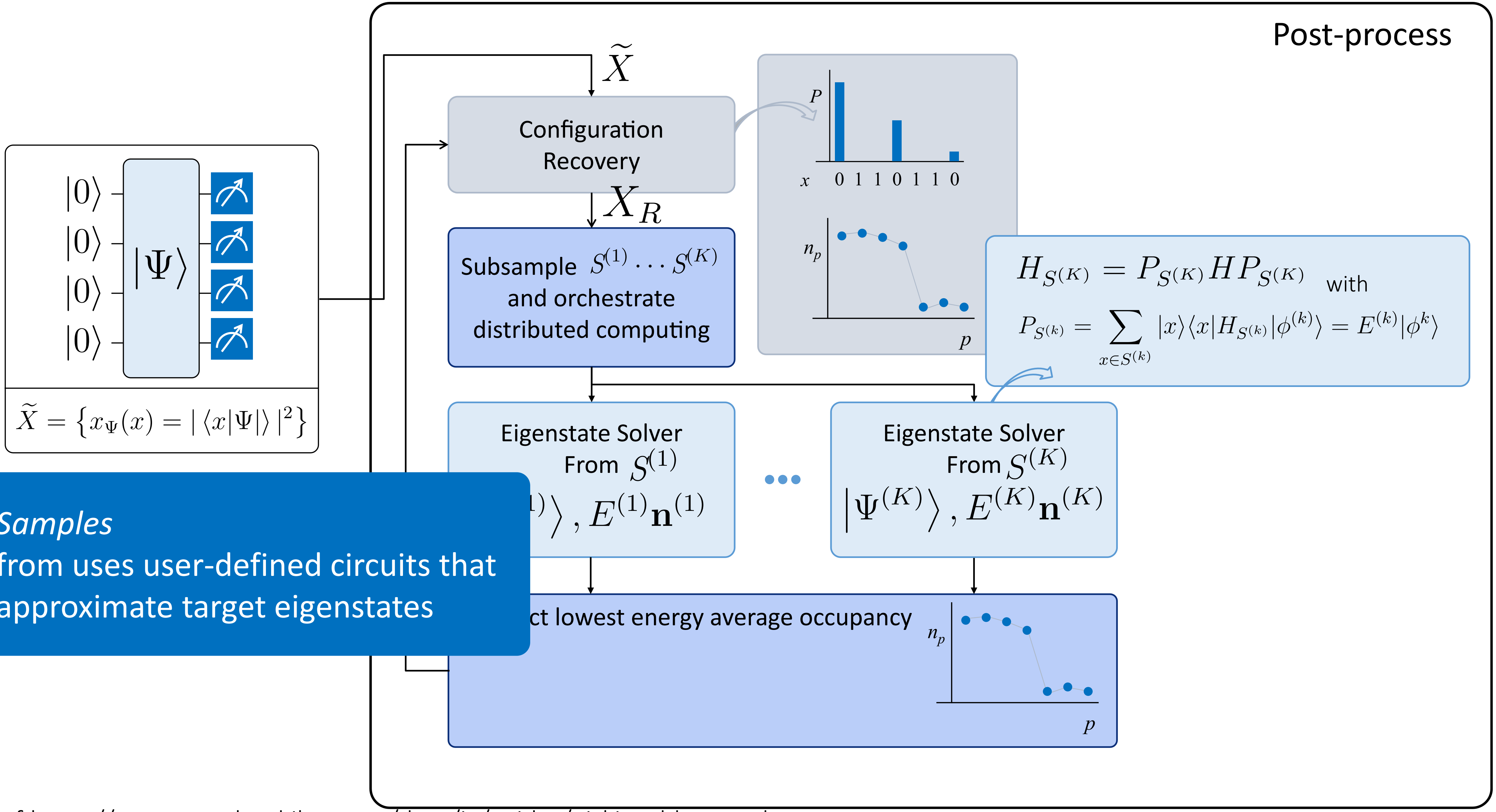
- Two experiences for Quantum-HPC Quantum Chemistry applications
  - **Ground state energy calculation of [4Fe-4S] clusters by Sample-based quantum diagonalization (SQD)**
    - Effort for Quantum-centric Supercomputing (QCSC) with IBM and RIKEN
    - SQD by Herion QPU and a large number of nodes of Fugaku (150K nodes)
    - Tightly-Coupled programming models and diagonalization by large-number of nodes.
  - **Biomolecular chemical reactions by QC-HPC hybrid computing workflow**
    - Effort on Biochemistry with Quantinuum and RIKEN
    - Loosely coupled programming models by Quantinuum TierKreis workflow tools
    - Photo-isomerization of retinal. Use NTChem developed by R-CCS executed in Fugaku for environment and QC for reaction centers

Sample-based quantum diagonalization (SQD)



ref:https://quantum.cloud.ibm.com/docs/ja/guides/qiskit-addons-sqd

Sample-based quantum diagonalization (SQD)

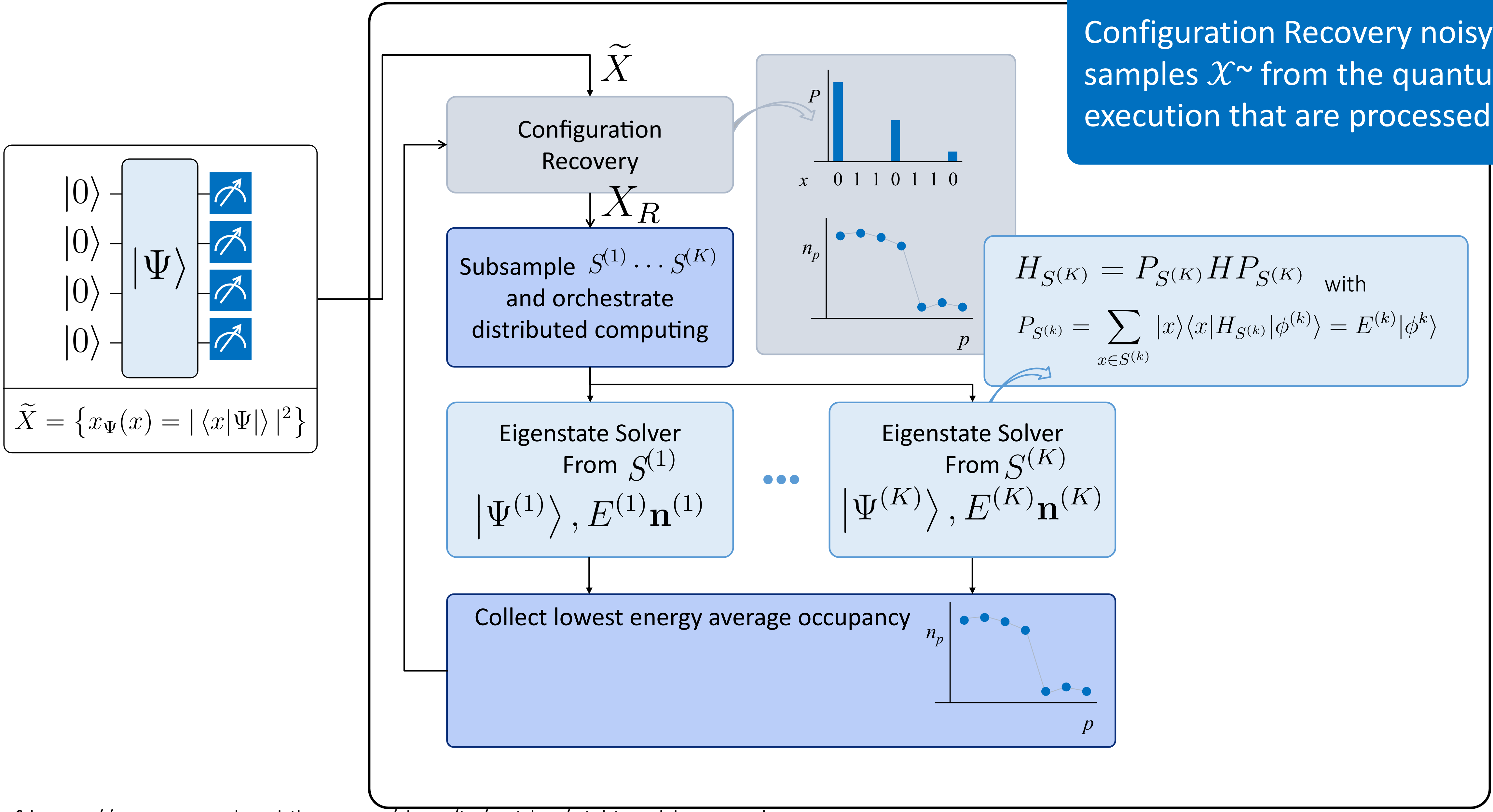


Samples
from uses user-defined circuits that approximate target eigenstates

ref:https://quantum.cloud.ibm.com/docs/ja/guides/qiskit-addons-sqd

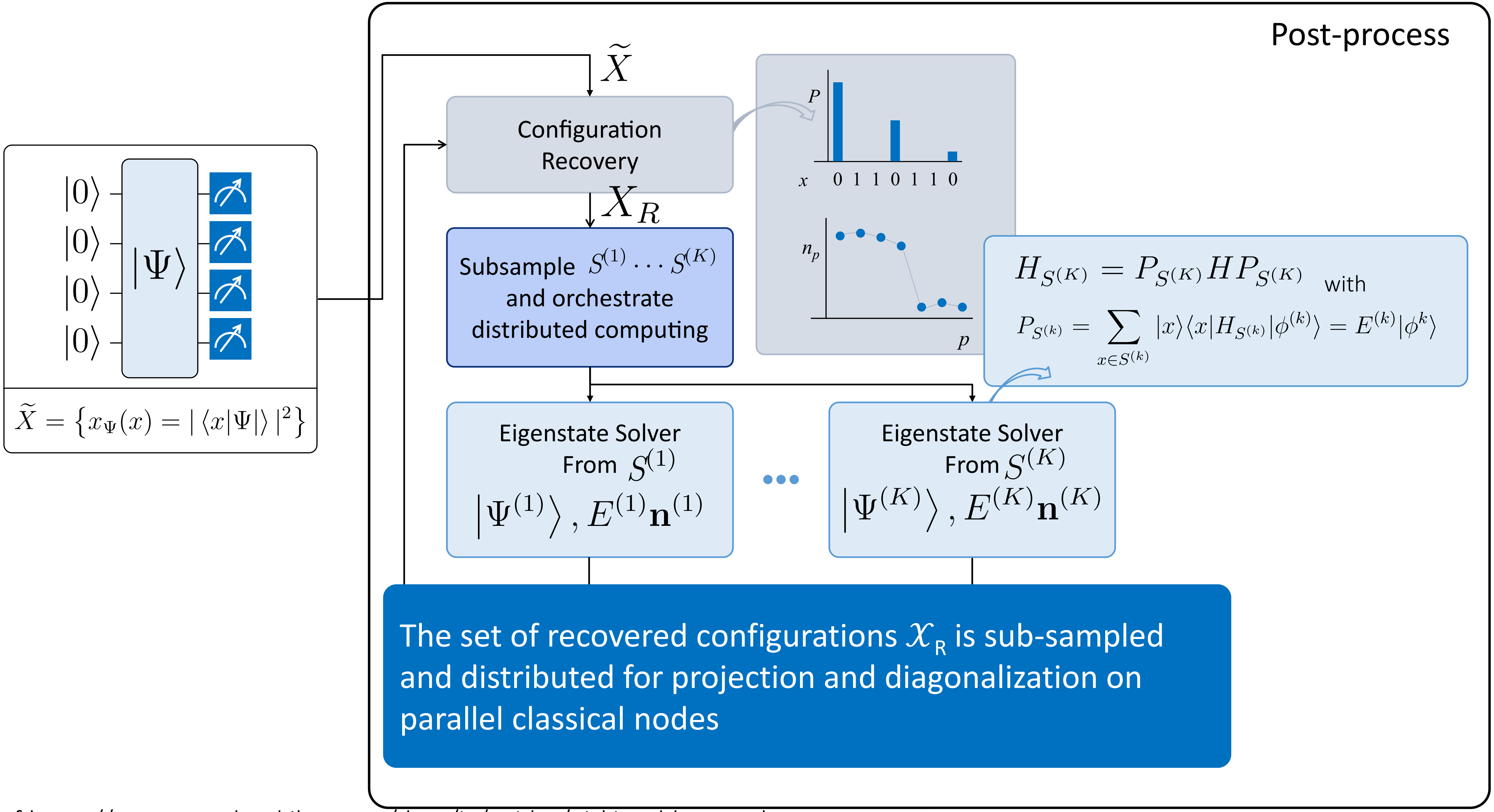
Sample-based quantum diagonalization (SQD)

Configuration Recovery noisy samples $\mathcal{X}$~ from the quantum execution that are processed



ref:https://quantum.cloud.ibm.com/docs/ja/guides/qiskit-addons-sqd

Sample-based quantum diagonalization (SQD)



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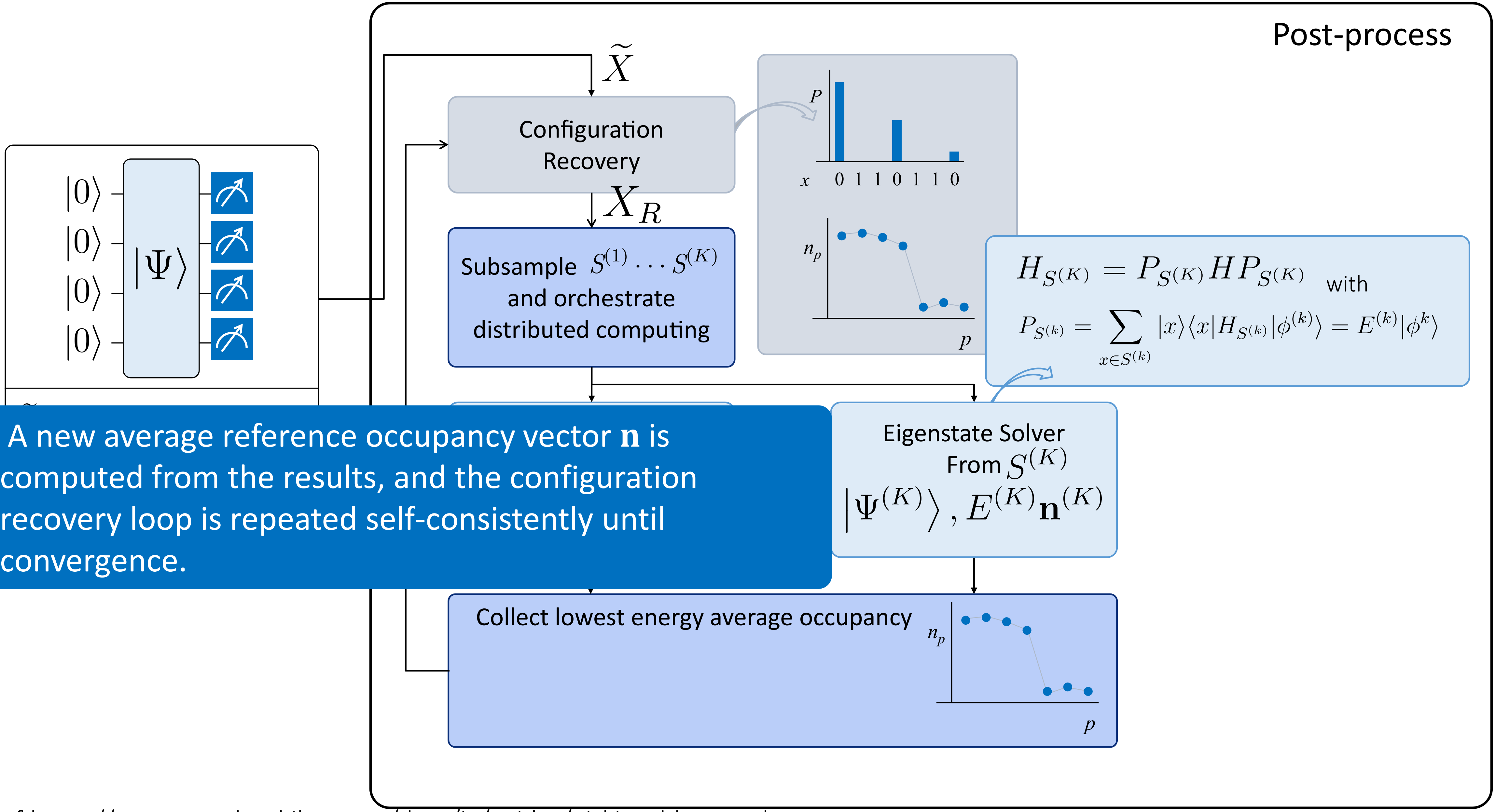
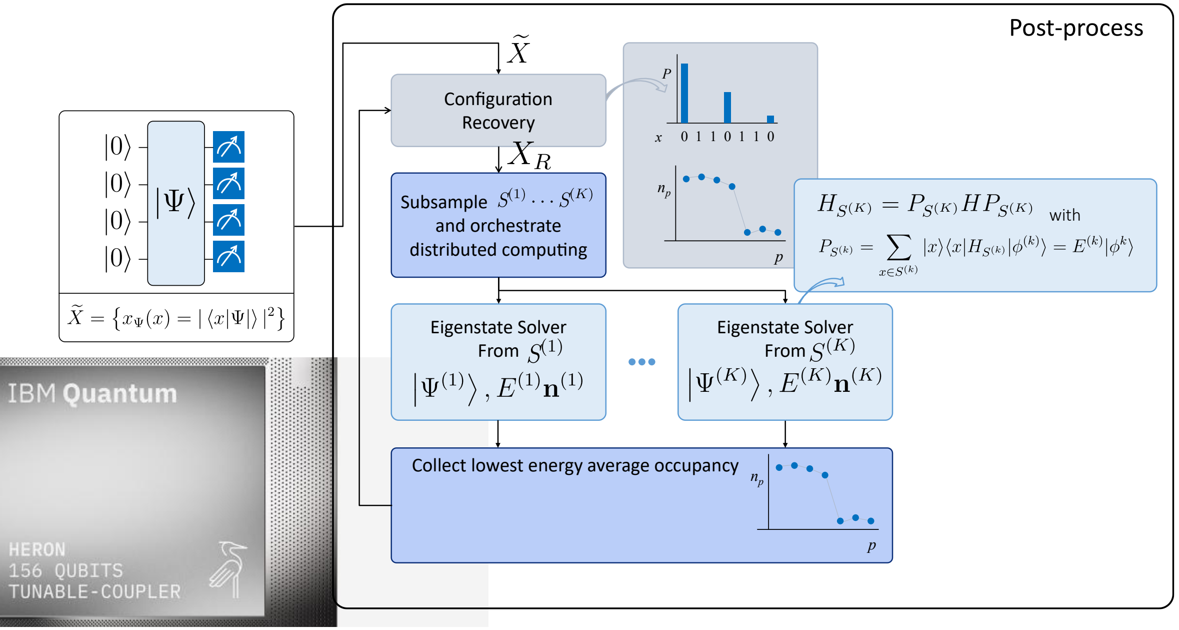
Sample-based quantum diagonalization (SQD)



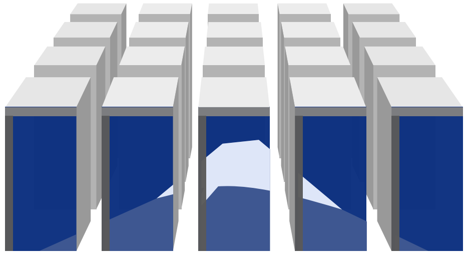
A new average reference occupancy vector $\mathbf{n}$ is computed from the results, and the configuration recovery loop is repeated self-consistently until convergence.

ref:https://quantum.cloud.ibm.com/docs/ja/guides/qiskit-addons-sqd

Quantum-HPC Hybrid Applications: Sample-based Quantum Diagonalization



58, 45, and 77 qubits of IBM Heron



6400 nodes of Fugaku

- incorporate quantum computations of chemistry in a quantum-centric supercomputing architecture, using up to 6400 nodes of the supercomputer Fugaku to assist a Heron superconducting quantum processor.
  - We simulate the N2 triple bond breaking in a correlation-consistent cc-pVDZ basis set, and the active-space electronic structure of [2Fe-2S] and [4Fe-4S] clusters, using 58, 45 and 77 qubits respectively, with quantum circuits of up to 10570 (3590 2-qubit) quantum gates.
- In this study, calculations are performed on a supercomputer using quantum computer results

- Execution with large-scale HPC: Iterative calculations were performed with tight integration by exchanging data at run-time with large-scale node of Fugaku

Figure: https://jp.newsroom.ibm.com/2024-11-14-ibm-launches-its-most-advanced-quantum-computers,-fueling-new-scientific-value-and-progress-towards-quantum-advantage

Evaluating energy for [4Fe-4S] with new diagonalization in a quantum subspace by using the latest devices and increasing the complexity of the workflow

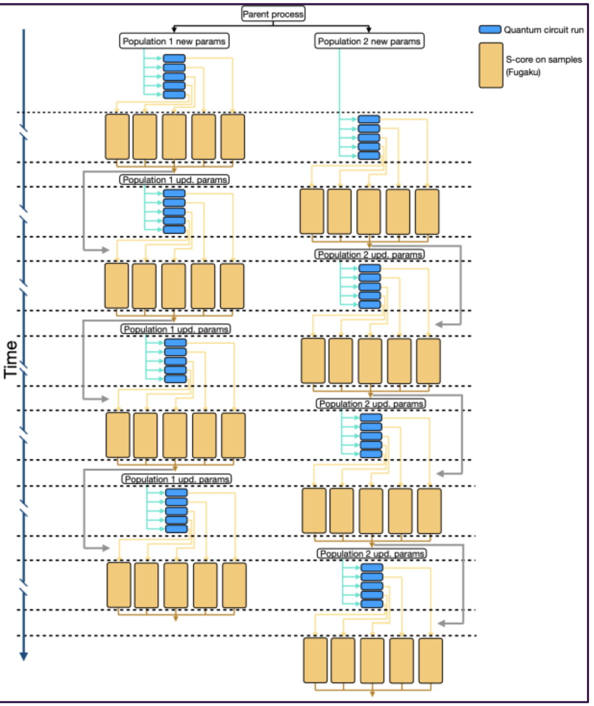
http://arxiv.org/abs/2511.00224s

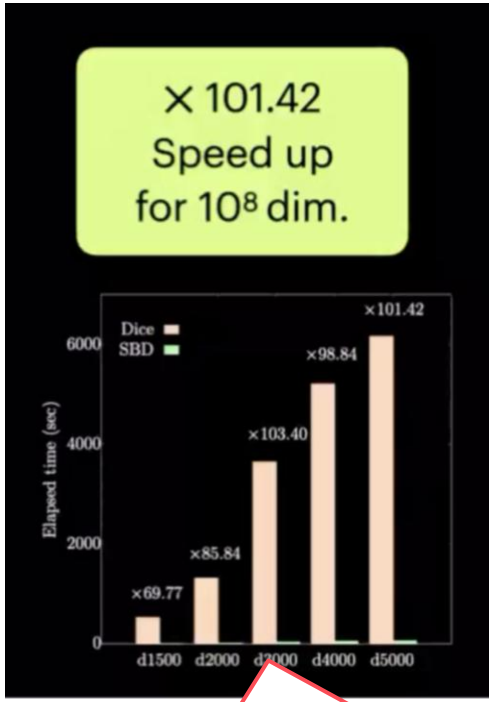
New algorithms
Optimize parameters of LUCJ circuits with iterations

New diagonalization
Fast diagonalization tool. 100x speedup

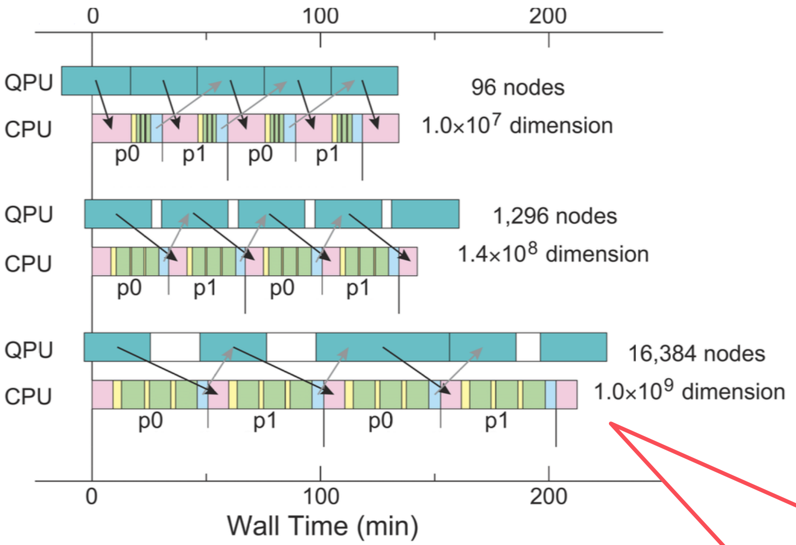
New QCSC workflow
Implementing the algorithms with feedback loop, tight coupling, orchestration of resources

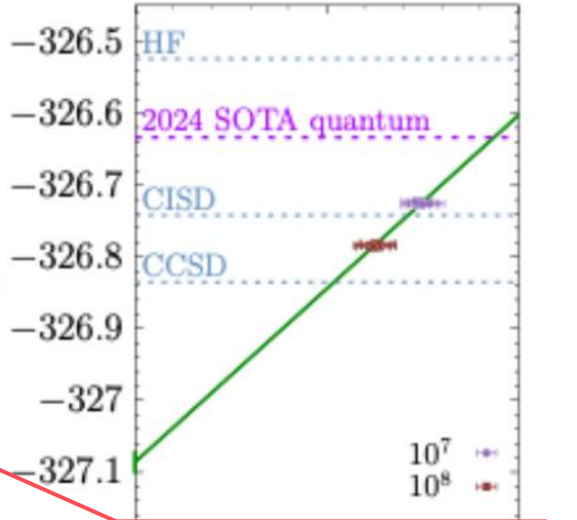
150 mEh improvement over 2024 demo
Efficiently utilize capabilities of Heron r2 (ibm_marrakesh) and 16K Fugaku computation nodes

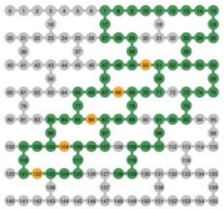




Implemented by MPI for using a large-scale of nodes in Fugaku







1.0 x 10^9 dimensions
Overlap between CPU and QPU computations by tight-coupled Use 16K nodes of Fugaku
integrations with Fugaku and Heron

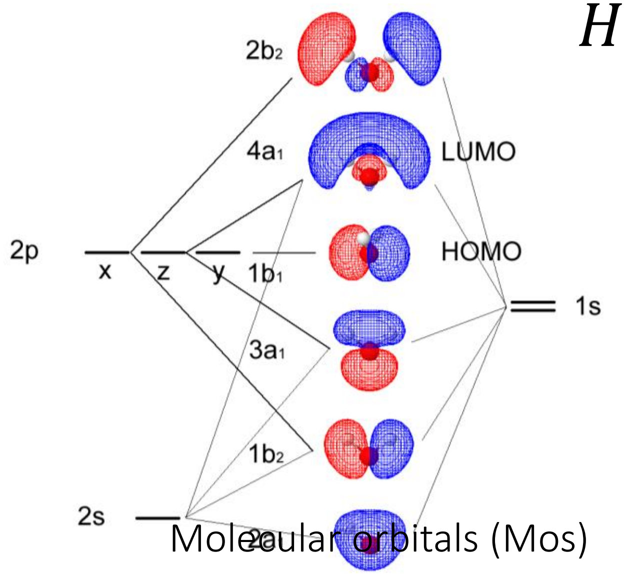
IBM **Quantum** RIKEN

Hybrid quantum-HPC computation of the biomolecular electronic excited states

Quantum chemistry

- Exact solution requires *exponentially* large classical computational resources
- To estimate chemical properties, solve the Schrödinger equation:

$$H|\Psi\rangle = E|\Psi\rangle \quad \text{with} \quad |\Psi\rangle = \sum_j C_j |\Phi_j\rangle$$



Molecular orbitals (Mos)

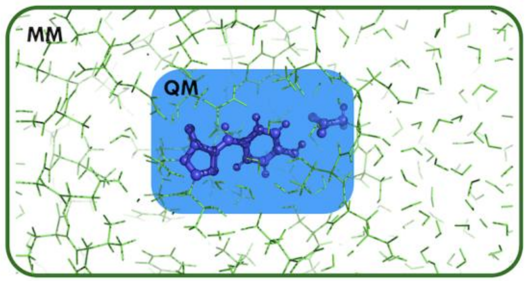
# of Mos	Size of Configuration Interactions (Cis)	Gbytes
4	36	0
8	4900	0
22	497634306624	58
30	24061445010950400	2,801,121

Quantum chemistry can benefit from quantum computing:

- Mapping of the electronic states: (# of qubits) = 2 x (# of MOs)

Quantum HPC Hybrid : hierarchical approaches like QM/MM, FMO, …

- Quantum for Active Space
- HPC for Environment Space



https://bioexcel.eu/events/virtual-workshop-best-practices-in-qm-mm-simulation-of-biomolecular-systems/

appears courtesy of Kentaro Yamamoto, Quantinuum

Hybrid quantum-HPC computation of the biomolecular electronic excited states

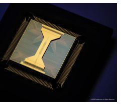
- Time Evolution Quantum Selected Configuration Interaction (TE-QSCI)

1. Solve the Complete Active Space Configuration Interaction (CASCI) (6e,6o) on the classical computer to draw the baseline

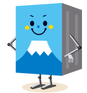
number of electrons

number of orbitals

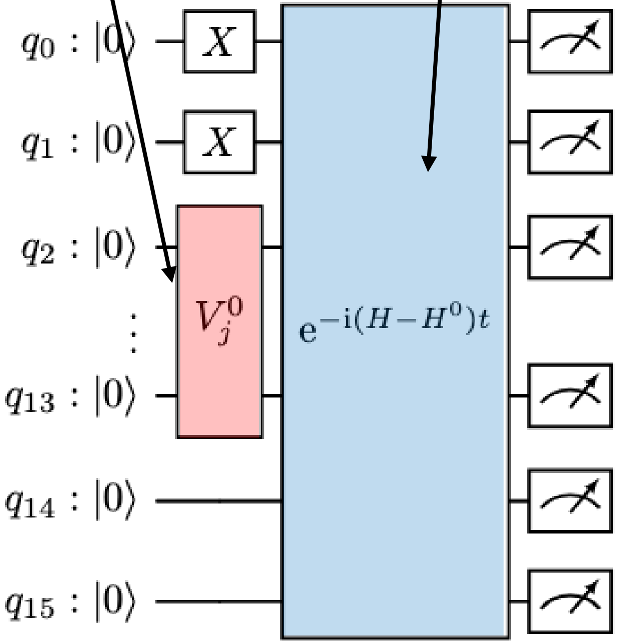
2. Approximately input the target eigenstate (V_j^0)

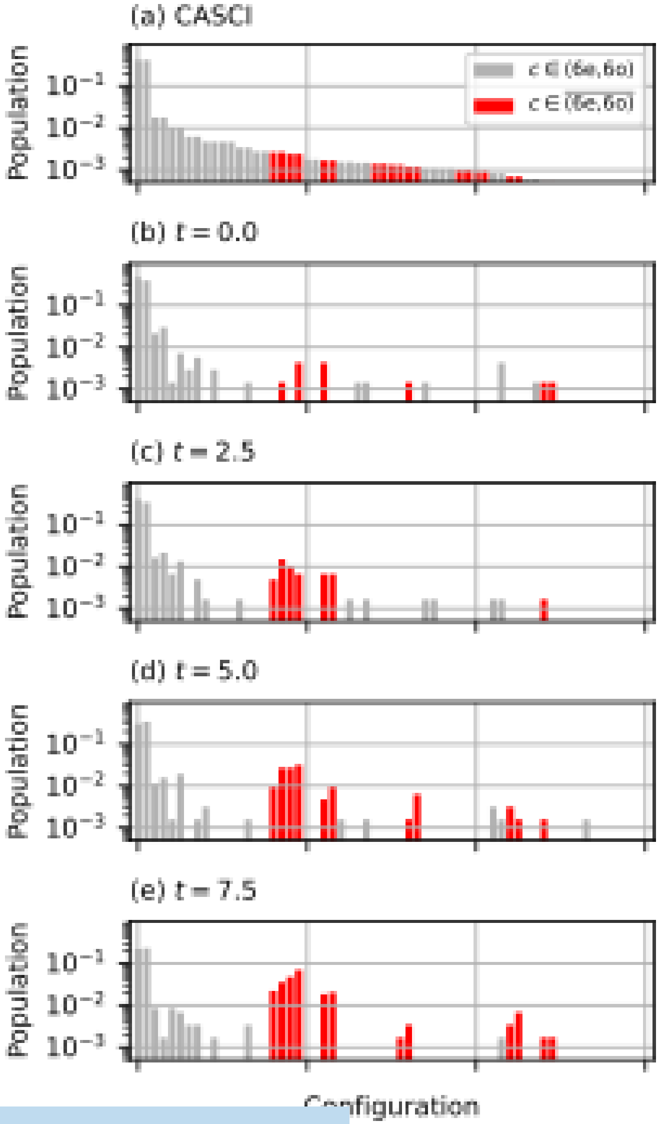


3. Time evolution to extend the configuration space for (8e,8o) active space



4. Diagonalize the subspace Hamiltonian





efficiently find the "important" configuration

Excitation energies (in eV)

Method	active space	T_0	S_1
CASCI	(6e,6o)	1.44	1.48
TE-QSCI	(8e,8o)	1.23	1.27
CASCI	(8e,8o)	1.26	1.29

Time-evolution with **truncated Hamiltonian** operator
Sample the configurations from the **Krylov subspace**

appears courtesy of Kentaro Yamamoto, Quantinuum

More Applications: Test User Program

- Call for application proposals to utilize the hybrid platform to research and develop quantum-HPC hybrid applications
- To obtain feedbacks on our hybrid platform
- 21 proposals are accepted
- 9 MOUs are concluded

User	Application area
JSR Corporation	Materials
Toyota Motor Corporation	Materials, Design & Manufacturing
SoftBank Corp.	Materials
Ochanomizu University	Natural Sciences
Toyota Central R&D Labs., Inc.	Design & Manufacturing
Kyoto University	Medical, Drug Discovery
Oita University	Medical, Drug Discovery
The University of Electro-Communications	Natural Sciences
Mitsubishi Chemical Corporation	Materials
and more ..	

Schedule

	FY2023	FY2024	FY2025	FY2026	FY2027	FY2028
	Remote QC use	Install QC in Kobe/Wako	End of Trial	Start full Operation		End of Operation
Installation and Operation of Quantum Computer	Facility design	Facility construction	Trial Operation	Operation	Operation	
		Deploy	Target: Construct the platform		Target: Multi-Platforms	
Development of Quantum-HPC Hybrid Software	Design	Implementation and test	Test with real hardware	Evaluation and Improvement	Extension for multi-platforms	
			Real utilization	Target: Validate the Platform w/ Hybrid Applications		
Development of Quantum-HPC Hybrid Application	Design	Implementation and test	Test with real hardware	Test with real applications	Evaluation and Improvement	
				Target: Commercial Use of Hybrid Applications		

Summary

- Four Japanese Quantum HPC projects are ongoing
- Some details about JHPC-Quantum project
  - Programming model: Workflow for Loosely coupled programs and Tightly coupled tasks
  - Software stack
  - Scheduler between quantum and HPC
  - Use cases
    - Ground state energy calculation of [4Fe-4S] clusters by Sample-based quantum diagonalization
    - Biomolecular chemical reactions by quantum-HPC hybrid computing workflow
    - Test user program

Acknowledgment

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- This work is based on results obtained from a project, JPNP20017, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).