Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

HIDE SLIDE WHEN PRESENTING

Talk Title: The Arrival, Applicability and Assessment of Quantum to HPC

Presentation Parameters

Submitted Abstract

Quantum systems are now entering HPC centers and their integration as accelerators into HPC workflows is underway. Given their early technological state, diverse architectures and rapid evolution, quantum accelerators pose unique challenges for reliable and useful benchmarks to characterize their performance and error profiles.

Further, as we integrate quantum processors into HPC, there is a growing need for benchmarks tailored to these hybrid workflows to accurately characterize the interplay of these resources and guide optimization and resource allocation.

This talk will explore the overall state of quantum-HPC integration, the challenges of benchmarking quantum and quantum-HPC systems, and our efforts at LRZ on these topics.

Event

2nd TQCI International Seminar on Benchmarks for Quantum Computers
https://teratec.eu/activites_quantiques/TQCI_240604_programme.html

Audience

QC benchmarking specialists

Objective

Provide an overview of the state of hybrid-quantum systems and how we are benchmarking them. Provide some insight into the challenges of benchmarking quantum-HPC complexes.

Quantum-HPC Benchmarking:

The Arrival, Applicability and Assessment of Quantum to HPC

04.06.2024 | Laura Schulz, Head of Quantum Computing and Technologies
Leibniz Supercomputing Centre (LRZ), Garching, Germany

lrz

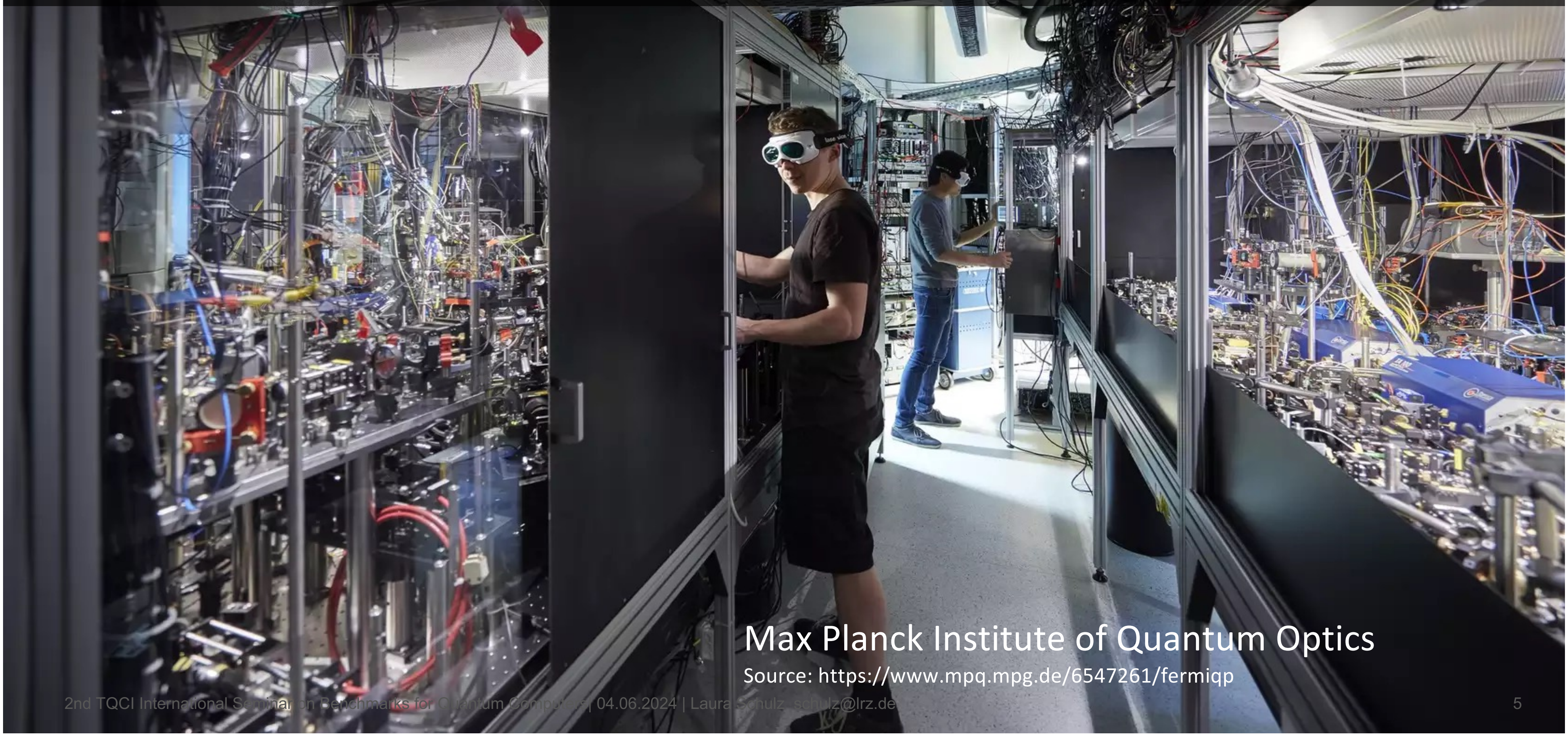
Munich Quantum Valley

Arrival, Applicability and Assessment of Quantum to HPC

The Stable(-ish) World of HPC

Arrival, Applicability and Assessment of Quantum to HPC

The New World of Quantum Computing

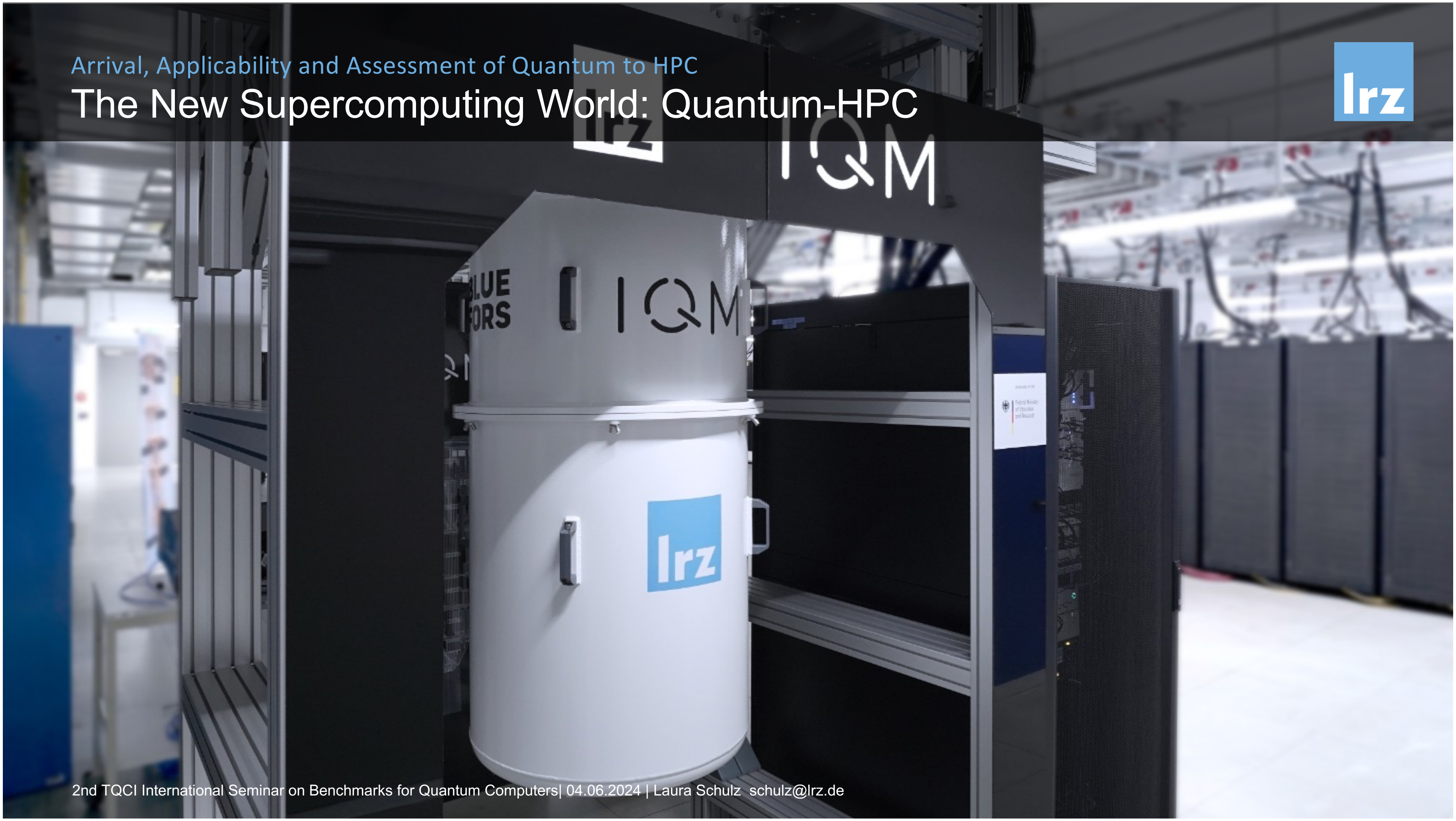


Max Planck Institute of Quantum Optics

Source: https://www.mpq.mpg.de/6547261/fermiqp

Arrival, Applicability and Assessment of Quantum to HPC

The New Supercomputing World: Quantum-HPC



2nd TQCI International Seminar on Benchmarks for Quantum Computers| 04.06.2024 | Laura Schulz schulz@lrz.de

Arrival, Applicability and Assessment of Quantum to HPC

The New Supercomputing: Quantum-HPC

Quantum-Accelerated HPC in PROGRESS

Achieved first submissions of hybrid application (VQE) via HPC compute node to quantum system using co-located, on prem HPC and QC systems.

The Quantum Systems of LRZ

Ion Trap

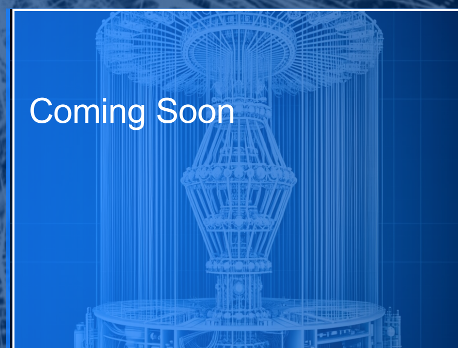
System 4:
20+ qubits

Superconducting

System 1:
5 qubits
System 2:
20 qubits
System 3:
20 qubits

Neutral Atoms

System 7:
1000 qubits*



Superconducting*

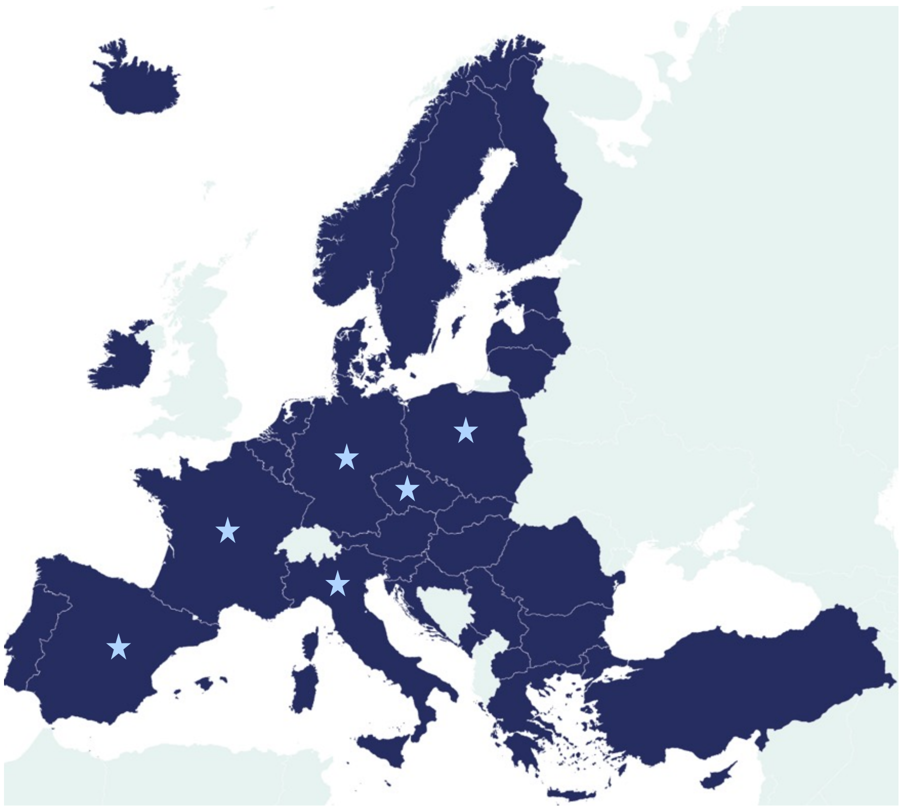
System 5:
50+ qubits
System 6:
100+ qubits

*EuroHPC procurement in progress

Many Different Qubit Types with Physics and Engineering Diversity

Type	Basis	Pros	Cons
Superconducting	Synthetic	High gate speeds and fidelities. Can leverage standard lithographic processes. Among first modalities so has a head start	Requires cryogenic cooling. Short coherence times. Microwave interconnect frequencies still not well understood
Trapped Ions	Natural	Extremely high gate fidelities and long coherence times. Extreme cryogenic cooling not required. Ions are perfect and consistent.	Slow gate times / operations are low connectivity between qubits. Lasers hard to align and scale. Ultra-high vacuum required. Ion charges may restrict scalability.
Photonics	Natural	Extremely fast gate speeds and promising fidelities. No cryogenics or vacuums required. Small overall footprint. Can leverage existing CMOS fabs.	Noise from photon loss. Each program requires its own chip. Photons don't naturally interact so 2Q gate challenges.
Neutral Atoms	Natural	Long coherence times. Atoms are perfect and consistent. Strong connectivity more than 2Q. External cryogenetics not required.	Requires ultra-high vacuums. Laser scaling is challenging.
Silicon Spin / Quantum Dots	Synthetic	Leverages existing semiconductor technology. Strong gate fidelities and speeds.	Requires cryogenics. Only a few entangled gates to date with low coherence time. Interference/cross talk
Nitrogen-vacancy in diamonds	Natural	Limited decoherence; room temperature; electron spin is easy to manipulate; many commodity laser components.	Diamonds not as easily produced as silicon – harder to etch. Scalability very low currently.

EuroHPC Joint Undertaking Mandate: Integrate QC into HPC Centers



EuroHPC Joint Undertaking

Six centers selected for hosting QC systems

- Germany: LRZ
- Spain: BSC
- Czechia: IT4Innovations (LUMI-Q)
- Italy: Cineca
- Poland: PSNC
- France: Genci

The Need for Quantum Benchmarking Increases

Multiple Ways to Make a Qubit

- Performance measurement
- Comparative assessment for specific computations

Progress Tracking

- Qualitative assessment of progress for hardware evolution
- Qualitative assessment of progress for algorithm evolution
- Indicates bottlenecks and improvement opportunities

Standardization

- Allows for consistent comparison
- Evaluation builds trust on reported capabilities

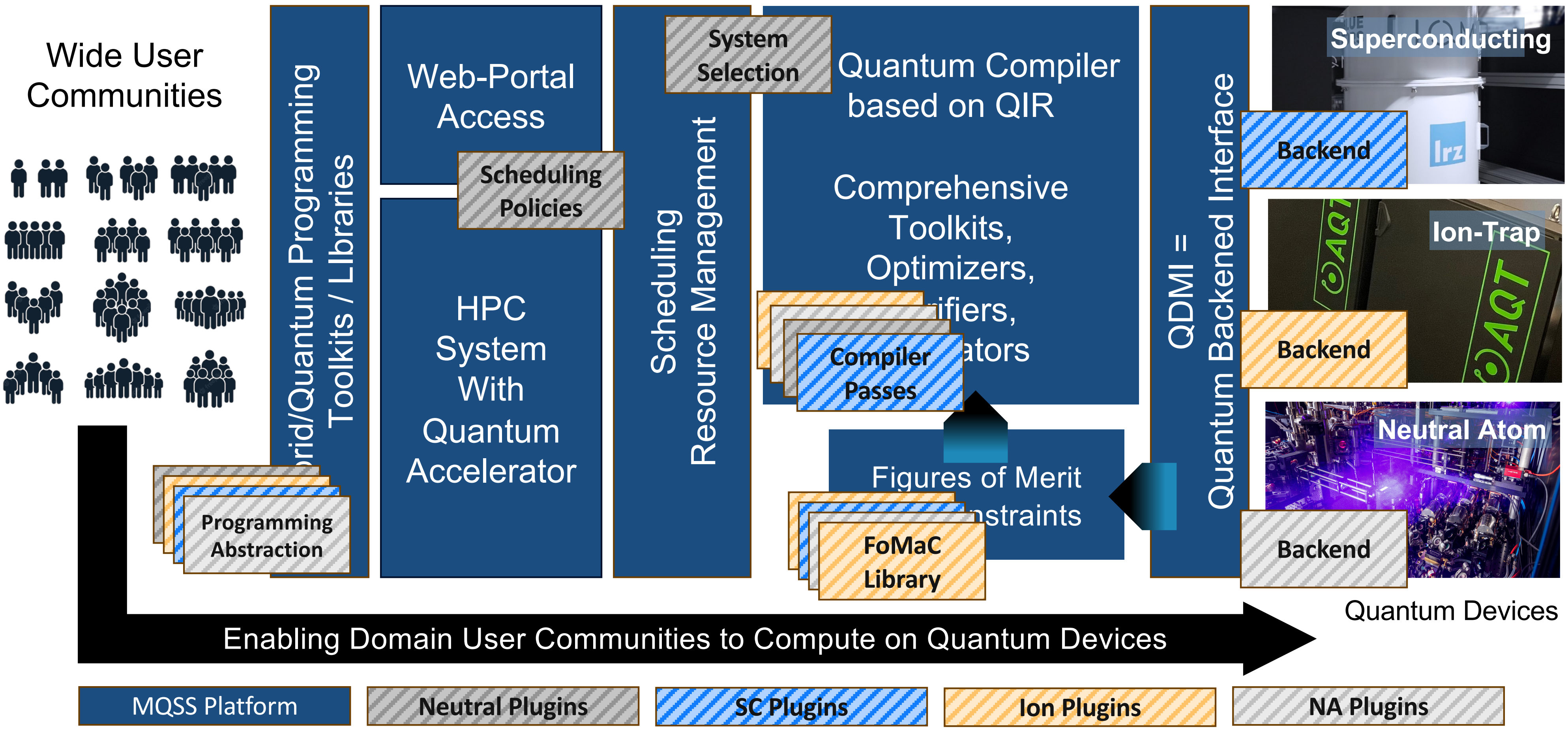
Procurements Underway

- Tenders need reliable, legally defendable comparison framework
- Funders need confidence in ROI

Combining HPC and QC Systems and Benchmarking

Parameter	HPC	Quantum
Technology	Portfolio of Matured Systems	Spectrum of Novice Modalities
Evolutionary Pace	Slower, iterative	Faster with paradigm shifts
Application Profile	Large application sets, multiple domains	No established large scale applications
Execution	Mostly Deterministic	Mostly Stochastic
Errors	Minimal	Heavily Error Prone
Metrics	System-level: Bandwidth, Comm. OH, … App-level: full end-to-end runtime	Physics-level: T1/2, Fidelities, QV, … App-level: not much presently
Dependencies	Can produce results alone	QC result is strongly dependent on classic compute

Munich Quantum Software Stack (MQSS)



HPC Benchmark Boss: Linpack

TOP 500 The List.

LINPACK (HPL)

- Benchmark to "reflect the *performance of a dedicated system for solving a dense system of linear equations."*

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,206.00	1,714.81	22,786
2	**Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States	9,264,128	1,012.00	1,980.01	38,698

HPC Benchmark Boss: Linpack

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- Benchmark to "*reflect the performance of a dedicated system for solving a dense system of linear equations.*"

Green500

- Energy Efficiency (Flops/Watt)

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
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Standardized Benchmark Suite for Algorithms & Applications

Conceptual Model: Algorithms
Berkeley's (7) 13 Dwarfs

Dense linear algebra
Sparse linear algebra
Spectral methods
N-body methods
Structural grids
Unstructured grids
MapReduce

Combinatorial logic
Graph traversal
Dynamic programming
Backtrack / Branch-and-bound
Graph models
Finite state machines

An algorithmic method that captures a pattern of computation and communication

The Landscape of Parallel Computing Research: A View from Berkeley, 2006

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What are the QC and HPC-QC "colossi"?

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Conceptual Model: Real Challenges
Problems looking for better compute

Fusion
Chemistry
Biology
Space

Drug Discovery
Fertilizers
Batteries
Carbon Capture
New Materials

Suitability of different quantum accelerators for applications under study

This spans the chain of:
- programming models
- frameworks
- compilers
- Optimisers
- Etc

End-to-end software stack and environment required to run these use cases on the HPC-QC systems

Two Complementary Benchmarking Objectives

Performance of the full-stack system for:

A given application
within a suite of benchmarks

Efficiency of a a system for an application

Analogous to benchmarking **CAPABILITY**

This is the most prominent HPC benchmarking approach now.

A workload
composed of a set of applications at a given time

Efficiency of a system in handling/serving a given workload scenario composed of multiple applications

Analogous to benchmarking **CAPACITY**

Not central focus to HPC now, but becoming more relevant as HPC systems support dynamic workflows concurrently from multiple applications

Some Thoughts and Caveats on HPCQC Benchmarks

To ensure we develop, purchase and optimize the best computational tools for our user communities in pursuit of significant science discovery:

We need a benchmark **portfolio** early on: A full house, no sole kings

We need to align on the **metrics** for HPC and QC (physics and system levels)

We need alignment on a representative, standardized suite of **application and application kernels** for QC and HPCQC

We need **end-to-end** (user-to-output) **benchmarks** covering overall performance
Including runtime (how long) and energy use (how much)

We should orient towards **"science/society impact" benchmarks**, i.e. "battery benchmark", "High Performance Climate and Weather (HPCW) benchmark"
→ helps communicating to public and policymakers
→ shows maybe impact of QC and HPCQC

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