PCCC AI/機械学習技術部会 第４回ワークショップ, HPC-AI AC
第３回日本カンファレンス 4月19日 2023年

Overview and plan for Quantum HPC hybrid computing platform in RIKEN R-CCS

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理化学研究所は、理研内横断プロジェクトとして「Transformative Research Innovation Platform of RIKEN platforms（TRIP）」を推進することとしており、その一環として、量子コンピュータ（Quantum Computing: QC）とスーパーコンピュータ（High Performance Computing:HPC）を連携するためのシステムソフトウエアの研究開発を進める計画です。本講演では、理研内の量子コンピュータの研究について紹介し、理化学研究所計算科学センターでの量子HPC連携プラットフォームの研究開発の概要と計画についてご説明いたします。

New division for QC-HPC hybrid computing in R-CCS

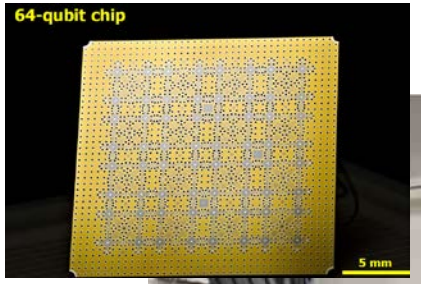
- **In R-CCS, Quantum HPC Hybrid Computing Platform Division was started from April, 2023**
  - Quantum computational technologies are expected to present the opportunity to tackle several problems that are currently infeasible to solve with supercomputers.
  - The mission is R&D to design and development the quantum HPC hybrid computing platform to make use of quantum computational technologies by the integration with high-end supercomputers (such as Fugaku).

- **Three Units**
  - Quantum-HPC Hybrid Software Environment Unit
  - Quantum Computing Simulation Unit
  - Quantum-HPC Hybrid Platform Operations Unit

- **Note:**
  - This division will focus mainly on the development of QC-HPC hybrid platform
  - Researches on Quantum-HPC Hybrid algorithm and application will be conducted by R-CCS and RIKEN research teams using this platform.

Quantum Computing Researches in RIKEN

- **RIKEN Center for Quantum Computing (RQC)**
  - The research and development of superconducting quantum computers
  - Research of optical quantum computers
  - Researches on quantum computing theory
- **RIKEN Center for Computational Science (R-CCS)**
  - Development of quantum computers simulators using Fugaku Supercomputer
  - R&D for hybrid computing system with Fugaku and quantum computers
  - Feasibility study on technologies for integration of quantum computers in the next flagship supercomputer project
- **iTHEMS (Interdisciplinary Theoretical and Mathematical Sciences Program)**
  - Researches on theory and algorithm of quantum computing
  - Quantum computing applications
- **Center for Advanced Intelligence Project (AIP)**
  - Research of quantum AI and optimization algorithms



QC Projects in R-CCS

- **RIKEN project "Transformative Research Innovation Platform of RIKEN platforms (TRIP)"**
  - R&D and deploy of SC-QC hybrid computing platform
- **MEXT "Feasibility Study Research on the next generation computing infrastructure", Feasibility Study Research for new computing paradigm**
  - Feasibility study on technologies including architecture, system software, algorithms, for integration of quantum computers in the next flagship supercomputer project
  - Keio Univ (Leader), RIKEN, Kyusyu Univ, Fujitsu, Tohoku Univ, NEC
- **COI-NEXT program: Center of Innovation for sustainable quantum AI (by software and HPC, simulation technologies) (leaded by Prof. Todo, U Tokyo)**
  - U. Tokyo, Keio Univ., RIKEN , OIST
  - R-CCS joins the research group of quantum-HPC computing and QC simulation technologies.
- **Moonshot project: R&D on scalable backend system for QC-FT (Dr. Sano)**

Transformative Research Innovation Platform of RIKEN platforms (TRIP)

Value Creation by Quantum-Classical Advanced Computing Platform for Accelerating Research DX

Pioneer predictive control science of the future by linking new types of computers, predictive algorithms, and data maintenance

High-quality data acquisition

Bioresources
Measurements using synchrotron radiation
Research DX specialists

SPring-8
SACLA

Bioresources

Develop into a pioneering research DX initiative

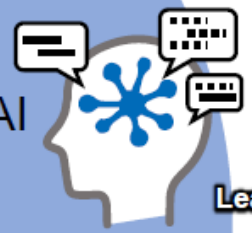
Data

AI

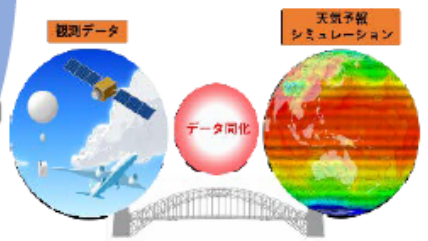
Super computer

Pioneer prediction science with AI x mathematics

Electronic state prediction / New functional materials
Transmutation of elements prediction / New energy creation
Ecosystem prediction / Recycling-oriented society



Learning theory

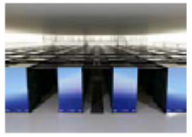


Data assimilation

Expansion of Computationally Viable Region

Quantum-classical hybrid computing

Improvement of usage environment
Next generation semiconductor
Development of EUV lithography



Supercomputer "Fugaku"

Quantum computing

Pioneer the "predictive control science of the future" across fields
(Predict social and global issues and control them through interventions)

Transformative Research Innovation Platform of RIKEN platforms（TRIP）

～ 研究DX加速のための量子古典Advanced Computingプラットフォームによる価値創成 ～

- ◆ 理研の最先端研究プラットフォーム（スパコン、放射光、バイオリソース等）をつなぐとともに、「AI×数理」、「量子古典ハイブリッドコンピューティング」の導入により、先駆的に研究DXを加速・発展
- ◆ 「未来の予測制御の科学」を開拓し、社会変革のエンジンを国内・国際社会へ提供

良質なデータ取得（蓄積・統合）

【プラットフォーム開発】
- 良質なデータ取得と多様なデータの蓄積・統合による解析基盤整備 など

多様な分野のデータを蓄積・統合

NII

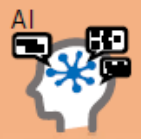
世界トップレベル研究から創出される研究データの連携

バイオリソース

SPring-8 SACLA

AI×数理（予測の科学）

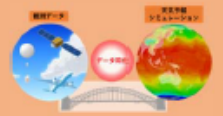
【プラットフォーム開発】
- 数理科学に、スパコン、AI、量子コンピュータをつなぎ、様々な分野における量子古典ハイブリッド計算のアルゴリズム開発を行い活用 など



学習理論

統数研

最先端のAI、数理解析と量子技術



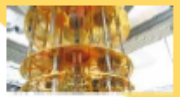
データ同化

研究DXの先駆的取組へ発展

量子古典ハイブリッドコンピューティング（計算可能領域の拡張）

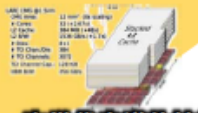
【プラットフォーム開発】
- 量子コンピュータとスパコンのハイブリッドコンピューティングの基盤を整備
- 次世代シリコン半導体やEUVリソグラフィー光源などの要素技術の開発 など

量子コンピュータとスパコン「富岳」のハイブリッド計算活用・基盤整備



量子コンピュータ

スパコン「富岳」



次世代半導体技術

プラットフォームで実現する新たな価値創成研究（ユースケース）

（元素変換の予測と制御 ―新たなエネルギー源の創成）
- 元素変換の新技術を開発し、新たなエネルギー源の創成等を実現

（電子状態の予測制御―新機能材料）
- 物質中の電子状態の高精度予測・制御を実現し、物質の機能・特性の向上や新たな機能を持つ材料の開発等を実現

（生態系の予測制御―循環型社会）
- 複雑な生態系ネットワークの統合モデルを開発し、循環型社会の実現に貢献

国家的・社会的に重要な先端技術を集中的に研究できる運営体制の整備
- 国内の大学・研究機関等の優れた研究者を結集（クロアポ等）
- 技術安全保障や研究インテグリティの管理体制を強化し、セキュアな研究環境で整備
- 新たに研究DXを推進する職を設け、研究DX人材を育成

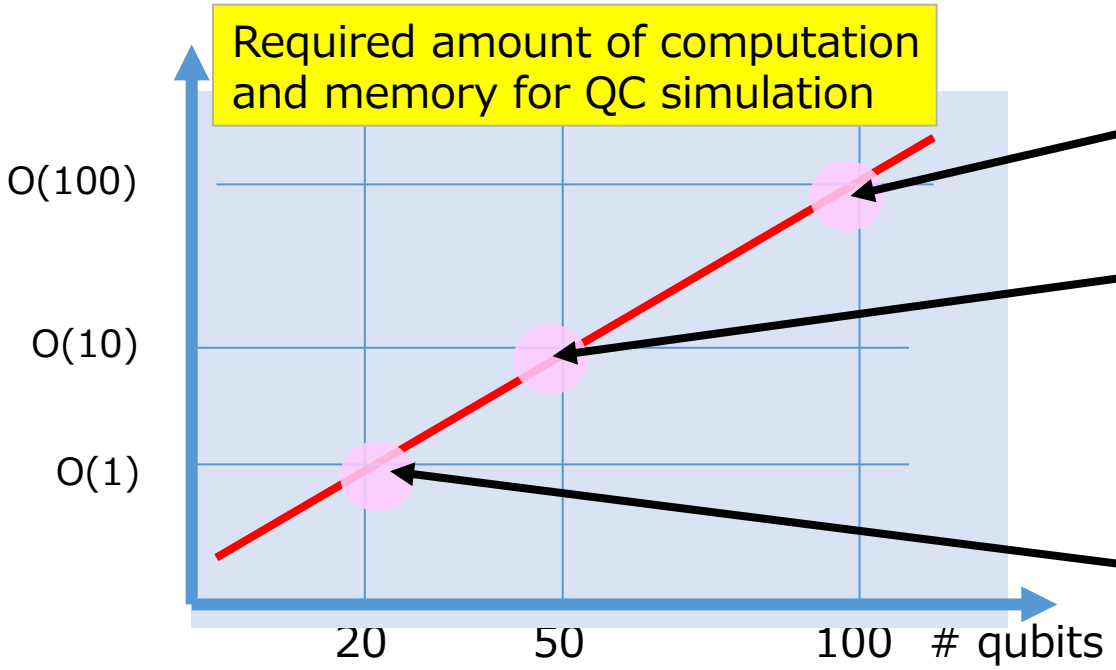
「未来の予測制御の科学」を分野の枠を超えて開拓

（社会や地球規模の課題の予測と介入による制御を実現）

QC-HPC (supercomputer) hybrid computing (1/3)

- **Offloading some useful computation onto QC from large-scale HPC applications**
  - Like GPUs! This is a final goal, but too early?

- **Supercomputers for large-scale QC simulation**
  - QC simulation is very important to design QC algorithms such as error mitigation
  - QC simulation with noise model, simulation for QC physical device will be useful.



methods such as tensor-network method are required even by supercomputer and GPUs.

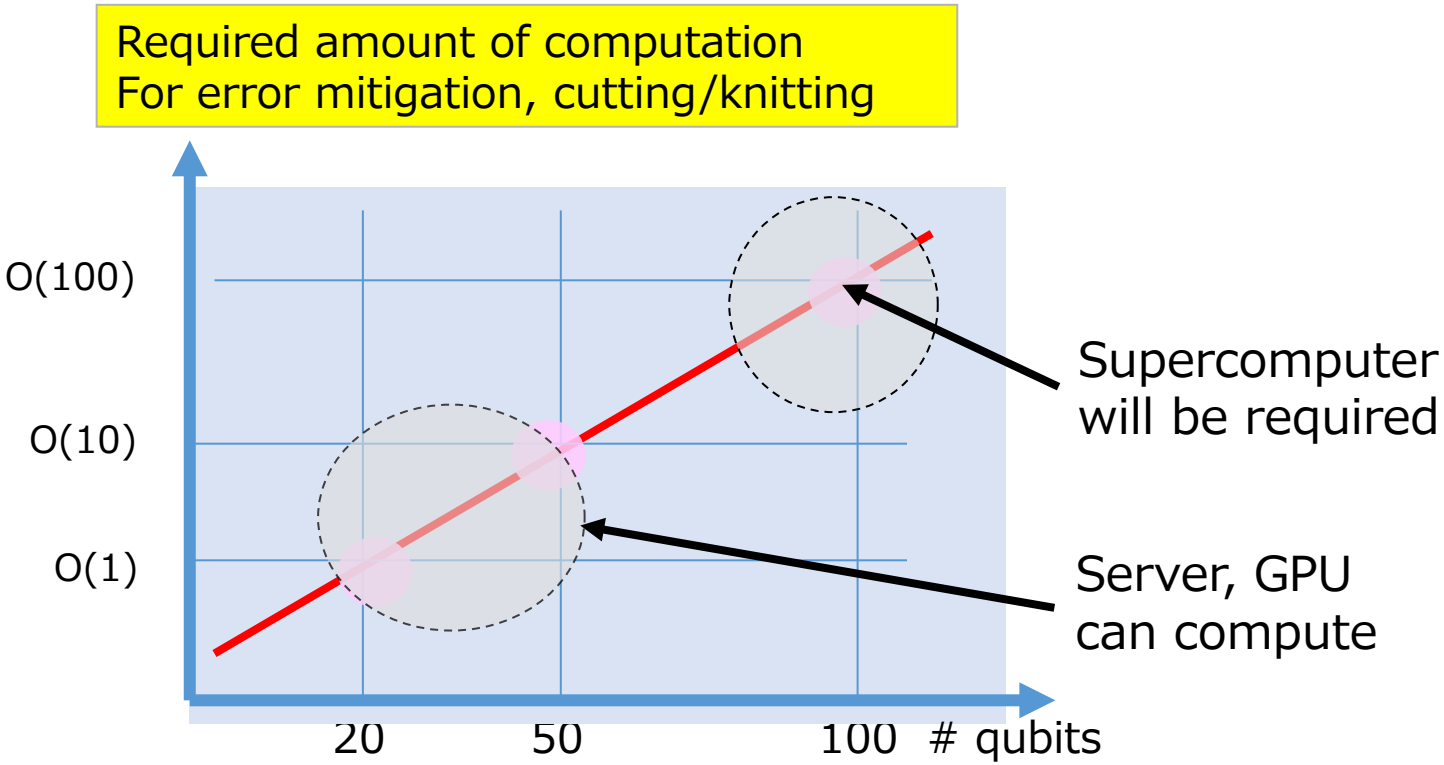
Maximum qubits can be simulated by supercomputer (Fugaku) using state-vector method

K. De Raedt; Massive Parallel Quantum Computer Simulator;Computer Physics Communications vol.176 (2007); pp.121-136. https://doi.org/10.1016/j.cpc.2006.08.007

PC and sever can simulate up to 30qubits

QC-HPC (supercomputer) hybrid computing (2/3)

- **Error mitigation for NISQ by HPC**
  - Error analysis requires the results by QC simulator on HPC
  - QC simulation with noise will be useful to study NISQ
- **Optimization and cutting/knitting of large quantum circuits by HPC**



- M3 error mitigation algorithm will require supercomputer for more than 100 qubits

  https://journals.aps.org/prxquantum/pdf/10.1103/PRXQuantum.2.040326

- Circuit cutting algorithm is a mixed-integer linear programming problem

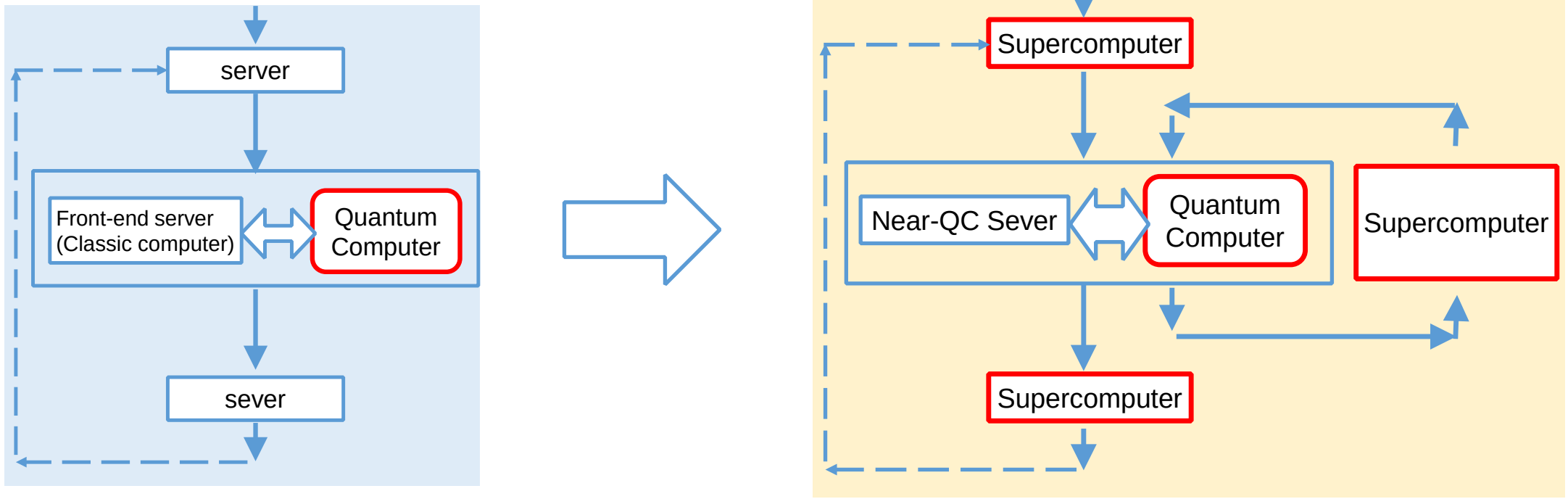
[1]https://arxiv.org/pdf/2012.02333.pdf

[2]https://arxiv.org/pdf/2205.05836.pdf

QC-HPC (supercomputer) hybrid computing (3/3)

- **Variational algorithms need many iterations of computation and communication between QC and HPC**
  - VQE: Variational Quantum Eigensolver, QAOA: Quantum Approximate Optimization Algorithms, …
  - Large problems of VA (with error mitigation) will need “supercomputer” via Tightly-coupled LAN (?)

Supercomputer Is bandwidth-oriented system
Not latency-oriented system



Plan for Quantum Hybrid Computing platform in R-CCS

Fugaku

Classical HPC Infrastructure

Dedicated Simulator Machine (classic) ~1000 GPUs

Hybrid Programming API & Workflow Scheduler

Tightly Coupled LAN or Internet (For variational algorithms, low latency, high BW)

Quantum SW Stack

Near-QC Hybrid Programming & API

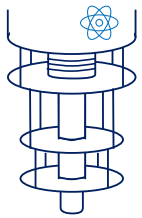
Unified IL for QC/Hybrid

Near QC server

Quantum Computers (Physical & Simulated)

FPGA

Directly observable



Quantum Machines (RQC, multiple vendors)

Multiple simulators on Fugaku (R-CCS/RQC)
(Mainly) State Vector
QULACS, BRAKET, QIBO, …

Dedicated Simulator Machine (Quantum Sim)
~1000 GPUs
Tensor Contraction
cuQuantum etc.

Algorithmic Descriptions

Hybrid Variational Algorithms

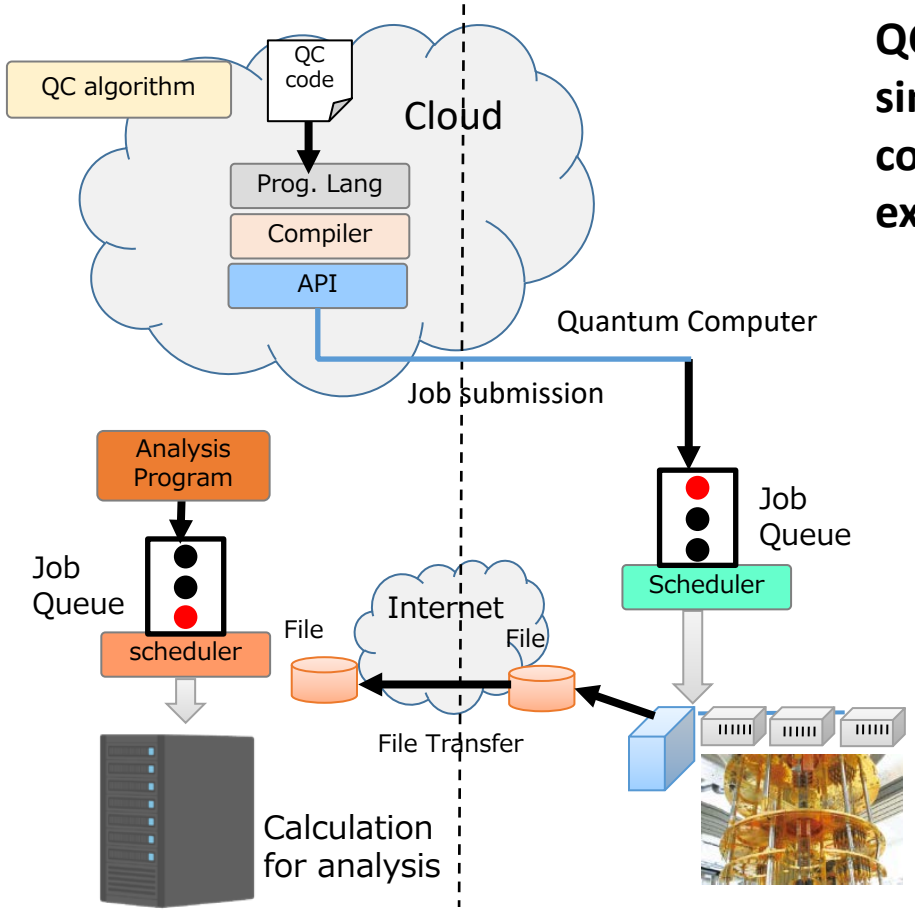
Quantum Alg.

NISQ Alg

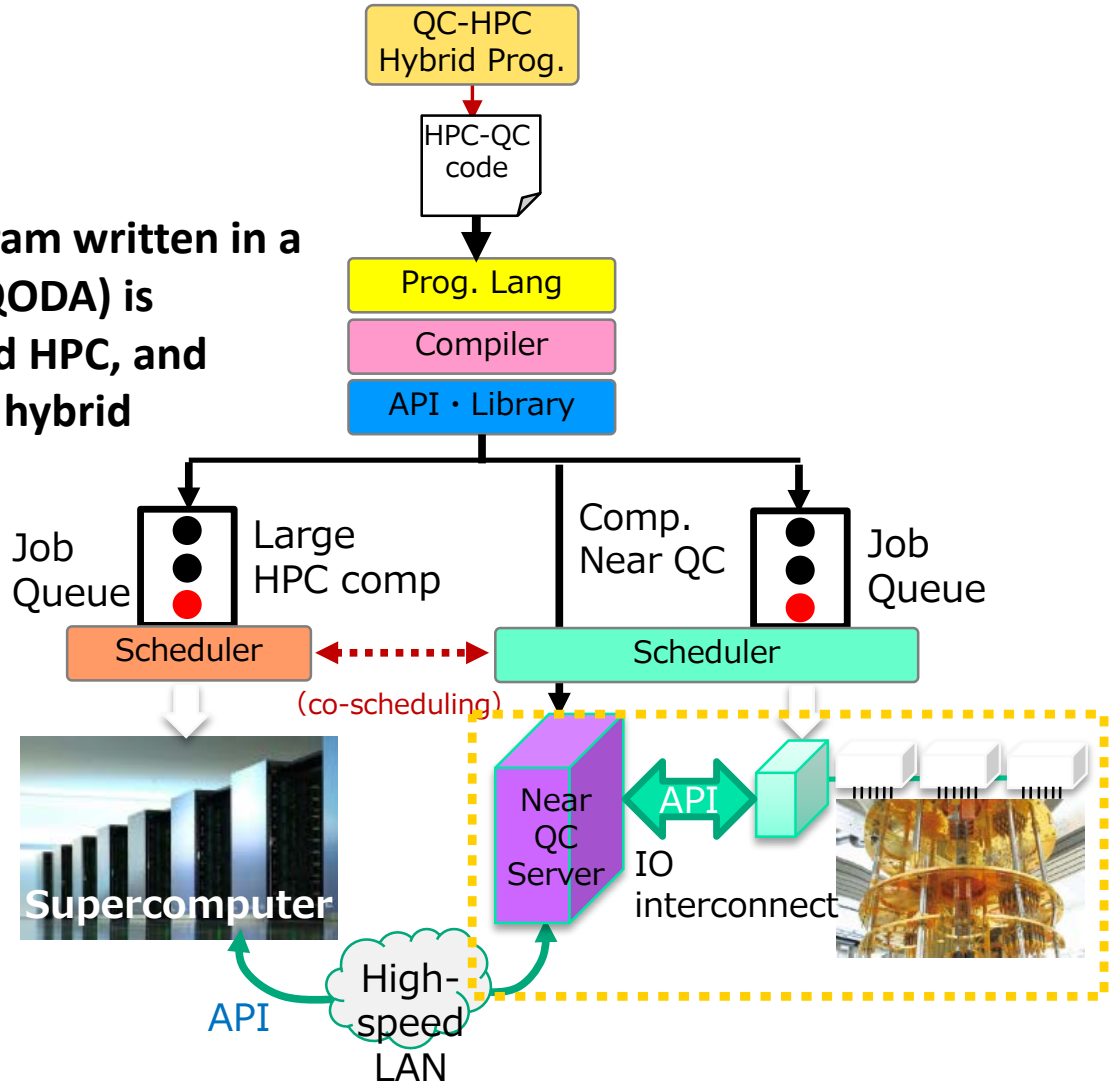
- Quantum BLAS
- Qiskit：IBM prog. Framework incl. transpiler
- Cirq：Google quantum prog. tool
- TensorFlow Quantum: Quantum ML
- Q#:Microsoft quantum prog. Tool.
- Qulacs：Osaka-u prog. Tool
- QunaSys　simulation
- Covalent: Agnostiq、quantum HPC workflow
- PyQubo：converts combinatorial optimization problem into QUBO

Design of QC-HPC hybrid system

In most current QC-Classic system, the workflow is limited: Compilation on cloud, submission to QC, and retrieve of result by file transfer followed by analysis on server.

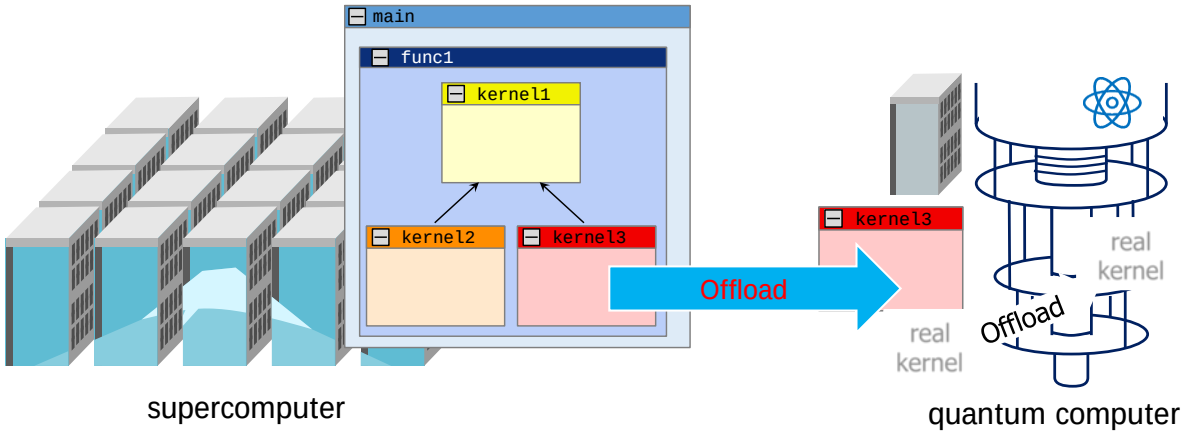


QC-HPC hybrid program written in a single source (as in QODA) is compiled into QC and HPC, and executed by HPC-QC hybrid



R&D for QC-HPC hybrid system

- **Programming models and framework for QC-HPC hybrid computing, and design and development of hybrid computing environment**
  - Single-source and unified programming system for QC-HPC hybrid applications
    - Some extension of Qiskit, QODA, Qibo …
  - Middleware to offload a part of an application -- kernel -- to a quantum computer
  - Use Task programming and Remote Procedure Call (RPC) framework for the offloading



Software stack for QC-HPC hybrid computing