Bringing together HPC and QC: it is mainly a software challenge!

Martin Schulz, TU Munich

IPELS/ISSS @ IPP Garching, August 8th, 2024

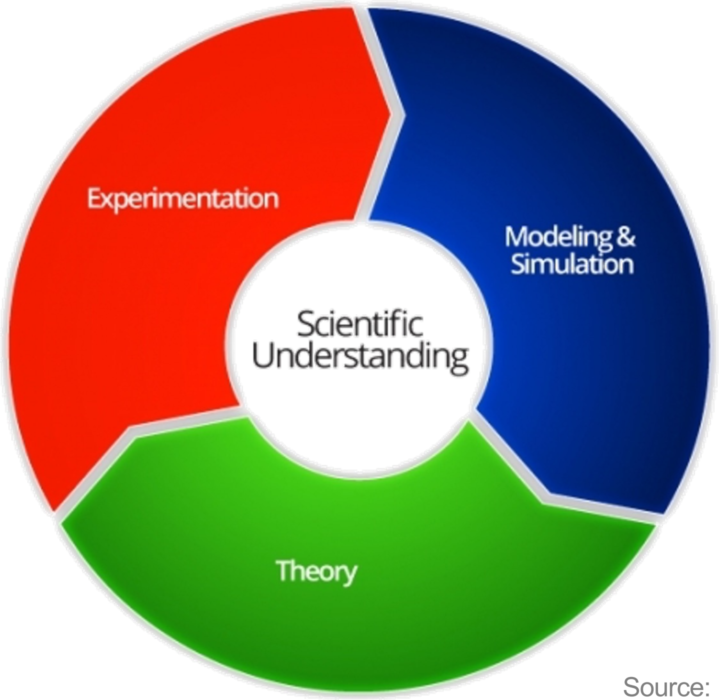
Munich Quantum Valley

Q-DESSI

Modeling and Simulation as the Third Leg of Scientific Discovery

HPC has become indispensible

- Supporting theory and experiments
- Fundamental to the scientific process



Source:
US Department of Energy

The role of HPC in Science and Industry

HPC as the Third Leg of Scientific Discovery

HPC has become indispensible

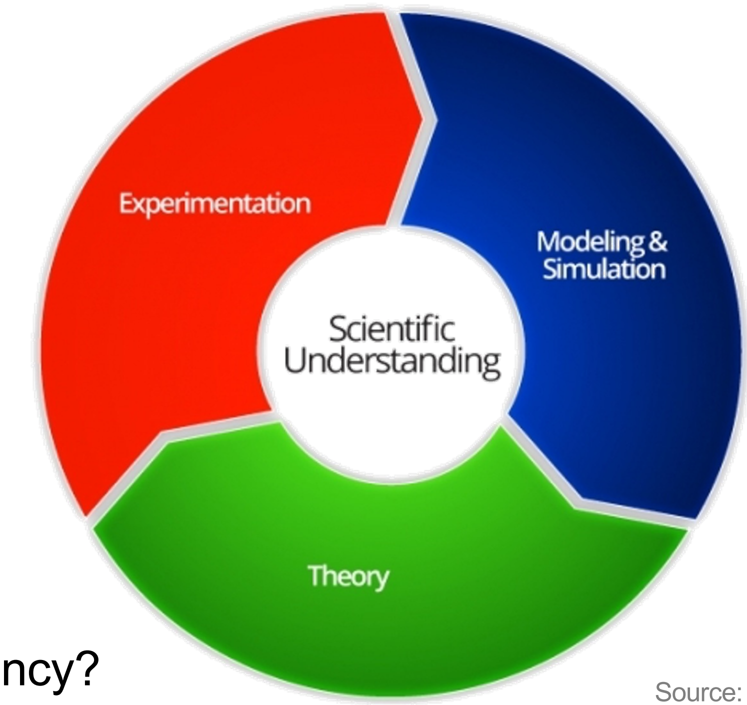
- Supporting theory and experiments
- Fundamental to the scientific process

Working with plasma simulation codes

- Collaboration on Gene and Gene-X codes at IPP
- PLASMA Center of Excellence
  - EuroHPC Center of Excellence

Goal: How to get more performance/science?

- In addition to algorithmic work done
- How to improve GPU utilization and energy efficiency?
- How to tune memory access patterns?
- How to optimize communication?



Source:
US Department of Energy

Top 500 HPC Systems

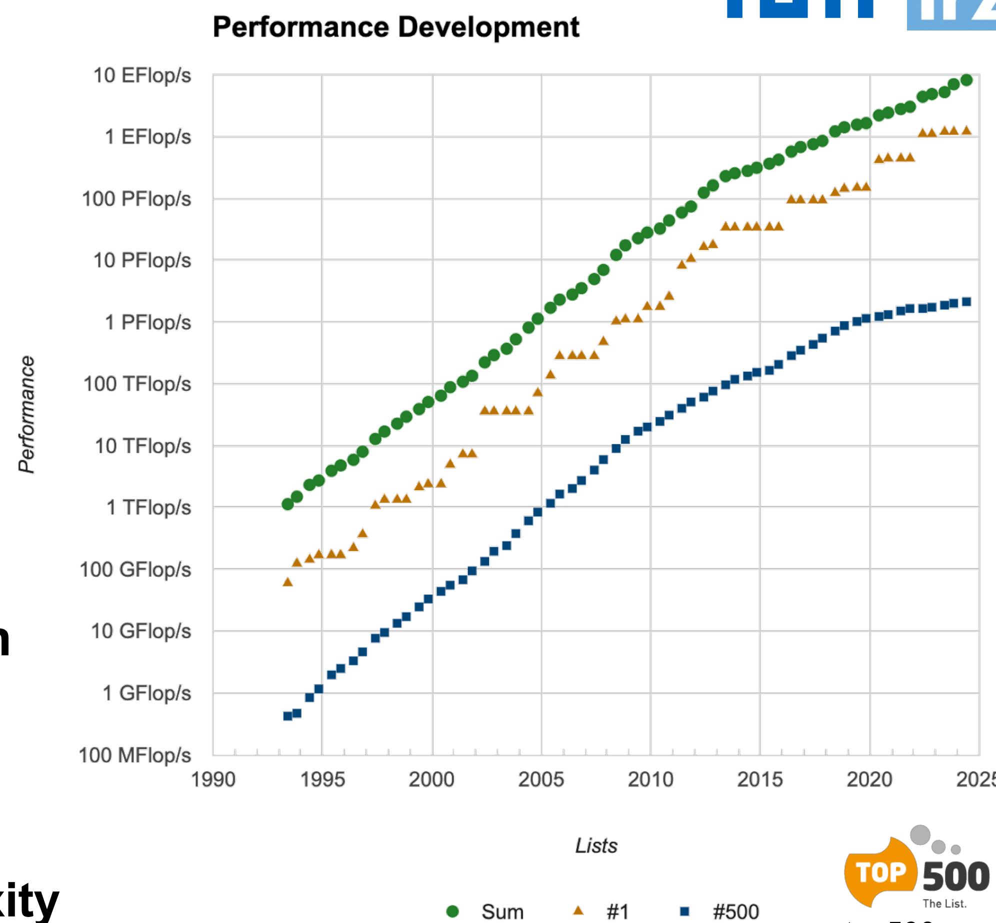
The Growth Trend is Slowing

Node performance growth is slowing
- End of Dennard Scaling
- Nearing the end of Moore's Law

System size growth is slowing
- Power and energy
- Physical limitations

Era of Acceleration via Specialization
- GPUs and FPGAs
- Specialized AI systems

But: No fundamental change in complexity



top500.org

The Promise of Quantum Computing

System working on quantum mechanical principles

- Superposition = Multiple States at one time (until measured)
- Entanglement = Correlation between states in a system
- Probabilistic

Basic unit = 1 Qubit

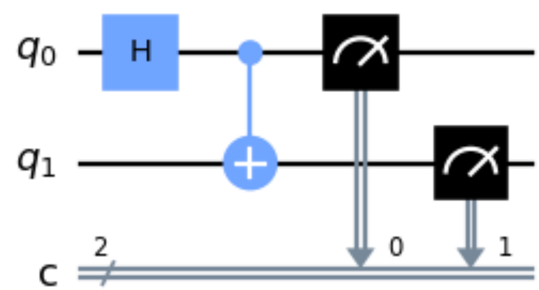
- Can be in superposed and/or entangled state
- When read: 0 or 1 only (rest collapses)

Programming with gates

- Operations on qubits
- Different systems have different gates

Quantum Advantage

- Some quantum algorithms require exponentially less steps than classical algorithms



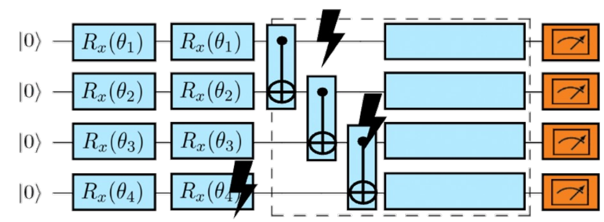
From: https://docs.quantum.ibm.com/api/qiskit/qiskit.circuit.QuantumCircuit

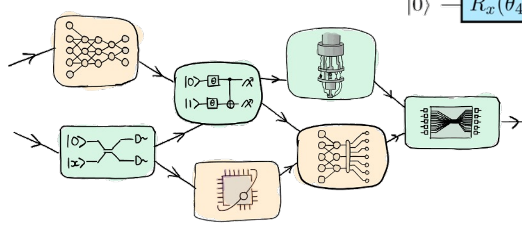
What is all the Fuzz About?

Applications for Quantum Computing

Main Application Domains
- Quantum simulation of quantum systems
- Quantum optimization
- Quantum machine learning
- Quantum linear systems

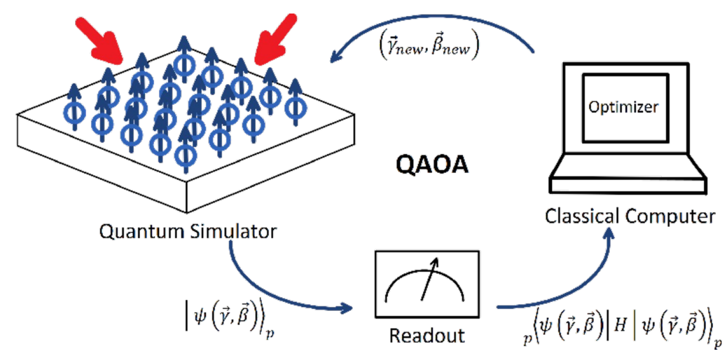
$$\mathcal{N}(\rho) = \sum_{i=0}^{n} K_i \rho K_i^{\dagger}$$





PENNYLANE

Problems:
- Small number of qubits
- Noisy systems
- Only few working algorithms
- Specialized programming
- Still treated as physics experiments



The Munich Quantum Valley initiative develops quantum computation and quantum technologies in Bavaria.

Superconducting. Ion. Neutral Atom. Quantum-HPC.

BAdW Bayerische Akademie der Wissenschaften · DLR · FAU Friedrich-Alexander-Universität Erlangen-Nürnberg · Fraunhofer · LMU Ludwig-Maximilians-Universität München · Max Planck Gesellschaft · Technische Universität München TUM

Quantum Computing ←→ HPC

Usage exclusively as accelerator for HPC workloads

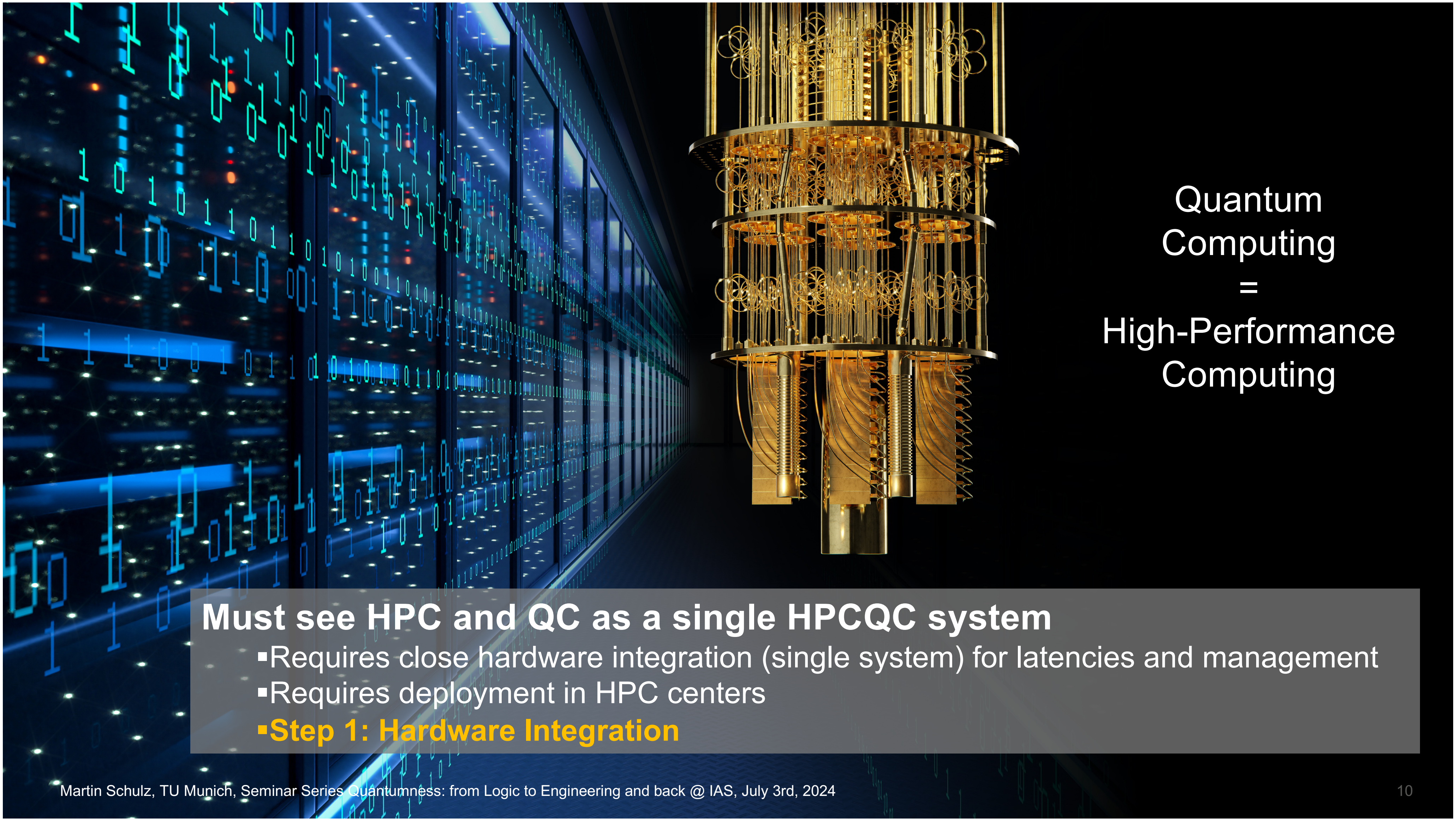
- Intended for fine-grained kernels within larger applications or workloads
- Need classic pre- and post-processing
- Only certain problems are suitable for quantum computing: optimization, quantum simulations

Goal: Use of QC similar to other accelerators

- On-node (like GPUs, FPGAs)
- Dissaggregated (like AI HW)

Quantum Computing as a stand-alone system not viable at growing scales

- Complex control systems
- Data staging and post-processing
- Targeted towards very specific workloads and kernels
- Tight interactions needed for variational algorithms
- Complex compilation and runtime environment with high demands need HPC



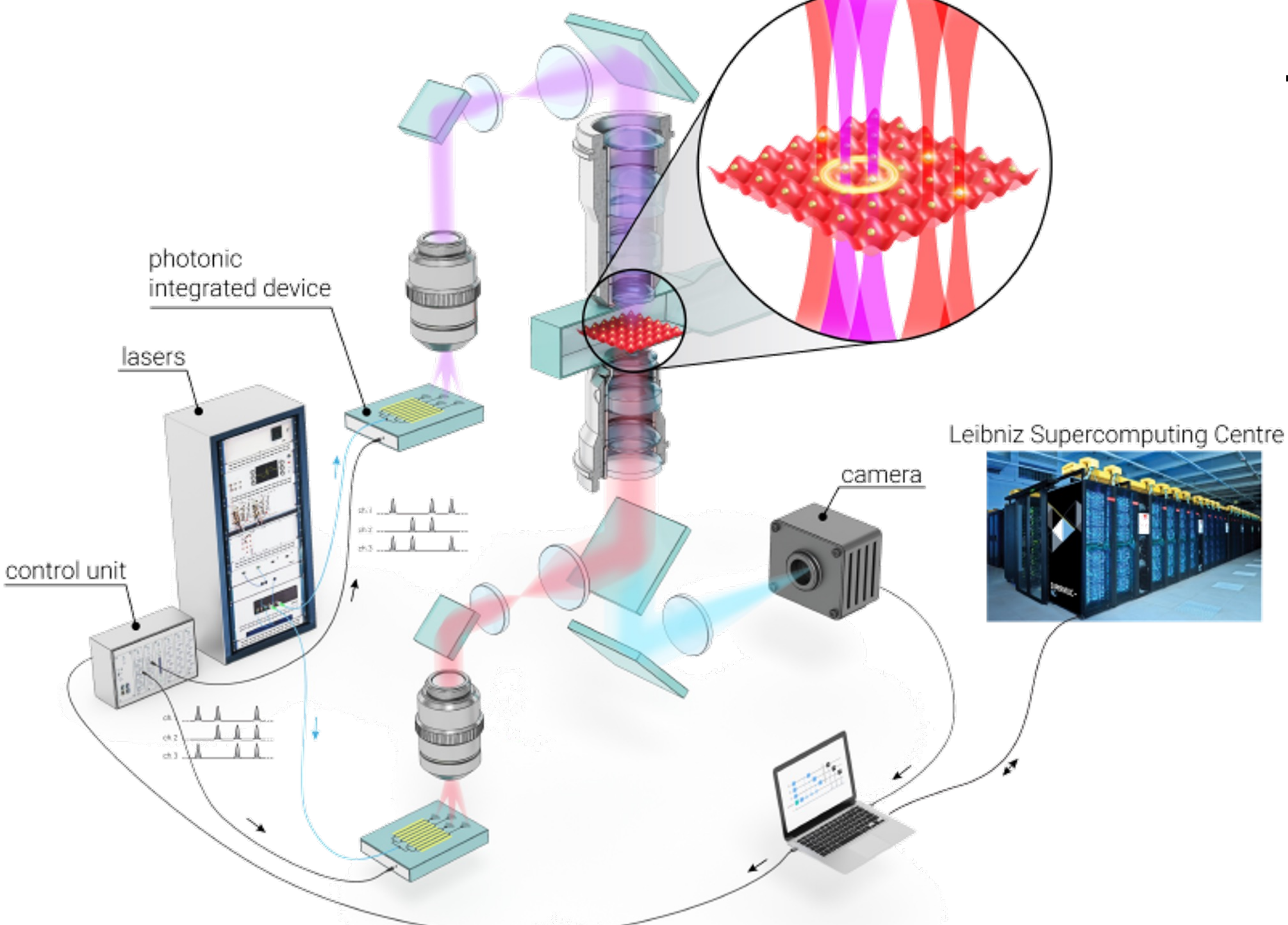
Quantum
Computing
=
High-Performance
Computing

Must see HPC and QC as a single HPCQC system

- Requires close hardware integration (single system) for latencies and management
- Requires deployment in HPC centers
- **Step 1: Hardware Integration**

Typical Quantum Computer Setup

Example: Neutral Atoms

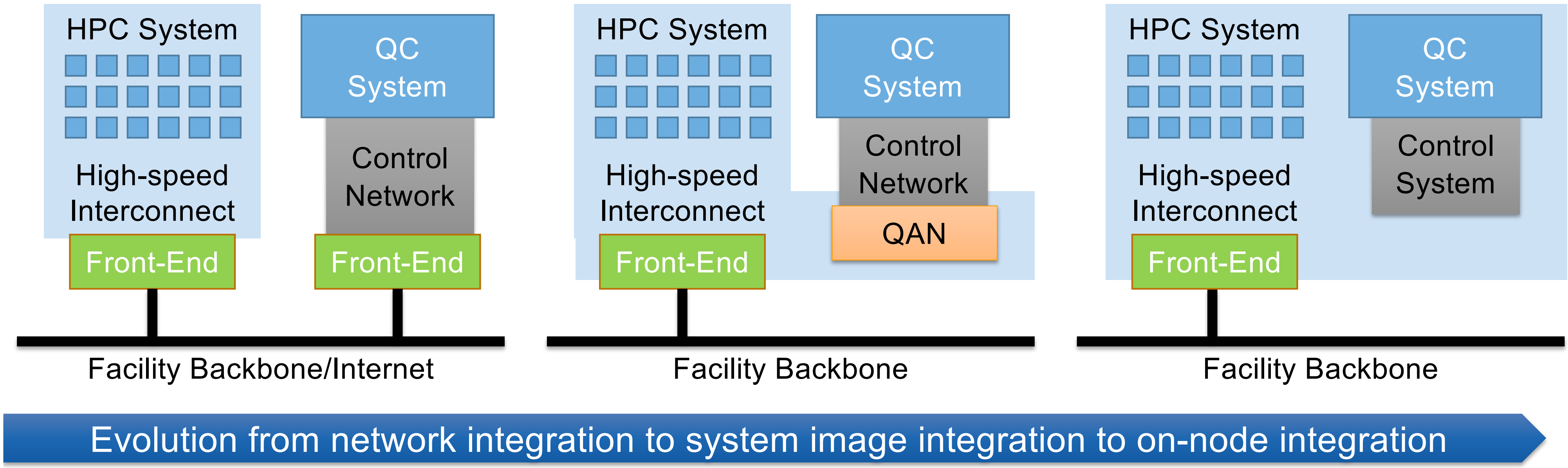


Typical Structure Today

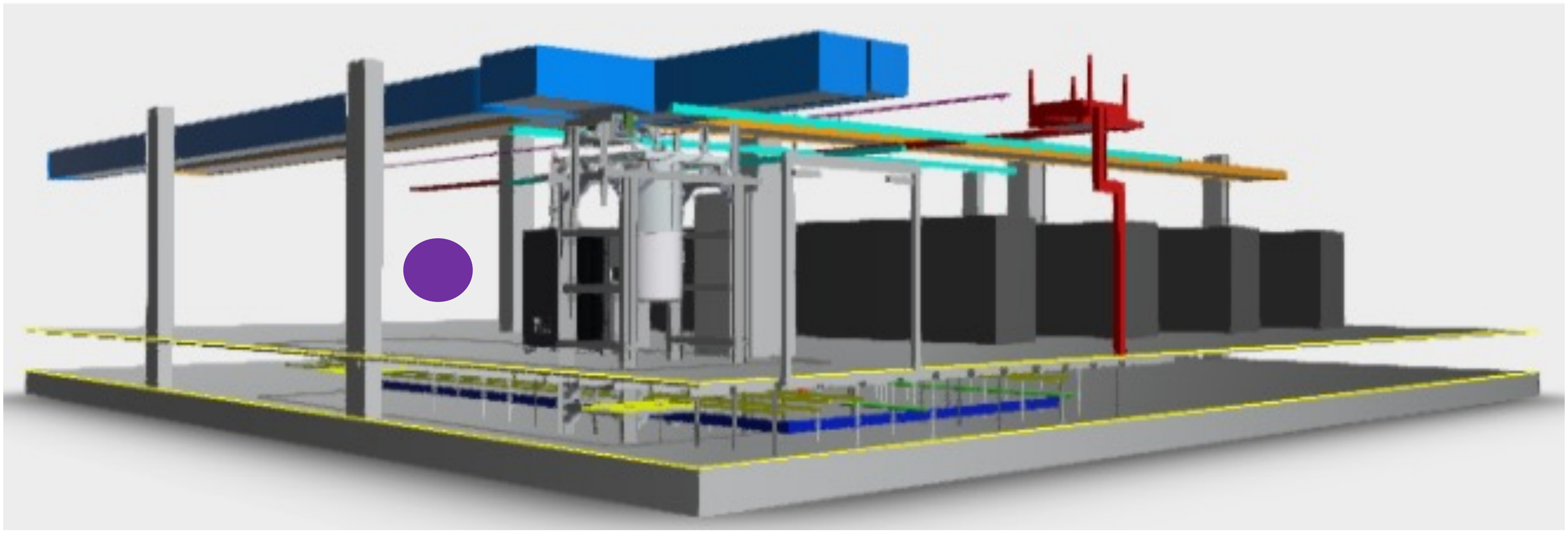
- ”Medium” for Qubits
- Control via external influence
  - Lasers, Microwaves, …
- Separate control system
- Connected to an access node
  - In lab settings, often simple
- Remote access from HPC to the access node

Source: MPQ

Reducing the Gap between Host and Accelerator



Location of Production QC systems in LRZ Compute Cube



Planned location of System Q-Exa (shown) and Euro-Q-Exa system (to the left of Q-Exa, purple dot).

Quantum Systems at LRZ

Superconducting

System 1: 5 qubits (R&D system)
Vendor: IQM
Up and running in QIC

System 2: ca. 20 qubits (R&D system)
Vendor: IQM
Up and running in QIC

System 3: 20 qubits (Production)
Vendor: IQM
Soon available to Bavarian,
German and European users in pilot phase

System 4: 50+ qubits (Euro-Q-Exa-1)
Vendor: TBD
Target: Bavarian, German and
European users
EuroHPC procurement in process

Phase 2: 100+ qubits (Euro-Q-Exa-2)
Vendor: TBD
Target: Bavaran, German and
European users
EuroHPC procurement in process

Quantum
Computing
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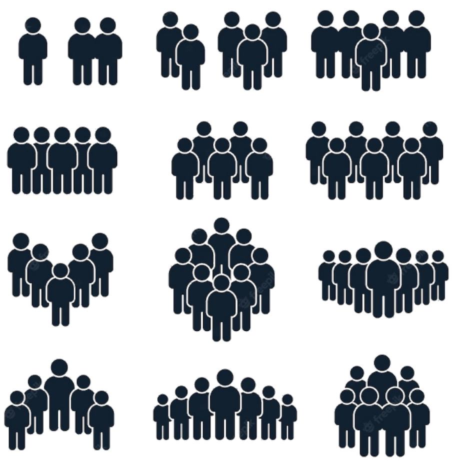
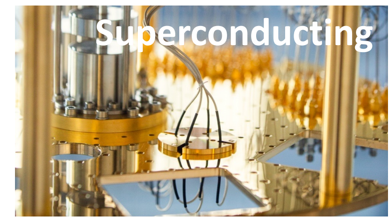
Must see HPC and QC as a single HPCQC system

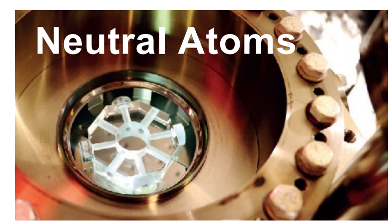
- Requires close hardware integration (single system) for latencies and management
- Requires deployment in HPC centers
- Requires integration into a single software stack and execution environment
- Requires unified user access/management/experience

Towards Support for Multiple Communities on Multiple Systems

Wide User Communities



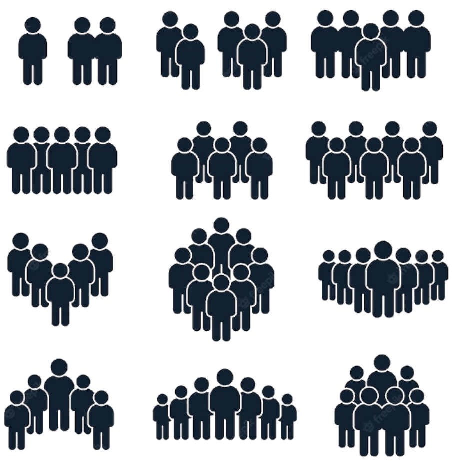




Many/Different Quantum Devices

How *not* to do it!

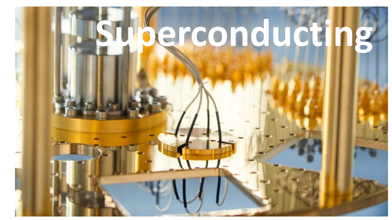
Wide User Communities

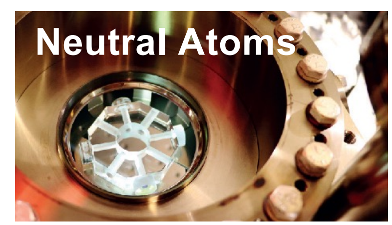


Stack for A

Stack for B

Stack for C



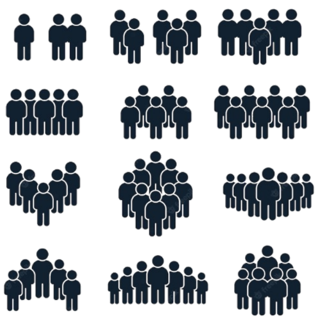


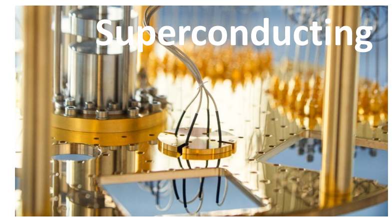
Many/Different Quantum Devices

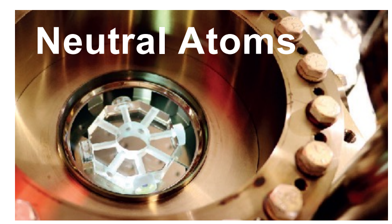
Connecting Users to Systems

Martin Schulz et. Al, Towards the Munich Quantum Software Stack, Poster at QCE Weel 2023

Wide HPC User Communities







Enabling Domain User Communities to Compute on Quantum Devices

QCs & Simulators

Front-End / Languages

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Wide HPC User Communities

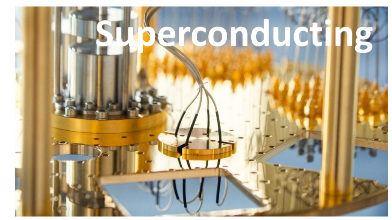
Hybrid/Quantum Programming Toolkits / Libraries

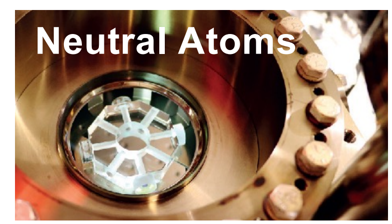
Different Programming Models

- Standard approaches like Qiskit/Pennylane
- Higher-level abstractions
- New developments
- HPCQC approaches, like OpenMP
- Domain specific support

Decoupled from compilation stack

- Multiple front-ends, one backend
- Translation into standard format
  - QIR establishing itself as standard
- Result: Templated circuits





Enabling Domain User Communities to Compute on Quantum Devices

QCs & Simulators

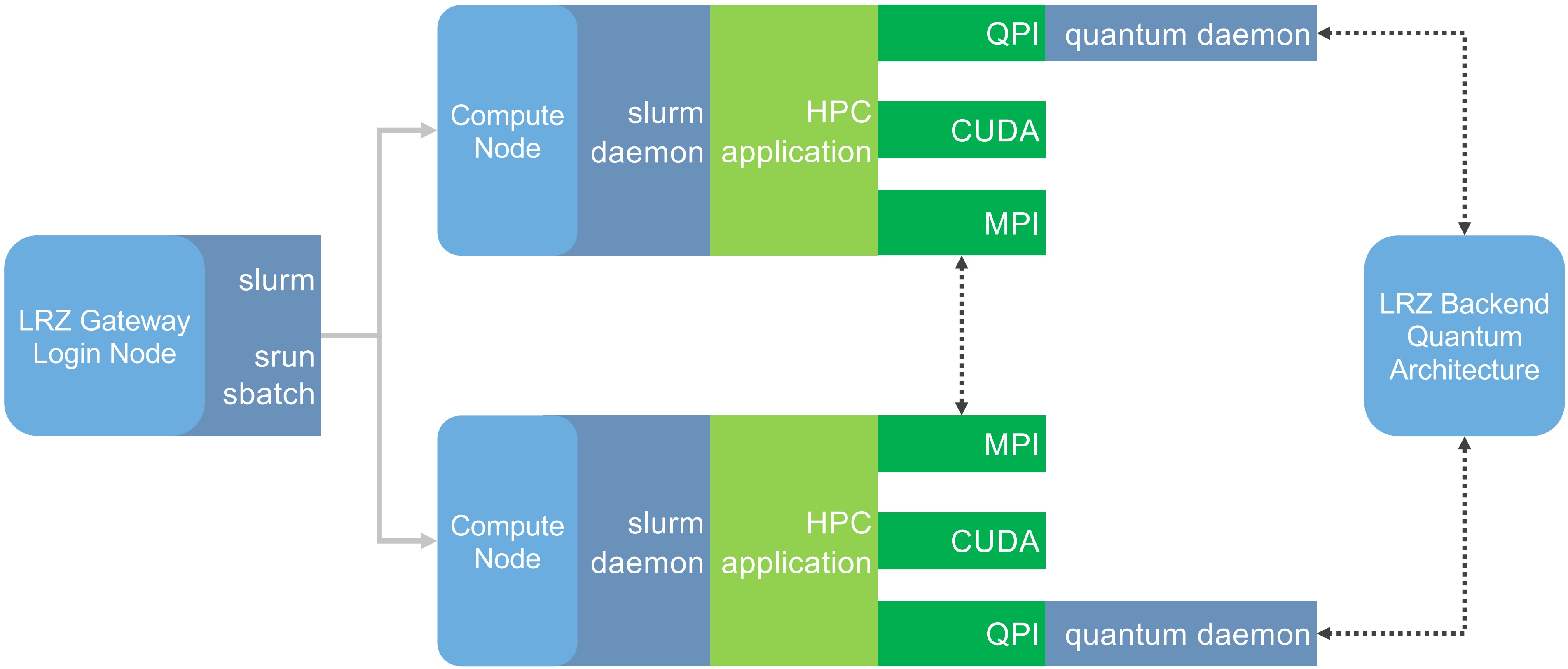
The Munich Quantum Software Stack (MQSS)

Quantum Programming Interface

- Aims to provide similar abstraction to Qiskit
- Abstracts architecture and vendors to avoid lock in
- Users are legacy HPC applications
- State machine interface for quantum task programming
- Maps well to task-offload model and doesn't force data structure

```c
#define QPI_1
#include <qpi.h>
#include <stdio.h>


void bell_0() {
    Qcircuit circuit;
    Qstatus status;

    int states = 4;
    int shots = 1000;

    // 4 states can exist with 2 qubits
    int output[states];

    qCircuitBegin(&circuit);

    qH(0);
    qCX(0, 1);

    qMeasure_all();

    qCircuitEnd();

    qExecute(circuit, shots, &status);
    qWait(status);

    qRead(status, QPI_READ_ALL_STATES, (int*)&output);

    for(int state_idx=0; state_idx < states; state_idx++) {
        printf("|%d>: %d", state_idx, output[state_idx]);
    }
}
```

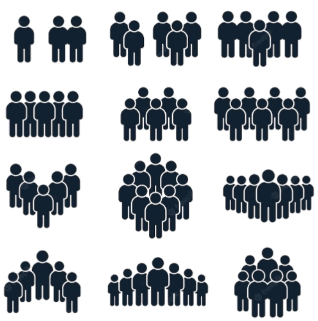
HPC Accessing QC via QPI



Access Modes

Martin Schulz et. Al, Towards the Munich Quantum Software Stack, Poster at QCE Weel 2023

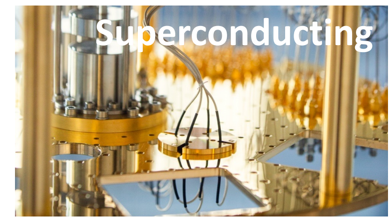
Wide HPC User Communities

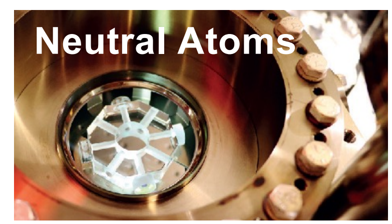


Hybrid/Quantum Programming Toolkits / Libraries

Web-Portal Access

HPC System With Quantum Accelerator





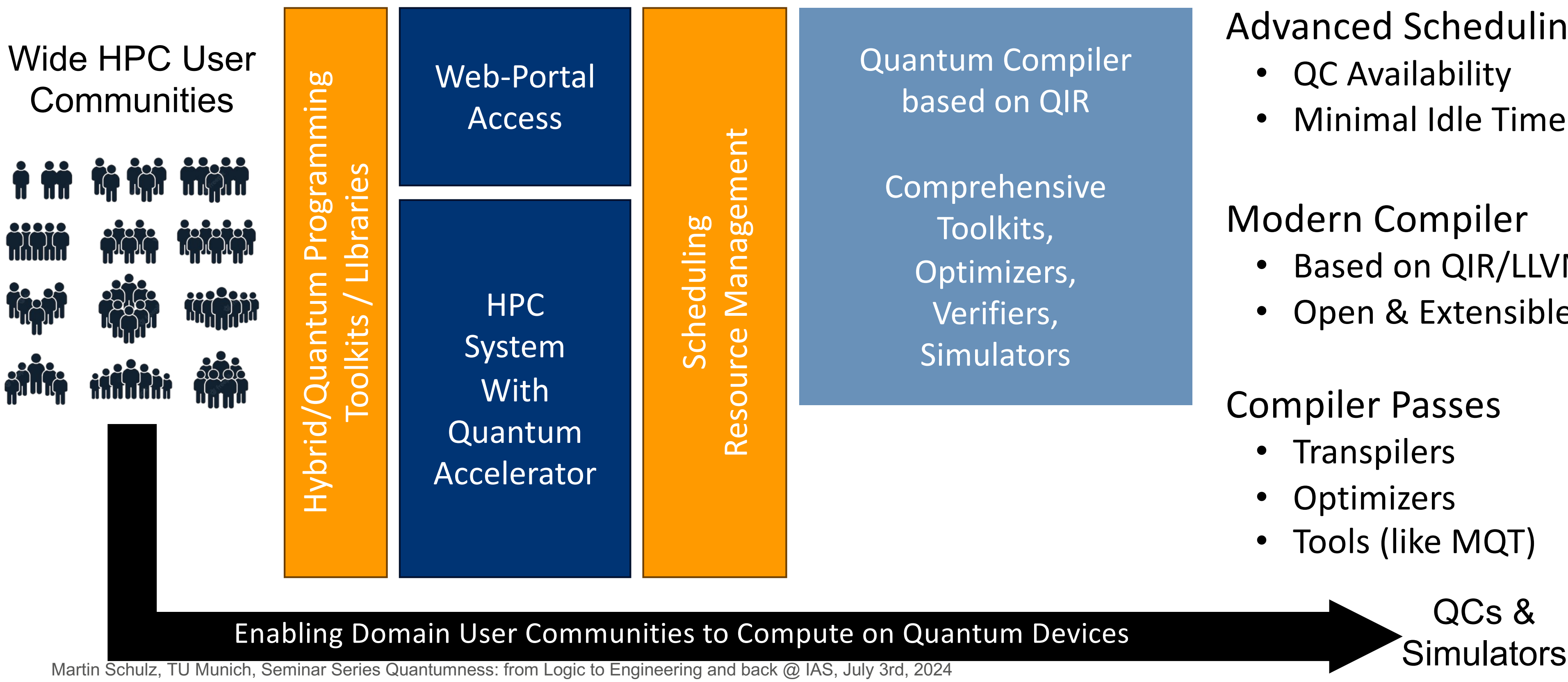
Enabling Domain User Communities to Compute on Quantum Devices

QCs & Simulators

The Munich Quantum Software Stack (MQSS)

Quantum Scheduler and Compiler

Martin Schulz et. Al, Towards the Munich Quantum Software Stack, Poster at QCE Weel 2023



Advanced Scheduling
- QC Availability
- Minimal Idle Times

Modern Compiler
- Based on QIR/LLVM
- Open & Extensible

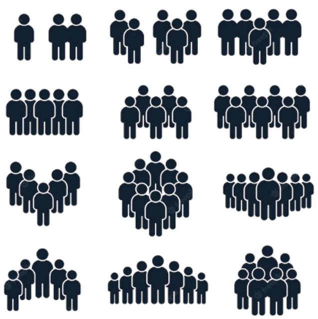
Compiler Passes
- Transpilers
- Optimizers
- Tools (like MQT)

A Comprehensive Runtime and Scheduling Software Stack

QDMI: API for System Control and Feedback

Martin Schulz et. Al, Towards the Munich Quantum Software Stack, Poster at QCE Weel 2023

Wide HPC User Communities



Hybrid/Quantum Programming Toolkits / Libraries

Web-Portal Access

HPC System With Quantum Accelerator

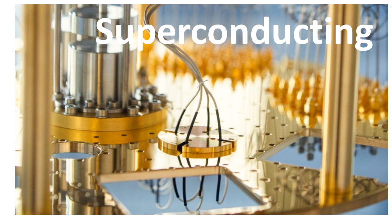
Scheduling Resource Management

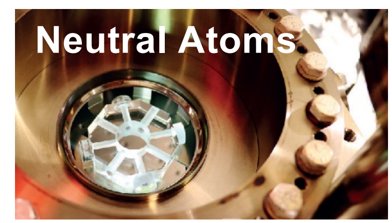
Quantum Compiler based on QIR

Comprehensive Toolkits, Optimizers, Verifiers, Simulators

Figures of Merit and Constraints

QDMI = Quantum Backened Interface





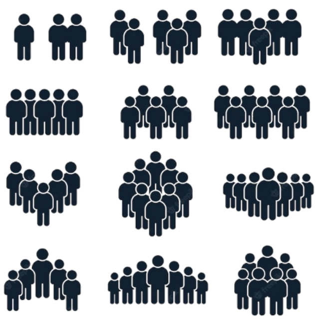
Enabling Domain User Communities to Compute on Quantum Devices

QCs & Simulators

What’s next?

Challenges for the End-User

Wide HPC User Communities



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HPC Access

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Quantum Compiler based on QIR

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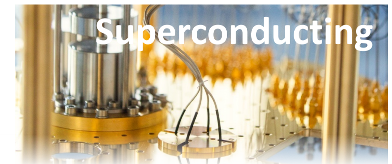
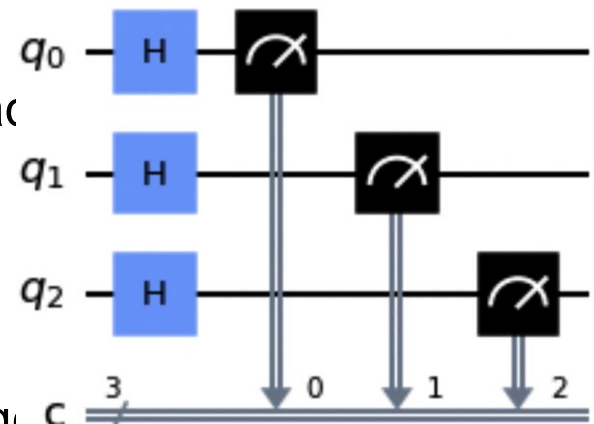


Finding the right kernels

- Substantial amount of work to “offloac
- Matching the right algorithm

Coding is currently very low-level

- Circuit-level
- Requires quantum-physics knowledg



Enabling Domain User Communities to Compute on Quantum Devices

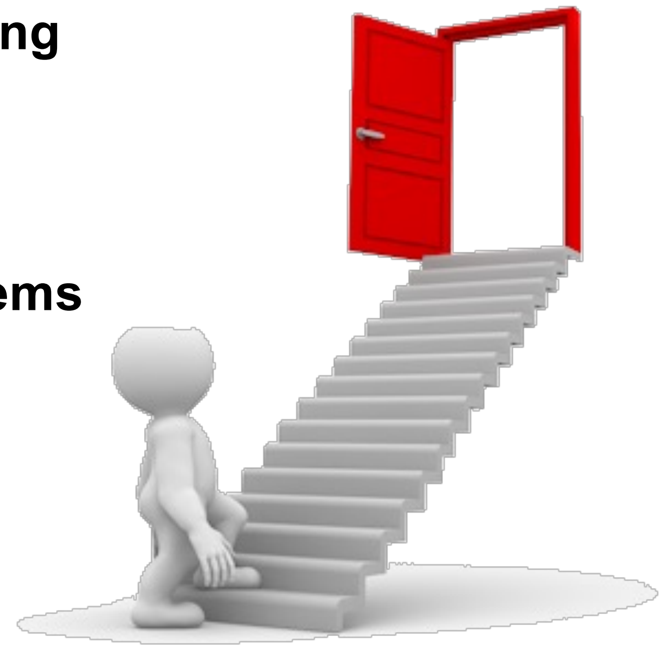
QCs & Simulators

Bringing together HPC and QC:

It is mainly a software challenge

Quantum Computing as one Option to Continue Scaling

- Further support computational demands for simulations
- New computational paradigm
- Applications and algorithms as well as size still very limited



A Comprehensive Software Stack is Key for QC Systems

- Enables wide range of user communities
- Delivers efficient workflows from code to optimized pulses
- Must be deeply integrated with HPC systems for hybrid usage
- ➢ Single stack build on top of established HPC technology

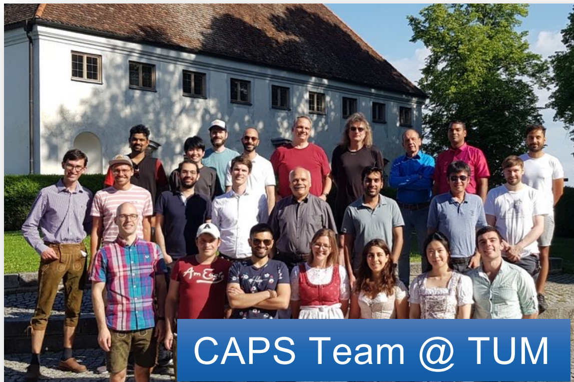
The Munich Quantum Computing Software Stack

- Portal and HPC access to heterogeneous backends
- New programming models for direct access
- Efficient compilers and optimizers
- Comprehensive tools for verification and optimization

Acknowledgements

It takes a team, or rather many teams!

Munich Quantum Valley



CAPS Team @ TUM

QCT Team @ LRZ

CDA Team @ TUM

From the MQV Review Meeting 2022

Bayerisches Staatsministerium für Wissenschaft und Kunst

Federal Ministry of Education and Research

Federal Ministry for Economic Affairs and Climate Action

European Commission

EuroHPC Joint Undertaking

https://www.hpcqc.org/ https://www.munich-quantum-valley.de/

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Munich Quantum Valley Q-DESSI

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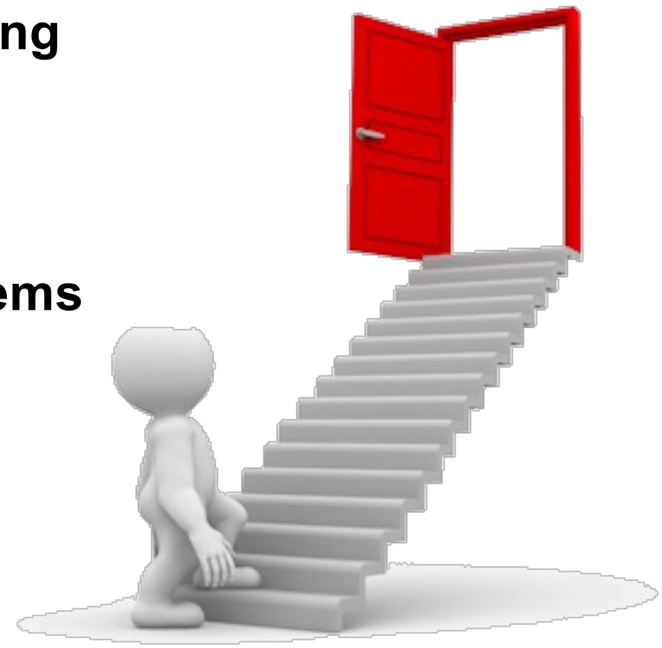

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MQV HPCQC MQT